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CHARGE DENSITY WAVES AND STRUCTURAL MODULATIONS
IN POLYTELLURIDE COMPOUNDS

presented by

Christos D. Malliakas

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Ph.D. degree in Chemistry

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CHARGE DENSITY WAVES AND STRUCTURAL MODULATIONS
IN POLYTELLURIDE COMPOUNDS

VOLUME I

By

Christos D. Malliakas

A DISSERTATION

Submitted to
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ABSTRACT

CHARGE DENSITY WAVES AND STRUCTURAL MODULATIONS IN POLYTELLURIDE COMPOUNDS

by

Christos D. Malliakas

A lattice of positive ions surrounded by a cloud of delocalized electrons is the classical description of a metal. Superconductivity and Charge Density Waves (CDWs) are the two known instabilities that break this diffuse character of the electronic sea into a more ordered picture. These two competing states arise in low quasi-dimensional systems from a phonon-electron coupling that is thermodynamically stable usually at low temperature. CDWs develop from a periodic modulation of the electron density that creates a new broken symmetry ground state through a so-called Peierls distortion.

Although the CDW phenomenon is well understood for one-dimensional systems theoretically no proper models have been developed for the two-dimensional cases. The study of CDWs is important, because a successful description of the coupled electronic lattice instability reflects on the broader issue of the electronic aspects of structural stability which is linked to several interesting phenomena including superconductivity.

In this work, a systematic study of CDW distorted polytelluride materials will be reported in order to understand and elucidate their structural modulations. CDWs are created in these materials due to extended hypervalent Te $\cdots$ Te bonding that occurs in the planar square nets of tellurium. The first family of compounds that will be presented in this Dissertation, RETe₃ (RE = Rare earth), revealed for the first time that the nature of

the CDW in these compounds varies subtly but significantly with RE element. Surprisingly, the temperature dependence of the modulated structures of RETe_3 compounds found to be anomalous. A change in cell volume with RE element has an opposite effect from comparable changes in volume caused by temperature. Furthermore, investigation of AMRETe_4 ($A = \text{Na, K; M} = \text{Cu, Ag; RE} = \text{La, Ce}$) that is structurally related to RETe_3 showed that cross-plane interactions play an import role on defining the CDW distortions in these materials. Additionally, variation of the cross-plane interactions in AM_2EuTe_4 ($A = \text{Na, K, Rb, Cs; M} = \text{Cu, Ag}$) with substitution of different alkali metal ions and europium atoms suggested that in-plane and cross-plane structural changes have different effects on the CDW distortions. Furthermore, the intergrowth $\text{Sm}_2\text{Te}_{5-x}$ that is composed by the substructures of SmTe_{2-x} and SmTe_3 represents a rare example of composite structure and posses two Te nets with different oxidation states showed a hybrid CDW distortion with two independent modulation vectors. A similar behavior of coexistence of two modulation vectors was found in $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10-x}$. Finally, CDW distortions in the linear Te chains of Cu_xUTe_3 found to depend strongly on the concentration of intercalated Cu atoms together with an unusual long range ordering of Cu atoms and vacancies into clusters.

The CDW modulations in the polytellurides that are reported in this thesis are not effected only by the average electron count as it was originally assumed. Temperature, size of atoms, and dimensionality play a very important role on the formation and stability of CDW modulations. Interactions along all three directions must be taken into account and the “quasi” description has to be used with caution.

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Dedicated to my family

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Figure 8.3. Overview of the modulation vectors of most of the known CDW distorted polytelluride phases.561

KEY TO ABBREVIATIONS

CDW	Charge Density Wave
DMF	N,N-Dimethylformamide
EDS	Energy Dispersive Spectroscopy
IR	InfraRed
PDF	Pair Distribution Function
RA-PDF	Rapid Acquisition - Pair Distribution Function
SAED	Selected Area Electron Diffraction
SEM	Scanning Electron Microscopy
TEM	Transmission Electron Microscopy
STM	Scanning Tunneling Microscopy
LT-STM	Low Temperature Scanning Tunneling Microscopy
FFT	Fast Fourier Transform
SQUID	Superconducting QUantum Interference Device
PPMS	Physical Property Measurement System
DFT	Density Functional Theory
FS	Fermi Surface
IC	InCommensurate
C	Commensurate
NIC	Near InCommensurate
e.s.d.	Estimated Standard Deviation
AC	Alternating Current

Chapter 1

Distortions in Planar Nets of Tellurium: Synthetic and Characterization Techniques

1.1 Introduction

Polychalcogenide compounds are defined by the occurrence of Q – Q bonds (Q = S, Se, Te) in the structure. These compounds have recognizable polychalcogenide $(Q_x)^{2-}$ units. As the chalcogen atoms become larger and heavier in addition to Q-Q bonds, ternary hypervalent $Q\cdots Q$ bonding interactions can develop.¹ These interactions evolve from being essentially van der Waals in nature in the lighter congeners, to becoming significant and prevalent in the tellurides giving rise to unusual non-classical arrangements such as oligomeric or polymeric anions and square nets (section 1.3). Compounds with these features can give rise to interesting physical properties such as charge density waves (CDW, section 1.4), anisotropic optical properties, and may even be interesting for thermoelectric investigations (section 1.5). In polytellurides extended hypervalent $Te\cdots Te$ bonding is frequently observed with flat square nets of tellurium. At first glance these nets are highly symmetric but a closer look almost always reveals subtle distortions associated with commensurately or incommensurately modulated superstructures.¹

A variety of experimental techniques like Electron Diffraction (ED), Superspace crystallography, and Pair Distribution Function analysis (PDF) along with theoretical calculations at the Density Functional Theory (DFT) level were used to properly characterize the CDW materials reported here. Since some of those techniques are not standard and commonly used a brief introduction for PDF analysis (section 1.6) and superspace approach (section 1.7) will be given in this Chapter.

1.2 Polychalcogenide and halide flux synthetic technique

A conventional solid state synthesis involves use of very high temperature (usually more than 1000 °C) and heating of elements or simple binaries phases at stoichiometric amounts based on the target compound. This so-called “heat and beat” synthetic method however has some limitations. The reaction of the starting materials depends on the diffusion between the solid particles. Therefore homogeneity is difficult to achieve since most of the times either one of the reaction components or the final product remain still in the solid state at the conditions of the reaction. Successive grinding and compression (pellet) of the mixture of reactants/products between heating cycles may be the only way to obtain homogeneous products. Since high temperature is required to facilitate as much as possible the diffusion between reactants the final products are usually the most thermodynamically stable ones. Compounds that are metastable and decompose at relative high temperature or whose formation is kinetically controlled are almost impossible to obtain via this classical synthetic approach. Growth of single crystals and characterization of those by X-ray diffraction methods is the “backbone” of any solid state science and essential to obtain structures in real space. The large number of reflections in the three-dimensional reciprocal space obtained by single crystal diffraction is preferable than the limited number of reflections present in a two-dimensional projection of a powder diffraction experiment. Since diffusion is relative limited in a typical solid state experiment single crystal growth is a major problem that makes the structural characterization of new phases rather difficult if not impossible.

Molten salts have been used for over 100 years as a high temperature recrystallization media for various binary and ternary compounds² to overcome the

limited diffusion problem of the conventional solid state synthesis. It was not until 1987 when a molten salt was used at lower temperature to synthesize new compounds.³ Since then a large number of new compounds have been reported. In this work, a rare earth metal is reacted with tellurium metal. The reaction between these two elements is extremely exothermic and the direct combination of them will always create an explosion of the glass container ($> 400\text{ }^{\circ}\text{C}$). The use of a halide (or polytelluride) flux in this case is important not only for crystal growth purposes but also as a heat absorber. A list of relative low melting point halide salts (and eutectic mixtures of them) and their corresponding melting point temperature are presented at the bottom of Table 1.1.

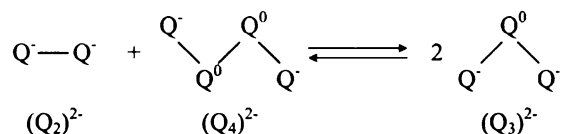
The use of molten alkali metal polychalcogenide A_2Q_x ($\text{A} = \text{Alkali metal}$, $\text{Q} = \text{S, Se, Te}$) flux as solvent has been very useful for the discovery of new (poly)chalcogenide materials.⁴ The reason for that is mainly the fact that the flux has a low melting point and the reactions immersed into it can be carried out at relative lower temperatures (lower than $700\text{ }^{\circ}\text{C}$). The melting points of several alkali metal/polychalcogenide salts (A_2Q_x) are given in Table 1.1. It is worth noted that most of the A_2Q_x ($x>2$) species have a melting point less than $500\text{ }^{\circ}\text{C}$ and in some cases even less than $200\text{ }^{\circ}\text{C}$. The molten flux acts as solvent and in many cases as reactant too, providing and incorporating the chalcogenide and/or the alkali metal into the final product. Importantly, the A_2Q_x fluxes remain nonvolatile over a wide temperature range which is a necessary requirement for a solvent. It can be used for various reaction temperatures above their melting point without concerning solvent loss. In addition, crystal growth is enhanced. Through a mineralization effect, small or poorly formed crystallites can be redissolved in the flux and reprecipitate as larger single crystals. Finally, the excess A_xQ_y salt that remained

from the flux can be easily washed off using any polar solvent such as methanol, N,N-Dimethylformamide or water.

Table 1.1. Melting points of some known alkali metal polychalcogenide (A_xQ_y where Q = S, Se and Te) species and halide salts.^{5,6,7}

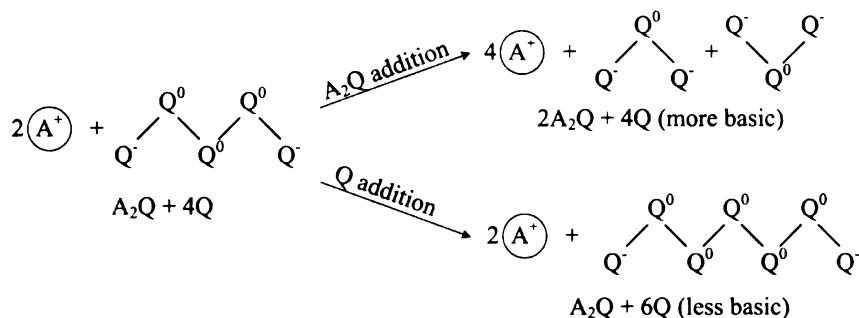
A_xQ_y	A_2Q	A_2Q_2	A_2Q_3	A_2Q_4	A_2Q_5	A_2Q_6
A_xS_y	Li ₂ S 900-975 °C	Li ₂ S ₂ 369 °C				
	Na ₂ S 1180 °C	Na ₂ S ₂ 490 °C	Na ₂ S ₃ 228 °C	Na ₂ S ₄ 275 °C	Na ₂ S ₅ 252 °C	
	K ₂ S 840 °C	K ₂ S ₂ 470 °C	K ₂ S ₃ 252 °C	K ₂ S ₄ 145 °C	K ₂ S ₅ 206 °C	K ₂ S ₆ 189 °C
	Rb ₂ S 530 °C	Rb ₂ S ₂ 420 °C	Rb ₂ S ₃ 213 °C	Rb ₂ S ₄ 160 °C	Rb ₂ S ₅ 225 °C	Rb ₂ S ₆ 201 °C
		Cs ₂ S ₂ 460 °C	Cs ₂ S ₃ 217 °C	Cs ₂ S ₄ 160 °C	Cs ₂ S ₅ 210 °C	Cs ₂ S ₆ 186 °C
A_xSe_y	Na ₂ Se >875 °C	Na ₂ Se ₂ 495 °C	Na ₂ Se ₃ 313 °C	Na ₂ Se ₄ 290 °C		Na ₂ Se ₆ 258 °C
		K ₂ Se ₂ 460 °C	K ₂ Se ₃ 380 °C	K ₂ Se ₄ 205 °C	K ₂ Se ₅ 190 °C	
A_xTe_y	Na ₂ Te 953 °C	Na ₂ Te ₂ 348 °C				Na ₂ Te ₆ 436
	K ₂ Te 900 °C		K ₂ Te ₃ 429 °C	K ₂ Te ₄ 266 °C	K ₂ Te ₅ 268 °C	K ₂ Te ₆ 264 °C
	Rb ₂ Te 775 °C		Rb ₂ Te ₃ 400 °C		Rb ₂ Te ₅ 270 °C	
	Cs ₂ Te 820 °C		Cs ₂ Te ₃ 395 °C	Cs ₂ Te ₄ 221-237 °C	Cs ₂ Te ₅ 235 °C	Cs ₂ Te ₆ 226 °C
Halide	LiF 848 °C	LiCl 610 °C	LiBr 552 °C	LiI 681 °C	Eutectic mixtures (molar fraction)	
	NaF 996 °C	NaCl 801 °C	NaBr 747 °C	NaI 660 °C	RbCl (42.2) – LiCl 313 °C	
	KF 858 °C	KCl 771 °C	KBr 734 °C	KI 469 °C	LiI (36.6) – KI 286 °C	
	RbF 833 °C	RbCl 720 °C	RbBr 693 °C	RbI 647 °C	LiCl (58) – CsCl 326 °C	
	CsF 703 °C	CsCl 646 °C	CsBr 636 °C	CsI 626 °C		

The reaction between A_2Q and Q (starting materials of the flux) occurs in situ and polychalcogenide chains $(Q_x)^{2-}$ with various lengths are formed. These chains consist of two terminal atoms that carry a charge of 1- and $x-2$ internal atoms with zero-valent charge. The negative charged terminal atoms behave like a Lewis base and coordinate to the metal (reactant) and the internal Q atoms at the same time oxidize the metal while they are being reduced. The internal atoms now become terminal chalcogens and the chains are splitted into smaller $(Q_x)^{2-}$ fragments. Furthermore, the polychalcogenide chains can undergo also self-redox equilibria of the type shown in Scheme 1.1.



Scheme 1.1: Self-redox equilibrium of the polychalcogenide flux.

The relative basicity of the reaction depends on the length of these polychalcogenide chains and it can be controlled by changing the A_2Q/Q ratio. If less A_2Q (or more Q) is used in the reaction mixture, longer polychalcogenide chains will form. The Q^0/Q^{1-} ratio will increase and therefore the resulting flux will be more oxidizing (less basic), Scheme 1.2.



Scheme 1.2: Control of the basicity with variation of the A_2Q/Q ratio.

The alkali metal polychalcogenide flux method became one of the most powerful synthetic tool for exploratory synthesis in the solid state community. The ability to control the basicity of the flux by varying the A_2Q/Q ratio gave the possibility to explore different chemical systems under a wide range of synthetic conditions. The flux conditions allow the reaction system to evolve without constraints and form either kinetic or thermodynamic stable products. The excess flux facilitates the synthesis of new compounds with no predefined stoichiometries and structure types. Metastable phases that could not be synthesized or predicted previously are now accessible.

1.3 Distortions in planar nets of tellurium

Moving across the VI group of elements in the periodic table, from S to Se and Te, the size and diffuse nature of the p-orbitals increases. Tellurium is the least electronegative element among the chalcogens and can stabilize longer than normal bond distances having a great tendency to associate through Te-Te bonding interactions. Roald Hoffmann described this behavior of tellurium as a “constant flirtation with other tellurium partners, in the range between a bond and no bond”.⁸ This has been illustrated in the alkali metal rich tellurides⁹ where such Te-Te “hyper-interactions” has resulted in the formation of one-dimensional infinite¹⁰ and spirocyclic¹¹ chains, cyclohexane-like Te_6 rings¹² and puckered crown shaped Te_8 rings.¹³

Low dimensional compounds with planar Te nets have been observed when a transition metal or a rare earth metal is added in the synthesis. These compounds have been found to undergo structural distortions located mainly in the planar nets of tellurium. Due to this distortion the planar Te net from an ideal square geometry breaks

down into oligomers of the form $(Q_x)^{2-}$. Some representative examples of compounds with planar Te nets include $K_{0.33}Ba_{0.67}AgTe_2$,¹⁴ $NdTe_3$,¹⁵ $SmTe_{1.84}$,¹⁶ ARE_3Te_8 ($A = K, Rb, Cs$; $RE = Ce, Nd$),¹⁷ $KCuCeTe_4$,¹⁸ $RbCuCeTe_4$,²⁰ $Na_{0.8}Ag_{1.2}CeTe_4$,²⁰ $K_{2.5}Ag_{4.5}Ce_2Te_9$,²⁰ $K_{2.5}Ag_{4.5}La_2Te_9$,²⁰ $Cu_{0.66}EuTe_2$,¹⁹ KCu_2EuTe_4 ,¹⁹ $Na_{0.2}Ag_{2.8}EuTe_4$,¹⁹ $K_{0.65}Ag_2Eu_{1.35}Te_4$ ²⁰ and Cu_xUTe_3 ($x = 0.25, 0.33$).²¹ In some cases the undistorted or distorted compounds possess one dimensional linear chains like $\alpha-UTe_3$ ²² and ATH_2Te_6 ($A = Cs, Cu$).²³ More examples of planar chalcogenide nets include $K_3Cu_8S_6$,²⁴ $LaSe_{1.9}$,²⁵ $DySe_{1.84}$,²⁶ and $RbDy_3Se_8$.²⁷ These structural distortions are not specific to square nets only but rather to the low-dimensional nature of the compounds that makes them susceptible to distort. Some typical examples include the chain-like transition metal trichalcogenides,²⁸ the layered transition metal dichalcogenides,²⁹ the red³⁰ and purple³¹ bronzes.

The physical properties of a system undoubtedly depend on its structure. An “ideal” square net of Te atoms should contact electrons and be metallic in nature. The electronic properties of compounds that contain planar Te nets should depend mainly on this diffuse nature of the Te p-orbitals which are considered to be delocalized across the net. Indeed, from theoretical calculations on most of the compounds mentioned above, the Fermi level is primarily made up of Te p-orbitals. When the formal oxidation state of all Te atoms in the net is -2, a stable square net is observed (e.g., $NaCuTe$).³² However, when the formal oxidation state is < -2 , or when there are atomic vacancies in the square net, structural distortions are possible leading to Te-Te bonding interactions and the formation of $(Te_x)^{2-}$ species within the net, Figure 1.1. The distortions in these electron deficient Te nets lower the total energy of the system by decreasing the energy of the filled Te p-orbitals and bringing the electrons into fully occupied bonding orbitals (Jahn-

Teller type distortion). Consequently, a gap opens up at the Fermi level and the material becomes a semiconductor or insulator.

The distortions in planar nets of Te can be created in a form of a Charge Density Wave (CDW) or Site Occupancy Wave (SOW) or combination of these two waves. In the case of CDW, an electron-photon coupling creates a sinusoidal (or combination of several sinusoidal waves) atomic displacement of the Te atoms. This coupling lowers the total energy and a gap is produced in the Fermi surface (Peierls distortion). The wave vector of the modulation (q-vector) can orient in principle to any direction in the reciprocal space. The energetically preferred orientation of the q-vector is the one that will create a greater stability (lower energy) or bigger band gap. The Fermi surface topology will determine this lower energy path and bands will span along that direction in order to create a gap. This nesting effect is thermodynamically favorable and the corresponding nesting vector dictates the wave vector of the electron density. Essentially, the q-vector of the distortion is the same with the nesting vector of the Fermi surface.

The result of this CDW modulation in the pattern of the Te net is the creation of oligomeric fragments of $(\text{Te}_x)^{2-}$, Figure 1.1. The length of each oligomer x will depend on the period of the modulation wave (1/2, 1/3, 1/4 etc.) and the average oxidation state of the net. In a commensurate case, a regular sequence of oligomers will form while electrons can be localized on the well separated fragments, Figures 1.1A, 1.1B. For example, LaTe_2 possesses a 2×2 supercell in the plane that contains the planar net and an average oxidation of 1- on the Te atoms in the net.³³ As expected, the supercell contains dimers of $(\text{Te}_2)^{2-}$. In an incommensurate case, the rationalization mentioned above is more difficult since there is no obvious “commensurate” periodicity in the system.

Therefore, the calculation of the average number of electrons is not trivial and it will always depend on the arbitrary rational approximation of the supercell. There is no easy way to localize electrons and the pattern of the $(\text{Te}_x)^{2-}$ species is more diffuse with aperiodic sequences, Figure 1.1C.

Site Occupancy Waves (SOWs) is another way of distortion. Usually vacancies may order in the net and create periodic holes in it. Around these vacant sites, Te atoms may move and displace in order to find a relaxed (energetically favorable) position. Therefore, SOWs are most of the times accompanied with positional modulations and in the case of planar Te nets coupled with CDWs. Some possible distorted Te patterns of SOWs and CDWs are shown in Figures 1.1D, 1.1E.

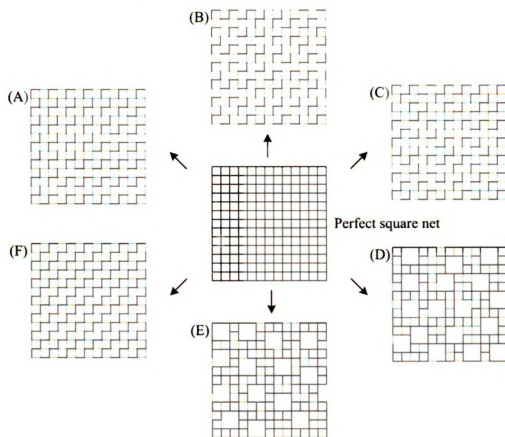


Figure 1.1. Schematic representation of some possible patterns of distortion of an ideal square net of tellurium atoms.

1.4 Charge-Density-Wave (CDW)

Almost 50 years ago R. Peierls³⁴ and H. Frohlich³⁵ independently suggested that a coupling of the electron and phonon systems in a one-dimensional metal is unstable with respect to a static lattice deformation of wavevector $Q = 2k_f$. A CDW is a modulation of the conduction electron density in a metal and an associated modulation of the lattice atoms positions. These kinds of modulations, which are giving rise to the unusual properties of quasi-one-dimensional metals, have three spatial features:

1. They are caused by instability of the metallic Fermi surface due to the electron-phonon interaction
2. They result in energy gaps at the Fermi surface and
3. Their wavelength λ_c is π/k_f where k_f is the Fermi wavevector

In an electron-localized description, Jahn-Teller distortion, the system usually adopts a commensurate superstructure in which covalent bonding between near neighbors leads to an insulating system. In a more electron-diffuse description, Peierls distortion, the Fermi surface driven distortion is stabilized by the formation of the CDW gap. The nesting vector may be incommensurate and the gap may remove states from only part of the Fermi surface.

1.4.1 Jahn-Teller distortion

Here the system is described as having local bonding between nearest neighbors and the distortion is energetically stabilized by the overlap of partially filled degenerate molecular orbitals. When the number of bonding neighbors in the distorted structure is equal to the number of unoccupied states, only energetically lowered states are occupied,

Figure 1.2. Fully occupied bonding and unoccupied antibonding orbitals are separated by an energy gap in the presence of the coordination-lowering distortion, leading to insulating behavior. This gap is equivalent to that derived from the Fermi surface driven sinusoidal distortion created from the Peierls transition. In both cases the distortion is stabilized by the lowering of occupied states.³⁶

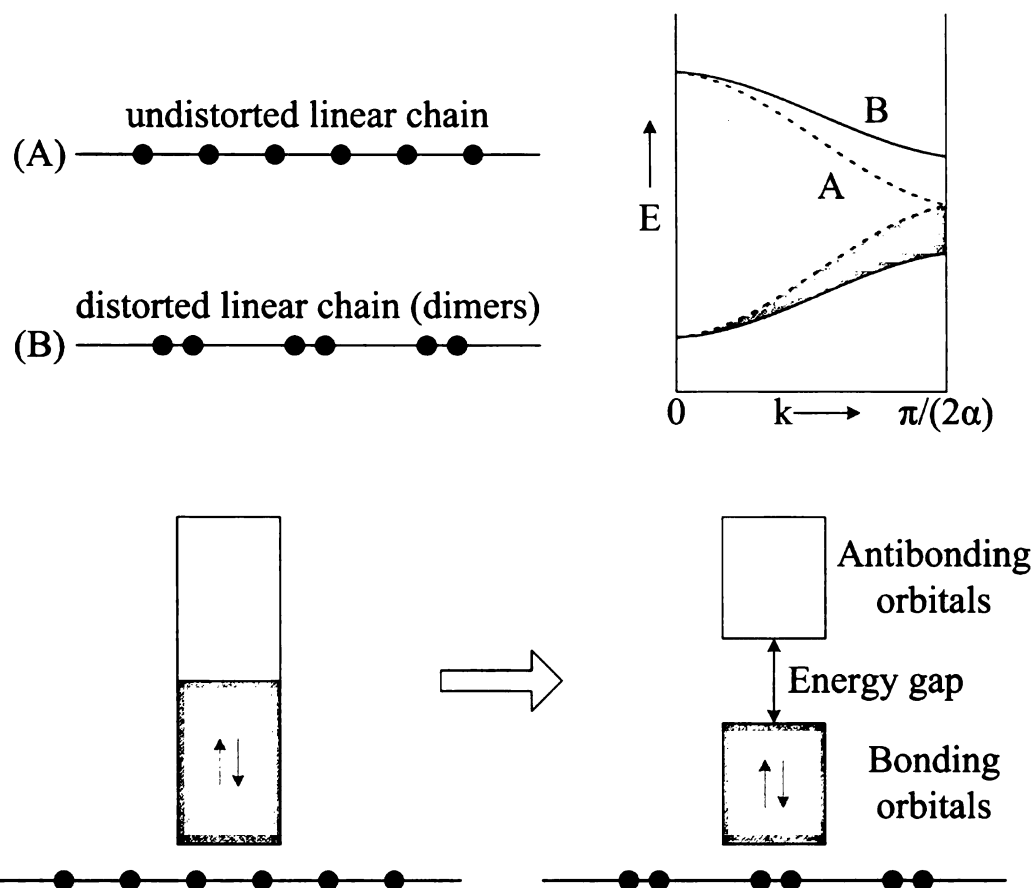


Figure 1.2. Schematic representation of the localized picture of Jahn-Teller distortion. (A) The undistorted linear chain of atoms and the corresponding metallic state. (B) Formation of dimers and a gap opening at the Fermi level. This picture creates fully occupied bonding orbital and unoccupied antibonding orbitals.

1.4.2 Peierls distortion and Charge-Density-Waves

Consider a quasi-one-dimensional metal with chains of equally spaced atoms. The conduction states form a band as shown in Figure 1.3A. If there is coupling between the conduction electrons and the lattice then a periodic displacement of the ions

$$dr_i = A_i \cos(\mathbf{q} \cdot \mathbf{r}_i) \quad (1.1)$$

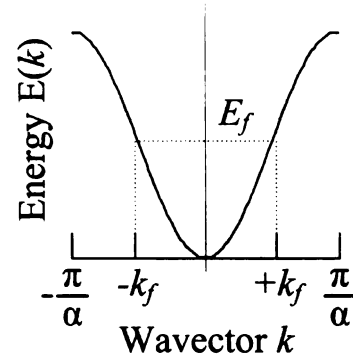
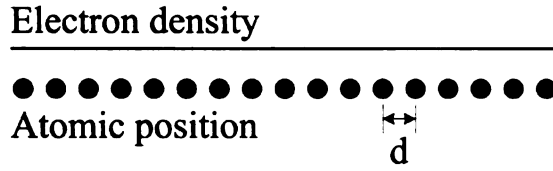
will produce a perturbation potential

$$V(\mathbf{r}) = V_0 \cos(\mathbf{q} \cdot \mathbf{r}) \quad (1.2)$$

seen by the conduction electrons. Here $\mathbf{q}$ is the wavevector of the distortion, lattice positions are given by $\mathbf{r}$ and the potential $V_0 \equiv g|A|$ is proportional to the distortion amplitude and the electron-phonon coupling constant. This perturbation splits the degenerate levels and produces a gap in the bandstructure at $\pm \mathbf{q}/2$. States with wavevectors just less than $\mathbf{q}/2$ will be lowered in energy while those with wavevector greater than $\mathbf{q}/2$ will be raised.

The distortion is most favorable when $\mathbf{q} = 2\mathbf{k}_f$ therefore the gap is produced at the Fermi surface. In this case the occupied states below $\mathbf{k}_f$ are lowered in energy while the raised states are unoccupied and the only energetic cost is the lattice strain. The energetic requirement for the distortion has implicit temperature dependence since increasing temperature will progressively populate the raised electronic states. Ultimately, above a transition temperature T_{CDW} the distortion will be lost and the system will return to its metallic undistorted condition. In this one-dimensional case any finite electron-phonon coupling leads to the adoption of a superstructure and a gap at E_f .³⁷

(A)



(B)

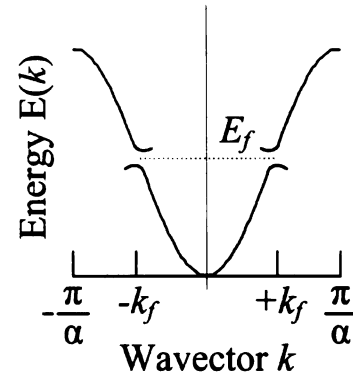
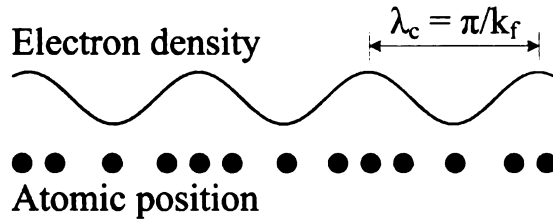


Figure 1.3. (A) A quasi-one-dimensional undistorted metal with interatomic spacing d (B) CDW modulated electrons and phonons and the creation of a gap at the Fermi level. The modulations are usually quite small with atomic displacements about 1% of the interatomic spacing and the conduction electron density varies by several percent.

1.5 Thermoelectric property

In order for a material to be useful for thermoelectric applications it must have a high figure of merit, ZT :

$$ZT = \frac{S^2 \sigma T}{\kappa} \quad (1.3)$$

where S is the thermopower, σ is the electrical conductivity and κ is the thermal conductivity. From equation ((1.3)) is apparent that in order to obtain a high ZT , the material must possess high thermopower, high electrical conductivity and low thermal

conductivity. Although this appears to be very straight forward the problem is actual more complicated because these variables are dependent of each other. Rising of thermopower is usually followed by decreasing of electrical conductivity and increasing of electrical conductivity is usually followed by increasing of thermal conductivity.³⁸

Although metallic materials may have high electrical conductivity, they generally have low thermopower. Wide band gap semiconductors may possess higher thermopower but their electrical conductivity is too low due to fewer carriers. Semimetals or narrow bandgap semiconductors with heavy metals seems to be the more promising materials for thermoelectric applications.³⁸ They have high electrical conductivity and low thermal conductivity due to low frequency lattice vibrations of the heavy elements.

The thermopower is given by the equation:

$$S = K \cdot \frac{d \ln \sigma(E)}{dE} \text{ at } E = E_f \quad (1.4)$$

where K is a constant and $\sigma(E)$ is the electrical conductivity as a function of Fermi energy, E_f . The thermopower can be seen as a measure of the difference of $\sigma(E)$ below and above the Fermi surface. The complexity of a band structure increases with the complexity of the electronic structure and furthermore the chances for a high $\sigma(E)$ at the Fermi level. Thereby, the thermopower can be increased.

1.6 Pair Distribution Function analysis (PDF)

Knowing the real structure of a material is very important in determining and explaining its properties and characteristics. The structure characterization of a solid usually involves X-ray diffraction study and crystallographic analysis. However, the crystal structure represents only the long-range order and the average unit cell.

Deviations from ideal “perfect” crystals - like mixed site occupation, impurities, distortions and defects – are very important for the properties of the materials. Sometimes, these structural deviations are being hidden into the average structure and short-range order characterization techniques are necessary to probe this kind of defects.

The pair distribution function method (PDF) is a powerful technique for local structure studies. Basically, the PDF describes the distribution of interatomic distances in a material. The power and the difference of PDF from other crystallographic techniques like Rietveld is that PDF is a total scattering technique which means both the Bragg and diffuse scattering are treated on an equal basic.

The experiments are straightforward X-ray or neutron powder diffraction measurements, Figure 1.4A. From the coherent part, $I^{coh}(Q)$, of the measured total diffracted intensity of the material we find the total scattering structure function, $S(Q)$

$$S(Q) = \frac{I^{coh}(Q) - \sum c_i |f_i(Q)|^2}{\left| \sum c_i f_i(Q) \right|^2} + 1 \quad (1.5)$$

where the coherent intensity is corrected for background and other experimental effects and normalized by the flux and number of atoms in the sample, Figure 1.4B. Here, c_i and f_i are the atomic concentration and X-ray atomic form factor, respectively, for the atomic species of type i . Momentum transfer, Q , is given by

$$Q = 4\pi \sin \vartheta / \lambda \quad (1.6)$$

By Fourier transforming the expression $Q[S(Q)-1]$ we have

$$G(r) = (2/\pi) \int_{Q=0}^{Q_{\max}} Q[S(Q) - 1] \sin(Q \cdot r) dQ \quad (1.7)$$

where $G(r)$ is the atomic pair distribution function which is also defined as

$$G(r) = 4\pi \cdot r [\rho(r) - \rho_0] \quad (1.8)$$

where ρ_0 is the average atomic number density, $\rho(r)$ is the atomic pair-density and r is a radial distance. The function $G(r)$ gives information about the number of atoms in a spherical shell of unit thickness at a distance r from a reference atom, Figure 1.4C.

Finally, the experimental $G(r)$ can be compared and refined against a theoretical $G(r)$ from a structural model given by

$$G(r) + 4\pi \cdot r \cdot \rho_0 = \frac{1}{r} \sum_{\nu} \sum_{\mu} \frac{f(0)_{\nu} f(0)_{\mu}}{\langle f(0) \rangle^2} \delta(r - r_{\nu\mu}) \quad (1.9)$$

In theory, $Q_{\max}$ from equation (1.7) should be infinite but experimentally is always a finite number. In order to have good resolution, values of $Q > 30 \text{ \AA}^{-1}$ are desirable therefore short wavelengths are necessary according to equation (1.6). X-rays of $> 45 \text{ KeV}$ ($\lambda = 0.27 \text{ \AA}$) and up to 130 KeV ($\lambda = 0.09 \text{ \AA}$) or neutrons are typically used.

As can be seen PDF is based on a conventional X-ray or neutron powder diffraction experiment and it's simply another representation of the diffraction data. The only difference is that PDF reflects both the long-range atomic structure, manifest in the Bragg reflections, and the local structure imperfections, manifest in the diffuse component of the diffraction pattern. The data analysis does not presume any periodicity therefore the PDF technique is very useful for examining if the distortions found in a specific single crystal are representative of the total bulk of the sample.³⁹

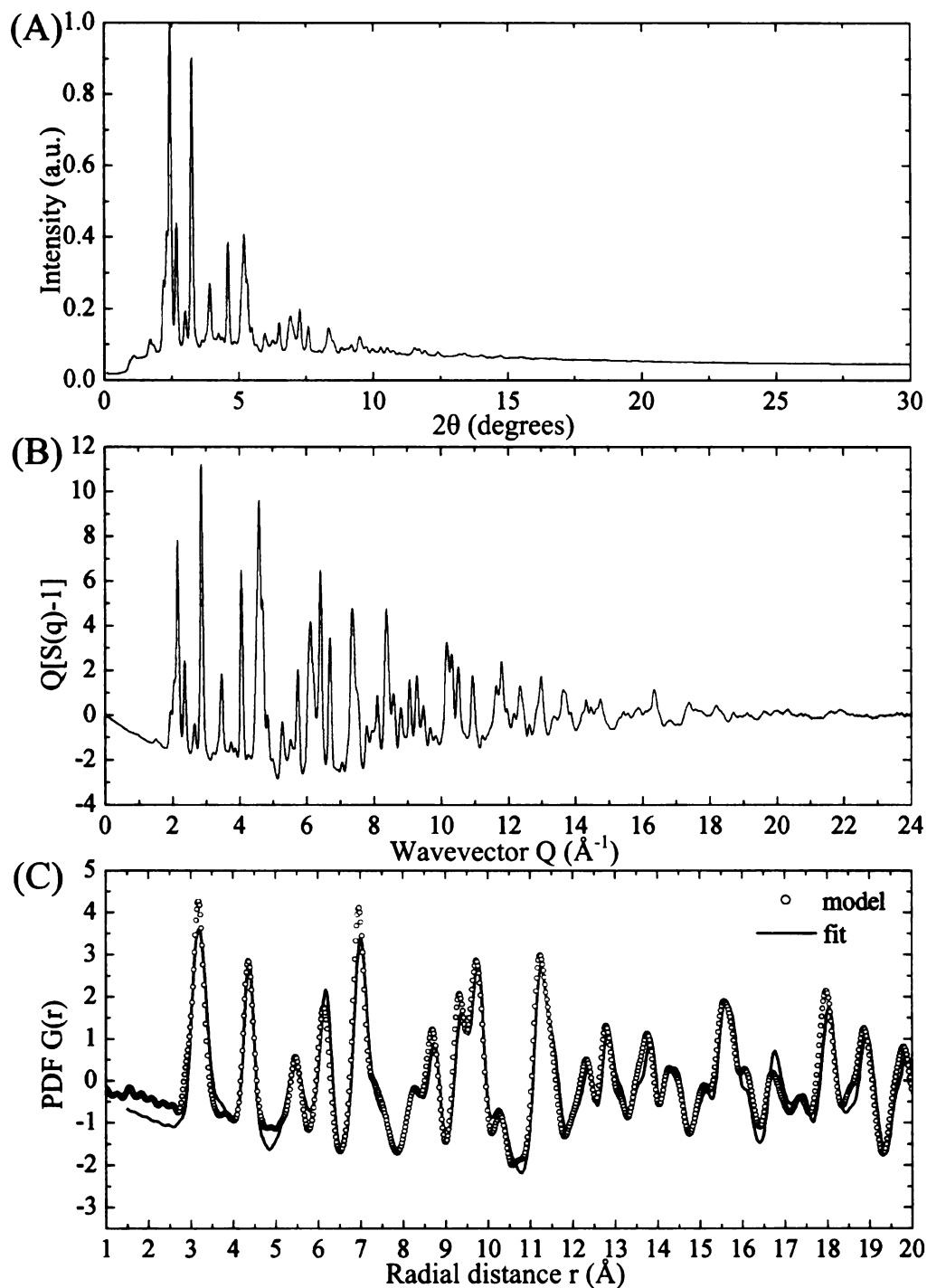


Figure 1.4. (A) Experimental x-ray diffraction pattern of CeTe_3 powder. (B) The corrected and reduced $Q[S(q)-1]$ plot and (C) the PDF $G(r)$ after the Fourier transform.

1.7 Superspace approach for modulated structures

Lattice periodicity is a fundamental concept in crystallography. This property is widely considered as essential for the characterization of the concept of a crystal. In recent decades, however, more and more long-range-ordered condensed-matter phases have been observed in nature that do not have lattice periodicity, so-called aperiodic systems. They only differ from normal crystal phases in very subtle and not easy to observe structural and physical properties. There are three main classes of compounds with aperiodic character. One is the family of commensurate or incommensurate modulated systems. Another one is the group of composite crystals in which at least two different structural motifs (substructures) are crystallized together and form an intergrowth modulated system. In that case, the reflections in reciprocal space of one substructure become supercell reflections of the other one and vice versa. Quasicrystals belong to the third family of aperiodic crystals. In that case symmetry elements like 5-fold, 7-fold, 9-fold etc. rotation axis are present in the diffraction pattern that cannot be described by the conventional crystallographic theory. In this work we will deal only with the first class of incommensurate modulated systems.

A modulation is considered to be a periodic deformation of a “basic structure” having spacegroup symmetry. If the periodicity of the modulation does not belong to the periodicities of the basic structure, the modulated crystal structure is called incommensurate. On the other hand, if the period of the distortion can be generated by a relative small integer number of repetitions of the basic structure, the supercell is called commensurate. This description is based on the observation in the diffraction pattern of

modulated structures of main reflections, situated on a reciprocal lattice, and additional reflections, generally of weaker intensity, called satellites.

1.7.1 Reciprocal space and superspace

Incommensurate crystals are characterized by Bragg reflection peaks in the diffraction pattern which are well separated but do not belong to a lattice and cannot be indexed by three-integer indices, Figure 1.5. Satellites are regularly spaced but they cannot be indexed with three reciprocal vectors. Diffraction pattern has no more three dimensional lattice character and the basic property of crystal, three dimensional translation symmetry, is violated but in a specific regular way. One or more additional, modulation vectors (q -vectors) have to be added to index all diffraction spots.⁴⁰

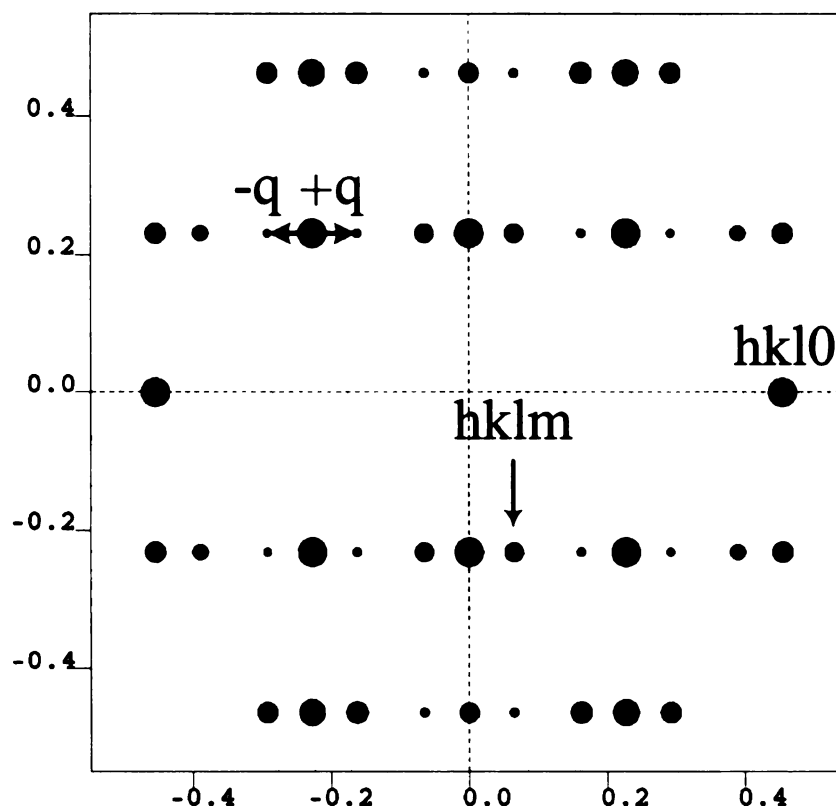


Figure 1.5. Typical diffraction pattern (reciprocal space) of a modulated system. The main strong reflections are indexed as $hkl0$ and the weaker satellite reflections are indexed as $hk1m$ where m is the $(3+1)$ dimensional index.

The positions of all the Bragg reflections can be described by

$$\mathbf{Q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q} = \mathbf{H} + m\mathbf{q} \quad (1.10)$$

where the modulation vector $\mathbf{q}$ can be expressed as a linear combination of $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$

$$\mathbf{q} = q_1\mathbf{a}^* + q_2\mathbf{b}^* + q_3\mathbf{c}^* \quad (1.11)$$

When $m = 0$ then the reflection belongs to the undistorted subcell and is called main reflection. When $m \neq 0$ then the reflection is characterized as satellite due to the supercell formation. In other words, if q_1 , q_2 and q_3 are rational numbers then we have a commensurate modulation otherwise for irrational q_1 , q_2 and q_3 numbers the modulation is incommensurate. It is difficult to prove irrationality only from the measured values of the length of the vectors. The higher the denominators the smaller difference between commensurate and incommensurate situation. But there are cases like $1/2$, $1/3$ where commensurability is easy to identify.

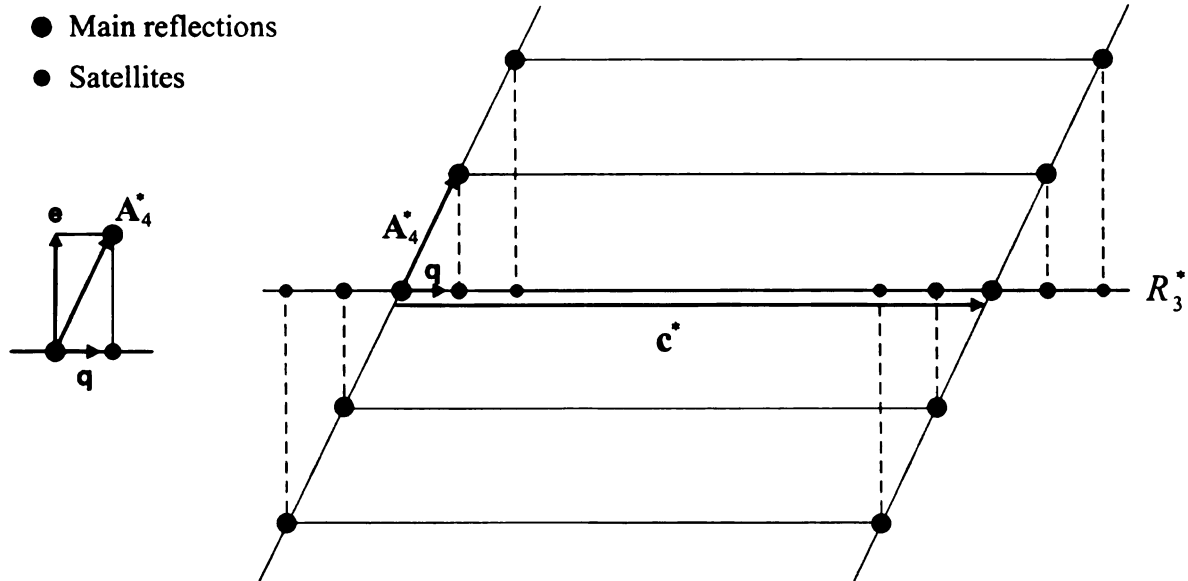


Figure 1.6. Schematic representation of real diffraction pattern (3D) by a projection from the (3+1) dimensional superspace.

Modulated, composite, and quasicrystals can be described in a (3+d) dimensional superspace. The theory has developed by P.M. DeWolff, A. Janner and T. Janssen⁴⁰ (Aminoff prize 1998). This theory allows to generalize concept of symmetry and also to modify all method used for structure determination and refinement of three dimensional systems for aperiodic crystals. The basic idea is that a real diffraction pattern can be seen as a projection from the (3+d) dimensional superspace, Figure 1.6. The additional vector $\mathbf{e}$, perpendicular to the real space $\mathbf{R}_3$, allows the description of the diffraction pattern as a four-dimensional lattice. Therefore, real reflections in the observed three-dimensional space can be understood as a projection along vector $\mathbf{e}$ from a four-dimensional lattice. Thus, the new four-dimensional reciprocal basis can be written as:

$$\mathbf{A}_i^* = \mathbf{a}_i^* \text{ for } i = 1, 2, 3 \text{ and } \mathbf{A}_4^* = \mathbf{q} + \mathbf{e} \quad (1.12)$$

1.7.2 Direct space and superspace

As the diffraction pattern has a four-dimensional lattice character, its Fourier transformation (direct or real space), which represents some generalized four-dimensional density, must fulfill the periodicity condition. Depending on the character of the modulation we shall get different four-dimensional maps. For a positional modulation we can get a map similar to that in Figure 1.7. The map has a translational character and the whole structure can be build up from one four-dimensional basic cell. Individual atoms are now represented by a modulation curve which has periodicity following the four-dimensional lattice. The direct four-dimensional basic vectors are related to the reciprocal ones by the orthonormality condition $\mathbf{A}_i \cdot \mathbf{A}_j^* = \delta_{ij}$ (where δ_{ij} is Kronecker's delta:

$\delta_{ij} = 1$ when $i = j$, and $\delta_{ij} = 0$ when $i \neq j$) which allows the derivation of relationships

between three and four-dimensional basis vectors:

$$\mathbf{A}_i = \mathbf{a}_i - (\mathbf{q} \cdot \mathbf{a}_i) \cdot \mathbf{e} \text{ for } i = 1, 2, 3 \text{ and } \mathbf{A}_4 = \mathbf{e} \quad (1.13)$$

The superspace description gives the possibility to describe a modulated structure in a similar way as a regular structure, Figure 1.7. The density can be again divided into "atoms" but they are not concentrated any more in a relatively small volume but in a so-called atomic domains (atomic strings). In analogy to a regular structure, the atomic domains are again described by a set of parameters which are now a function of the internal coordinate x_4 . For the incommensurate case all sections through the atomic domain are realized in some cell in R_3 , for the commensurate case only some specific values are realized.

A useful coordinate t that characterizes and describes the real three dimensional structure constructed as a perpendicular intersection with the $\mathbf{A}_4$ axis is defined as:

$$t = x_4 - \mathbf{q} \cdot \mathbf{r} \quad (1.14)$$

All different t sections for the incommensurate case are equivalent to only the "first" cell chosen in a different way. On the other hand selection of the t coordinate plays a crucial role in commensurate cases where it can lead to different space groups.

The superspace approach includes all methods for solution and refinement of aperiodic crystals. It enables the use of the tools used in structure analysis of regular crystals such as direct methods, Fourier maps, least squares, distance and angle calculations, bond valence summations, maximum entropy method etc. so that they can be used in a similar way like in standard crystallography.

1.7.3 Symmetry in superspace

There are 775 superspace groups and they were derived and listed by de Wolff, Janssen and Janner in the *International Tables of Crystallography, Volume C* for (3+1) dimensional modulated systems. There are several notations, for example:

$$B^{Pmna}_{s1\bar{1}} \quad \text{or} \quad B : Pmna.s1\bar{1}$$

The first symbol denotes a Bravais class where the four-dimensional centering vectors for each symbol are:

P (000)	A ($\frac{1}{2}, 0, 0$)	B ($0, \frac{1}{2}, 0$)	C ($0, 0, \frac{1}{2}$)
R ($\frac{1}{3}, \frac{1}{3}, 0$)	L (1,0,0)	M (0,1,0)	N (0,0,1)
	U ($0, \frac{1}{2}, \frac{1}{2}$)	V ($\frac{1}{2}, 0, \frac{1}{2}$)	W ($\frac{1}{2}, \frac{1}{2}, 0$)

When there is no three-dimensional analog of a certain centering vector usually along the x_4 , for example ($0, 0, \frac{1}{2}, \frac{1}{2}$), the Bravais class notation becomes “X”.

The symbols introduced in the original paper were later modified and, according to *International Tables Vol. C*, the superspace group mentioned above is written as *Pnma*(01/2 γ)s00. This means that both, the rational and irrational part of the modulation vector are given explicitly. In this notation, the first symbols before the parentheses contain the elements of the three-dimensional space group, *Pnma*. In the parentheses, the components of the modulation q-vector (α, β, γ parameters of equation (1.11)) are introduced. Finally, after parentheses values of translational vectors τ in the fourth-

dimension for each generator that appears in the three-dimensional space group are introduced. A letter symbolizes the value of τ according to:

τ	0	1/2	$\pm 1/3$	$\pm 1/4$	$\pm 1/6$
symbol	0	s	t	q	h

In our example, the notation of the superspace group $Pnma(0\frac{1}{2}\gamma)s00$ means that the undistorted subcell structure has a $Pnma$ symmetry with a rational component of the q-vector of $\frac{1}{2}$ along the b^* and an incommensurate component (γ) along the c^* . Furthermore, there is a non-primitive translation of $\frac{1}{2}$ associated on the n-glide plane along the a^* axis $(\frac{1}{2}a, 0) = (\frac{1}{2}000)$. There are no extra centering conditions along the mirror plane and α -glide plane of b^* and c^* axis respectively.

Similar formalism has been adopted for modulation with two and three q-vectors. Although the corresponding superspace groups were derived by Akiji Yamamoto for (3+2)-dimensions⁴¹ and (3+3)-dimensions⁴² still they are not tabulated in the *International Tables of Crystallography*.

1.7.4 Refinement of modulated structures

The calculation of the structure factors for a modulated crystal comes from an integration procedure since the cells in three-dimensional space are generally different along the modulation. This can be done either numerically or analytically. The numerical procedures are based on Gaussian,⁴³ or FFT⁴⁴ integration and the analytical ones usually on Bessel functions.⁴⁵ Three different programs REMOS,⁴³ MSR⁴⁶ and Jana^{36,47} were developed for the refinement of modulated structures.

The refinement programs use a periodic modulation function $p(x_4) = p(x_4 + n)$, where n is an integer number, to describe the changes of the basic structural parameters along the modulation vector. Due to the periodicity, the distortion (positional, occupational, temperature parameter, etc.) of a given atomic parameter x_4 of the subcell can be expressed by a periodic modulation function $p(x_4)$ in a form of a Fourier expansion:

$$p(k + x_4) = \sum_{n=1}^m A_{sn} \sin[2\pi \cdot \bar{q}_n (k + x_4)] + \sum_{n=1}^m A_{cn} \cos[2\pi \cdot \bar{q}_n (k + x_4)] \quad (1.15)$$

where A_{sn} is the sinusoidal coefficient of the given Fourier term, A_{cn} the cosine coefficient, n the number of modulation waves used for the refinement and k the lattice translation. $\bar{q}_n = \sum_{i=1}^d \alpha_{ni} \mathbf{q}_i$ where α_{ni} integer numbers for the linear combination of the incommensurate modulation vectors $\mathbf{q}_i$. The number of terms used depends on the complexity of the modulation function and therefore on the order of the observed satellites, Figure 1.8A-B.

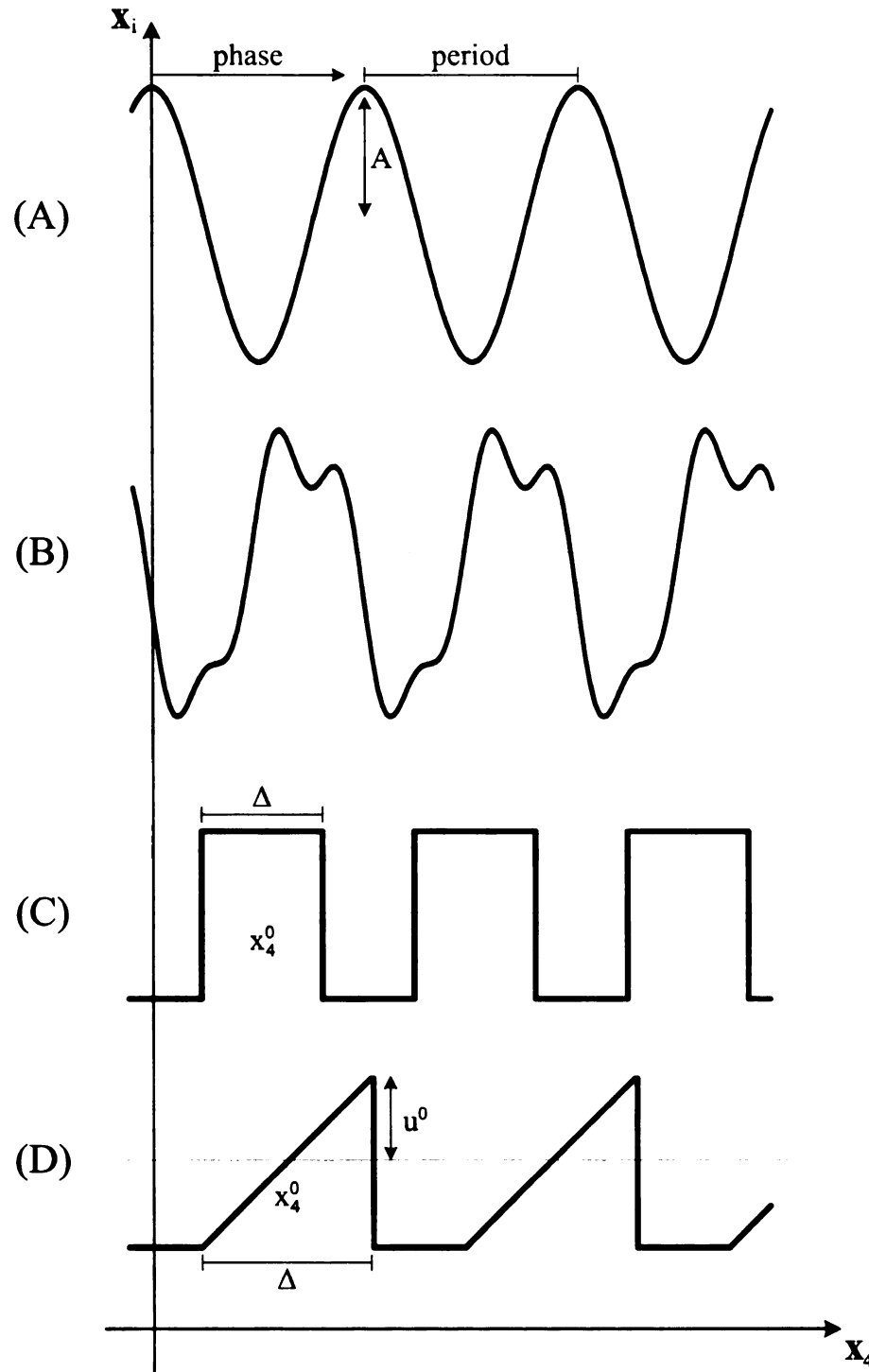


Figure 1.8. (A) Illustration of a harmonic function composed of a single wave with an amplitude A . The period and phase are indicated. (B) A complex square-like harmonic function composed of three waves. (C) A square function (crenel) with center x_4^0 and width Δ . (D) A sawtooth function with center x_4^0 , width Δ and maximal displacement u_0 . Both crenel and sawtooth functions repeat periodically along the x_4 direction.

1.7.5 Positional modulation

The positional modulation affects intensities in a relative complex way. The kinematical theory of diffraction allows derivation of diffracted intensities for harmonic modulation waves. A combination of static waves is used for describing modulated structures in a similar derivation fashion like the expression of thermal vibrations in the crystal. The independent derivations for various cases were made by several authors.^{34,36,48,49} For a simple harmonic modulation wave the modulation displacement $\mathbf{u}$ and the corresponding structure factor F can be expressed as:

$$\mathbf{u} = \mathbf{U} \cos(2\pi \mathbf{q} \cdot \mathbf{r}) \text{ and } F = f \exp(2\pi i \cdot \mathbf{Q} \cdot \mathbf{r}) J_m(2\pi \mathbf{U} \cdot \mathbf{H}) \quad (1.16)$$

The symbol J_m stands for the m -th order Bessel function, m being the satellite index. The argument is a scalar product of the diffraction vector $\mathbf{H}$ with the modulation amplitude $\mathbf{U}$. Therefore, all satellites with $\mathbf{H}$ perpendicular to $\mathbf{U}$ are unobserved. This makes it possible to draw some conclusions concerning the modulation amplitude directly from the diffraction pattern.

1.7.6 Substitutional modulation

There are cases that a single crystallographic site is occupied by two or more atoms. Assuming that the probability of finding a given atom on that site is a harmonic function of the x_4 coordinate, the atomic form factor can be described as

$$f_v = \frac{f_{1v} + f_{2v}}{2} + \frac{f_{1v} - f_{2v}}{2} \sin(2\pi \cdot \mathbf{q} \cdot \mathbf{r}_v) \quad (1.17)$$

This gives rise to main reflections and first order satellites:

$$\begin{aligned}
F_{\nu}(hkl0) &= \frac{f_{1\nu} + f_{2\nu}}{2} \exp(2\pi \cdot i \cdot \mathbf{Q} \cdot \mathbf{r}_{\nu}) \\
F_{\nu}(hkl \pm 1) &= \frac{f_{1\nu} - f_{2\nu}}{2} \exp(2\pi \cdot i \cdot \mathbf{Q} \cdot \mathbf{r}_{\nu})
\end{aligned}
\tag{1.18}$$

The diffraction pattern has isotropic character and satellites are generally present in all positions predicted by the $\mathbf{q}$ vector. Their intensity depends on differences in the form factors of two atoms. The main reflections are also modified and their structure factors are the average of two limiting cases.

Furthermore, it is possible to have positional and occupational modulations on the same structure. This situation creates a more ordered picture with the presence of higher order satellite reflections. The shape of the overall modulation function is rather complex and in general it takes a combination of a lot of harmonic waves in order to fully describe the observed distortion. Special functions have been deployed for describing possible discontinues substitutional patterns (Crenel function) or discontinues positional and occupational distortions (Sawtooth function).

1.7.7 Crenel function

Occupational distortions sometimes cannot be described by a relative small number of harmonic waves as we assumed in the previous case. The occupational modulation pattern may look like a step-like discontinuous function with sharp changes on the occupied fraction from 0 to 1, Figure 1.8C. The so-called crenel functions are discontinuous periodic functions constructed for the description of such cases. The occupational modulation often occurs as atomic blocks that are occupied by one kind of

atom. These blocks can have different width and order. Such a model can be described by a periodic discontinuous modulation function:⁵⁰

$$\begin{aligned} p(x_4) &= 1 \text{ for } x_4 \in \langle x_4^0 - \Delta/2, x_4^0 + \Delta/2 \rangle \\ p(x_4) &= 0 \text{ for } x_4 \notin \langle x_4^0 - \Delta/2, x_4^0 + \Delta/2 \rangle \end{aligned} \quad (1.19)$$

where Δ and x_4^0 are the width and center of the crenel function. The Fourier transform of this function gives

$$P_m(\Delta, x_4^0) = \exp\left(2\pi \cdot i \cdot m \cdot x_4^0\right) \sin(\pi \cdot m \cdot \Delta) / \pi \cdot m \quad (1.20)$$

that modifies the atomic contribution to the structure factor. Such a modulation induces strong satellites up to very high order. Similarly as for the harmonic modulation, the diffraction pattern has isotropic character but the number of observable satellites is much higher. According to equation (1.20) intensities of satellites are dropping off as $1/m^2$. The crenel like modulation was originally introduced to account for a strong occupation modulation in one special structure⁵¹ but nowadays plays a very important role as it allows the description of a general discontinuity in a modulated structure.

The substitutional modulation naturally induces some periodic incommensurate tension in the crystal as the two different atoms cannot generally fit to the same position and coordination. This often causes an additional positional modulation. The Crenel function is applied on the last wave of the overall modulation (possible combination of waves for positional distortion) and it significantly reduces the number of parameters compared to the use of a large number of Fourier series of harmonic waves.

1.7.8 Sawtooth function

Similar to the picture of distortions with discontinuous occupational waves, we may have cases in which the positional parameters behave discontinuously. The corresponding function that can describe this behavior is called sawtooth function, Figure 1.8D. The width Δx_4 is defined as the length of the projection of the sawtooth function on the x_4 -axis. It repeats periodically along the horizontal direction x_4 , causing a linear displacement of $-\Delta x_i$ to $+\Delta x_i$ in a range of width Δx_4 centered at x_4^0 on the internal direction where $i = 1, 2, 3$ for $x_4 \in \left\langle x_4^0 - \Delta/2, x_4^0 + \Delta/2 \right\rangle$.

$$p(x_4) = 2\Delta x_4^0 \left(\frac{x_4 - x_4^0}{\Delta} \right) \quad (1.21)$$

In addition, the sawtooth function has an occupational character. The value of the width Δ can be less than one and in that case the occupation will have a step-like character as we saw in the crenel case. Similarly, the number of satellite reflections is much higher than those observed for a single harmonic wave.

1.7.9 Examples of continues and discontinues distortions in real space

A few illustrations of how distortions may look like in real space can be found in Figures 1.9-1.11. A single harmonic positional wave of atoms may occur at any direction in the three-dimensional space. On an undistorted square pattern of atoms, Figure 1.9A, a positional distortion can be along a longitudinal direction and create in-plane

displacements along the direction of the net, Figure 1.9B. Another possibility is to have a transverse distortion and the creation of out-of-plane displacements as can be seen in Figure 1.9C. The overall modulation will create a new periodicity in the system and this can be apparent from the examination of the reciprocal diffraction pattern of Figure 1.9D. Extra satellite reflections will be present indicative of the periodic distortion.

In a more complex system we can have a combination of positional and occupational modulation with discontinuous character, Figures 1.10-1.11. Let's assume domain 1 with a concentration of $2/3$ which possesses a positional modulation of the complex shape shown in Figure 1.10. The complementary fraction of $1/3$ is occupied by domain 2 which is not distorted (flat line). The four-dimensional unit cell is notated (see Figure 1.7 as well). The resulting sequence of atoms (position and occupation) in the real space will depend on the specific value of the t -coordinate we choose. The "cuts" for two T -values of 0.26 and 0.59 are shown at the bottom of Figure 1.10. The component of the q -vector in this case is 0.24. Note the difference of the atomic sequences between the two T -values in terms of position and occupancy. Let's examine now a situation in which the length of the q -vector changes, Figure 1.11. The atomic domains and four-dimensional unit cell are exactly the same like in the previous example. The observed sequence of atoms now is quite different from the one observed before even if we choose the same t -sections. The q -vector component in the later case is 0.13.

It is amazing how a small variation of modulation parameters (q -vector, occupancy, etc.) can dramatically affect the real space picture. From the other hand, it's apparent how the superspace approach can successfully describe a complex modulated structure with a small number of parameters.

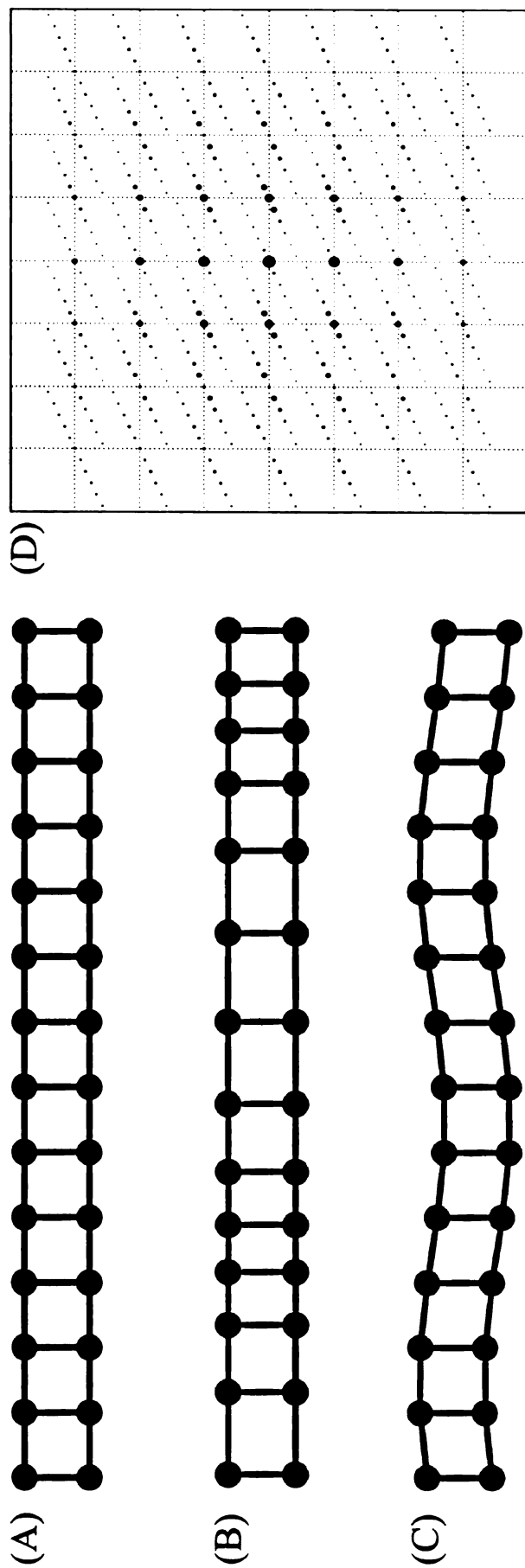
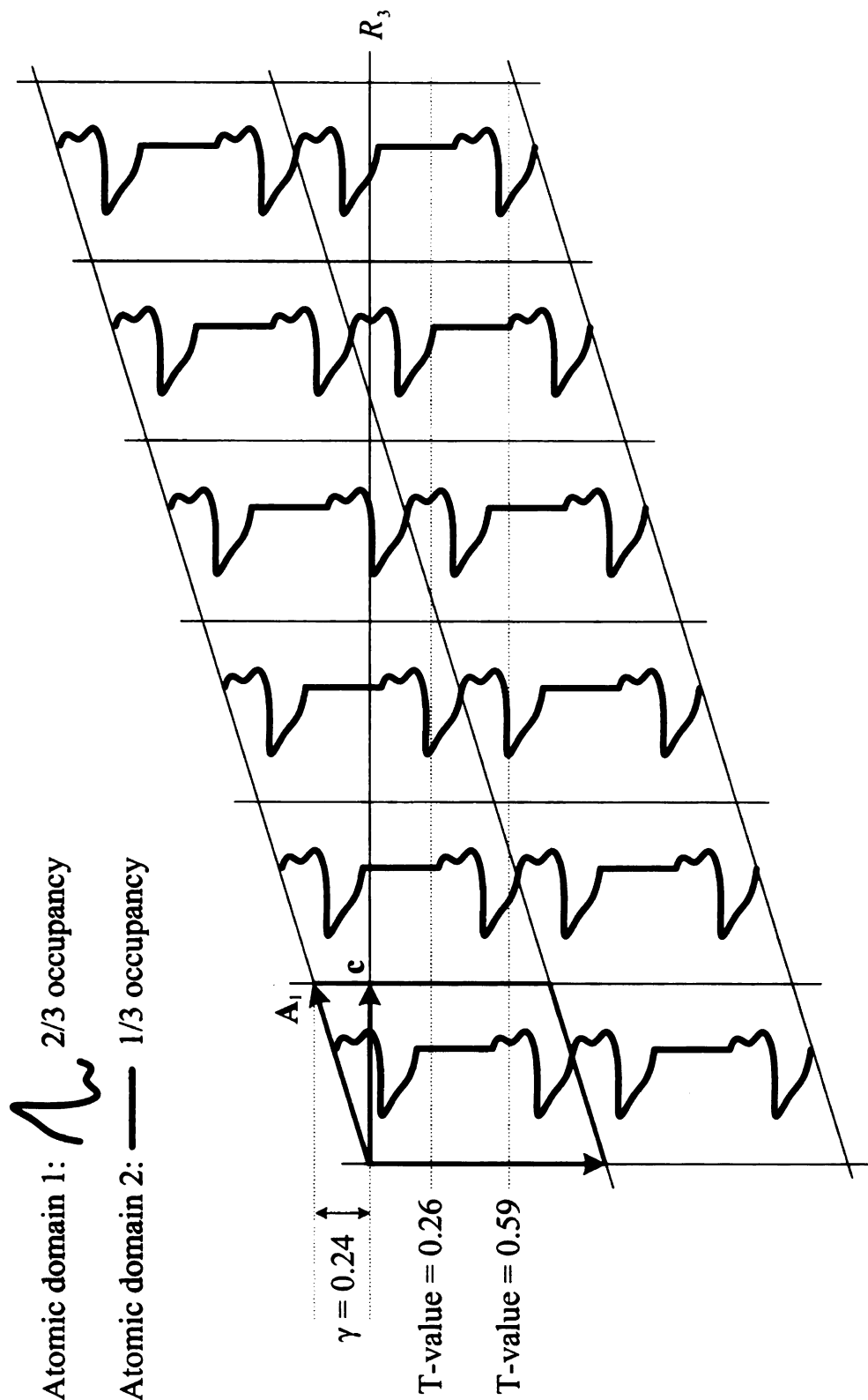


Figure 1.9. (A) Undistorted pattern of atoms. (B) Longitudinal positional modulation in direct space. (C) Transverse positional modulation in direct space. (D) Diffraction pattern of the modulated patterns.



Resulting sequence for:

T-value = 0.26 $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$

T-value = 0.59 $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$ $\bullet$

Figure 1.10. Combination of a harmonic modulation wave and a crenel function in real space. The resulting sequence of atoms is shown for two different t-sections with a q-vector component of 0.24.

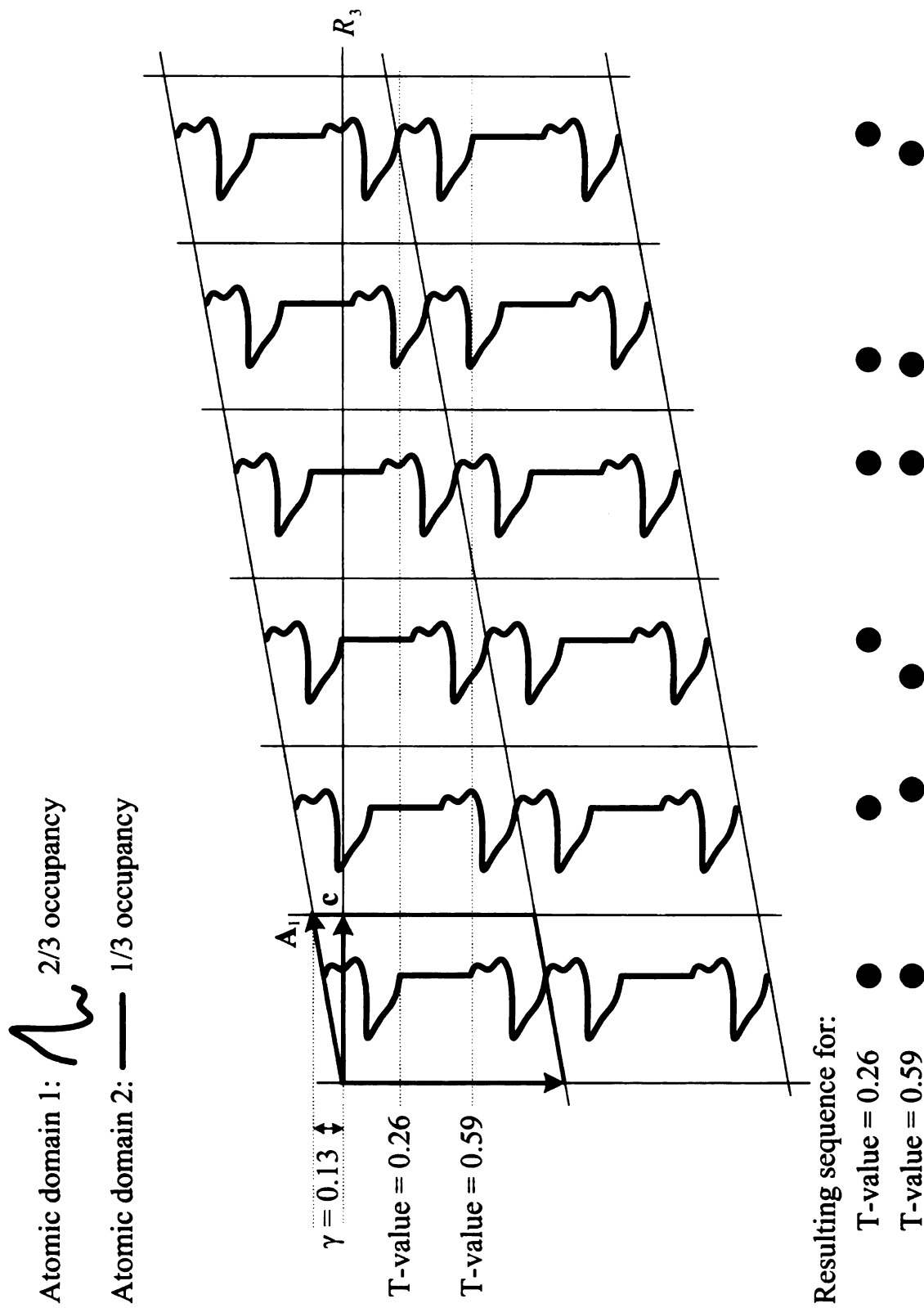


Figure 1.11. Combination of a harmonic modulation wave and a crenel function in real space. The resulting sequence of atoms is shown for two different t-sections with a q-vector component of 0.13.

1.7.10 Structure solution of modulated crystals

The structure solution of modulated systems can be divided into two steps. First we have to find the structure of the subcell that is described by the electron density coming from the main reflections of the experimental reciprocal space. The average undistorted cell of the main reflections can be solved using traditional ways for solution like direct and heavy atom methods. The structure solution can be performed by programs such as SHELX⁵² or SIR.⁵³ The quality of the refinement of the subcell depends on the magnitude of the distortion. For weakly modulated systems (atomic displacements less than 0.1 Å) the refinement is usually reasonable or sometimes so good that no evidence of distortion is present. Usually structural indications reminiscent of distortion in the refined subcell can be relative large harmonic ADP parameters, anharmonicity or splitting. For strongly modulated systems the solution of the average structure can be a big problem. In that case, the intensities of the main reflections have to be corrected for the presence of satellites. The simplest method that works well for simple modulations is to add the intensities of the satellite reflections to the intensity of main reflections.

Since the structure of the subcell has been found the next step is to describe the modulation coming from the intensity of the satellite reflections. Trial and error is a typical tool in order to find a proper starting point (superspace group, modulation waves, etc.) for the refinement of modulated structures. The smaller the displacements in the distorted structure, the more insensitive the refinement to the quality of the starting point. Often we start refining the modulated structure just from small displacements. The situation is similar to the refinement of ADP harmonic parameters for a regular structure.

In analogy to regular structures, both direct⁵⁴ and heavy atom⁵⁵ methods for solution of modulated structures have been developed. Both methods start from the known average structure.

If all trials to solve a modulated structure fail, we have to use some supercell approximation and try to solve the structure in a large cell. This can be a difficult task that often requires advanced direct methods. The supercell solution then can be used as a starting point for the final modulated refinement.

1.7.11 Special books, literature and resources on superspace concept

The basic physical and mathematical concepts of modulated structures were briefly described in this chapter in order to help the reader to understand the results reported in this thesis. For a detailed description of the theory of aperiodic systems I strongly recommend the following material:

- van Smaalen, S. "*Incommensurate Crystallography*", Oxford University Press, **2007**.
- Janssen, T.; Chapuis, G. and de Boissieu, M. "*Aperiodic Crystals: From Modulated Phases to Quasicrystals*", Oxford University Press, **2007**.

Some more references can be found in the review articles bellow:

- International Tables for Crystallography, Volume C - Mathematical, Physical and Chemical Tables in the chapter "*Incommensurate and Commensurate Modulated Structures*" by Janssen, T.; Janner, A.; Looijenga-Vos, A.; de Wolff, P. M.
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- Pérez-Mato, J.; Zúñiga, F. and Madariaga, G. E. "*Superspace description of commensurately modulated structures. Methods of structural analysis of modulated structures and quasicrystals*", World Scientific. Singapore, New Jersey, London, Hong Kong, **1991**, p. 117.
- Pérez-Mato, J. M.; Madariaga, G.; Zúñiga, F. J. and Garcia Arribas, A. "*On the structure and symmetry of incommensurate phases. A practical formulation*", *Acta Cryst.* **1987**, *A43*, 216.

Finally, some resources that I found very helpful for preparing this introductory part:

- Web site of Ivan Orlov and Gervais Chapuis at <http://lcr.epfl.ch/>.
- Ivan Orlov's thesis. EPFL, Switzerland, 2007.
- Hanna Lind's thesis. University of Stockholm, Stockholm, 2004.

1.8 Conventions of the thesis

Detailed crystallographic data reports for all the solved and refined modulated structures can be found in the individual chapter of this thesis. All the Fourier coefficients of the general harmonic equation (1.15) were freely refined based on the superspace symmetry conditions for every case. The Fourier term A_{cn} was notated as cos, n in the crystallographic tables and the term A_{sn} as sin, n . For examples, the sinusoidal coefficient of the second harmonic waves was symbolized as "sin, 2". The minimum, maximum and average values of the distribution of bond distances and angles between atoms are given instead of "static" three dimensional lengths. Each distribution was calculated for the first period of the t -section with a resolution of 0.1. The bonding cutoff between atoms was 3.5 Å.

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Chapter 2

Reactions of Rare-Earth Metals (RE) and Tellurium: Size Effect of Rare Earth to the Distortions of the Tellurium Net of RETe_3

“Square Nets of Tellurium: Rare-Earth Dependent Variation in the Charge-Density Wave of RETe_3 (RE = Rare-Earth Element)”, Malliakas, C. D.; Billinge, S. J. L.; Kim, H. J.; Kanatzidis, M. G. *J. Am. Chem. Soc.* **2005**, *127*, 6510-6511. American Chemical Society (ACS) is gratefully acknowledged for the permission to include this reprint in the Thesis.

2.1. Introduction

The tritellurides RETe_3 (RE = rare earth element)^{1,2} were originally reported to crystallize in the layered so-called NdTe_3 structure type, however recently they were recognized to be two-dimensional CDW materials. A salient feature of this structure is monolayers of Te atoms that appear to define “perfect” square nets. All Te-Te distances in the net are ~ 3.1 Å, too long to be normal bonds yet too short to be ignored as non-bonding. Because of the novel bonding implications of a square net it would be rather exciting if ideal square nets of Te actually existed in the entire absolute temperature range. This picture, however, is incorrect and deceptive as it masks completely the true underlying structure.³ Square net arrangements of atoms are predicted theoretically⁴ to be unstable and prone to charge density waves (CDW) and therefore systems which feature them, such as RETe_3 , are of great interest. Electron diffraction studies on several RETe_3 compounds revealed evidence for the presence of long range ordering.⁵ This casts doubt on the “perfect” square net picture and raises the possibility of lattice distortions of the charge density wave (CDW) type in RETe_3 .⁶ Electrical conductivity measurements on RETe_3 systems indicate metallic behavior and absence of a band gap in these materials.⁷ Therefore detailed knowledge of the long range modulations is necessary to correctly understand the properties of RETe_3 . Modulations in Te nets have been found in more complex multinary compounds such as KBaAgTe_2 ³, and LaTe_2Se ⁸ which show oligomerization within the net to Te_x^{2-} fragments where x varies depending on electrons per Te atom. Complicating further the structural issue is that the distortions can be incommensurate with the underlying sublattice, which historically has frustrated attempts at a complete crystallographic analysis.

2.2. Experimental Section

2.2.1. Reagents

The following reagents were used as obtained. All rare-earth metals, 99.9% pure, fillings from ingot, Chinese Rare Earth Information Center, Inner Mongolia, China; Tellurium shots, 99.9% pure, Tellurex Corporation, Traverse City, MI; Rubidium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Lithium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Lithium Iodide, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Potassium Iodide, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; N, N – Dimethylformamide (DMF), ACS reagent grade, Spectrum Chemicals, New Brunswick, NJ; Diethyl ether anhydrous, ACS reagent grade, Columbus Chemical Industries, Columbus, WI.

2.2.2. Synthesis

$RETe_3$ ($RE = La, Ce, Pr, Nd, Sm, Gd, Tb$ and Dy) – All manipulations were carried out under dry nitrogen atmosphere in a Vacuum Atmospheres Dri-Lab glovebox. Stoichiometric amounts of rare earth (~ 0.3 g) and tellurium (~ 0.82 g) were loaded into quartz tubes under nitrogen together with a double amount (~ 2 g) of halide flux (0.42:0.58 molar mixtures of RbCl and LiCl). The tubes were sealed under vacuum ($<10^{-4}$ torr) and heated to 650 °C at 12 hours for 6 days. The tubes were then cooled down to room temperature at a rate of 4 °C $\cdot$ min $^{-1}$. The halide flux was dissolved in water and the crystals were washed with acetone and dried under nitrogen environment. The morphology of the crystals is that of thin plates with a brown (copper-like) color.

Electron microprobe energy dispersive spectroscopy (EDS) was performed on several crystals of the compound and confirmed the 1:3 ratio of the rare earth to tellurium and the absence of other elements of the flux. Compounds found to be X-ray pure and moisture sensitive after exposure to air for a few days.

RETe₃ (RE = Ho, Er, Tm and Y) – In the case of the heavier rare earths the RbCl/LiCl halide flux reacts with the elements producing Rb_xRE_yTe_z compounds. Instead, an eutectic halide of LiI and KI (0.37:0.63 molar mixtures) was used to synthesize the target RETe₃ binaries. Similarly, stoichiometric amounts of rare earth (~ 0.3 g) and tellurium (~ 0.82 g) were loaded into quartz tubes under nitrogen together with a double amount (~ 2 g) of the halide flux. The tubes were sealed under vacuum (<10⁻⁴ torr) and heated to 650 °C at 12 hours for 6 days. The tubes were then cooled down to room temperature at a rate of 4 °C·min⁻¹. The halide flux was dissolved in DMF since the crystals found to be extremely moisture sensitive (surface becomes black after a few seconds of exposure to water / moisture) and the crystals were washed with ether and dried under nitrogen environment. The morphology of the crystals is that of thin plates with a brown (copper-like) color. Electron microprobe energy dispersive spectroscopy (EDS) was performed on several crystals of the compound and confirmed the 1:3 ratio of the rare earth to tellurium and the absence of other elements of the flux. Compounds found to be X-ray pure.

2.2.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran

Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – A single crystal of each RETe₃ member was mounted with glue on the tip of a glass fiber. Intensity data were collected on a STOE IPDS II diffractometer equipped with a graphite monochromatized Mo radiation ($\lambda = 0.71073\text{\AA}$) and an Image Plate (IP) detector. The data were collected with an ω -scan technique from 0-180° and an arbitrary ϕ -angle. Data reduction was performed with the X-Area package.⁹ The length determination and refinement of the q-vectors was performed with the Peaklist 1.06 software part of the X-Area suite using a least square refinement algorithm. An analytical absorption correction was performed (X-Shape within X-Area) and all structures were refined with JANA2000 software.¹⁰ Direct methods of SHELXTL software¹¹ were used to find the atomic positions in the subcell.

Satellite reflections of first order were observed and used for the refinement. A single modulation wave for positional parameters was used. Only the symmetry allowed Fourier terms were refined. The pseudo-tetragonal character of the crystal system allows the plates to stack and twin in a merohedral fashion. Therefore high electronic densities were observed in different positions from the calculated ones for some of the RETe₃ members. By applying a twin law of a rotation of 90° along *b*-axis

$$\begin{bmatrix} a' \\ b' \\ c' \end{bmatrix} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \text{ the R factors for all the reflections (R}_1\text{/wR}_2\text{) in the refinement}$$

significantly dropped (for the case of the NdTe₃ subcell from 11.97/28.90 to 2.62/5.83).

The complete data collection parameters and details of the structure solution and

refinement for all RETe_3 members at 300 K are given in Tables 2.1-2.73. Temperature was controlled by an Oxford Cryostream 700 Plus cryostat.

Transmission Electron Microscopy of CeTe_3 – Selected area electron diffraction (SAED) studies were carried out on a JEOL 2010F (Japan Electron Optics Laboratories) 200 kV field emission TEM at the Center for Advanced Microscopy of Michigan State University. A thin plate crystal of CeTe_3 was polished and ion-milled in order to be thin enough for TEM study. The crystal was mounted on a copper aperture grid. For the cross section diffraction experiment a stack of plate crystals was sandwiched between two thin carbon plates and polished / ion-milled.

Infrared (IR) Spectroscopy – Optical diffuse reflectance measurements were performed on single crystals of all RETe_3 members at room temperature. The spectra were recorded in the Mid-IR region ($6000 - 400 \text{ cm}^{-1}$) with a Nicolet 6700 FT-IR Spectrometer equipped with a diffuse reflectance collector from Spectra-Tech Inc.

Pair Distribution Function of RETe_3 ($\text{RE} = \text{Ce}, \text{Pr}$ and Nd) – Powder samples of RETe_3 ($\text{R} = \text{Ce}, \text{Pr}$ and Nd) were packed in 1.0 mm thick flat plates sealed between kapton tapes. The X-ray scattering experiments were conducted on the RETe_3 samples with 99.8 KeV ($\lambda = 0.1242 \text{ \AA}$) X-ray at the 6-ID-D beam line at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL). Powder diffraction data were collected at 300 K using the recently developed rapid acquisition pair distribution function (RA-PDF) technique. In order to avoid the saturation of the detector, each measurement was made for 4 seconds, and repeated 5 times to improve counting statistics. All the corrections, the total scattering structure function $S(Q)$ and PDF $G(r)$ were obtained using the program PDFgetX 2.0.¹²

2.3. Results and Discussion

Subcell Description of RETe_3 – The average structure of RETe_3 adopts the space group Cmcm . It consists of puckered double layers of (RETe) that are sandwiched by the planar nets of Te making a RETe_3 slab. The slabs then stack along the b -axis creating van der Waals gaps. The formula can be more expressly written as $(\text{RETe})^+(\text{Te}_2)^-$, Figure 2.1A. The RE atom is in a monocapped tetragonal antiprism of Te atoms, Figure 2.1B. The apparent Te-Te distances in the square net are $3.1034(6)$ Å (for CeTe_3), Figure 2.1C.

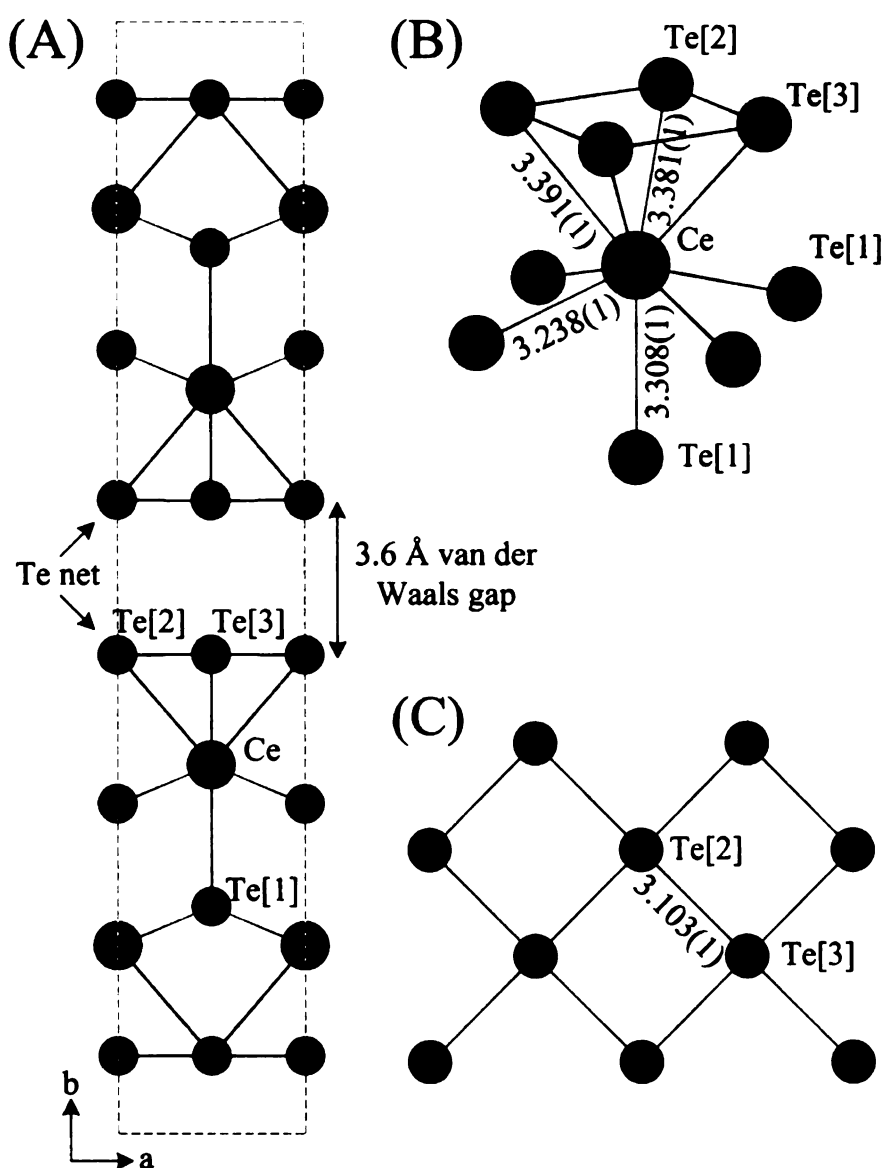


Figure 2.1. (A) Undistorted structure of CeTe_3 . (B) Coordination geometry and environment of Ce. (C) Ideal square net of Te atoms in the CeTe_3 subcell.

Electron Transmission Microscopy of CeTe₃ – Electron diffraction studies on CeTe₃ revealed a commensurate 7-fold superstructure along the ac-plane, Figure 2.3A. The superstructure has an approximate cell of $c_{\text{sup}} = 7c_{\text{sub}}$ due to the presence of relative weak in intensity satellite reflections along the c^* direction. A densitometric intensity scan along the ($h1-1$) row of reflections is shown in Figure 2.3B with the satellite reflections located at a distance of $0.285c^*$ from the main (01-1) spot. The electron diffraction pattern along the ab-plane (cross-section) shows that there is no modulation along the b^* direction since there are no supplementary supercell spots, Figure 2.4A.

Commensurate Supercell Description of RETe₃ (RE = Ce, Pr and Nd) – The TEM results led us to single crystal x-ray diffraction studies which confirmed the supercell of $c = 7c_{\text{sub}}$ axis in space group Ama2 (Figure 2.2A) for RETe₃ (RE = Ce, Pr and Nd) analogs, Table 2.1. The modulation is mostly located on the tellurium net and results in a wide distribution of distances between the Te atoms. For CeTe₃ the minimum Te-Te distance in the net is 2.939(8) Å and the maximum 3.266(3) Å. For PrTe₃ these distances are 2.939(6) Å and 3.201(6) Å respectively, and for NdTe₃ they are 2.959(7) Å and 3.214(7) Å respectively. By taking less than 3.020 Å to be the Te-Te bonding threshold, the square net contains V-shaped trimers and N-shaped tetramers, Figure 2.2B. For the Ce analog, the Te-Te distances within the two different V-shaped trimers are 2.985(8) and 2.979(8) Å respectively, whereas within the N-shaped tetramers are 2.939(8), 3.001(8) and 3.002(9) Å. The sequence of trimers and tetramers found to be the same for the RETe₃ (RE = Ce, Pr and Nd) members using the commensurate solution. These Te-Te distances are much longer than those found in classical isolated Te₃²⁻ and Te₄²⁻ polytelluride anions.¹³ In the latter normal Te-Te bonds are in the order of 2.8 Å. The

longer Te-Te distances observe in the V-shaped trimers and N-shaped tetramers of the net may be the result of averaging over a wider distribution of different oligomers than those observed crystallographically and also due to significant inter- polytelluride interactions³ that tend to disturb the normal order of the intra-polytelluride bonding. The calculated electron diffraction pattern of the model we obtained from the single crystal X-ray refinement matches with the experimental one, Figure 2.4B.

By using the Zintl-Klemm concept and considering rare-earth atoms to be RE^{3+} ions and the Te atoms in the $(\text{RETe})^+$ part to be 2^- , each Te atom in the net must have an average charge of -0.5 according to the formula $[(\text{CeTe})^+]_7[\text{Te}_{14}]^{7-}$. However if we assume the V-shaped trimers and N-shaped tetramers to be Te_3^{2-} and Te_4^{2-} polytellurides units then we can expect the over all charge of the Te-net to be $[\text{Te}_{14}]^{8-}$ which is one electron rich compared to the expected $[(\text{CeTe})^+]_7[\text{Te}_{14}]^{7-}$. If the extra electron is located randomly on Te_3^{2-} or Te_4^{2-} units then this will also be an additional reason for lengthening the average Te-Te bonds in the net.

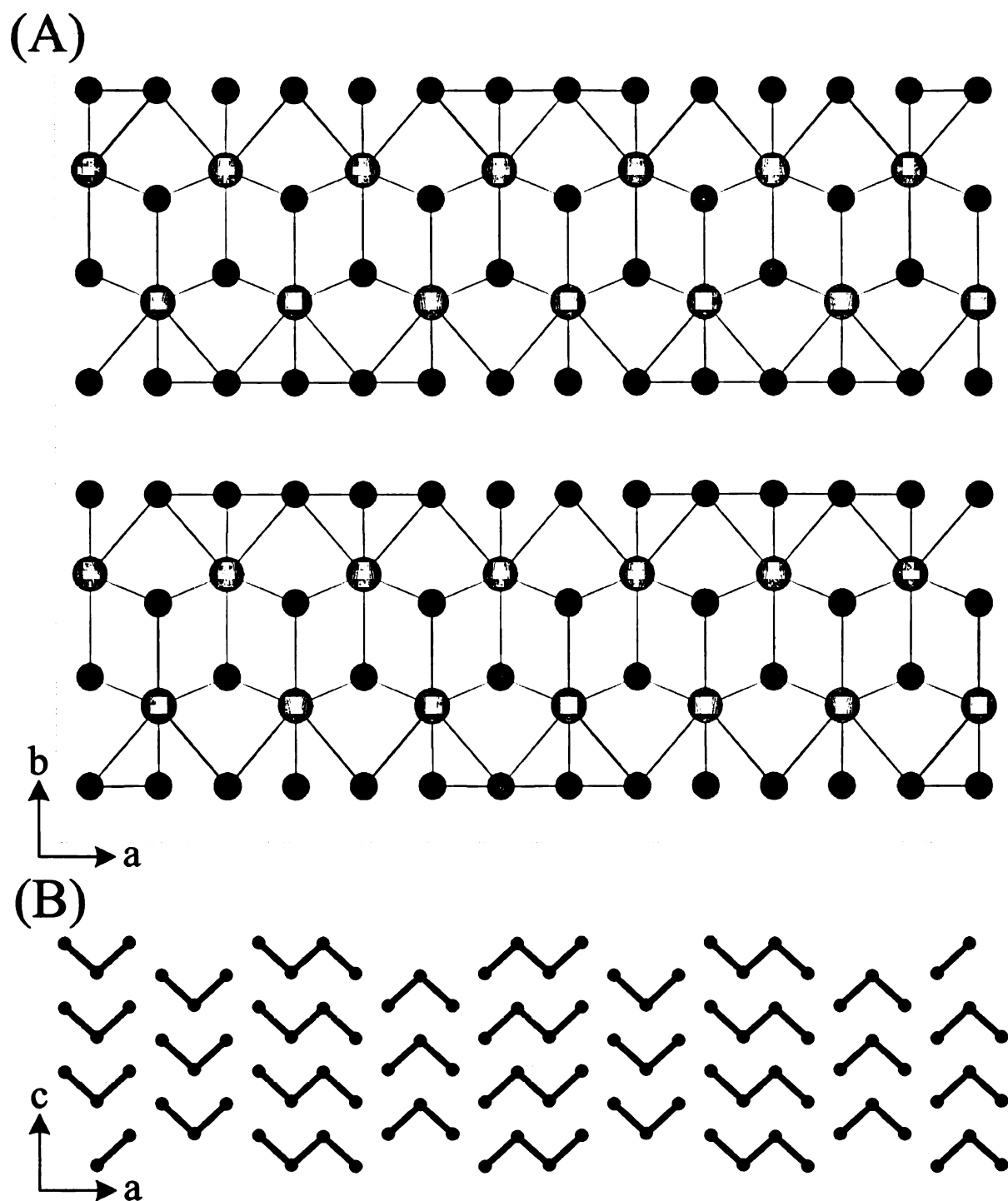


Figure 2.2. ORTEP representation of the (A) commensurate 7-fold supercell of CeTe_3 as seen down the c -axis (95% probability ellipsoids). (B) Distorted tellurium net at a threshold of 3.020 Å.

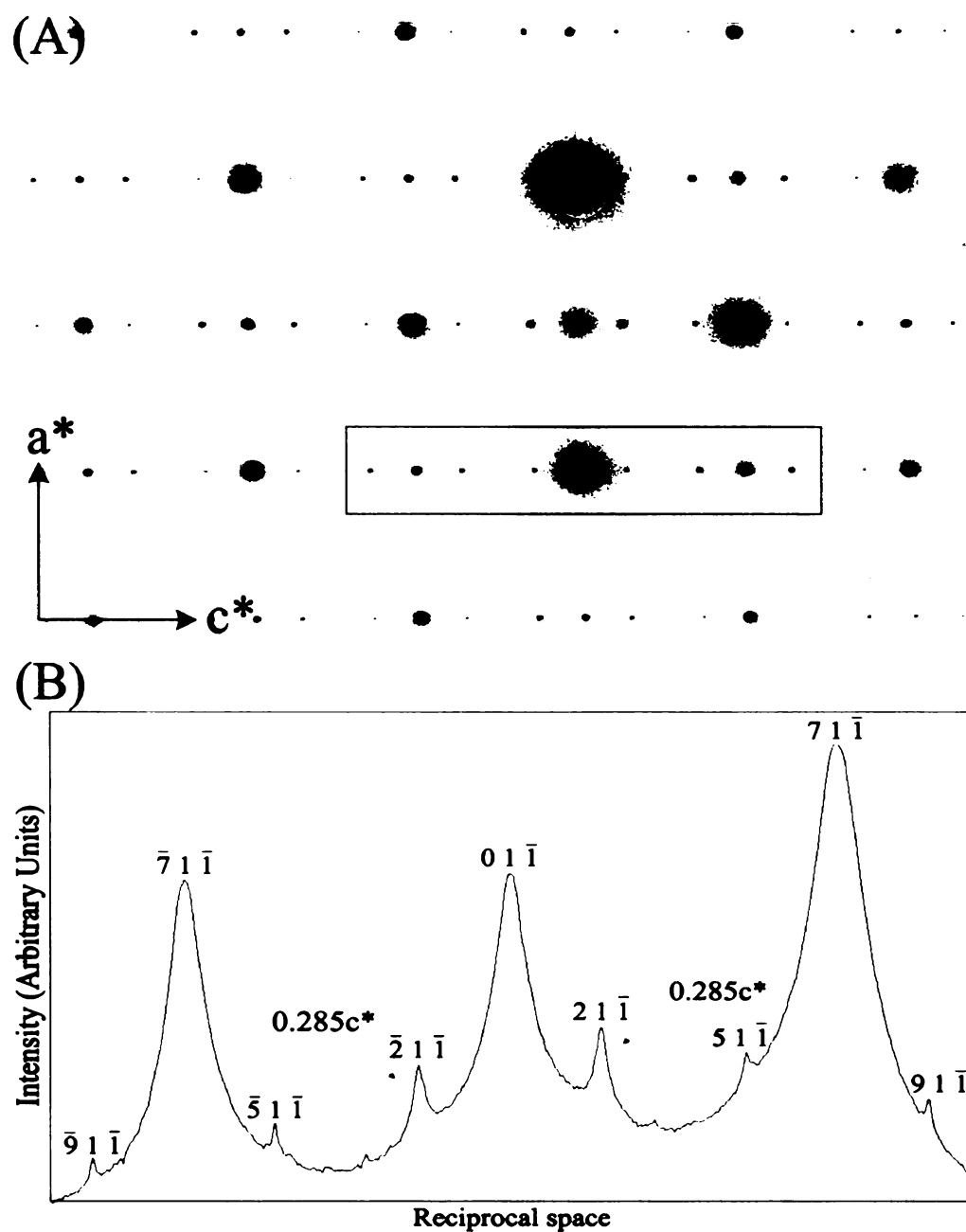


Figure 2.3. (A) Selected area electron diffraction (SAED) pattern for CeTe_3 at the $[010]$ orientation showing the 7-fold superlattice. (B) Intensity scan along the c^* axis of the SAED pattern (shown in rectangular box) and approximate indexing based on supercell. The q -vector is also indicated.

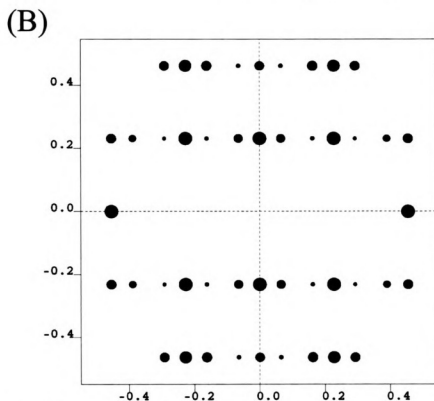
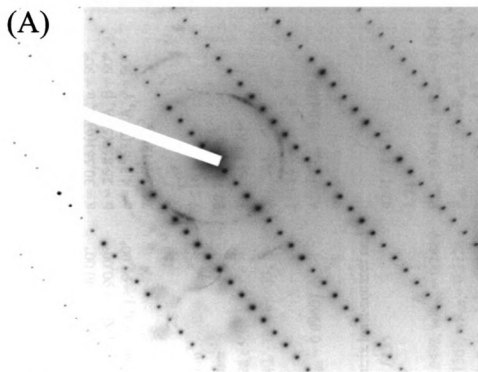


Figure 2.4. (A) Cross section selected area electron diffraction (SAED) pattern for CeTe_3 at the $[100]$ orientation. (B) Theoretical calculated diffraction pattern based on the commensurate supercell model.

Table 2.1. Crystal data and structure refinement for CeTe₃, PrTe₃ and NdTe₃ using the commensurate solution at 300 K.

Empirical formula	CeTe ₃	PrTe ₃	NdTe ₃
Formula weight	522.9	523.71	527
Crystal system		Orthorhombic	
Space group		Ama2	
Unit cell dimensions	a = 30.800(8) Å, α = 90° b = 26.055(7) Å, β = 90° c = 4.3810(12) Å, γ = 90°	a = 30.640(8) Å, α = 90.00° b = 25.915(7) Å, β = 90.00° c = 4.3598(11) Å, γ = 90.00°	a = 30.561(6) Å, α = 90° b = 25.859(5) Å, β = 90° c = 4.3563(9) Å, γ = 90°
Volume	3515.8(16) Å ³	3461.9(15) Å ³	3442.7(12) Å ³
Z		28	
Density (calculated)	6.913 g/cm ³	7.034 g/cm ³	7.116 g/cm ³
Absorption coefficient	26.023 mm ⁻¹	26.998 mm ⁻¹	27.789 mm ⁻¹
Theta range for data collection	1.32 to 28.48°	1.33 to 28.65°	1.33 to 28.61°
Index ranges		-40<= <i>h</i> <=40, -33<= <i>k</i> <=33, -5<= <i>l</i> <=5	
Reflections collected	19997	17728	15114
Independent reflections	4258 [R _{int} = 0.0351]	4254 [R _{int} = 0.0960]	4201 [R _{int} = 0.0448]
Completeness to θ = 28.48°	97%	97%	97%
Refinement method		Full-matrix least-squares on F ²	
Data / restraints / parameters	4258 / 1 / 135	4254 / 1 / 135	4201 / 1 / 135
Goodness-of-fit on F ²	1.79	1.74	1.74
Final R indices [I>2σ(I)]	R _{obs} = 0.0379, wR _{obs} = 0.0881	R _{obs} = 0.0498, wR _{obs} = 0.1469	R _{obs} = 0.0482, wR _{obs} = 0.1243
R indices (all data)	R _{all} = 0.0927, wR _{all} = 0.1001	R _{all} = 0.1567, wR _{all} = 0.2124	R _{all} = 0.1119, wR _{all} = 0.1421
Largest diff. peak and hole	2.53 and -3.81 e.Å ⁻³	3.49 and -3.40 e.Å ⁻³	4.94 and -4.07 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{\Sigma[w(F_o)^2 - F_c ^2] / \Sigma[w(F_o)^4]\}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$			

Table 2.2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Ce[1]	3214(1)	3306(1)	4128	1	9(1)
Ce[2]	3929(1)	1685(1)	9178(12)	1	9(1)
Ce[3]	2549	1686(2)	9096(19)	1	10(1)
Ce[4]	4643(1)	3310(1)	4226(12)	1	7(1)
Te[1]	3931(1)	2954(1)	9181(16)	1	9(1)
Te[2]	3214(1)	2036(1)	4167(9)	1	9(1)
Te[3]	2549	2956(2)	9169(19)	1	12(1)
Te[4]	4641(1)	2041(1)	4177(13)	1	7(1)
Te[5]	2549	4300(3)	4495(20)	1	16(2)
Te[6]	3213(2)	694(1)	9377(11)	1	15(1)
Te[7]	4644(2)	4300(2)	9459(14)	1	14(1)
Te[8]	3930(1)	697(2)	4283(18)	1	13(1)
Te[9]	3929(1)	4298(2)	4125(20)	1	12(1)
Te[10]	3212(2)	4296(1)	9088(9)	1	10(1)
Te[11]	2549	694(2)	3995(20)	1	7(1)
Te[12]	4645(1)	697(2)	8935(16)	1	7(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce[1]	11(1)	9(1)	7(1)	1(1)	1(2)	8(1)
Ce[2]	6(1)	12(1)	8(1)	0(1)	0(1)	-3(2)
Ce[3]	5(2)	13(2)	11(2)	0	0	-1(2)
Ce[4]	9(1)	9(1)	5(1)	0(1)	1(2)	6(1)
Te[1]	13(2)	8(2)	5(1)	2(1)	2(1)	2(2)
Te[2]	3(1)	12(1)	11(1)	1(2)	0(2)	4(1)
Te[3]	18(2)	12(2)	6(1)	0	0	3(3)
Te[4]	5(1)	9(1)	6(1)	2(1)	-1(2)	0(2)
Te[5]	19(3)	17(2)	13(3)	0	0	5(2)
Te[6]	9(1)	20(1)	17(2)	0(2)	-1(2)	2(1)
Te[7]	14(2)	15(2)	13(2)	1(2)	1(2)	2(2)

Table 2.3. (cont'd) Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[8]	9(2)	16(2)	14(2)	0(1)	2(2)	1(2)
Te[9]	12(2)	15(2)	10(1)	0(2)	-3(1)	3(2)
Te[10]	13(1)	9(1)	7(1)	0(2)	1(2)	5(1)
Te[11]	5(2)	6(2)	9(2)	0	0	1(2)
Te[12]	5(2)	7(1)	9(2)	0(1)	1(2)	1(1)

Table 2.4. Selected bond distances [$\text{\AA}$] for CeTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Ce[1] - Te[1]	3.226(6)	Ce[3] - Te[11]	3.360(10)
Ce[1] - Te[1]	3.258(6)	Ce[4] - Te[1]	3.250(7)
Ce[1] - Te[2]	3.309(3)	Ce[4] - Te[1]	3.223(7)
Ce[1] - Te[3]	3.224(6)	Ce[4] - Te[4]	3.307(4)
Ce[1] - Te[3]	3.248(6)	Ce[4] - Te[4]	3.254(6)
Ce[1] - Te[5]	3.401(6)	Ce[4] - Te[4]	3.225(6)
Ce[1] - Te[9]	3.396(5)	Ce[4] - Te[7]	3.318(6)
Ce[1] - Te[10]	3.395(4)	Ce[4] - Te[7]	3.451(7)
Ce[1] - Te[10]	3.373(4)	Ce[4] - Te[9]	3.387(5)
Ce[2] - Te[1]	3.307(5)	Ce[4] - Te[12]	3.394(5)
Ce[2] - Te[2]	3.241(5)	Te[5] - Te[10] x 2	3.227(8)
Ce[2] - Te[2]	3.234(5)	Te[5] - Te[10] x 2	2.979(8)
Ce[2] - Te[4]	3.237(6)	Te[6] - Te[8]	3.138(8)
Ce[2] - Te[4]	3.236(6)	Te[6] - Te[8]	3.080(8)
Ce[2] - Te[6]	3.396(5)	Te[6] - Te[11]	3.222(9)
Ce[2] - Te[8]	3.349(8)	Te[6] - Te[11]	2.986(8)
Ce[2] - Te[8]	3.408(8)	Te[7] - Te[9]	3.213(9)
Ce[2] - Te[12]	3.391(5)	Te[7] - Te[9]	3.002(9)
Ce[3] - Te[2] x 2	3.214(7)	Te[7] - Te[12]	3.264(8)
Ce[3] - Te[2] x 2	3.257(7)	Te[7] - Te[12]	2.940(8)
Ce[3] - Te[3]	3.308(6)	Te[8] - Te[12]	3.216(9)
Ce[3] - Te[6] x 2	3.394(5)	Te[8] - Te[12]	3.001(8)
Ce[3] - Te[11]	3.417(10)	Te[9] - Te[10]	3.119(9)

Table 2.5. Selected bond angles [°] for CeTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Ce[1] - Te[5] - Ce[1] x 2	80.60(16)	Ce[4] - Te[7] - Te[12]	65.35(15)
Ce[1] - Te[5] - Te[10] x 2	61.56(11)	Te[9] - Te[7] - Te[9] x 2	89.6(2)
Ce[1] - Te[5] - Te[10] x 2	63.41(11)	Te[9] - Te[7] - Te[12]	85.4(2)
Ce[1] - Te[5] - Te[10] x 2	113.8(2)	Te[9] - Te[7] - Te[12]	175.1(3)
Ce[1] - Te[5] - Te[10] x 2	120.3(3)	Te[9] - Te[7] - Te[12]	175.0(3)
Te[10] - Te[5] - Te[10] x 4	89.72(13)	Te[9] - Te[7] - Te[12]	95.3(3)
Te[10] - Te[5] - Te[10] x 2	85.7(3)	Te[12] - Te[7] - Te[12] x 2	89.7(2)
Te[10] - Te[5] - Te[10] x 4	175.4(3)	Ce[2] - Te[8] - Ce[2] x 2	80.82(16)
Te[10] - Te[5] - Te[10] x 2	94.9(3)	Ce[2] - Te[8] - Te[6]	62.87(16)
Ce[2] - Te[6] - Ce[3]	80.80(9)	Ce[2] - Te[8] - Te[6]	117.92(17)
Ce[2] - Te[6] - Te[8]	61.52(16)	Ce[2] - Te[8] - Te[12]	61.50(16)
Ce[2] - Te[6] - Te[8]	63.29(16)	Ce[2] - Te[8] - Te[12]	116.51(18)
Ce[2] - Te[6] - Te[11]	115.07(18)	Ce[2] - Te[8] - Te[6]	116.66(17)
Ce[2] - Te[6] - Te[11]	119.66(19)	Ce[2] - Te[8] - Te[6]	63.03(16)
Ce[3] - Te[6] - Te[8]	115.27(19)	Ce[2] - Te[8] - Te[12]	117.86(17)
Ce[3] - Te[6] - Te[8]	119.11(19)	Ce[2] - Te[8] - Te[12]	64.28(17)
Ce[3] - Te[6] - Te[11]	62.13(19)	Te[6] - Te[8] - Te[6] x 2	89.57(17)
Ce[3] - Te[6] - Te[11]	63.17(19)	Te[6] - Te[8] - Te[12]	89.0(3)
Te[8] - Te[6] - Te[8] x 2	89.6(2)	Te[6] - Te[8] - Te[12]	178.5(3)
Te[8] - Te[6] - Te[11]	87.6(2)	Te[6] - Te[8] - Te[12]	178.6(3)
Te[8] - Te[6] - Te[11]	177.3(3)	Te[6] - Te[8] - Te[12]	91.9(3)
Te[8] - Te[6] - Te[11]	177.2(3)	Te[12] - Te[8] - Te[12] x 2	89.52(18)
Te[8] - Te[6] - Te[11]	93.1(2)	Ce[1] - Te[9] - Ce[4]	80.92(12)
Te[11] - Te[6] - Te[11] x 2	89.7(2)	Ce[1] - Te[9] - Te[7]	118.5(2)
Ce[4] - Te[7] - Ce[4] x 2	80.64(14)	Ce[1] - Te[9] - Te[7]	116.4(2)
Ce[4] - Te[7] - Te[9]	60.97(15)	Ce[1] - Te[9] - Te[10]	62.65(12)
Ce[4] - Te[7] - Te[9]	116.76(19)	Ce[1] - Te[9] - Te[10]	62.36(12)
Ce[4] - Te[7] - Te[12]	60.64(14)	Ce[4] - Te[9] - Te[7]	62.24(15)
Ce[4] - Te[7] - Te[12]	116.46(18)	Ce[4] - Te[9] - Te[7]	62.99(15)
Ce[4] - Te[7] - Te[9]	117.18(18)	Ce[4] - Te[9] - Te[10]	117.9(2)
Ce[4] - Te[7] - Te[9]	64.57(16)	Ce[4] - Te[9] - Te[10]	116.8(2)
Ce[4] - Te[7] - Te[12]	117.96(17)	Te[7] - Te[9] - Te[7] x 2	89.58(18)

Table 2.5. (cont'd) Selected bond angles [°] for CeTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[7] - Te[9] - Te[10]	92.2(3)	Ce[3] - Te[11] - Te[6] x 2	116.30(17)
Te[7] - Te[9] - Te[10] x 2	178.2(3)	Ce[3] - Te[11] - Te[6] x 2	61.41(17)
Te[7] - Te[9] - Te[10]	88.7(3)	Te[6] - Te[11] - Te[6] x 4	89.69(14)
Te[10] - Te[9] - Te[10] x 2	89.56(16)	Te[6] - Te[11] - Te[6] x 2	94.7(3)
Ce[1] - Te[10] - Ce[1] x 2	80.68(6)	Te[6] - Te[11] - Te[6] x 4	175.6(3)
Ce[1] - Te[10] - Te[5]	64.41(16)	Te[6] - Te[11] - Te[6] x 2	85.9(3)
Ce[1] - Te[10] - Te[5]	118.42(18)	Ce[2] - Te[12] - Ce[4]	80.82(11)
Ce[1] - Te[10] - Te[9]	63.12(14)	Ce[2] - Te[12] - Te[7]	120.2(2)
Ce[1] - Te[10] - Te[9]	117.11(17)	Ce[2] - Te[12] - Te[7]	114.3(2)
Ce[1] - Te[10] - Te[5]	116.34(19)	Ce[2] - Te[12] - Te[8]	62.84(16)
Ce[1] - Te[10] - Te[5]	61.75(14)	Ce[2] - Te[12] - Te[8]	62.04(15)
Ce[1] - Te[10] - Te[9]	117.20(17)	Ce[4] - Te[12] - Te[7]	62.71(15)
Ce[1] - Te[10] - Te[9]	62.67(13)	Ce[4] - Te[12] - Te[7]	62.40(14)
Te[5] - Te[10] - Te[5] x 2	89.7(2)	Ce[4] - Te[12] - Te[8]	120.0(2)
Te[5] - Te[10] - Te[9]	92.8(2)	Ce[4] - Te[12] - Te[8]	114.5(2)
Te[5] - Te[10] - Te[9]	177.6(3)	Te[7] - Te[12] - Te[7] x 2	89.68(19)
Te[5] - Te[10] - Te[9]	177.4(2)	Te[7] - Te[12] - Te[8]	95.4(3)
Te[5] - Te[10] - Te[9]	87.9(2)	Te[7] - Te[12] - Te[8]	175.1(3)
Te[9] - Te[10] - Te[9] x 2	89.6(2)	Te[7] - Te[12] - Te[8]	174.9(3)
Ce[3] - Te[11] - Ce[3] x 2	80.5(2)	Te[7] - Te[12] - Te[8]	85.4(2)
Ce[3] - Te[11] - Te[6] x 2	64.35(18)	Te[8] - Te[12] - Te[8] x 2	89.5(2)
Ce[3] - Te[11] - Te[6] x 2	117.87(17)		

Table 2.6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Pr[1]	3214(1)	3305(1)	3151(8)	1	11(1)
Pr[2]	3929(1)	1687(1)	8229(9)	1	10(1)
Pr[3]	2500	1687(2)	-1847(10)	1	12(1)
Pr[4]	4646(1)	3308(1)	3252(5)	1	9(1)
Te[1]	3930(1)	2952(2)	8198(10)	1	10(1)
Te[2]	3216(1)	2038(1)	3180(9)	1	10(1)
Te[3]	2500	2950(3)	8194(13)	1	13(1)

Table 2.6. (cont'd) Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[4]	4642(1)	2041(2)	13188(7)	1	8(1)
Te[5]	2500	4293(3)	3471(16)	1	17(2)
Te[6]	3215(2)	696(2)	8388(10)	1	17(1)
Te[7]	4645(2)	4297(2)	-1530(9)	1	16(1)
Te[8]	3929(2)	699(2)	3347(14)	1	15(1)
Te[9]	3929(1)	4296(2)	3135(13)	1	13(1)
Te[10]	3213(1)	4292(2)	-1849(9)	1	10(1)
Te[11]	2500	696(3)	-6912(14)	1	8(1)
Te[12]	4644(1)	701(2)	7992(10)	1	9(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr[1]	8(1)	13(2)	13(1)	1(1)	0(1)	2(2)
Pr[2]	6(2)	14(2)	9(1)	-1(1)	0(1)	-3(2)
Pr[3]	7(2)	14(2)	14(2)	0	0	-3(2)
Pr[4]	6(1)	14(2)	5(1)	-1(1)	0(1)	4(1)
Te[1]	11(2)	9(2)	8(1)	0(2)	1(1)	-4(2)
Te[2]	5(2)	13(2)	12(2)	0(2)	-1(2)	2(2)
Te[3]	12(3)	14(3)	14(2)	0	0	-7(2)
Te[4]	3(1)	12(2)	7(1)	1(2)	1(2)	0(2)
Te[5]	12(3)	17(4)	22(4)	0	0	1(3)
Te[6]	14(2)	20(2)	18(3)	0(2)	-1(2)	2(2)
Te[7]	12(2)	18(3)	18(3)	1(2)	1(2)	1(2)
Te[8]	12(2)	18(2)	13(2)	-1(2)	1(2)	-2(2)
Te[9]	7(2)	18(2)	15(2)	1(2)	-2(2)	0(2)
Te[10]	10(2)	11(2)	9(2)	0(2)	1(2)	0(2)
Te[11]	5(2)	7(3)	12(3)	0	0	-8(2)
Te[12]	6(1)	14(2)	8(2)	-1(2)	-2(2)	2(1)

Table 2.8. Bond distances [Å] for PrTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Pr[1] - Te[1]	3.210(5)	Te[1] - Pr[1]	3.210(5)
Pr[1] - Te[3]	3.209(5)	Te[1] - Pr[4]	3.243(5)
Pr[1] - Te[3]	3.234(6)	Te[2] - Pr[3]	3.215(5)
Pr[1] - Te[1]	3.238(5)	Te[2] - Pr[2]	3.202(5)
Pr[1] - Te[2]	3.284(5)	Te[3] - Pr[1] x 2	3.209(5)
Pr[1] - Te[10] x 2	3.361(5)	Te[3] - Pr[1]	3.234(6)
Pr[1] - Te[9]	3.375(6)	Te[3] - Pr[3]	3.275(9)
Pr[1] - Te[5]	3.371(6)	Te[4] - Pr[4]	3.196(5)
Pr[2] - Te[2]	3.202(5)	Te[4] - Pr[2]	3.233(5)
Pr[2] - Te[4]	3.208(5)	Te[4] - Pr[4]	3.234(5)
Pr[2] - Te[2]	3.231(5)	Te[4] - Pr[4]	3.285(6)
Pr[2] - Te[4]	3.233(5)	Te[5] - Te[10] x 2	2.990(6)
Pr[2] - Te[1]	3.279(6)	Te[5] - Te[10] x 2	3.187(6)
Pr[2] - Te[8]	3.331(6)	Te[5] - Pr[1]	3.372(6)
Pr[2] - Te[6]	3.373(6)	Te[6] - Te[11]	2.999(5)
Pr[2] - Te[12]	3.369(6)	Te[6] - Te[8]	3.077(6)
Pr[2] - Te[8]	3.397(6)	Te[6] - Te[8]	3.102(7)
Pr[3] - Te[2] x 2	3.214(5)	Te[6] - Te[11]	3.184(6)
Pr[3] - Te[2] x 2	3.231(5)	Te[6] - Pr[3]	3.376(6)
Pr[3] - Te[3]	3.275(9)	Te[7] - Te[12]	2.939(6)
Pr[3] - Te[11]	3.349(8)	Te[7] - Te[9]	2.992(6)
Pr[3] - Te[6] x 2	3.376(6)	Te[7] - Te[9]	3.198(6)
Pr[3] - Te[11]	3.386(8)	Te[7] - Pr[4]	3.426(5)
Pr[4] - Te[4]	3.196(5)	Te[8] - Te[12]	2.982(6)
Pr[4] - Te[1]	3.211(5)	Te[8] - Te[6]	3.077(6)
Pr[4] - Te[4]	3.234(5)	Te[8] - Te[12]	3.201(6)
Pr[4] - Te[1]	3.243(5)	Te[8] - Pr[2]	3.397(6)
Pr[4] - Te[4]	3.285(6)	Te[9] - Te[10] x 2	3.086(6)
Pr[4] - Te[7]	3.303(5)	Te[9] - Te[7]	3.198(6)
Pr[4] - Te[9]	3.373(6)	Te[10] - Te[5]	2.990(6)
Pr[4] - Te[12]	3.369(5)	Te[10] - Te[9]	3.096(6)
Pr[4] - Te[7]	3.426(5)	Te[10] - Pr[1]	3.361(5)

Table 2.8. (cont'd) Bond distances [Å] for PrTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[11] - Te[6] x 2	2.999(5)	Te[12] - Te[7]	2.939(6)
Te[11] - Te[6] x 2	3.184(6)	Te[12] - Te[8]	3.201(6)
Te[11] - Pr[3]	3.349(8)		

Table 2.9. Selected bond angles [°] for PrTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[10] - Te[5] - Te[10]	93.9(2)	Te[9] - Te[7] - Pr[4]	116.82(17)
Te[10] - Te[5] - Te[10] x 2	176.33(18)	Te[9] - Te[7] - Pr[4]	61.10(12)
Te[10] - Te[5] - Te[10] x 2	89.74(12)	Pr[4] - Te[7] - Pr[4]	80.75(12)
Te[10] - Te[5] - Te[10]	86.6(2)	Te[12] - Te[8] - Te[6]	178.1(2)
Te[10] - Te[5] - Pr[1] x 2	63.47(13)	Te[12] - Te[8] - Te[6]	92.12(18)
Te[10] - Te[5] - Pr[1] x 2	120.1(2)	Te[6] - Te[8] - Te[6]	89.75(16)
Te[10] - Te[5] - Pr[1] x 2	114.5(2)	Te[12] - Te[8] - Te[12]	89.60(16)
Te[10] - Te[5] - Pr[1] x 2	61.59(12)	Te[6] - Te[8] - Te[12]	88.52(18)
Pr[1] - Te[5] - Pr[1]	80.91(19)	Te[6] - Te[8] - Te[12]	178.3(2)
Te[11] - Te[6] - Te[8]	92.26(14)	Te[12] - Te[8] - Pr[2]	64.22(14)
Te[11] - Te[6] - Te[8]	177.98(19)	Te[6] - Te[8] - Pr[2]	116.75(17)
Te[8] - Te[6] - Te[8]	89.75(16)	Te[6] - Te[8] - Pr[2]	63.14(14)
Te[11] - Te[6] - Te[11]	89.63(12)	Te[12] - Te[8] - Pr[2]	117.73(17)
Te[8] - Te[6] - Te[11]	178.10(17)	Te[12] - Te[8] - Pr[2]	116.43(17)
Te[8] - Te[6] - Te[11]	88.35(14)	Te[6] - Te[8] - Pr[2]	62.58(14)
Te[11] - Te[6] - Pr[3]	63.06(16)	Te[6] - Te[8] - Pr[2]	117.80(17)
Te[8] - Te[6] - Pr[3]	118.78(17)	Te[12] - Te[8] - Pr[2]	61.32(13)
Te[8] - Te[6] - Pr[3]	115.77(17)	Pr[2] - Te[8] - Pr[2]	80.78(13)
Te[11] - Te[6] - Pr[3]	62.06(15)	Te[7] - Te[9] - Te[10]	92.43(19)
Te[11] - Te[6] - Pr[2]	119.16(17)	Te[7] - Te[9] - Te[10]	177.9(2)
Te[8] - Te[6] - Pr[2]	63.36(14)	Te[10] - Te[9] - Te[10]	89.69(15)
Te[8] - Te[6] - Pr[2]	61.74(13)	Te[7] - Te[9] - Te[7]	89.49(16)
Te[11] - Te[6] - Pr[2]	115.52(17)	Te[10] - Te[9] - Te[7]	178.1(2)
Pr[3] - Te[6] - Pr[2]	80.86(12)	Te[10] - Te[9] - Te[7]	88.40(16)
Te[12] - Te[7] - Te[9]	95.06(16)	Te[7] - Te[9] - Pr[4]	62.18(13)
Te[12] - Te[7] - Te[9]	175.45(19)	Te[10] - Te[9] - Pr[4]	118.08(17)

Table 2.9. (cont'd) Selected bond angles [°] for PrTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[9] - Te[7] - Te[9]	89.49(16)	Te[10] - Te[9] - Pr[4]	116.61(19)
Te[12] - Te[7] - Pr[4]	65.03(13)	Te[7] - Te[9] - Pr[4]	62.79(13)
Te[9] - Te[7] - Pr[4]	64.58(14)	Te[7] - Te[9] - Pr[1]	118.55(17)
Te[9] - Te[7] - Pr[4]	117.32(18)	Te[10] - Te[9] - Pr[1] x 2	62.50(13)
Te[12] - Te[7] - Pr[4]	116.52(17)	Te[7] - Te[9] - Pr[1]	116.38(19)
Pr[4] - Te[9] - Pr[1]	81.09(13)	Te[6] - Te[11] - Te[6] x 2	89.63(12)
Te[5] - Te[10] - Te[9]	178.26(17)	Te[6] - Te[11] - Te[6]	86.92(19)
Te[5] - Te[10] - Te[9]	92.03(13)	Te[6] - Te[11] - Pr[3] x 2	63.97(15)
Te[9] - Te[10] - Te[9]	89.69(15)	Te[6] - Te[11] - Pr[3] x 2	117.81(17)
Te[5] - Te[10] - Te[5]	89.74(12)	Te[6] - Te[11] - Pr[3] x 2	116.47(17)
Te[9] - Te[10] - Te[5]	88.54(13)	Te[6] - Te[11] - Pr[3] x 2	61.75(13)
Te[9] - Te[10] - Te[5]	178.21(17)	Pr[3] - Te[11] - Pr[3]	80.69(18)
Te[5] - Te[10] - Pr[1]	63.81(14)	Te[7] - Te[12] - Te[8]	95.11(17)
Te[9] - Te[10] - Pr[1] x 2	117.29(16)	Te[7] - Te[12] - Te[8]	175.3(2)
Te[9] - Te[10] - Pr[1] x 2	62.87(13)	Te[8] - Te[12] - Te[8]	89.60(16)
Te[5] - Te[10] - Pr[1]	118.24(17)	Te[7] - Te[12] - Pr[4]	62.71(13)
Te[5] - Te[10] - Pr[1]	116.35(19)	Te[8] - Te[12] - Pr[4]	119.92(17)
Te[5] - Te[10] - Pr[1]	61.91(15)	Te[8] - Te[12] - Pr[4]	114.76(16)
Pr[1] - Te[10] - Pr[1]	80.86(11)	Te[7] - Te[12] - Pr[2]	120.10(17)
Te[6] - Te[11] - Te[6]	93.8(2)	Te[8] - Te[12] - Pr[2]	62.91(14)
Te[6] - Te[11] - Te[6] x 2	176.56(17)	Te[8] - Te[12] - Pr[2]	62.21(13)

Table 2.10. Atomic coordinates (x10⁴) and equivalent isotropic displacement parameters (Å²x10³) for NdTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U _{eq} [*]
Nd[1]	7549	3310(2)	2775	1	8(1)
Nd[2]	6786(2)	1693(1)	7765(20)	1	7(1)
Nd[3]	6071(1)	3310(2)	2725(30)	1	10(1)
Nd[4]	5357(2)	1693(1)	7683(11)	1	11(1)
Te[1]	7549	2043(3)	2705(30)	1	6(2)
Te[2]	6786(3)	2960(1)	-2285(20)	1	8(1)
Te[3]	6073(1)	2047(2)	2715(30)	1	9(2)
Te[4]	5356(2)	2953(2)	-2285(20)	1	12(1)

Table 2.10. (cont'd) Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[5]	7549	4306(5)	-2125(30)	1	11(2)
Te[6]	6786(4)	703(2)	2815(20)	1	11(1)
Te[7]	7549	715(4)	7465(40)	1	11(2)
Te[8]	6071(2)	4298(5)	-2355(30)	1	15(2)
Te[9]	6788(5)	4295(2)	2575(20)	1	15(1)
Te[10]	6072(2)	705(4)	7775(30)	1	12(2)
Te[11]	5357(4)	709(3)	2515(20)	1	13(2)
Te[12]	5357(3)	4303(3)	2925(20)	1	8(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Nd[1]	10(3)	10(2)	3(2)	0	0	-3(2)
Nd[2]	3(1)	11(1)	7(2)	1(2)	1(3)	-2(1)
Nd[3]	11(3)	10(2)	8(2)	1(1)	0(2)	-3(2)
Nd[4]	9(2)	11(2)	13(1)	2(2)	0(3)	0(2)
Te[1]	0(3)	9(3)	8(3)	0	0	-6(3)
Te[2]	16(1)	3(1)	4(2)	0(2)	1(3)	0(1)
Te[3]	4(3)	14(3)	9(2)	-1(2)	0(2)	-5(3)
Te[4]	12(3)	14(2)	9(2)	-1(2)	0(4)	2(2)
Te[5]	7(5)	13(3)	12(4)	0	0	-18(3)
Te[6]	6(2)	14(2)	14(2)	0(4)	0(4)	8(1)
Te[7]	9(5)	4(3)	21(4)	0	0	0(3)
Te[8]	13(5)	18(3)	12(3)	1(2)	1(2)	-13(3)
Te[9]	14(2)	14(2)	16(2)	0(4)	-1(4)	-1(2)
Te[10]	8(4)	14(3)	15(3)	1(2)	-2(3)	-6(2)
Te[11]	12(4)	14(2)	14(3)	1(3)	0(4)	13(2)
Te[12]	7(3)	10(2)	8(2)	0(3)	-1(3)	0(2)

Table 2.12. Bond distances [$\text{\AA}$] for NdTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Nd[1] - Te[1]	3.276(9)	Nd[3] - Te[12]	3.371(10)
Nd[1] - Te[2] x 2	3.234(9)	Nd[4] - Te[3] x 2	3.213(11)
Nd[1] - Te[2] x 2	3.195(9)	Nd[4] - Te[4]	3.258(6)
Nd[1] - Te[5]	3.348(14)	Nd[4] - Te[4] x 2	3.207(10)
Nd[1] - Te[5]	3.399(14)	Nd[4] - Te[10]	3.362(10)
Nd[1] - Te[9] x 2	3.351(11)	Nd[4] - Te[11]	3.399(10)
Nd[2] - Te[1]	3.232(12)	Nd[4] - Te[11]	3.300(10)
Nd[2] - Te[1]	3.196(12)	Nd[4] - Te[12]	3.378(10)
Nd[2] - Te[2]	3.275(4)	Te[5] - Te[9] x 2	3.173(15)
Nd[2] - Te[3]	3.231(13)	Te[5] - Te[9] x 2	2.989(15)
Nd[2] - Te[3]	3.198(12)	Te[6] - Te[7]	3.190(16)
Nd[2] - Te[6]	3.349(10)	Te[6] - Te[7]	2.980(16)
Nd[2] - Te[6]	3.374(10)	Te[6] - Te[10] x 2	3.094(15)
Nd[2] - Te[7]	3.344(9)	Te[8] - Te[9]	3.110(16)
Nd[2] - Te[10]	3.360(10)	Te[8] - Te[9]	3.067(16)
Nd[3] - Te[2] x 2	3.217(13)	Te[8] - Te[12]	2.997(15)
Nd[3] - Te[3]	3.265(8)	Te[8] - Te[12]	3.173(15)
Nd[3] - Te[4] x 2	3.223(13)	Te[10] - Te[11]	3.168(15)
Nd[3] - Te[8]	3.381(16)	Te[10] - Te[11]	3.007(15)
Nd[3] - Te[8]	3.335(16)	Te[11] - Te[12]	2.958(15)
Nd[3] - Te[9]	3.361(11)		

Table 2.13. Selected bond angles [$^\circ$] for NdTe_3 (commensurate) at 300 K with e.s.d.'s in parentheses.

Label	Angle	Label	Angle
Nd[1] - Te[5] - Nd[1] x 2	80.4(3)	Nd[3] - Te[8] - Te[12]	64.1(3)
Nd[1] - Te[5] - Te[9] x 2	61.2(3)	Nd[3] - Te[8] - Te[12] x 2	118.0(4)
Nd[1] - Te[5] - Te[9] x 2	116.1(3)	Nd[3] - Te[8] - Te[12]	61.8(3)
Nd[1] - Te[5] - Te[9] x 2	117.2(3)	Te[9] - Te[8] - Te[9] x 3	89.7(4)
Nd[1] - Te[5] - Te[9] x 2	63.6(3)	Te[9] - Te[8] - Te[12]	91.5(5)
Te[9] - Te[5] - Te[9] x 4	89.9(3)	Te[9] - Te[8] - Te[12] x 2	178.7(5)
Te[9] - Te[5] - Te[9] x 2	86.6(4)	Nd[3] - Te[9] - Te[8]	61.9(4)

Table 2.13. (cont'd) Selected bond angles [°] for NdTe₃ (commensurate) at 300 K with e.s.d.'s in parentheses.

Te[9] - Te[5] - Te[9] x 4	176.4(5)	Te[5] - Te[9] - Te[5] x 2	89.9(4)
Te[9] - Te[5] - Te[9] x 2	93.5(5)	Te[5] - Te[9] - Te[8]	92.3(4)
Nd[2] - Te[1] - Nd[2] x 4	147.3(3)	Nd[2] - Te[10] - Te[11]	116.4(4)
Nd[2] - Te[6] - Te[10] x 2	62.4(3)	Nd[2] - Te[10] - Te[11]	118.0(4)
Nd[2] - Te[6] - Te[10] x 3	117.2(4)	Nd[4] - Te[10] - Te[6]	117.0(4)
Nd[2] - Te[6] - Te[7]	63.5(3)	Nd[4] - Te[10] - Te[6]	117.9(4)
Te[7] - Te[6] - Te[7] x 2	89.8(4)	Nd[4] - Te[10] - Te[11]	62.6(2)
Te[7] - Te[6] - Te[10]	88.0(4)	Nd[4] - Te[10] - Te[11]	62.1(2)
Te[7] - Te[6] - Te[10] x 2	177.8(5)	Te[6] - Te[10] - Te[6] x 2	89.9(3)
Te[7] - Te[6] - Te[10]	92.3(4)	Te[6] - Te[10] - Te[11]	88.9(4)
Te[10] - Te[6] - Te[10] x 2	89.9(4)	Te[6] - Te[10] - Te[11] x 2	178.6(5)
Nd[2] - Te[7] - Nd[2] x 2	81.5(3)	Te[6] - Te[10] - Te[11]	91.5(4)
Nd[2] - Te[7] - Te[6] x 2	63.6(2)	Te[11] - Te[10] - Te[11] x 2	89.7(3)
Nd[2] - Te[7] - Te[6] x 2	62.1(2)	Nd[4] - Te[11] - Nd[4] x 2	81.1(2)
Nd[2] - Te[7] - Te[6] x 2	120.8(4)	Nd[4] - Te[11] - Te[10]	64.2(3)
Nd[2] - Te[7] - Te[6] x 2	115.2(4)	Nd[4] - Te[11] - Te[10] x 3	117.6(4)
Te[6] - Te[7] - Te[6] x 4	89.8(3)	Nd[4] - Te[11] - Te[12]	65.1(3)
Te[6] - Te[7] - Te[6] x 2	94.2(5)	Te[12] - Te[8] - Te[12] x 2	89.8(3)
Te[6] - Te[7] - Te[6] x 4	175.9(5)	Nd[1] - Te[9] - Nd[3]	81.20(13)
Te[6] - Te[7] - Te[6] x 2	86.3(5)	Nd[1] - Te[9] - Te[5]	63.4(3)
Nd[3] - Te[8] - Nd[3] x 2	80.9(4)	Nd[1] - Te[9] - Te[5]	62.7(3)
Nd[3] - Te[8] - Te[9] x 2	62.8(3)	Nd[1] - Te[9] - Te[8]	119.0(3)
Nd[3] - Te[8] - Te[9] x 2	116.6(4)	Nd[1] - Te[9] - Te[8]	116.1(3)
Nd[3] - Te[9] - Te[5]	119.7(4)	Nd[3] - Te[12] - Te[8] x 2	62.1(3)
Nd[3] - Te[9] - Te[5]	116.1(4)	Nd[3] - Te[12] - Te[11]	114.3(4)
Nd[3] - Te[9] - Te[8]	63.3(4)	Nd[3] - Te[12] - Te[11]	119.1(4)
Nd[4] - Te[11] - Te[12]	118.4(3)	Nd[4] - Te[12] - Te[8]	114.8(3)
Nd[4] - Te[11] - Te[10] x 2	61.5(3)	Nd[4] - Te[12] - Te[8]	119.2(4)
Te[10] - Te[11] - Te[10] x 2	89.7(4)	Nd[4] - Te[12] - Te[11] x 2	62.0(3)
Te[10] - Te[11] - Te[12]	94.2(4)	Te[8] - Te[12] - Te[8] x 2	89.8(4)
Te[10] - Te[11] - Te[12] x 2	176.0(5)	Te[8] - Te[12] - Te[11]	86.2(4)
Te[10] - Te[11] - Te[12]	86.4(4)	Te[8] - Te[12] - Te[11] x 2	175.9(5)
Te[12] - Te[11] - Te[12] x 2	89.7(4)	Te[8] - Te[12] - Te[11]	94.3(4)
Nd[3] - Te[12] - Nd[4]	80.57(18)	Te[11] - Te[12] - Te[11] x 2	89.7(4)

Supercell Description of RETe₃ Based on a Modulation q-vector – Although the commensurate supercell approach gave a much better view of the distortions in these compounds it is, however, still inadequate as it “glosses over” some important details of the structure. A more accurate description was obtained when the four-dimensional superspace crystallographic approach was used to refine the structures based on the existence of a modulation q vector. X-ray diffraction gave accurate q values which in fact vary slightly but significantly with the RE element (e.g. $q = 0.2801(4)$, $0.2821(4)$ and $0.2831(4)$ respectively for Ce, Pr and Nd) and this has consequences on the observed distortion. The length of the q -vector increases with decreasing RE size (from La to Dy) as can be seen in Figure 2.5. Interestingly, the CDW for the three heaviest RE (Ho, Er and Tm) disappears judging from the vanishing of the q -vector.

The superspace crystallographic analysis gave for CeTe₃ the minimum Te-Te distance in the net to be 2.999(2) Å and the maximum 3.198(2) Å. For PrTe₃ these distances are 2.956(3) Å and 3.214(3) Å respectively, and for NdTe₃ 2.9454(14) Å and 3.2104(15) Å respectively. By arbitrarily taking 3.035 Å to be the Te-Te bonding threshold, the square net of CeTe₃ can be easily viewed as a sequence of V-shaped “trimers” and N-shaped “tetramers” and, infrequently, even “single” Te atoms, Figure 2.11. The Te-Te distances within the oligomers are shorter than the average 3.1034(6) Å found in the original Cmc₂m structure.

The most surprising finding of the superspace analysis is that the RETe₃ analogs do not have identical CDW distortions. A closer look at the pattern of the Te nets reveals substantial differences in the way the nets distort as the RE element changes, Figures 2.11-2.17. The net does not simply shrink to follow the lanthanide contraction. Instead,

the long-short bond alternation among the Te atoms varies from Ce to Pr to Nd e.g. forming different oligomeric patterns. Starting from the left of Figure 2.11, we can see that the net for the three compounds is identical up to a certain distance (shown by the boxed area). After that point there is divergence; in CeTe_3 for example, Te atoms form two tetramers thereby breaking the trimer-to-tetramer order, Figure 2.11A. In contrast, the order of oligomers in PrTe_3 and NdTe_3 continues identical until the appearance of single Te atoms in PrTe_3 (shown in the dotted boxed area), Figure 2.11B and Figure 2.11C. At this point the patterns of PrTe_3 and NdTe_3 diverge. Every distorted Te net within the RETe_3 series is unique as can be seen in Figures 2.11 – 2.17.

The distortion is mainly located at the tellurium planar net creating a wide distribution of Te-Te distances as can be seen in Figure 2.6. The atomic displacement of the Te atoms (Te[2] and Te[3]) in the planar net along the a -axis (x direction) is at least two orders of magnitude larger than the displacements found along the other two directions, Figure 2.7. Along the b and c -axis (y and z directions respectively), Ce and Te1 have the largest displacement as a result of the respond of the $[\text{RETe}]$ layer to the CDW distortion of the Te net, Figures 2.8-2.9.

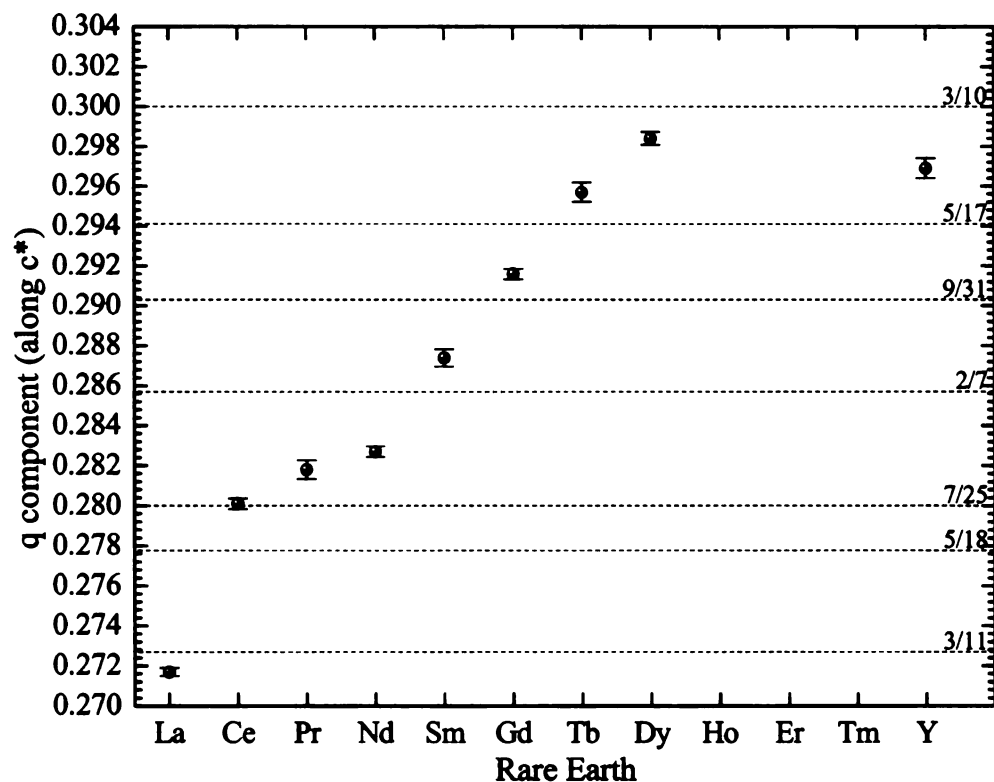


Figure 2.5. Plot of the q-vector dependence as a function of RE size at 300K. Parallel dashed lines notate some possible low index commensurate approximants.

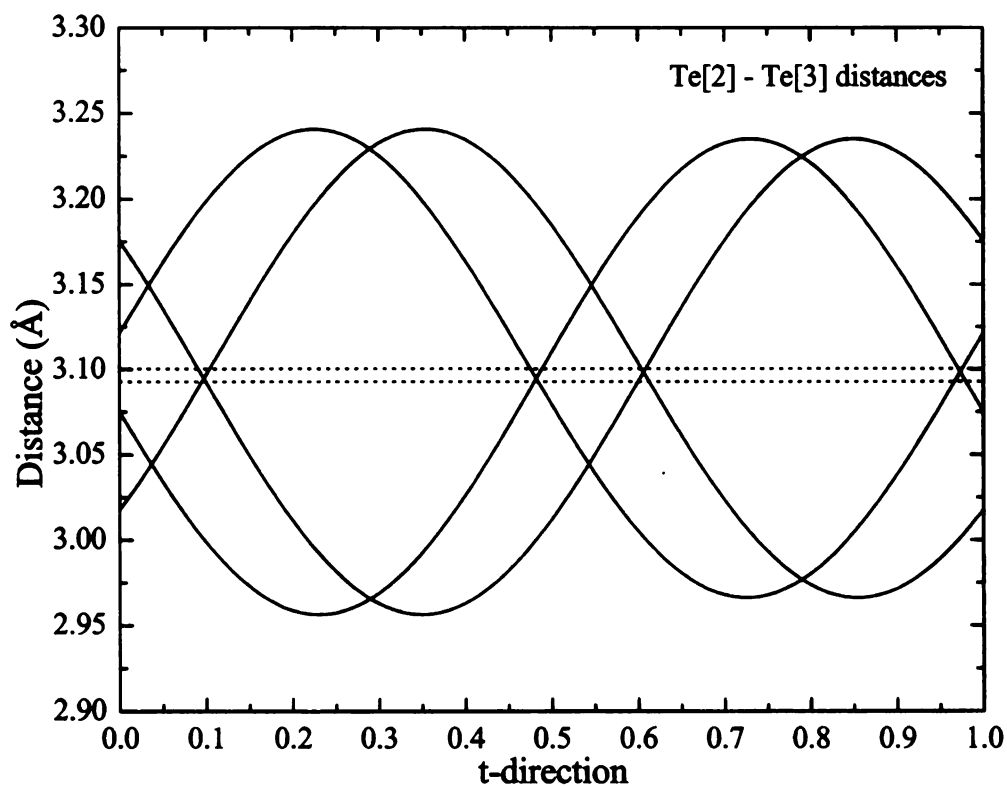


Figure 2.6. Representative plot of the Te[2]-Te[3] distances found in the distorted net of CeTe_3 from the superspace analysis based on a q-vector as a function of t-direction. Dashed lines represent the average (undistorted) Te-Te distances.

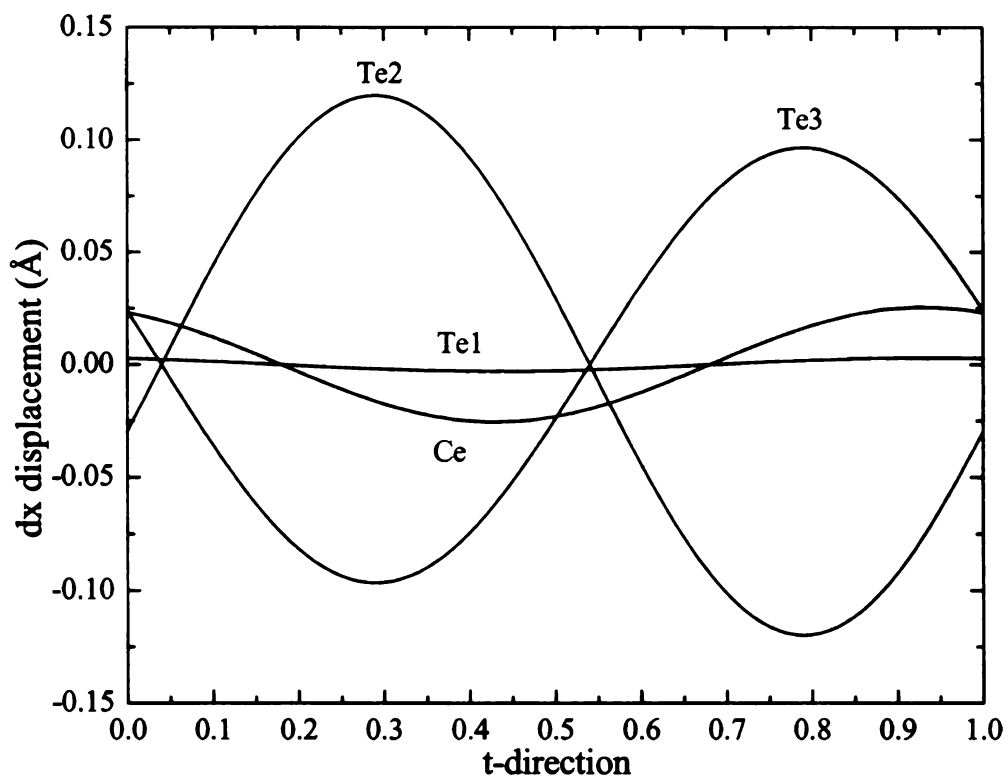


Figure 2.7. Plot of the positional displacement (Å) along x-axis of all the atoms in the CeTe_3 supercell as a function of t-direction.

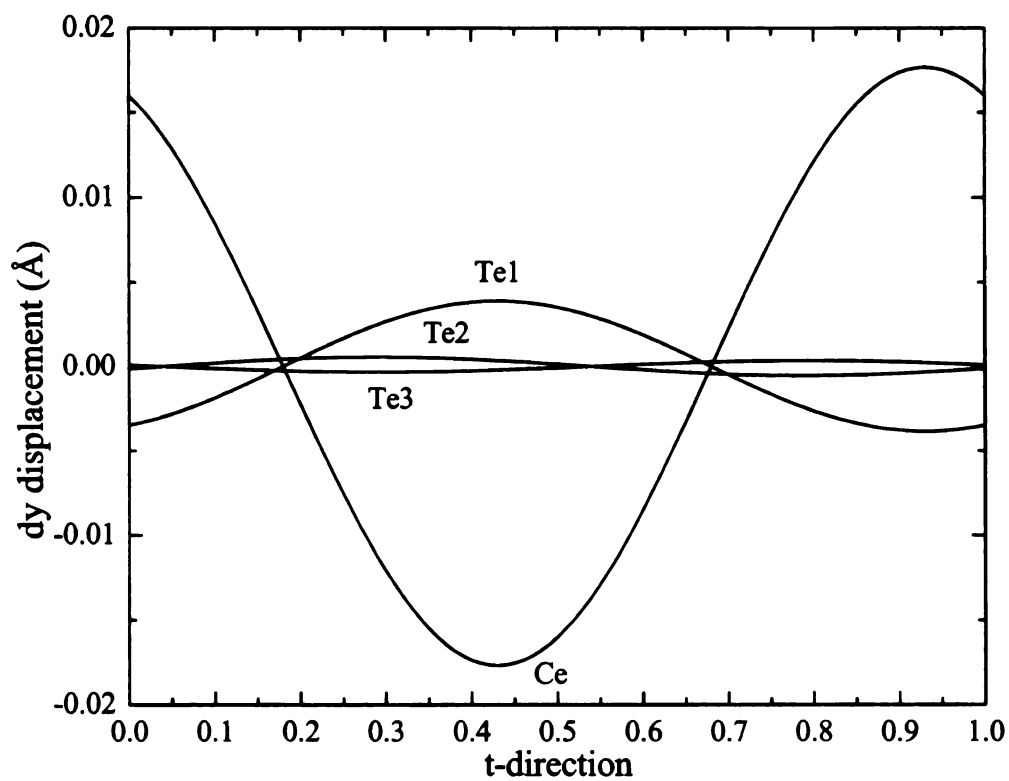


Figure 2.8. Plot of the positional displacement (Å) along y-axis of all the atoms in the CeTe_3 supercell as a function of t-direction.

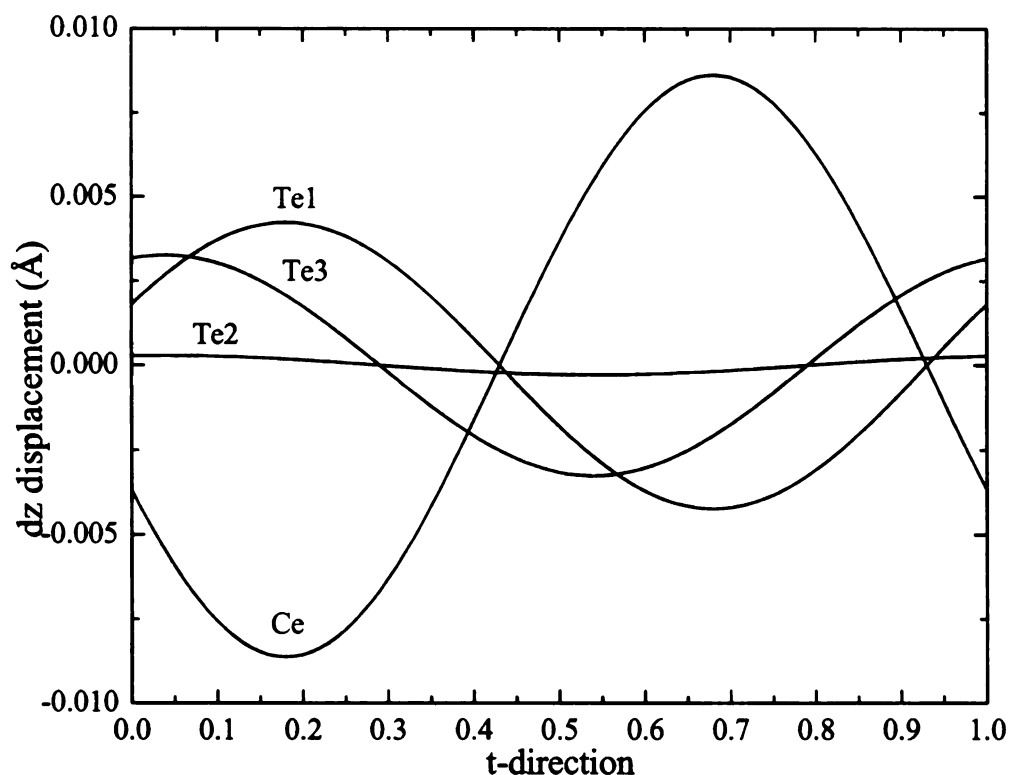


Figure 2.9. Plot of the positional displacement (Å) along z-axis of all the atoms in the CeTe_3 supercell as a function of t-direction.

Pair Distribution Function Analysis of RETe_3 ($\text{RE} = \text{Ce}, \text{Pr}$ and Nd) – In order to ensure that the observed modulations were representative of the bulk and not of isolated single crystal domains sampled selectively by our electron or X-ray diffraction experiments, we sought a total scattering technique to check the entire sample. The PDF technique is a powerful and unique tool for the characterization and structure refinement of crystalline materials with intrinsic disorder.¹⁴ The technique has proven successful in determining the structure of crystalline materials exhibiting local deviations from the average structure arising from different degrees of disorder or long range modulations. The experimental PDF of all three RETe_3 systems were studied show a pronounced shoulder on the first peak at ~ 2.9 Å and it is due to the Te-Te bonds in the oligomers. The average Cmcm structure cannot account for this peak because it has no distance < 3.1 Å,

Figure 2.18B. This feature is much larger than the noise and is also apparent in data collected from PrTe_3 and NdTe_3 (Figure 2.19 and Figure 2.20). This proves that the distortion in the Te-net is a bulk phenomenon of the RETe_3 systems.

Furthermore, the amplitude of local distortions in the model obtained from PDF analysis found to be larger than those determined crystallographically. The results were reconciled within the discommensuration model where phase slips of the CDW exist between commensurate regions resulting in an incommensurate wavevector on the average, Figure 2.10. This work was done in collaboration with HyunJeong Kim and Simon J. L. Billinge at the Department of Physics at Michigan State University.¹⁵

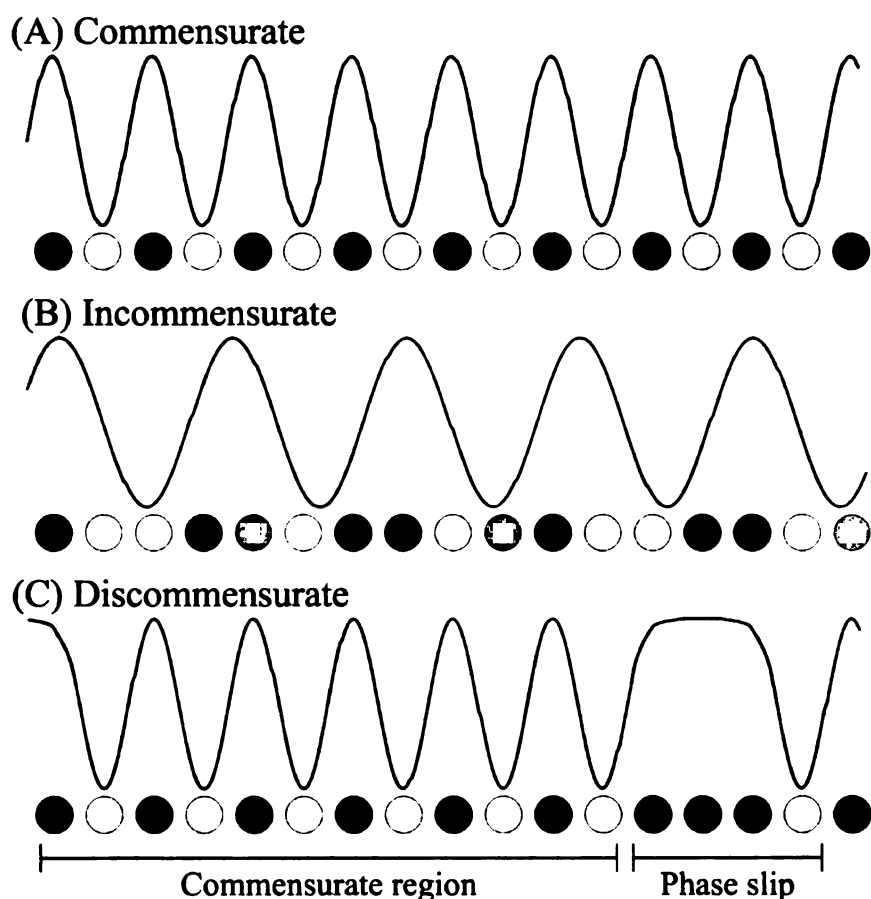


Figure 2.10. General scheme of (A) Commensurate, (B) Incommensurate and (C) Discommensurate Charge Density Wave. Circles represent the crystal lattice and solid lines the electron density. A discommensurate wave can be seen as a combination of a commensurate wave and a phase slip. The average long range result is the same with an incommensurate wave but locally the two cases are very different.

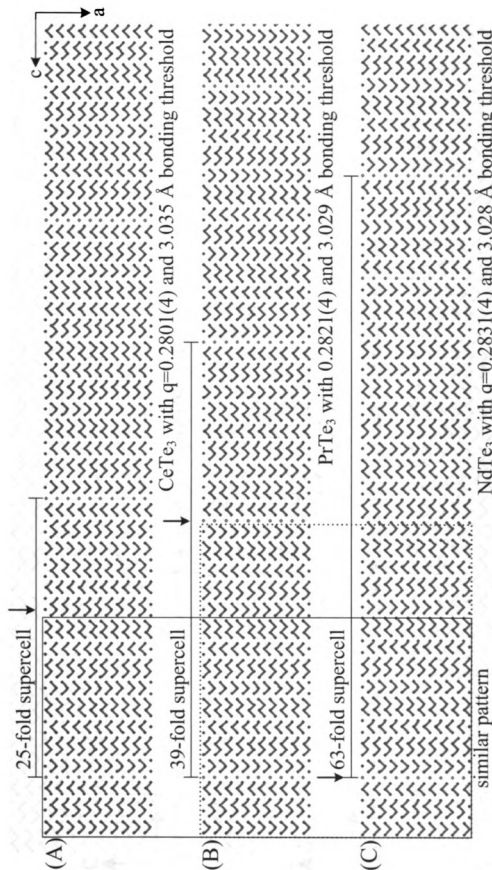


Figure 2.11. (A) Resolved structure of the Te net of CeTe_3 at a threshold of $3.035 \text{ \AA}$ showing V- and N-shaped oligomers. (B) Te net of PrTe_3 at a threshold of $3.029 \text{ \AA}$. (C) Te net of NdTe_3 at a threshold of $3.028 \text{ \AA}$. The q-vectors correspond to an approximate 25-fold, 39-fold and 63-fold supercell respectively. The boxed areas represent regions where identical domains are encountered between RETe_3 members.

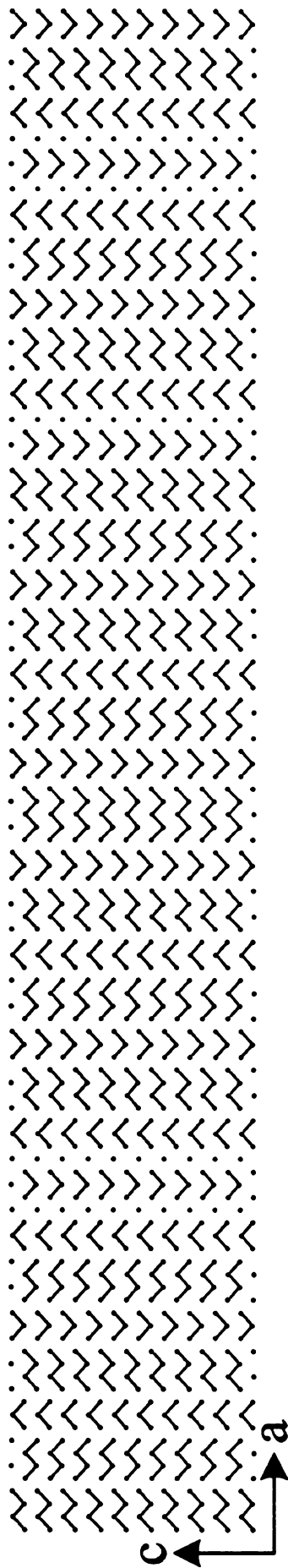


Figure 2.12. Distorted Te net of LaTe_3 at 300 K with $q=0.2717(6)$ and 3.043 Å bonding threshold.

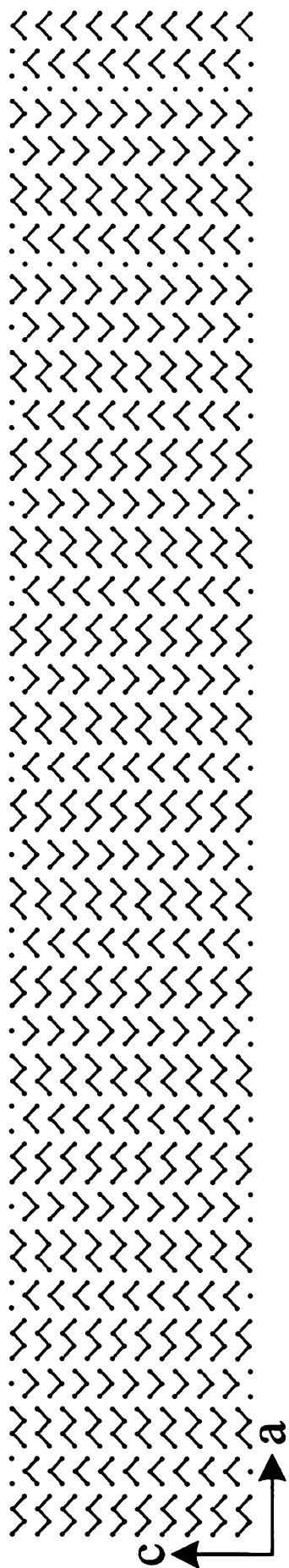


Figure 2.13. Distorted Te net of SmTe_3 at 300 K with $q=0.2874(4)$ and 3.018 Å bonding threshold.

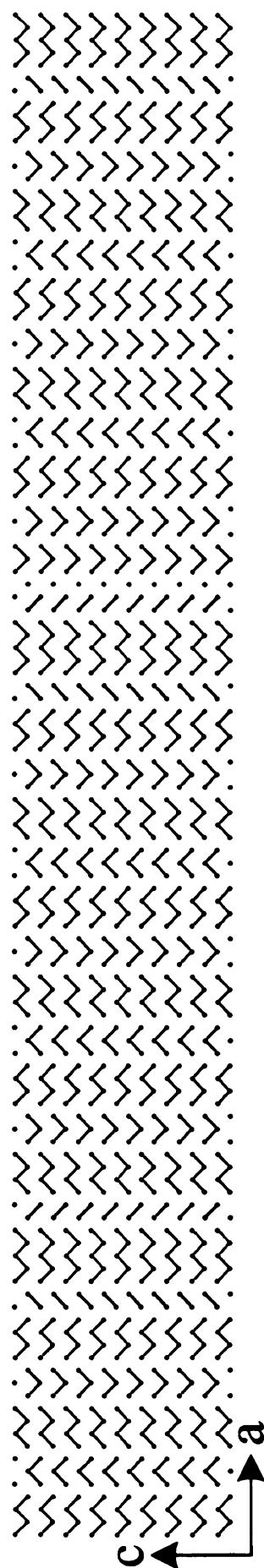


Figure 2.14. Distorted Te net of GdTe_3 at 300 K with $q=0.2916(3)$ and 3.003 Å bonding threshold.

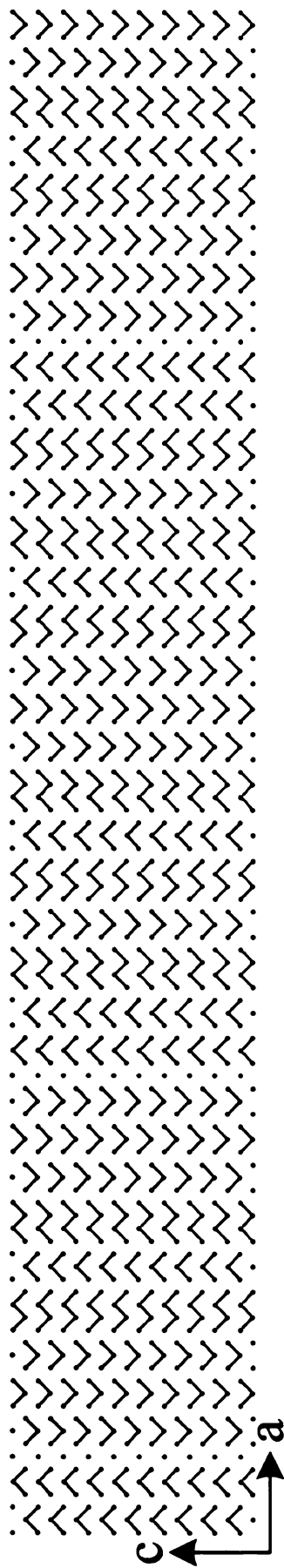


Figure 2.15. Distorted Te net of TbTe_3 at 300 K with $q=0.2957(5)$ and 3.019 Å bonding threshold.

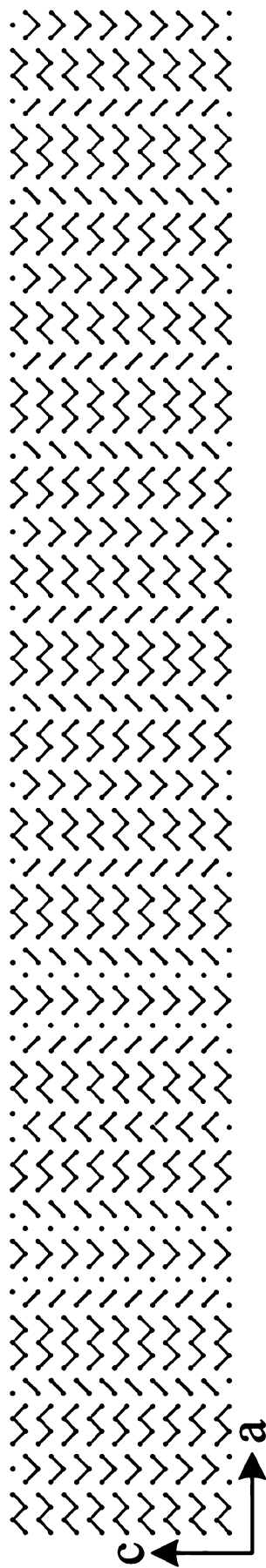


Figure 2.16. Distorted Te net of DyTe_3 at 300 K with $q=0.2984(3)$ and 3.023 Å bonding threshold.

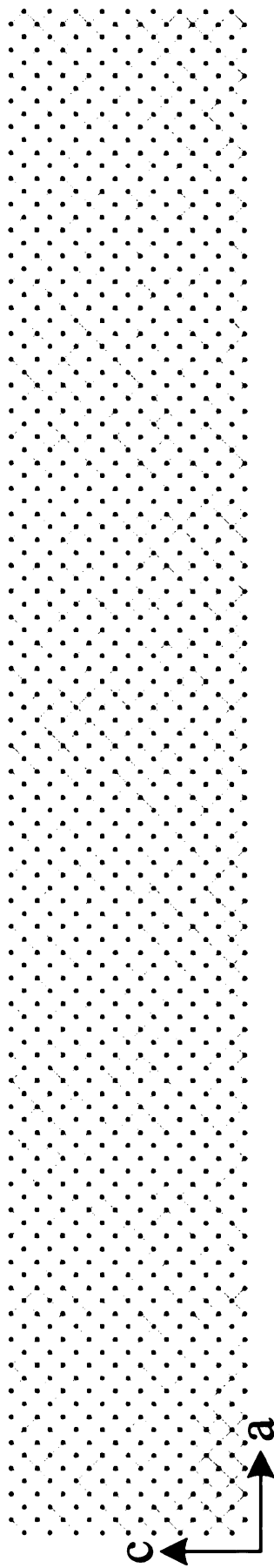


Figure 2.17. Te net of HoTe_3 , ErTe_3 and TmTe_3 at 300 K with no observable q -vector.

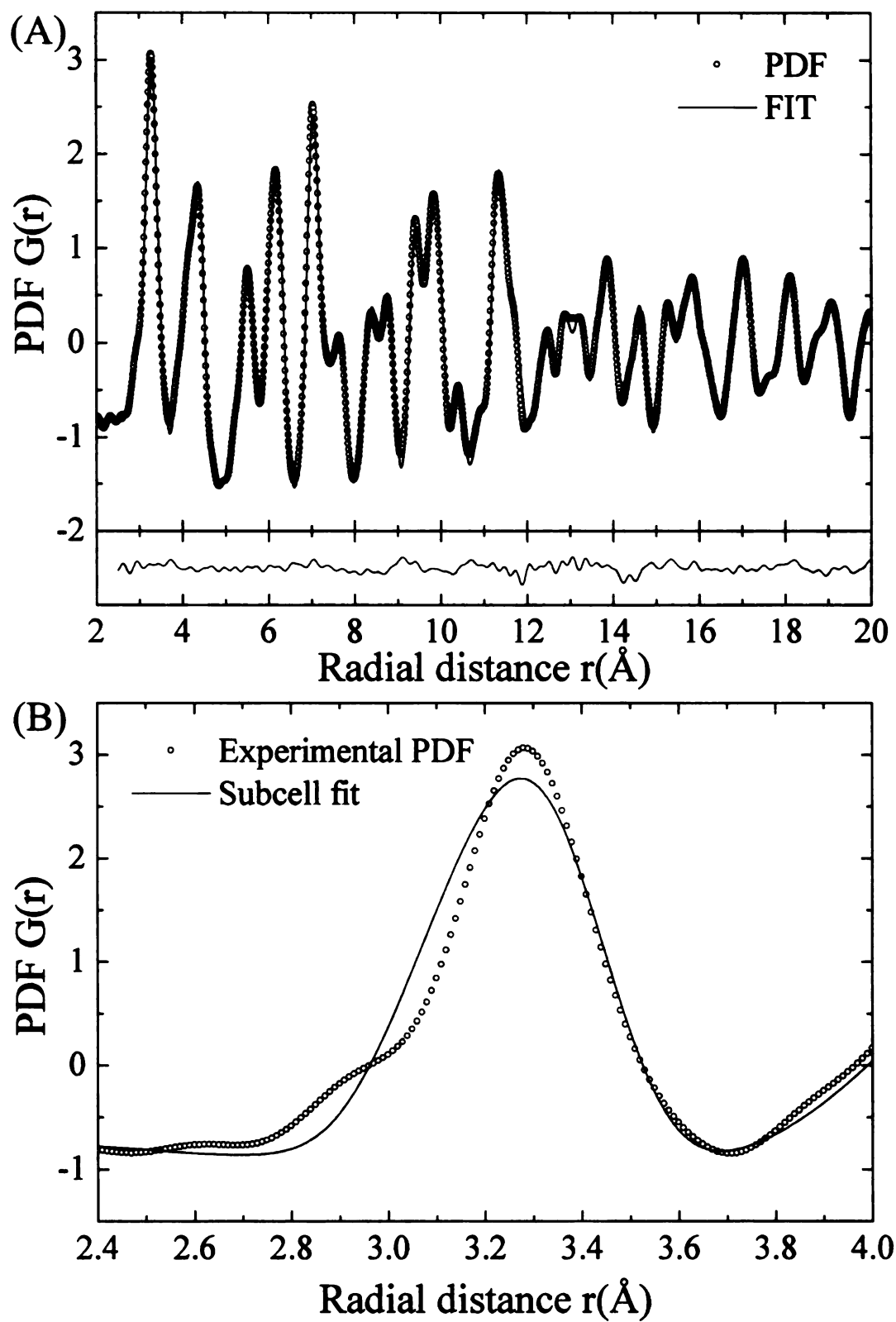


Figure 2.18. (A) Fit of the experimental PDF data in the range of 2-20 $\text{\AA}$ (B) First PDF peak which represents the local structure of the CeTe_3 . The solid line represents the average structural model and the circles the experimental data.

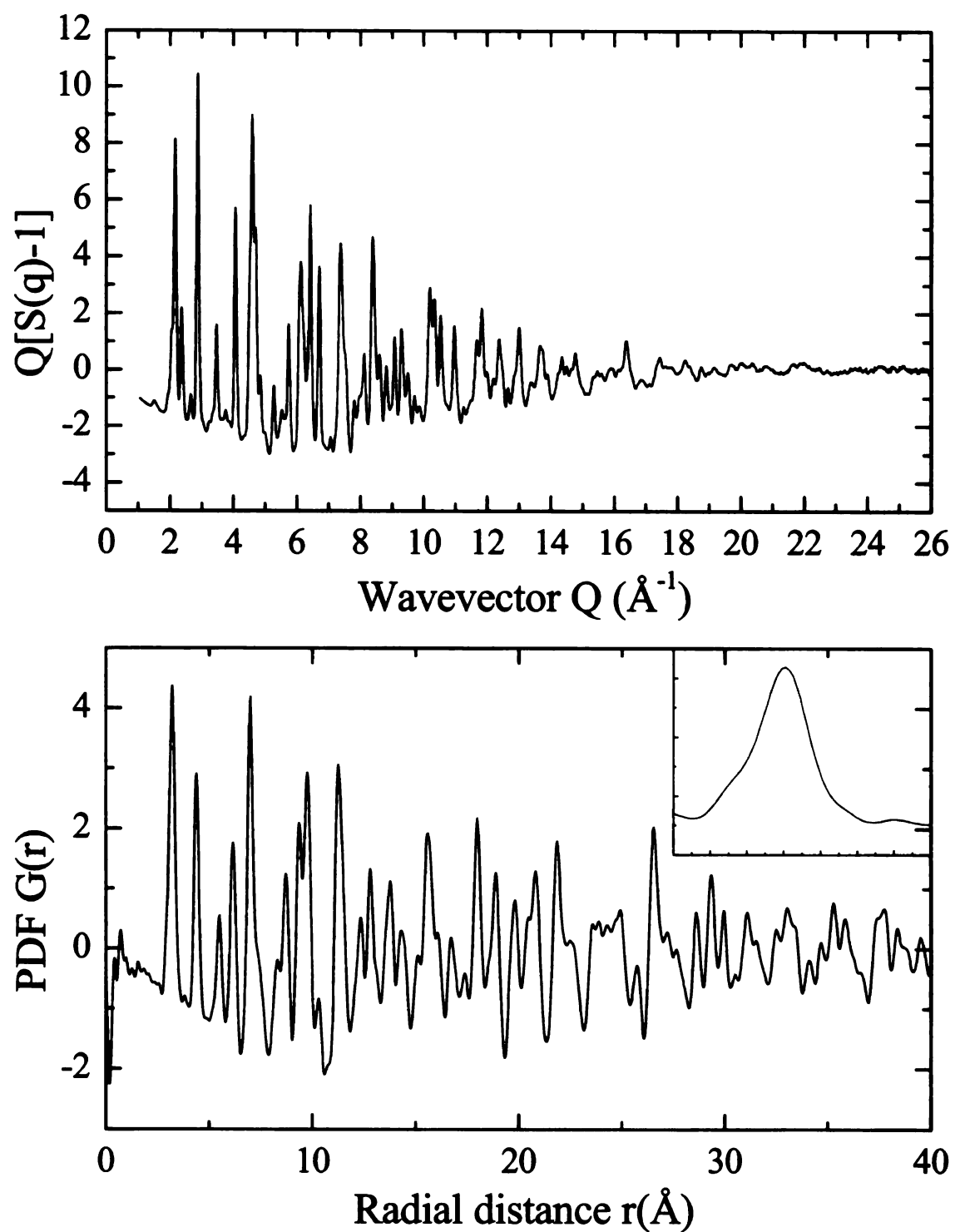


Figure 2.19. The reduced $Q[S(q)-1]$ and PDF $G(r)$ plots of PrTe_3

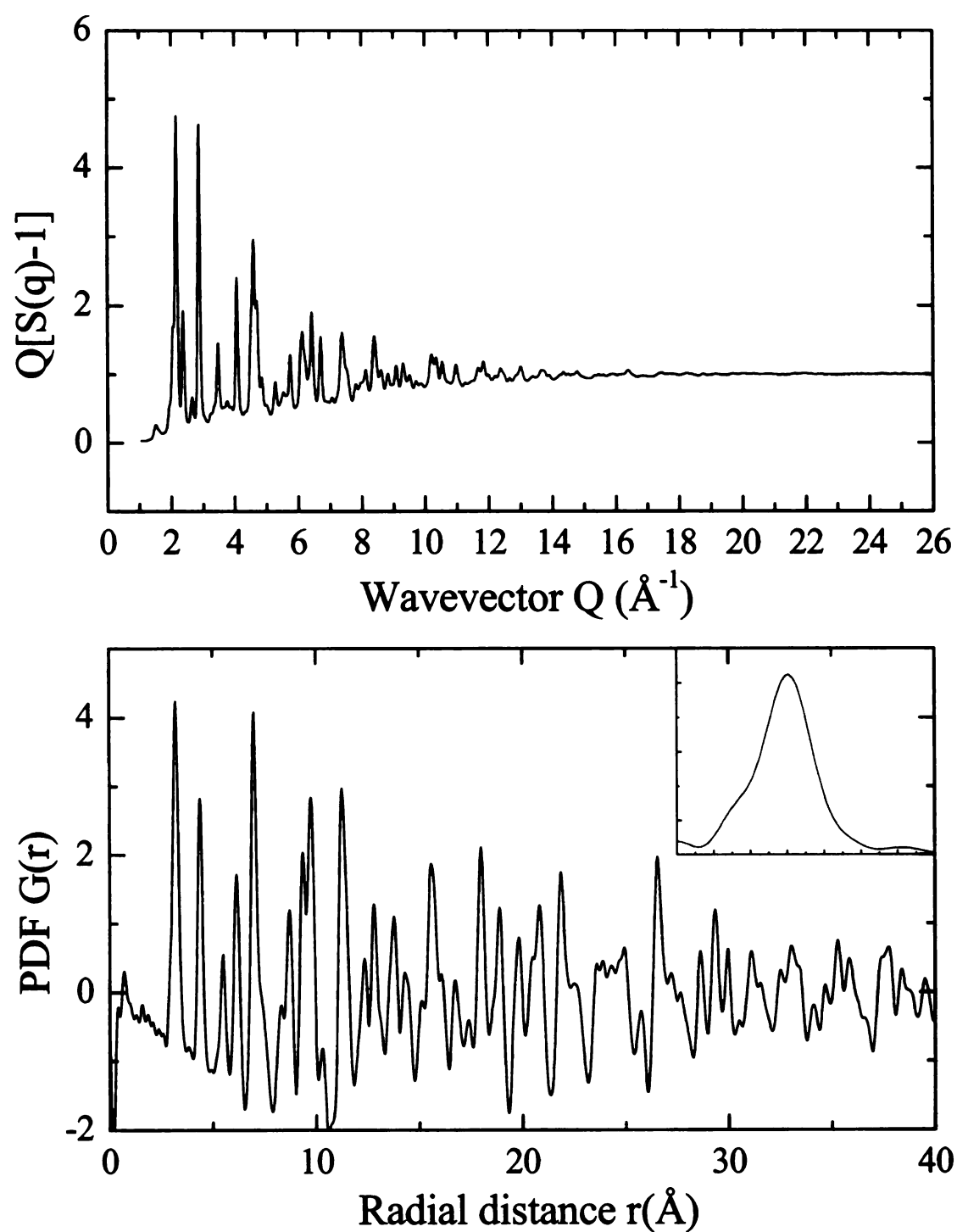


Figure 2.20. The reduced $Q[S(q)-1]$ and PDF $G(r)$ plots of NdTe_3

Band structure calculation of LaTe₃ – The calculations were performed using the self-consistent full-potential linearized augmented plane wave method (LAPW)¹⁶ and the generalized gradient approximation (GGA)¹⁷ for the exchange and correlation potential. The experimental cell constants (Table 2.14) and atomic coordinates (Table 2.15) from the crystal structure refinement of LaTe₃ in Cmc₂m were used. Directions in the Brillouin zone (BZ) are shown in Figure 2.23A.¹⁸ Interatomic forces were minimized within 0.1 mRy/bohr using a reverse-communication trust-region quasi-Newton method from the Port library.¹⁹ Scalar relativistic corrections were included and a spin-orbit interaction was incorporated using a second variational procedure.²⁰ The values of the atomic radii were taken to be: 2.7 a.u. for La atom and 2.5 a.u. for Te atoms, where a.u. is the atomic unit (0.529 Å). Convergence of the self-consistent iterations was performed for 30 k points inside the irreducible BZ to within 0.0001 Ry with a cutoff of -6.0 Ry between the valence and the core states. The calculations were performed using WIEN2K program.²¹

The bands of p_x and p_z orbitals of Te[2] and Te[3] (atoms in the net) are highly dispersive crossing the Fermi surface, Figure 2.21. This is a clear indication of the metallic character of LaTe₃. Partial density of states (DOS) of the p orbital of Te[3] (Figure 2.22A) and total DOS of the subcell (Figure 2.22B) were also calculated showing no gap at the Fermi level. The Fermi surface topology favors the formation of a nesting vector (q-vector) along the c^* direction with a value of $\sim 0.28(2)$ which is consistent with our experimental observation, Figure 2.23B

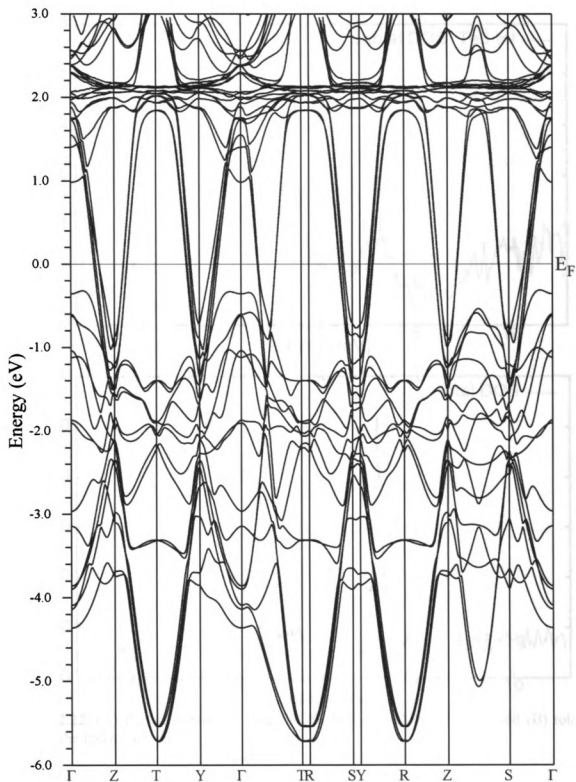


Figure 2.21. Band structure of LaTe_3 near the Fermi level.

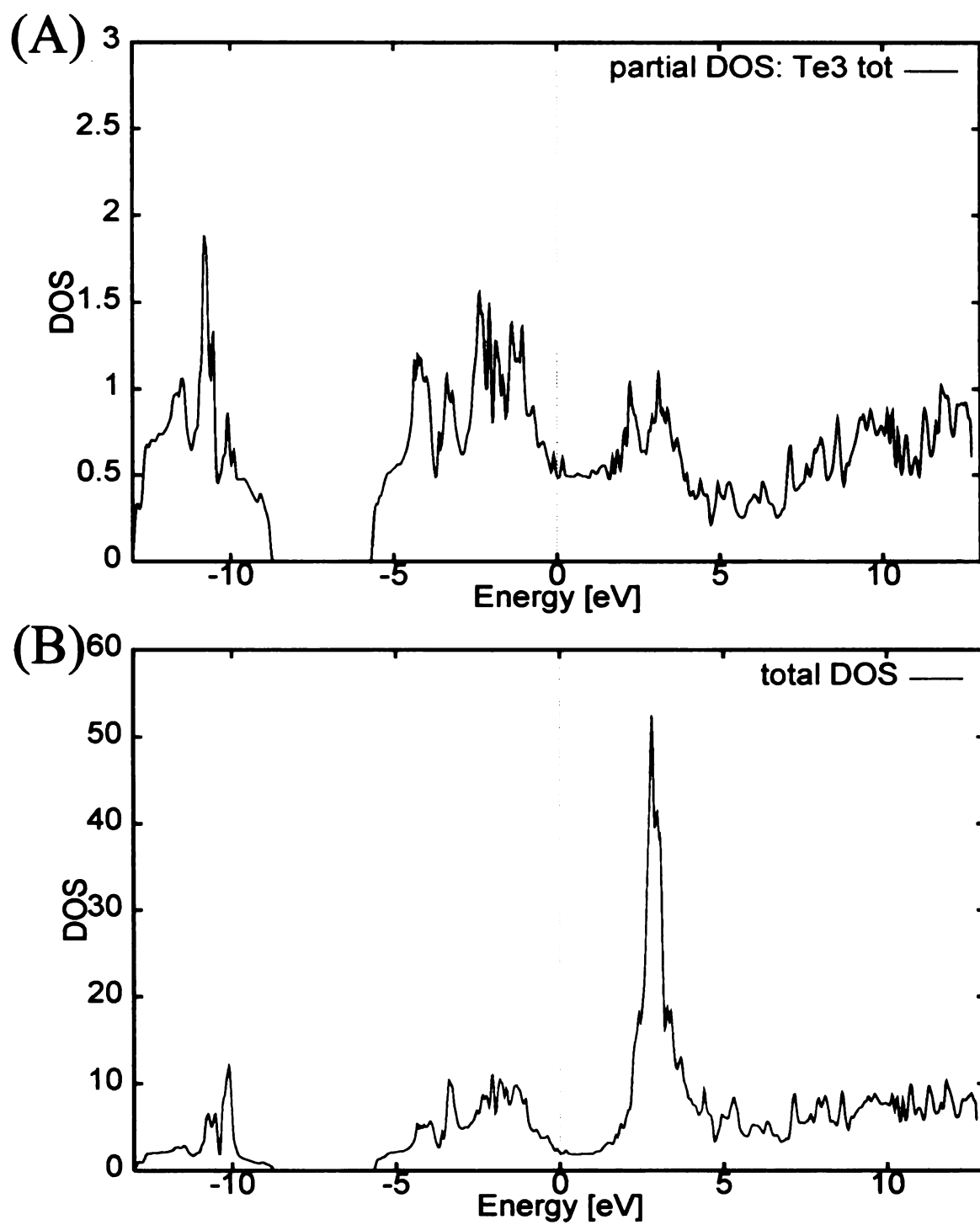


Figure 2.22. (A) Partial density of state (DOS) of the p orbital of Te[3] and (B) total DOS of the LaTe_3 subcell.

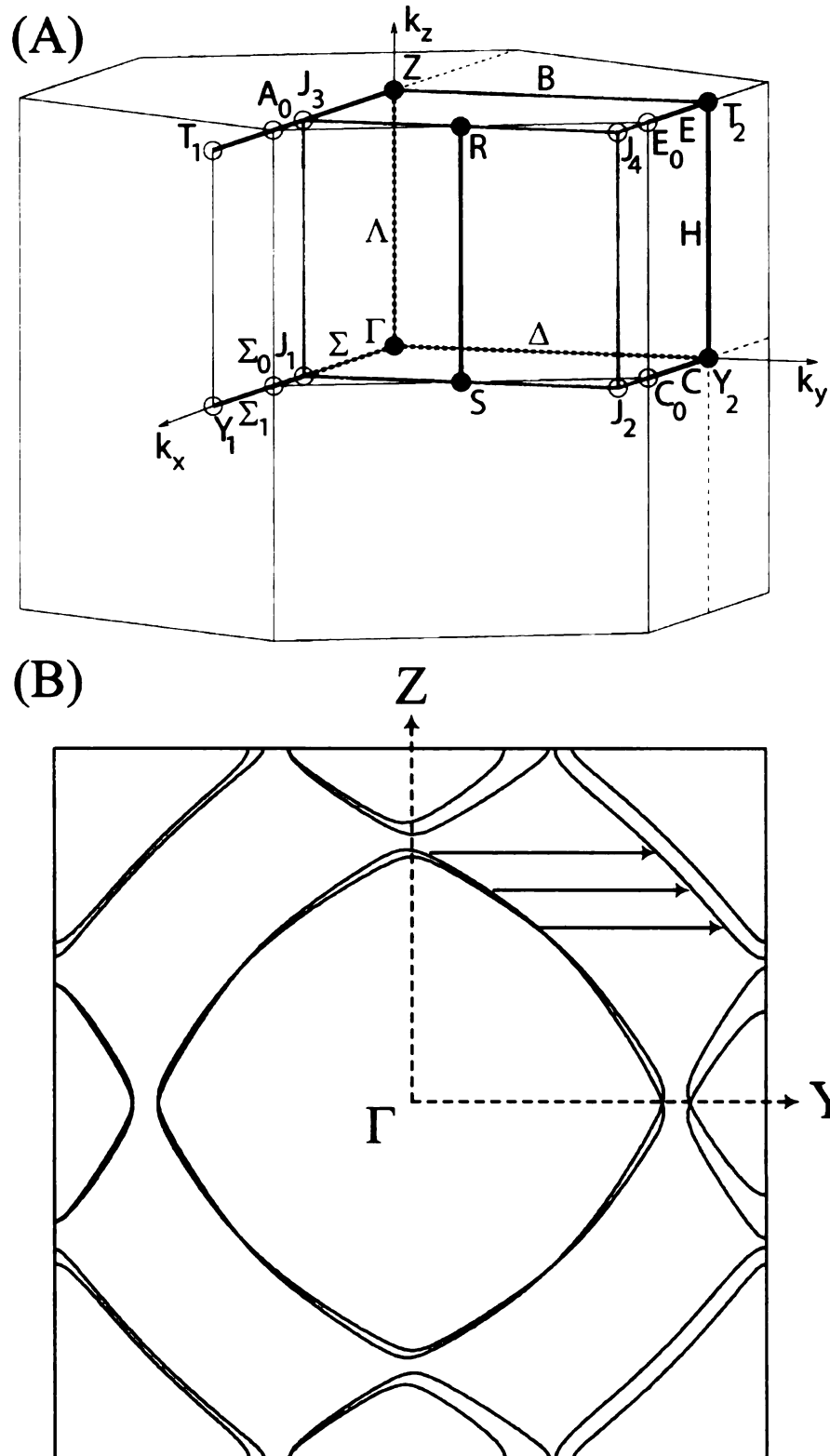


Figure 2.23. (A) Brillouin zone of $Cmcm$ space group (B) Fermi surface topology of $LaTe_3$ with an average nesting vector of 0.28(2) (solid arrows).

2.4. Conclusions

Charge density waves (CDWs) are broken symmetry states of mostly strongly anisotropic quasi-one dimensional metals.²² As a result of a Peierls instability their ground state is a coherent superposition of electron-hole pairs which results in a periodic spatial modulation of the charge density. The study of CDWs is important, because a successful description of the coupled electronic lattice instability reflects on the broader issue of the electronic aspects of structural stability which is linked to several interesting phenomena including superconductivity. The CDW state has not received the same level of attention as superconductivity, although the phenomenon is potentially equally important. The vast majority of CDW studies focused on quasi one-dimensional systems partly because two-dimensional counterparts are scarce.

The resolution of the modulated structures of RETe₃ compounds sheds light on the subtle details of their CDW distortion(s). Furthermore, it reveals for the first time that the nature of the CDW wave in these compounds varies subtly yet detectably with RE element. This result is surprising given that the substitution of one RE for the next is isoelectronic in nature and therefore should presage an identical distortion pattern.²³

Because of the fine differences found in CDW distortions across the RE series, the structural characterization of the remaining members of the RETe₃ family is now justified. It is necessary to apply the superspace group crystallographic approach in order to successfully decipher these subtle differences. The new information reported here regarding the CDW distortions opens fresh perspectives on how to think about these systems and provides new possibilities for more informed theoretical interpretations of their physical properties.

Table 2.14. Crystal data and structure refinement for LaTe₃ at 300 K.

Empirical formula	LaTe ₃
Formula weight	521.7
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3944(8) Å, α = 90° b = 26.227(4) Å, β = 90° c = 4.4076(7) Å, γ = 90°
q-vector(1)	0.2751(4)c*
Volume	507.99(14) Å ³
Z	4
Density (calculated)	6.8193 g/cm ³
Absorption coefficient	25.075 mm ⁻¹
F(000)	852
Crystal size	0.10 x 0.06 x 0.01 mm ³
Theta range for data collection	2.00 to 29.26°
Index ranges	-6<=h<=6, -36<=k<=30, -6<=l<=6, -1<=m<=1
Reflections collected	7195 (2397 main + 4798 satellites)
Independent reflections	2123 (758 main + 1365 satellites) [R _{int} = 0.0783]
Completeness to θ = 29.26°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2123 / 0 / 38
Goodness-of-fit on F ²	1.68
Final R indices [I>2σ(I)]	R _{obs} = 0.0514, wR _{obs} = 0.1190
R indices (all data)	R _{all} = 0.0827, wR _{all} = 0.1267
Final R main indices [I>2σ(I)]	R _{obs} = 0.0410, wR _{obs} = 0.1054
R main indices (all data)	R _{all} = 0.0430, wR _{all} = 0.1059
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1146, wR _{obs} = 0.1723
R 1 st order satellites (all data)	R _{all} = 0.2533, wR _{all} = 0.2004
Extinction coefficient	0.00050(6)
T _{min} and T _{max} coefficients	0.1189 and 0.9333
Largest diff. peak and hole	3.41 and -3.22 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.15. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for LaTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
La	0	9349	1688(1)	2549	17(1)
	sin, 1	0	0	-1(5)	
	cos, 1	59(2)	2(1)	0	
Te[1]	0	9296(8)	2960(1)	2549	17(1)
	sin, 1	0	0	13(6)	
	cos, 1	10(2)	-1(1)	0	
Te[2]	0	9282(11)	691(1)	7549	21(1)
	sin, 1	0	0	-20(8)	
	cos, 1	-308(4)	-3(1)	0	
Te[3]	0	9339(9)	4306(1)	7549	21(1)
	sin, 1	0	0	-51(8)	
	cos, 1	240(4)	-11(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LaTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	13(1)	25(1)	13(1)	0(1)	0	0
Te[1]	13(1)	25(1)	14(1)	0(1)	0	0
Te[2]	20(1)	28(1)	16(1)	4(2)	0	0
Te[3]	18(1)	27(1)	17(1)	-2(1)	0	0

Table 2.17. Bond lengths distributions [$\text{\AA}$] for LaTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[1]	3.336(3)	3.328(5)	3.343(5)
La - Te[1] x 4	3.247(3)	3.229(3)	3.264(3)
La - Te[2] x 2	3.423(3)	3.414(3)	3.433(3)
La - Te[3]	3.398(3)	3.329(5)	3.468(5)
La - Te[3]	3.421(3)	3.388(5)	3.454(5)
Te[2] - Te[3] x 2	3.095(5)	2.934(5)	3.261(5)
Te[2] - Te[3] x 2	3.133(5)	2.988(5)	3.280(5)

Table 2.18. Bond angles distributions [°] for LaTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - La - Te[1] x 8	73.48(6)	73.40(7)	73.57(7)
Te[1] - La - Te[2] x 2	139.85(7)	139.59(6)	140.03(6)
Te[1] - La - Te[3] x 2	140.08(8)	139.68(9)	140.48(9)
Te[1] - La - Te[1] x 8	85.49(7)	85.14(7)	85.85(8)
Te[1] - La - Te[1] x 4	147.00(7)	146.79(10)	147.19(10)
Te[1] - La - Te[2] x 4	77.18(8)	75.52(9)	78.88(9)
Te[1] - La - Te[2] x 4	130.75(10)	128.15(9)	133.37(9)
Te[1] - La - Te[3] x 4	77.50(7)	77.14(7)	77.86(7)
Te[1] - La - Te[3] x 4	130.91(9)	130.27(8)	131.54(8)
Te[2] - La - Te[2] x 2	80.21(7)	79.75(8)	80.57(8)
Te[2] - La - Te[3] x 4	53.96(9)	51.32(9)	56.67(10)
Te[3] - La - Te[3] x 2	80.24(9)	79.72(11)	80.73(11)
La - Te[1] - La x 8	106.53(7)	106.24(8)	106.81(8)
La - Te[1] - La x 8	85.57(9)	85.28(9)	85.85(9)
La - Te[1] - La x 4	147.00(7)	146.84(4)	147.15(4)
La - Te[2] - La x 2	80.17(6)	79.86(8)	80.38(8)
La - Te[2] - Te[3] x 4	62.57(6)	61.92(6)	63.34(7)
La - Te[2] - Te[3] x 4	117.23(12)	114.45(13)	119.90(14)
Te[3] - Te[2] - Te[3] x 2	90.98(16)	86.14(15)	96.00(18)
Te[3] - Te[2] - Te[3] x 6	89.68(11)	89.19(9)	90.18(11)
Te[3] - Te[2] - Te[3] x 4	176.52(16)	173.86(16)	179.79(8)
La - Te[3] - La x 2	80.24(5)	79.72(8)	80.73(8)
La - Te[3] - Te[2] x 2	62.80(8)	61.20(8)	64.43(9)
La - Te[3] - Te[2] x 4	117.12(8)	116.97(8)	117.38(9)
La - Te[3] - Te[2] x 2	63.46(8)	61.01(8)	65.99(9)
Te[2] - Te[3] - Te[2] x 6	89.64(15)	84.57(14)	94.90(17)
Te[2] - Te[3] - Te[2] x 4	176.64(15)	174.06(15)	180
Te[2] - Te[3] - Te[2] x 2	90.98(15)	86.11(14)	95.97(17)

Table 2.19. Crystal data and structure refinement for CeTe₃ at 300 K.

Empirical formula	CeTe ₃
Formula weight	522.9
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3732(5) Å, α = 90° b = 25.973(4) Å, β = 90° c = 4.3849(5) Å, γ = 90°
q-vector(1)	0.2801(3)c*
Volume	498.07(11) Å ³
Z	4
Density (calculated)	6.9714 g/cm ³
Absorption coefficient	26.242 mm ⁻¹
F(000)	856
Crystal size	0.79 x 0.34 x 0.01 mm ³
Theta range for data collection	3.13 to 31.68°
Index ranges	-6 ≤ h ≤ 6, -38 ≤ k ≤ 38, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	7356 (2167 main + 5189 satellites)
Independent reflections	2475 (822 main + 1653 satellites) [R _{int} = 0.0286]
Completeness to θ = 31.68°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2475 / 0 / 38
Goodness-of-fit on F ²	1.50
Final R indices [I > 2σ(I)]	R _{obs} = 0.0334, wR _{obs} = 0.0919
R indices (all data)	R _{all} = 0.0584, wR _{all} = 0.1028
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0171, wR _{obs} = 0.0592
R main indices (all data)	R _{all} = 0.0181, wR _{all} = 0.0600
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0996, wR _{obs} = 0.1496
R 1 st order satellites (all data)	R _{all} = 0.1932, wR _{all} = 0.1732
Extinction coefficient	0.033(8)
T _{min} and T _{max} coefficients	0.0722 and 0.7368
Largest diff. peak and hole	2.95 and -2.68 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.20. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for CeTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Ce	0	9249	1689(1)	2549	7(1)
	sin, 1	0	0	-20(4)	
	cos, 1	58(1)	7(1)	0	
Te[1]	0	9179(3)	2958(1)	2549	7(1)
	sin, 1	0	0	10(4)	
	cos, 1	7(1)	-1(1)	0	
Te[2]	0	9234(4)	697(1)	7549	11(1)
	sin, 1	0	0	1(5)	
	cos, 1	-274(1)	0(1)	0	
Te[3]	0	9222(3)	4300(1)	7549	11(1)
	sin, 1	0	0	7(5)	
	cos, 1	221(1)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.21. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	7(1)	9(1)	6(1)	0(1)	0	0
Te[1]	7(1)	9(1)	6(1)	0(1)	0	0
Te[2]	11(1)	12(1)	10(1)	-4(1)	0	0
Te[3]	11(1)	11(1)	11(1)	-1(1)	0	0

Table 2.22. Bond lengths distributions [$\text{\AA}$] for CeTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[1]	3.2963(11)	3.2750(19)	3.3180(19)
Ce - Te[1] x 2	3.2353(15)	3.2190(17)	3.2515(17)
Ce - Te[1] x 2	3.2228(15)	3.2042(12)	3.2418(12)
Ce - Te[2] x 2	3.3847(15)	3.3690(16)	3.3985(15)
Ce - Te[3]	3.3670(13)	3.3355(18)	3.3998(18)
Ce - Te[3]	3.3801(13)	3.3198(18)	3.4395(18)
Te[2] - Te[3] x 2	3.101(2)	2.9662(16)	3.2407(18)
Te[2] - Te[3] x 2	3.095(2)	2.9564(16)	3.2350(17)

Table 2.23. Bond angles distributions [°] for CeTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Ce - Te[1] x 8	73.44(3)	73.35(3)	73.54(3)
Te[1] - Ce - Te[2] x 2	139.57(5)	139.15(5)	139.94(7)
Te[1] - Ce - Te[3] x 2	139.57(3)	138.84(4)	140.29(4)
Te[1] - Ce - Te[1] x 6	85.32(4)	85.03(4)	85.62(4)
Te[1] - Ce - Te[1] x 4	147.05(3)	146.51(4)	147.58(4)
Te[1] - Ce - Te[2] x 2	77.24(4)	75.73(4)	78.78(4)
Te[1] - Ce - Te[2] x 2	131.12(4)	128.60(4)	133.67(4)
Te[1] - Ce - Te[3] x 4	77.13(4)	76.72(4)	77.54(4)
Te[1] - Ce - Te[3] x 4	131.01(5)	130.63(5)	131.39(5)
Te[1] - Ce - Te[1] x 2	85.74(4)	84.98(4)	86.49(4)
Te[1] - Ce - Te[2] x 2	76.87(4)	75.19(4)	78.52(4)
Te[1] - Ce - Te[2] x 2	130.86(4)	128.78(4)	132.89(4)
Te[2] - Ce - Te[2] x 2	80.79(4)	80.37(4)	81.12(4)
Te[2] - Ce - Te[3] x 4	54.67(4)	52.26(4)	57.17(4)
Te[3] - Ce - Te[3] x 2	80.80(3)	80.39(4)	81.20(4)
Ce - Te[1] - Ce x 4	106.62(4)	106.20(4)	107.04(4)
Ce - Te[1] - Ce x 4	106.33(4)	105.68(4)	106.99(4)
Ce - Te[1] - Ce x 8	85.24(4)	85.01(3)	85.48(3)
Ce - Te[1] - Ce x 4	147.05(3)	146.80(4)	147.29(4)
Ce - Te[2] - Ce x 2	80.75(4)	80.30(5)	81.12(5)
Ce - Te[2] - Te[3] x 2	62.35(3)	61.59(3)	63.08(3)
Ce - Te[2] - Te[3] x 2	116.93(5)	113.96(6)	119.84(6)
Ce - Te[2] - Te[3] x 2	62.68(3)	62.11(3)	63.26(3)
Ce - Te[2] - Te[3] x 2	117.41(5)	114.24(6)	120.56(6)
Te[3] - Te[2] - Te[3] x 4	90.14(6)	85.40(6)	95.02(7)
Te[3] - Te[2] - Te[3] x 4	89.73(5)	89.58(4)	89.92(7)
Te[3] - Te[2] - Te[3] x 4	176.96(7)	175.09(7)	179.69(3)
Ce - Te[3] - Ce x 2	80.80(2)	80.39(4)	81.20(4)
Ce - Te[3] - Te[2] x 4	62.87(3)	61.13(3)	64.70(3)
Ce - Te[3] - Te[2] x 4	117.42(4)	116.30(4)	118.48(4)
Te[2] - Te[3] - Te[2] x 4	90.40(6)	85.93(6)	95.01(6)
Te[2] - Te[3] - Te[2] x 4	89.73(6)	89.58(5)	89.92(7)
Te[2] - Te[3] - Te[2] x 4	177.10(7)	175.31(6)	179.70(3)

Table 2.24. Crystal data and structure refinement for PrTe₃ at 300 K.

Empirical formula	PrTe ₃
Formula weight	523.7
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3569(9) Å, α = 90° b = 25.896(5) Å, β = 90° c = 4.3666(9) Å, γ = 90°
q-vector(1)	0.2818(4)c*
Volume	492.67(17) Å ³
Z	4
Density (calculated)	7.058 g/cm ³
Absorption coefficient	26.945 mm ⁻¹
F(000)	860
Crystal size	0.32 x 0.31 x 0.02 mm ³
Theta range for data collection	2.05 to 29.17°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	5753 (3116 main + 6667 satellites)
Independent reflections	1914 (1094 main + 2046 satellites) [R _{int} = 0.0337]
Completeness to θ = 29.17°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1914 / 0 / 38
Goodness-of-fit on F ²	1.57
Final R indices [I > 2σ(I)]	R _{obs} = 0.0308, wR _{obs} = 0.0964
R indices (all data)	R _{all} = 0.0530, wR _{all} = 0.1077
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0402, wR _{obs} = 0.1191
R main indices (all data)	R _{all} = 0.0419, wR _{all} = 0.1224
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1200, wR _{obs} = 0.2178
R 1 st order satellites (all data)	R _{all} = 0.2453, wR _{all} = 0.3103
Extinction coefficient	0.00184(9)
T _{min} and T _{max} coefficients	0.0091 and 0.5931
Largest diff. peak and hole	2.30 and -2.07 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.25. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for PrTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Pr	0	9249	1691(1)	2549	5(1)
	sin, 1	0	0	3(3)	
	cos, 1	53(1)	1(1)	0	
Te[1]	0	9188(5)	2957(1)	2549	5(1)
	sin, 1	0	0	4(4)	
	cos, 1	6(1)	0(1)	0	
Te[2]	0	9213(5)	701(1)	7549	9(1)
	sin, 1	0	0	-13(5)	
	cos, 1	-246(2)	6(1)	0	
Te[3]	0	9267(4)	4297(1)	7549	8(1)
	sin, 1	0	0	-5(5)	
	cos, 1	205(2)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.26. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr	5(1)	6(1)	5(1)	-1(1)	0	0
Te[1]	5(1)	6(1)	5(1)	2(1)	0	0
Te[2]	10(1)	9(1)	8(1)	0(1)	0	0
Te[3]	8(1)	9(1)	8(1)	3(1)	0	0

Table 2.27. Bond lengths distributions [$\text{\AA}$] for PrTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Pr - Te[1]	3.2772(14)	3.275(2)	3.279(2)
Pr - Te[1] x 2	3.2201(17)	3.2051(16)	3.2349(16)
Pr - Te[1] x 2	3.2127(17)	3.1984(16)	3.2274(16)
Pr - Te[2] x 2	3.3690(15)	3.3589(15)	3.3815(15)
Pr - Te[3]	3.3424(17)	3.304(2)	3.382(2)
Pr - Te[3]	3.3808(17)	3.334(2)	3.428(2)
Te[2] - Te[3] x 2	3.068(3)	2.943(2)	3.197(2)
Te[2] - Te[3] x 2	3.103(3)	2.980(2)	3.227(2)

Table 2.28. Bond angles distributions [°] for PrTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Pr - Te[1] x 8	73.47(3)	73.34(4)	73.60(4)
Te[1] - Pr - Te[2] x 2	139.56(4)	139.35(5)	139.77(6)
Te[1] - Pr - Te[3]	139.90(5)	139.34(5)	140.46(5)
Te[1] - Pr - Te[3]	139.32(4)	138.90(5)	139.76(5)
Te[1] - Pr - Te[1] x 6	85.38(4)	84.96(4)	85.81(4)
Te[1] - Pr - Te[1] x 4	147.03(4)	146.94(6)	147.12(5)
Te[1] - Pr - Te[2] x 4	77.12(4)	75.55(5)	78.71(5)
Te[1] - Pr - Te[2] x 4	131.01(5)	128.99(5)	133.04(5)
Te[1] - Pr - Te[3] x 2	77.36(4)	76.92(4)	77.79(4)
Te[1] - Pr - Te[3] x 2	131.11(5)	130.70(5)	131.52(5)
Te[1] - Pr - Te[1] x 2	85.62(4)	85.08(4)	86.16(4)
Te[1] - Pr - Te[3] x 2	130.72(5)	130.16(5)	131.28(5)
Te[1] - Pr - Te[3] x 2	76.90(4)	76.50(4)	77.32(4)
Te[2] - Pr - Te[2] x 2	80.82(4)	80.72(5)	80.88(3)
Te[2] - Pr - Te[3] x 2	54.40(5)	52.38(5)	56.47(5)
Te[2] - Pr - Te[3] x 2	54.74(5)	52.62(5)	56.85(5)
Te[3] - Pr - Te[3] x 2	80.78(4)	80.64(5)	80.90(5)
Pr - Te[1] - Pr x 8	106.57(4)	106.30(5)	106.83(5)
Pr - Te[1] - Pr x 8	85.26(3)	85.25(2)	85.27(2)
Pr - Te[1] - Pr x 4	147.04(4)	146.89(2)	147.18(2)
Pr - Te[2] - Pr x 2	80.79(3)	80.40(5)	81.12(5)
Pr - Te[2] - Te[3] x 4	117.34(6)	114.18(7)	120.48(7)
Pr - Te[2] - Te[3] x 4	62.81(3)	62.32(3)	63.34(3)
Te[3] - Te[2] - Te[3] x 2	90.85(8)	86.59(8)	95.23(9)
Te[3] - Te[2] - Te[3] x 6	89.77(6)	89.63(5)	89.96(7)
Te[3] - Te[2] - Te[3] x 4	177.18(8)	175.04(8)	179.72(4)
Pr - Te[3] - Pr x 2	80.78(3)	80.64(4)	80.90(4)
Pr - Te[3] - Te[2] x 2	62.46(4)	60.59(4)	64.42(4)
Pr - Te[3] - Te[2] x 4	117.32(4)	116.20(4)	118.38(4)
Pr - Te[3] - Te[2] x 2	63.25(4)	61.80(4)	64.71(4)
Te[2] - Te[3] - Te[2] x 6	89.60(7)	85.45(7)	93.87(8)
Te[2] - Te[3] - Te[2] x 4	177.31(8)	175.23(8)	179.77(3)
Te[2] - Te[3] - Te[2] x 2	90.85(7)	86.83(7)	94.96(8)

Table 2.29. Crystal data and structure refinement for NdTe₃ at 300 K.

Empirical formula	NdTe ₃
Formula weight	527
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3433(6) Å, α = 90° b = 25.809(4) Å, β = 90° c = 4.3538(5) Å, γ = 90°
q-vector(1)	0.2827(3)c*
Volume	488.04(12) Å ³
Z	4
Density (calculated)	7.1705 g/cm ³
Absorption coefficient	28.004 mm ⁻¹
F(000)	864
Crystal size	0.34 x 0.23 x 0.01 mm ³
Theta range for data collection	2.05 to 29.14°
Index ranges	-5<=h<=5, -34<=k<=34, -6<=l<=5, -1<=m<=1
Reflections collected	12410 (1865 main + 4340 satellites)
Independent reflections	1991 (685 main + 1301 satellites) [R _{int} = 0.0256]
Completeness to θ = 29.14°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1991 / 0 / 38
Goodness-of-fit on F ²	1.59
Final R indices [I>2σ(I)]	R _{obs} = 0.0259, wR _{obs} = 0.0899
R indices (all data)	R _{all} = 0.0431, wR _{all} = 0.1019
Final R main indices [I>2σ(I)]	R _{obs} = 0.0172, wR _{obs} = 0.0653
R main indices (all data)	R _{all} = 0.0174, wR _{all} = 0.0653
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.0847, wR _{obs} = 0.1414
R 1 st order satellites (all data)	R _{all} = 0.2019, wR _{all} = 0.1729
Extinction coefficient	0.00096(7)
T _{min} and T _{max} coefficients	0.0151 and 0.6913
Largest diff. peak and hole	2.23 and -1.95 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.30. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for NdTe₃ at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Nd	0	9249	1692(1)	2549	6(1)
	sin, 1	0	0	-1(3)	
	cos, 1	53(1)	0(1)	0	
Te[1]	0	9202(3)	2956(1)	2549	6(1)
	sin, 1	0	0	-4(3)	
	cos, 1	6(1)	0(1)	0	
Te[2]	0	9264(4)	703(1)	7549	9(1)
	sin, 1	0	0	-6(4)	
	cos, 1	-230(1)	8(1)	0	
Te[3]	0	9209(3)	4295(1)	7549	9(1)
	sin, 1	0	0	20(4)	
	cos, 1	191(2)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.31. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Nd	6(1)	7(1)	5(1)	-1(1)	0	0
Te[1]	6(1)	7(1)	6(1)	-3(1)	0	0
Te[2]	10(1)	10(1)	8(1)	0(1)	0	0
Te[3]	9(1)	9(1)	9(1)	4(1)	0	0

Table 2.32. Bond lengths distributions [$\text{\AA}$] for NdTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Nd - Te[1]	3.2618(10)	3.2605(17)	3.2632(17)
Nd - Te[1] x 4	3.2063(12)	3.1928(12)	3.2196(12)
Nd - Te[2] x 2	3.3544(11)	3.3393(11)	3.3717(11)
Nd - Te[3]	3.3451(12)	3.3080(16)	3.3832(16)
Nd - Te[3]	3.3507(12)	3.3100(16)	3.3908(16)
Te[2] - Te[3] x 2	3.0922(19)	2.9787(16)	3.2095(17)
Te[2] - Te[3] x 2	3.0598(18)	2.9420(16)	3.1786(17)

Table 2.33. Bond angles distributions [°] for NdTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Nd - Te[1] x 8	73.52(3)	73.35(3)	73.69(3)
Te[1] - Nd - Te[2] x 2	139.49(3)	139.26(4)	139.70(5)
Te[1] - Nd - Te[3] x 2	139.63(3)	139.18(3)	140.08(3)
Te[1] - Nd - Te[1] x 4	85.52(3)	85.02(3)	86.03(3)
Te[1] - Nd - Te[1] x 4	85.25(4)	85.21(3)	85.29(3)
Te[1] - Nd - Te[1] x 4	147.02(3)	147.01(3)	147.042(18)
Te[1] - Nd - Te[2] x 2	77.32(3)	75.85(3)	78.80(4)
Te[1] - Nd - Te[2] x 2	131.45(4)	129.57(4)	133.33(4)
Te[1] - Nd - Te[3] x 4	77.15(3)	76.75(3)	77.54(3)
Te[1] - Nd - Te[3] x 4	130.96(4)	130.49(4)	131.42(3)
Te[1] - Nd - Te[2] x 2	76.70(3)	75.50(3)	77.87(3)
Te[1] - Nd - Te[2] x 2	130.62(4)	128.58(4)	132.64(4)
Te[2] - Nd - Te[2] x 2	80.96(3)	80.70(4)	81.15(4)
Te[2] - Nd - Te[3] x 2	54.96(4)	53.20(4)	56.78(4)
Te[2] - Nd - Te[3] x 2	54.31(4)	52.18(4)	56.42(4)
Te[3] - Nd - Te[3] x 2	80.88(3)	80.83(4)	80.91(4)
Nd - Te[1] - Nd x 8	106.48(3)	106.17(3)	106.78(3)
Nd - Te[1] - Nd x 8	85.49(4)	85.23(4)	85.74(4)
Nd - Te[1] - Nd x 4	147.02(3)	146.899(19)	147.152(19)
Nd - Te[2] - Nd x 2	80.93(3)	80.45(3)	81.35(3)
Nd - Te[2] - Te[3] x 4	62.35(3)	61.64(2)	63.04(2)
Nd - Te[2] - Te[3] x 2	116.79(4)	113.68(5)	119.88(5)
Nd - Te[2] - Te[3] x 2	117.82(4)	115.72(5)	119.86(5)
Te[3] - Te[2] - Te[3] x 6	89.60(6)	85.49(6)	93.80(6)
Te[3] - Te[2] - Te[3] x 4	177.38(6)	175.25(6)	179.89(6)
Te[3] - Te[2] - Te[3] x 2	90.84(6)	87.03(6)	94.79(6)
Nd - Te[3] - Nd x 2	80.878(19)	80.83(3)	80.91(3)
Nd - Te[3] - Te[2] x 2	62.93(3)	61.07(3)	64.88(3)
Nd - Te[3] - Te[2] x 4	117.08(3)	116.71(3)	117.38(3)
Nd - Te[3] - Te[2] x 2	62.67(3)	61.42(3)	63.93(3)
Te[2] - Te[3] - Te[2] x 2	90.85(6)	86.95(5)	94.85(6)
Te[2] - Te[3] - Te[2] x 6	89.77(5)	89.56(5)	90.13(5)
Te[2] - Te[3] - Te[2] x 4	177.51(6)	175.47(6)	180

Table 2.34. Crystal data and structure refinement for SmTe₃ at 300 K.

Empirical formula	SmTe ₃
Formula weight	533.2
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3218(6) Å, α = 90° b = 25.609(5) Å, β = 90° c = 4.3342(8) Å, γ = 90°
q-vector(1)	0.2874(4)c*
Volume	479.69(14) Å ³
Z	4
Density (calculated)	7.380 g/cm ³
Absorption coefficient	29.889 mm ⁻¹
F(000)	872
Crystal size	0.17 x 0.11 x 0.01 mm ³
Theta range for data collection	2.08 to 29.19°
Index ranges	-5<=h<=5, -34<=k<=34, -6<=l<=6, -1<=m<=1
Reflections collected	6599 (2048 main + 4551 satellites)
Independent reflections	1937 (663 main + 1274 satellites) [R _{int} = 0.0285]
Completeness to θ = 29.19°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1937 / 0 / 37
Goodness-of-fit on F ²	1.61
Final R indices [I>2σ(I)]	R _{obs} = 0.0267, wR _{obs} = 0.1044
R indices (all data)	R _{all} = 0.0507, wR _{all} = 0.1123
Final R main indices [I>2σ(I)]	R _{obs} = 0.0157, wR _{obs} = 0.0650
R main indices (all data)	R _{all} = 0.0159, wR _{all} = 0.0651
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1177, wR _{obs} = 0.2307
R 1 st order satellites (all data)	R _{all} = 0.2544, wR _{all} = 0.2551
Extinction coefficient	0.00169(8)
T _{min} and T _{max} coefficients	0.0501 and 0.6404
Largest diff. peak and hole	2.35 and -2.33 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2} \text{ and } w=1/(\sigma^2(I)+0.0016I^2)$	

Table 2.35. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for SmTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Sm	0	9449	1694(1)	2549	7(1)
	sin, 1	0	0	-18(4)	
	cos, 1	42(1)	6(1)	0	
Te[1]	0	9399(5)	2952(1)	2549	6(1)
	sin, 1	0	0	-6(4)	
	cos, 1	4(1)	0(1)	0	
Te[2]	0	9394(6)	708(1)	7549	10(1)
	sin, 1	0	0	14(5)	
	cos, 1	-144(2)	-2(1)	0	
Te[3]	0	4354(5)	709(1)	2549	9(1)
	sin, 1	0	0	13(5)	
	cos, 1	187(2)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.36. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SmTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	7(1)	7(1)	7(1)	1(1)	0	0
Te[1]	6(1)	6(1)	7(1)	1(1)	0	0
Te[2]	11(1)	10(1)	9(1)	2(1)	0	0
Te[3]	8(1)	10(1)	9(1)	3(1)	0	0

Table 2.37. Bond lengths distributions [$\text{\AA}$] for SmTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm - Te[1]	3.2216(13)	3.207(2)	3.236(2)
Sm - Te[1] x 4	3.1917(18)	3.1839(19)	3.1996(19)
Sm - Te[2] x 2	3.3289(16)	3.3117(16)	3.3455(16)
Sm - Te[3]	3.3359(19)	3.306(2)	3.367(2)
Sm - Te[3]	3.3107(19)	3.259(2)	3.362(2)
Te[2] - Te[3] x 2	3.073(3)	2.986(2)	3.162(3)
Te[2] - Te[3] x 2	3.050(3)	2.955(2)	3.144(3)

Table 2.38. Bond angles distributions [°] for SmTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Sm - Te[1] x 8	73.52(4)	73.41(4)	73.63(4)
Te[1] - Sm - Te[2] x 2	139.36(4)	139.05(5)	139.67(6)
Te[1] - Sm - Te[3]	139.18(5)	138.49(5)	139.87(5)
Te[1] - Sm - Te[3]	139.71(5)	139.33(5)	140.10(5)
Te[1] - Sm - Te[1] x 4	85.53(4)	85.23(5)	85.82(5)
Te[1] - Sm - Te[1] x 4	85.24(5)	85.01(5)	85.47(5)
Te[1] - Sm - Te[1] x 4	147.06(4)	146.57(5)	147.54(5)
Te[1] - Sm - Te[2] x 4	76.84(5)	76.01(4)	77.69(4)
Te[1] - Sm - Te[2] x 4	131.04(5)	129.50(5)	132.61(5)
Te[1] - Sm - Te[3] x 2	76.82(4)	76.47(5)	77.17(5)
Te[1] - Sm - Te[3] x 4	130.86(5)	130.53(5)	131.19(5)
Te[1] - Sm - Te[3] x 2	77.19(4)	76.63(4)	77.77(4)
Te[2] - Sm - Te[2] x 2	81.25(4)	80.97(5)	81.50(5)
Te[2] - Sm - Te[3] x 4	54.90(5)	53.35(5)	56.49(5)
Te[3] - Sm - Te[3] x 2	81.11(5)	80.80(6)	81.41(6)
Sm - Te[1] - Sm x 8	106.48(5)	106.24(4)	106.72(5)
Sm - Te[1] - Sm x 4	85.55(5)	85.42(6)	85.68(6)
Sm - Te[1] - Sm x 4	85.24(3)	85.01(3)	85.47(3)
Sm - Te[1] - Sm x 4	147.06(4)	146.77(6)	147.34(6)
Sm - Te[2] - Sm x 2	81.24(4)	80.77(5)	81.69(5)
Sm - Te[2] - Te[3] x 2	62.65(4)	62.28(4)	63.06(4)
Sm - Te[2] - Te[3] x 4	117.34(6)	115.72(7)	118.94(8)
Sm - Te[2] - Te[3] x 2	62.35(4)	62.07(4)	62.65(4)
Te[3] - Te[2] - Te[3] x 6	89.77(9)	86.72(8)	92.86(9)
Te[3] - Te[2] - Te[3] x 4	178.09(9)	176.56(9)	179.90(5)
Te[3] - Te[2] - Te[3] x 2	90.66(9)	87.81(8)	93.59(9)
Sm - Te[3] - Sm x 2	81.11(3)	80.80(5)	81.41(5)
Sm - Te[3] - Te[2] x 2	62.97(5)	61.76(4)	64.23(5)
Sm - Te[3] - Te[2] x 4	117.28(5)	116.67(4)	117.89(4)
Sm - Te[3] - Te[2] x 2	62.45(5)	60.94(5)	63.95(5)
Te[2] - Te[3] - Te[2] x 2	90.64(8)	87.64(8)	93.78(9)
Te[2] - Te[3] - Te[2] x 6	89.78(7)	89.63(6)	89.86(6)
Te[2] - Te[3] - Te[2] x 4	177.96(9)	176.38(9)	179.91(4)

Table 2.39. Crystal data and structure refinement for GdTe₃ at 300 K.

Empirical formula	GdTe ₃
Formula weight	540
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3083(4) Å, α = 90° b = 25.528(2) Å, β = 90° c = 4.3154(5) Å, γ = 90°
q-vector(1)	0.2916(3)c*
Volume	474.61(8) Å ³
Z	4
Density (calculated)	7.5556 g/cm ³
Absorption coefficient	31.821 mm ⁻¹
F(000)	880
Crystal size	0.11 x 0.10 x 0.01 mm ³
Theta range for data collection	2.10 to 29.09°
Index ranges	-5<=h<=5, -34<=k<=34, -6<=l<=6, -1<=m<=1
Reflections collected	6851 (2246 main + 4605 satellites)
Independent reflections	1932 (682 main + 1250 satellites) [R _{int} = 0.0898]
Completeness to θ = 29.09°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1932 / 0 / 39
Goodness-of-fit on F ²	1.47
Final R indices [I>2σ(I)]	R _{obs} = 0.0406, wR _{obs} = 0.1025
R indices (all data)	R _{all} = 0.0652, wR _{all} = 0.1081
Final R main indices [I>2σ(I)]	R _{obs} = 0.0376, wR _{obs} = 0.0991
R main indices (all data)	R _{all} = 0.0379, wR _{all} = 0.0994
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.0867, wR _{obs} = 0.1516
R 1 st order satellites (all data)	R _{all} = 0.2907, wR _{all} = 0.2095
Extinction coefficient	0.00020(5)
T _{min} and T _{max} coefficients	0.0590 and 0.8188
Largest diff. peak and hole	2.62 and -2.10 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2} \text{ and } w=1/(\sigma^2(I)+0.0016I^2)$	

Table 2.40. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for GdTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Gd	0	9000	1696(1)	2549	11(1)
	sin, 1	0	0	2(3)	
	cos, 1	-40(1)	0(1)	0	
Te[1]	0	8989(5)	2948(1)	2549	10(1)
	sin, 1	0	0	-8(5)	
	cos, 1	-5(2)	0(1)	0	
Te[2]	0	9015(5)	711(1)	7549	14(1)
	sin, 1	0	0	5(5)	
	cos, 1	150(4)	9(1)	0	
Te[3]	0	4082(5)	712(1)	2549	13(1)
	sin, 1	0	0	40(5)	
	cos, 1	-132(4)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.41. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for GdTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd	10(1)	16(1)	6(1)	0(1)	0	0
Te[1]	9(1)	15(1)	6(1)	3(1)	0	0
Te[2]	14(1)	18(1)	8(1)	-3(1)	0	0
Te[3]	13(1)	19(1)	8(1)	-1(1)	0	0

Table 2.42. Bond lengths distributions [$\text{\AA}$] for GdTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Gd - Te[1]	3.1951(18)	3.195(3)	3.196(3)
Gd - Te[1] x 2	3.1847(18)	3.1719(19)	3.1978(19)
Gd - Te[1] x 2	3.1784(18)	3.1696(17)	3.1871(17)
Gd - Te[2] x 2	3.3146(18)	3.299(2)	3.331(2)
Gd - Te[3]	3.287(2)	3.261(3)	3.313(3)
Gd - Te[3]	3.332(2)	3.307(3)	3.359(3)
Te[2] - Te[3] x 2	3.030(3)	2.946(2)	3.113(3)
Te[2] - Te[3] x 2	3.069(3)	2.999(2)	3.142(3)

Table 2.43. Bond angles distributions [°] for GdTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Gd - Te[1] x 8	73.35(4)	73.23(4)	73.48(4)
Te[1] - Gd - Te[2] x 2	139.36(5)	139.04(5)	139.67(5)
Te[1] - Gd - Te[3] x 2	139.02(5)	138.77(5)	139.28(5)
Te[1] - Gd - Te[1] x 8	85.30(5)	85.02(5)	85.58(5)
Te[1] - Gd - Te[1] x 4	146.79(5)	146.77(5)	146.82(4)
Te[1] - Gd - Te[2] x 4	77.12(5)	76.40(5)	77.82(5)
Te[1] - Gd - Te[2] x 4	131.23(5)	129.81(5)	132.65(5)
Te[1] - Gd - Te[3] x 2	77.36(5)	77.05(4)	77.67(4)
Te[1] - Gd - Te[3] x 2	131.34(5)	130.98(5)	131.70(5)
Te[1] - Gd - Te[3] x 2	130.89(6)	130.48(6)	131.29(6)
Te[1] - Gd - Te[3] x 2	76.79(5)	76.47(5)	77.10(5)
Te[2] - Gd - Te[2] x 2	81.24(5)	80.89(6)	81.57(6)
Te[2] - Gd - Te[3] x 2	54.64(5)	53.04(5)	56.22(5)
Te[2] - Gd - Te[3] x 2	55.00(5)	53.95(5)	56.08(5)
Te[3] - Gd - Te[3] x 2	81.20(5)	81.19(7)	81.21(4)
Gd - Te[1] - Gd x 8	106.68(5)	106.46(6)	106.90(6)
Gd - Te[1] - Gd x 8	85.51(5)	85.34(6)	85.68(6)
Gd - Te[1] - Gd x 4	146.80(5)	146.70(3)	146.89(3)
Gd - Te[2] - Gd x 2	81.23(4)	80.72(6)	81.72(6)
Gd - Te[2] - Te[3] x 4	62.21(4)	61.93(4)	62.51(4)
Gd - Te[2] - Te[3] x 4	117.48(6)	116.34(8)	118.60(8)
Te[3] - Te[2] - Te[3] x 2	90.90(8)	88.60(9)	93.25(9)
Te[3] - Te[2] - Te[3] x 4	89.86(6)	89.48(5)	90.28(6)
Te[3] - Te[2] - Te[3] x 4	178.17(8)	176.44(9)	180
Te[3] - Te[2] - Te[3] x 2	89.37(8)	86.42(8)	92.36(9)
Gd - Te[3] - Gd x 2	81.20(3)	81.19(6)	81.21(2)
Gd - Te[3] - Te[2] x 2	62.21(5)	61.43(5)	62.98(5)
Gd - Te[3] - Te[2] x 4	117.48(5)	117.21(5)	117.79(5)
Gd - Te[3] - Te[2] x 2	63.15(5)	61.76(4)	64.60(5)
Te[2] - Te[3] - Te[2] x 2	89.39(8)	86.81(8)	91.97(9)
Te[2] - Te[3] - Te[2] x 4	89.86(6)	89.48(7)	90.28(8)
Te[2] - Te[3] - Te[2] x 4	178.24(8)	176.59(9)	180
Te[2] - Te[3] - Te[2] x 2	90.88(8)	88.37(8)	93.47(9)

Table 2.44. Crystal data and structure refinement for TbTe₃ at 300 K.

Empirical formula	TbTe ₃
Formula weight	541.7
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2995(8) Å, α = 90° b = 25.420(6) Å, β = 90° c = 4.3078(9) Å, γ = 90°
q-vector(1)	0.2957(5)c*
Volume	470.82(17) Å ³
Z	4
Density (calculated)	7.640 g/cm ³
Absorption coefficient	33.11 mm ⁻¹
F(000)	884
Crystal size	0.28 x 0.20 x 0.03 mm ³
Theta range for data collection	2.12 to 29.09°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6061 (1886 main + 4175 satellites)
Independent reflections	1912 (664 main + 1248 satellites) [R _{int} = 0.0953]
Completeness to θ = 29.09°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1912 / 0 / 39
Goodness-of-fit on F ²	2.32
Final R indices [I > 2σ(I)]	R _{obs} = 0.0680, wR _{obs} = 0.1658
R indices (all data)	R _{all} = 0.0931, wR _{all} = 0.1711
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0647, wR _{obs} = 0.1646
R main indices (all data)	R _{all} = 0.0648, wR _{all} = 0.1646
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1346, wR _{obs} = 0.1959
R 1 st order satellites (all data)	R _{all} = 0.3717, wR _{all} = 0.2925
Extinction coefficient	0.00093(9)
T _{min} and T _{max} coefficients	0.0286 and 0.3198
Largest diff. peak and hole	7.80 and -5.93 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.45. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for TbTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Tb	0	9000	1697(1)	2549	10(1)
	sin, 1	0	0	-13(7)	
	cos, 1	26(2)	6(1)	0	
Te[1]	0	9014(7)	2948(1)	2549	9(1)
	sin, 1	0	0	9(9)	
	cos, 1	2(2)	-1(1)	0	
Te[2]	0	9043(7)	714(1)	7549	12(1)
	sin, 1	0	0	9(9)	
	cos, 1	-104(5)	0(1)	0	
Te[3]	0	9026(7)	4285(1)	7549	12(1)
	sin, 1	0	0	0(9)	
	cos, 1	83(5)	-1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.46. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TbTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tb	6(1)	18(1)	6(1)	8(1)	0	0
Te[1]	4(1)	18(1)	5(1)	-1(1)	0	0
Te[2]	7(1)	22(1)	7(1)	2(1)	0	0
Te[3]	7(1)	21(1)	8(1)	2(1)	0	0

Table 2.47. Bond lengths distributions [$\text{\AA}$] for TbTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Tb - Te[1] x 3	3.178(2)	3.161(4)	3.196(4)
Tb - Te[1] x 2	3.170(3)	3.162(4)	3.178(4)
Tb - Te[2] x 2	3.299(3)	3.285(3)	3.312(3)
Tb - Te[3]	3.288(3)	3.281(4)	3.295(4)
Tb - Te[3]	3.303(3)	3.277(4)	3.328(4)
Te[2] - Te[3] x 2	3.048(4)	2.999(4)	3.099(4)
Te[2] - Te[3] x 2	3.039(4)	2.987(4)	3.090(4)

Table 2.48. Bond angles distributions [°] for TbTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Tb - Te[1] x 8	73.53(6)	73.39(6)	73.66(6)
Te[1] - Tb - Te[2] x 2	139.23(9)	138.91(11)	139.53(11)
Te[1] - Tb - Te[3]	139.54(7)	139.26(8)	139.81(8)
Te[1] - Tb - Te[3]	139.02(7)	139.02(7)	139.03(8)
Te[1] - Tb - Te[1] x 8	85.59(8)	85.55(8)	85.64(8)
Te[1] - Tb - Te[1] x 4	146.95(6)	146.50(8)	147.38(8)
Te[1] - Tb - Te[2] x 4	77.04(8)	76.44(7)	77.66(7)
Te[1] - Tb - Te[2] x 2	131.54(8)	130.45(7)	132.64(7)
Te[1] - Tb - Te[3] x 4	77.09(7)	76.98(8)	77.20(8)
Te[1] - Tb - Te[3] x 4	131.14(9)	130.92(10)	131.35(10)
Te[1] - Tb - Te[2] x 2	130.84(8)	130.10(7)	131.56(7)
Te[2] - Tb - Te[2] x 2	81.53(7)	81.29(8)	81.77(8)
Te[2] - Tb - Te[3] x 4	55.13(8)	54.14(8)	56.15(8)
Te[3] - Tb - Te[3] x 2	81.44(7)	81.16(9)	81.72(9)
Tb - Te[1] - Tb x 8	106.43(8)	106.11(9)	106.75(9)
Tb - Te[1] - Tb x 8	85.33(9)	85.26(9)	85.39(9)
Tb - Te[1] - Tb x 4	146.94(7)	146.78(10)	147.10(10)
Tb - Te[2] - Tb x 2	81.53(7)	81.21(9)	81.83(10)
Tb - Te[2] - Te[3] x 2	62.25(6)	61.90(6)	62.59(6)
Tb - Te[2] - Te[3] x 2	117.21(10)	116.14(12)	118.26(12)
Tb - Te[2] - Te[3] x 2	62.66(6)	62.47(6)	62.84(6)
Tb - Te[2] - Te[3] x 2	117.82(10)	116.53(12)	119.11(12)
Te[3] - Te[2] - Te[3] x 8	89.94(13)	88.19(13)	91.70(14)
Te[3] - Te[2] - Te[3] x 4	178.88(14)	178.04(13)	180
Tb - Te[3] - Tb x 2	81.44(5)	81.16(9)	81.72(9)
Tb - Te[3] - Te[2] x 4	62.53(7)	61.95(7)	63.14(7)
Tb - Te[3] - Te[2] x 4	117.58(8)	117.15(7)	118.02(7)
Te[2] - Te[3] - Te[2] x 8	90.32(13)	88.74(13)	91.92(14)
Te[2] - Te[3] - Te[2] x 4	178.94(14)	178.14(13)	180

Table 2.49. Crystal data and structure refinement for DyTe₃ at 300 K.

Empirical formula	DyTe ₃
Formula weight	545.3
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2994(6) Å, α = 90° b = 25.353(5) Å, β = 90° c = 4.2930(6) Å, γ = 90°
q-vector(1)	0.2984(3)c*
Volume	467.95(13) Å ³
Z	4
Density (calculated)	7.738 g/cm ³
Absorption coefficient	34.139 mm ⁻¹
F(000)	888
Crystal size	0.23 x 0.15 x 0.03 mm ³
Theta range for data collection	2.14 to 28.96°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	5835 (1643 main + 4192 satellites)
Independent reflections	1859 (614 main + 1245 satellites) [R _{int} = 0.0361]
Completeness to θ = 28.96°	97%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1859 / 0 / 37
Goodness-of-fit on F ²	1.64
Final R indices [I > 2σ(I)]	R _{obs} = 0.0308, wR _{obs} = 0.1070
R indices (all data)	R _{all} = 0.0655, wR _{all} = 0.1228
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0244, wR _{obs} = 0.0996
R main indices (all data)	R _{all} = 0.0245, wR _{all} = 0.0996
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.2032, wR _{obs} = 0.3535
R 1 st order satellites (all data)	R _{all} = 0.4911, wR _{all} = 0.5517
Extinction coefficient	0.00115(10)
T _{min} and T _{max} coefficients	0.0234 and 0.3079
Largest diff. peak and hole	2.81 and -2.40 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.50. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for DyTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Dy	0	9449	1699(1)	2549	7(1)
	sin, 1	0	0	13(4)	
	cos, 1	16(2)	5(1)	0	
Te[1]	0	9366(3)	2946(1)	2549	6(1)
	sin, 1	0	0	-12(5)	
	cos, 1	-9(2)	-1(1)	0	
Te[2]	0	9407(4)	715(1)	7549	9(1)
	sin, 1	0	0	9(5)	
	cos, 1	-67(5)	1(1)	0	
Te[3]	0	4450(4)	716(1)	2549	9(1)
	sin, 1	0	0	-9(5)	
	cos, 1	57(5)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.51. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DyTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Dy	8(1)	6(1)	7(1)	0(1)	0	0
Te[1]	7(1)	5(1)	6(1)	3(1)	0	0
Te[2]	10(1)	10(1)	9(1)	-1(1)	0	0
Te[3]	10(1)	9(1)	9(1)	-1(1)	0	0

Table 2.52. Bond lengths distributions [$\text{\AA}$] for DyTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Dy - Te[1]	3.1616(12)	3.148(2)	3.176(2)
Dy - Te[1] x 2	3.1782(16)	3.1700(17)	3.1863(17)
Dy - Te[1] x 2	3.1580(16)	3.1452(18)	3.1710(18)
Dy - Te[2] x 2	3.2907(16)	3.2801(14)	3.3012(14)
Dy - Te[3]	3.2771(18)	3.275(3)	3.279(3)
Dy - Te[3]	3.3056(18)	3.284(3)	3.326(3)
Te[2] - Te[3] x 2	3.025(3)	2.991(2)	3.059(3)
Te[2] - Te[3] x 2	3.051(3)	3.017(2)	3.085(3)

Table 2.53. Bond angles distributions [°] for DyTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Dy - Te[1] x 4	73.38(3)	73.24(3)	73.52(3)
Te[1] - Dy - Te[1] x 4	73.65(3)	73.33(3)	73.97(3)
Te[1] - Dy - Te[2] x 4	139.28(5)	139.01(7)	139.55(7)
Te[1] - Dy - Te[1] x 2	84.97(4)	84.76(5)	85.17(5)
Te[1] - Dy - Te[1] x 6	85.46(5)	85.17(5)	85.75(5)
Te[1] - Dy - Te[1] x 4	147.03(3)	146.66(4)	147.40(4)
Te[1] - Dy - Te[2] x 4	76.96(4)	76.46(4)	77.47(4)
Te[1] - Dy - Te[2] x 4	130.96(4)	130.18(4)	131.74(4)
Te[1] - Dy - Te[3] x 4	76.87(4)	76.77(4)	76.96(4)
Te[1] - Dy - Te[3] x 2	131.35(5)	131.14(6)	131.56(6)
Te[1] - Dy - Te[3] x 2	130.95(5)	130.55(5)	131.35(5)
Te[2] - Dy - Te[2] x 2	81.43(4)	81.26(5)	81.60(5)
Te[2] - Dy - Te[3] x 4	54.84(5)	54.11(5)	55.59(5)
Te[3] - Dy - Te[3] x 2	81.56(4)	81.27(6)	81.85(6)
Dy - Te[1] - Dy x 4	106.73(4)	106.68(4)	106.77(4)
Dy - Te[1] - Dy x 4	106.24(4)	105.96(4)	106.52(4)
Dy - Te[1] - Dy x 6	85.64(5)	85.29(5)	85.98(5)
Dy - Te[1] - Dy x 4	147.03(4)	146.80(6)	147.26(6)
Dy - Te[1] - Dy x 2	84.97(5)	84.97(5)	84.97(5)
Dy - Te[2] - Dy x 2	81.43(4)	81.43(5)	81.43(3)
Dy - Te[2] - Te[3] x 2	62.35(4)	62.13(4)	62.56(4)
Dy - Te[2] - Te[3] x 4	117.50(5)	116.71(7)	118.29(7)
Dy - Te[2] - Te[3] x 2	62.69(4)	62.56(3)	62.82(3)
Te[3] - Te[2] - Te[3] x 6	90.42(7)	89.34(9)	91.51(9)
Te[3] - Te[2] - Te[3] x 4	179.17(8)	178.33(9)	179.91(4)
Te[3] - Te[2] - Te[3] x 2	89.42(7)	88.20(8)	90.66(9)
Dy - Te[3] - Dy x 2	81.56(3)	81.27(5)	81.85(5)
Dy - Te[3] - Te[2] x 2	62.20(4)	61.85(5)	62.56(5)
Dy - Te[3] - Te[2] x 4	117.60(5)	117.31(5)	117.88(5)
Dy - Te[3] - Te[2] x 2	62.81(4)	62.24(5)	63.37(5)
Te[2] - Te[3] - Te[2] x 2	89.42(8)	88.42(9)	90.44(9)
Te[2] - Te[3] - Te[2] x 6	90.08(6)	89.90(7)	90.27(7)
Te[2] - Te[3] - Te[2] x 4	179.20(8)	178.39(9)	179.91(5)

Table 2.54. Crystal data and structure refinement for HoTe₃ at 300 K.

Empirical formula	HoTe ₃
Formula weight	547.7
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 4.2862(6) Å, α = 90° b = 25.304(3) Å, β = 90° c = 4.2883(4) Å, γ = 90°
Volume	465.09(10) Å ³
Z	4
Density (calculated)	7.8198 g/cm ³
Absorption coefficient	35.33 mm ⁻¹
F(000)	892
Crystal size	0.24 x 0.20 x 0.04 mm ³
Theta range for data collection	3.22 to 29.09°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 5
Reflections collected	1999
Independent reflections	380 [R _{int} = 0.1024]
Completeness to θ = 29.09°	95%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	380 / 0 / 19
Goodness-of-fit on F ²	2.97
Final R indices [I > 2σ(I)]	R _{obs} = 0.0415, wR _{obs} = 0.1217
R indices (all data)	R _{all} = 0.0415, wR _{all} = 0.1217
Extinction coefficient	0.090(12)
Largest diff. peak and hole	3.05 and -4.37 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.55. Atomic coordinates (x10⁴) and equivalent isotropic displacement parameters (Å²x10³) for HoTe₃ at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U _{eq} [*]
Ho	0	1701(1)	2549	1	12(1)
Te[1]	0	2946(1)	2549	1	10(1)

Table 2.55. (cont'd) Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for HoTe_3 at 300 K with e.s.d.'s in parentheses.

Te[2]	0	4282(1)	7549	1	14(1)
Te[3]	0	717(1)	7549	1	14(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.56. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for HoTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ho	10(1)	13(1)	12(1)	0	0	0
Te[1]	7(1)	13(1)	11(1)	0	0	0
Te[2]	11(1)	16(1)	15(1)	0	0	0
Te[3]	9(1)	19(1)	14(1)	0	0	0

Table 2.57. Bond distances [$\text{\AA}$] for HoTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Ho - Te[1]	3.1496(10)	Ho - Te[3] x 2	3.2852(8)
Ho - Te[1] x 4	3.1608(3)	Te[2] - Te[3] x 4	3.0315
Ho - Te[2] x 2	3.2825(8)		

Table 2.58. Bond angles [$^\circ$] for HoTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[1] - Ho - Te[1] x 8	73.555(18)	Ho - Te[1] - Ho x 4	85.378(9)
Te[1] - Ho - Te[2] x 2	139.241(11)	Ho - Te[1] - Ho x 4	147.11(3)
Te[1] - Ho - Te[3] x 2	139.257(11)	Ho - Te[2] - Ho x 2	81.52(2)
Te[1] - Ho - Te[1] x 4	85.429(8)	Ho - Te[2] - Te[3] x 4	62.556(16)
Te[1] - Ho - Te[1] x 4	85.378(8)	Ho - Te[2] - Te[3] x 4	117.53(2)
Te[1] - Ho - Te[1] x 4	147.11(3)	Te[3] - Te[2] - Te[3] x 4	90.028
Te[1] - Ho - Te[2] x 4	76.807(15)	Te[3] - Te[2] - Te[3] x 4	89.972
Te[1] - Ho - Te[2] x 4	131.078(16)	Te[3] - Te[2] - Te[3] x 4	179.90(4)
Te[1] - Ho - Te[3] x 4	76.806(15)	Ho - Te[3] - Ho x 2	81.49(2)
Te[1] - Ho - Te[3] x 4	131.088(16)	Ho - Te[3] - Te[2] x 4	62.466(16)
Te[2] - Ho - Te[2] x 2	81.518(19)	Ho - Te[3] - Te[2] x 4	117.45(2)

Table 2.58. (cont'd) Bond angles [°] for HoTe₃ at 300 K with e.s.d.'s in parentheses.

Te[2] - Ho - Te[3] x 4	54.978(11)	Te[2] - Te[3] - Te[2] x 4	90.028
Te[3] - Ho - Te[3] x 2	81.485(19)	Te[2] - Te[3] - Te[2] x 4	89.972
Ho - Te[1] - Ho x 8	106.445(18)	Te[2] - Te[3] - Te[2] x 4	179.90(4)
Ho - Te[1] - Ho x 4	85.429(9)		

Table 2.59. Crystal data and structure refinement for ErTe₃ at 300 K.

Empirical formula	ErTe ₃
Formula weight	550.1
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 4.2994(6) Å, α = 90° b = 25.275(6) Å, β = 90° c = 4.2787(8) Å, γ = 90°
Volume	462.55(16) Å ³
Z	4
Density (calculated)	7.896 g/cm ³
Absorption coefficient	36.603 mm ⁻¹
F(000)	896
Crystal size	0.50 x 0.32 x 0.03 mm ³
Theta range for data collection	3.22 to 31.82°
Index ranges	-6 ≤ h ≤ 6, -37 ≤ k ≤ 37, -6 ≤ l ≤ 6
Reflections collected	2718
Independent reflections	492 [R _{int} = 0.1125]
Completeness to θ = 31.82°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	492 / 0 / 19
Goodness-of-fit on F ²	3.62
Final R indices [I > 2σ(I)]	R _{obs} = 0.0591, wR _{obs} = 0.1764
R indices (all data)	R _{all} = 0.0616, wR _{all} = 0.1770
Extinction coefficient	0.029(8)
Largest diff. peak and hole	10.64 and -6.94 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w=1/(σ ² (I)+0.0016I ²)	

Table 2.60. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ErTe_3 at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Er	0	3298(1)	7549	1	17(1)
Te[1]	0	2057(1)	7549	1	15(1)
Te[2]	5000	4280(1)	7549	1	22(1)
Te[3]	0	4282(1)	2549	1	21(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.61. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ErTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Er	15(1)	24(1)	13(1)	0	0	0
Te[1]	14(1)	22(1)	11(1)	0	0	0
Te[2]	23(1)	26(1)	17(1)	0	0	0
Te[3]	21(1)	26(1)	16(1)	0	0	0

Table 2.62. Bond distances [$\text{\AA}$] for ErTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Er - Te[1]	3.138(2)	Er - Te[3] x 2	3.2796(16)
Er - Te[1] x 4	3.1550(6)	Te[2] - Te[3] x 4	3.025
Er - Te[2] x 2	3.2767(17)		

Table 2.63. Bond angles [$^\circ$] for ErTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[1] - Er - Te[1] x 8	73.50(3)	Er - Te[1] - Er x 4	85.353(17)
Te[1] - Er - Te[2] x 2	139.26(3)	Er - Te[1] - Er x 4	146.99(6)
Te[1] - Er - Te[3] x 2	139.28(2)	Er - Te[2] - Er x 2	81.49(5)
Te[1] - Er - Te[1] x 4	85.390(16)	Er - Te[2] - Te[3] x 4	62.57(4)
Te[1] - Er - Te[1] x 4	85.353(16)	Er - Te[2] - Te[3] x 4	117.53(5)
Te[1] - Er - Te[1] x 4	146.99(6)	Te[3] - Te[2] - Te[3] x 4	90.02
Te[1] - Er - Te[2] x 4	76.87(3)	Te[3] - Te[2] - Te[3] x 4	89.98
Te[1] - Er - Te[2] x 4	131.12(3)	Te[3] - Te[2] - Te[3] x 4	179.87(9)

Table 2.63. (cont'd) Bond angles [°] for ErTe₃ at 300 K with e.s.d.'s in parentheses.

Te[1] - Er - Te[3] x 4	76.88(3)	Er - Te[3] - Er x 2	81.43(5)
Te[1] - Er - Te[3] x 4	131.12(3)	Er - Te[3] - Te[2] x 4	62.47(4)
Te[2] - Er - Te[2] x 2	81.49(4)	Er - Te[3] - Te[2] x 4	117.42(5)
Te[2] - Er - Te[3] x 4	54.95(2)	Te[2] - Te[3] - Te[2] x 4	90.02
Te[3] - Er - Te[3] x 2	81.43(4)	Te[2] - Te[3] - Te[2] x 4	89.98
Er - Te[1] - Er x 8	106.50(3)	Te[2] - Te[3] - Te[2] x 4	179.87(8)
Er - Te[1] - Er x 4	85.390(17)		

Table 2.64. Crystal data and structure refinement for TmTe₃ at 300 K.

Empirical formula	TmTe ₃
Formula weight	551.7
Temperature	300.0(3) K
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 4.2995(8) Å, α = 90° b = 25.190(3) Å, β = 90° c = 4.2804(7) Å, γ = 90°
Volume	460.60(11) Å ³
Z	4
Density (calculated)	7.9537 g/cm ³
Absorption coefficient	37.763 mm ⁻¹
Crystal size	0.43 x 0.40 x 0.04 mm ³
Theta range for data collection	3.23 to 31.69°
Index ranges	-5 ≤ h ≤ 6, -36 ≤ k ≤ 36, -5 ≤ l ≤ 6
Reflections collected	2369
Independent reflections	437 [R _{int} = 0.0386]
Completeness to θ = 31.69°	90%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	437 / 0 / 18
Goodness-of-fit on F ²	3.02
Final R indices [I > 2σ(I)]	R _{obs} = 0.0312, wR _{obs} = 0.1259
R indices (all data)	R _{all} = 0.0312, wR _{all} = 0.1259
Largest diff. peak and hole	4.17 and -2.63 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.65. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TmTe_3 at 300 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Tm	0	1704(1)	2549	1	11(1)
Te[1]	0	2943(1)	2549	1	9(1)
Te[2]	0	4279(1)	7549	1	13(1)
Te[3]	0	721(1)	7549	1	13(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.66. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TmTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tm	10(1)	10(1)	12(1)	0	0	0
Te[1]	8(1)	10(1)	10(1)	0	0	0
Te[2]	12(1)	14(1)	13(1)	0	0	0
Te[3]	10(1)	15(1)	12(1)	0	0	0

Table 2.67. Bond distances [$\text{\AA}$] for TmTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Tm - Te[1]	3.1223(9)	Tm - Te[3] x 2	3.2734(7)
Tm - Te[1] x 4	3.1517(3)	Te[2] - Te[3] x 4	3.0237(5)
Tm - Te[2] x 2	3.2701(7)		

Table 2.68. Bond angles [°] for TmTe₃ at 300 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[1] - Tm - Te[1] x 8	73.611(16)	Tm - Te[1] - Tm x 4	85.327(8)
Te[1] - Tm - Te[2] x 2	139.220(10)	Tm - Te[1] - Tm x 4	147.22(3)
Te[1] - Tm - Te[3] x 2	139.170(11)	Tm - Te[2] - Tm x 2	81.560(19)
Te[1] - Tm - Te[1] x 4	85.540(7)	Tm - Te[2] - Te[3] x 4	62.533(15)
Te[1] - Tm - Te[1] x 4	85.327(7)	Tm - Te[2] - Te[3] x 4	117.49(2)
Te[1] - Tm - Te[1] x 4	147.22(3)	Te[3] - Te[2] - Te[3] x 4	90.115
Te[1] - Tm - Te[2] x 4	76.762(14)	Te[3] - Te[2] - Te[3] x 4	89.885
Te[1] - Tm - Te[2] x 4	131.018(15)	Te[3] - Te[2] - Te[3] x 4	180
Te[1] - Tm - Te[3] x 4	76.674(14)	Tm - Te[3] - Tm x 2	81.661(20)
Te[1] - Tm - Te[3] x 4	131.107(15)	Tm - Te[3] - Te[2] x 4	62.424(15)
Te[2] - Tm - Te[2] x 2	81.560(16)	Tm - Te[3] - Te[2] x 4	117.56(2)
Te[2] - Tm - Te[3] x 4	55.044(10)	Te[2] - Te[3] - Te[2] x 4	90.115
Te[3] - Tm - Te[3] x 2	81.661(17)	Te[2] - Te[3] - Te[2] x 4	89.885
Tm - Te[1] - Tm x 8	106.389(16)	Te[2] - Te[3] - Te[2] x 4	180
Tm - Te[1] - Tm x 4	85.540(8)		

Table 2.69. Crystal data and structure refinement for YTe₃ at 300 K.

Empirical formula	YTe ₃
Formula weight	471.7
Temperature	300.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2947(7) Å, α = 90° b = 25.404(4) Å, β = 90° c = 4.2968(9) Å, γ = 90°
q-vector(1)	0.2969(5)c*
Volume	468.79(15) Å ³
Z	4
Density (calculated)	6.681 g/cm ³
Absorption coefficient	30.826 mm ⁻¹
F(000)	780
Crystal size	0.29 x 0.27 x 0.02 mm ³
Theta range for data collection	1.60 to 29.22°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6521 (2086 main + 4435 satellites)
Independent reflections	1929 (667 main + 1262 satellites) [R _{int} = 0.0482]
Completeness to θ = 29.22°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1929 / 0 / 39
Goodness-of-fit on F ²	1.25
Final R indices [I > 2σ(I)]	R _{obs} = 0.0307, wR _{obs} = 0.0818
R indices (all data)	R _{all} = 0.0516, wR _{all} = 0.0890
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0248, wR _{obs} = 0.0693
R main indices (all data)	R _{all} = 0.0251, wR _{all} = 0.0696
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1151, wR _{obs} = 0.1496
R 1 st order satellites (all data)	R _{all} = 0.2887, wR _{all} = 0.1815
Extinction coefficient	0.00054(8)
T _{min} and T _{max} coefficients	0.0410 and 0.7092
Largest diff. peak and hole	1.49 and -1.84 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 2.70. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for YTe_3 at 300 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Y	0	9012(3)	1701(1)	2549	12(1)
	sin, 1	0	0	2(4)	
	cos, 1	25(1)	1(1)	0	
Te[1]	0	9000	2946(1)	2549	11(1)
	sin, 1	0	0	-2(3)	
	cos, 1	2(1)	0(1)	0	
Te[2]	0	9015(2)	714(1)	7549	14(1)
	sin, 1	0	0	-5(3)	
	cos, 1	-101(2)	6(1)	0	
Te[3]	0	9045(2)	4285(1)	7549	14(1)
	sin, 1	0	0	-26(3)	
	cos, 1	86(2)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2.71. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for YTe_3 at 300 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Y	11(1)	14(1)	13(1)	-1(1)	0	0
Te[1]	9(1)	13(1)	10(1)	2(1)	0	0
Te[2]	13(1)	15(1)	13(1)	1(1)	0	0
Te[3]	13(1)	16(1)	13(1)	0(1)	0	0

Table 2.72. Bond lengths distributions [$\text{\AA}$] for YTe_3 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Y - Te[1] x 3	3.1646(11)	3.1608(19)	3.1686(19)
Y - Te[1] x 2	3.1709(14)	3.1651(12)	3.1765(12)
Y - Te[2] x 2	3.3011(13)	3.2912(12)	3.3116(12)
Y - Te[3]	3.2894(14)	3.2760(19)	3.3032(19)
Y - Te[3]	3.3083(14)	3.2874(19)	3.3289(19)
Te[2] - Te[3] x 2	3.0283(12)	2.9733(11)	3.0842(11)
Te[2] - Te[3] x 2	3.0474(12)	3.0002(11)	3.0944(11)

Table 2.73. Bond angles distributions [°] for YTe₃ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Y - Te[1] x 8	73.49(3)	73.44(3)	73.55(3)
Te[1] - Y - Te[2] x 2	139.39(4)	139.18(6)	139.59(6)
Te[1] - Y - Te[3] x 2	139.48(5)	139.26(5)	139.71(5)
Te[1] - Y - Te[1] x 6	85.30(4)	85.08(4)	85.53(4)
Te[1] - Y - Te[1] x 4	147.08(4)	146.99(6)	147.17(6)
Te[1] - Y - Te[2] x 4	76.94(3)	76.21(3)	77.68(3)
Te[1] - Y - Te[2] x 4	131.00(5)	130.14(5)	131.85(5)
Te[1] - Y - Te[3] x 4	77.01(4)	76.82(3)	77.21(3)
Te[1] - Y - Te[3] x 4	131.13(4)	130.89(4)	131.38(4)
Te[1] - Y - Te[1] x 2	85.54(4)	85.30(4)	85.78(4)
Te[2] - Y - Te[2] x 2	81.21(3)	81.10(4)	81.30(4)
Te[2] - Y - Te[3] x 2	54.70(3)	53.81(3)	55.61(3)
Te[2] - Y - Te[3] x 2	54.91(3)	54.08(3)	55.74(3)
Te[3] - Y - Te[3] x 2	81.22(3)	81.11(4)	81.33(4)
Y - Te[1] - Y x 8	106.54(3)	106.42(3)	106.67(3)
Y - Te[1] - Y x 8	85.54(4)	85.39(4)	85.69(4)
Y - Te[1] - Y x 4	147.08(3)	147.01(2)	147.16(2)
Y - Te[2] - Y x 2	81.20(3)	80.87(4)	81.53(4)
Y - Te[2] - Te[3] x 2	62.45(3)	61.98(3)	62.91(3)
Y - Te[2] - Te[3] x 4	117.45(4)	115.99(4)	118.92(4)
Y - Te[2] - Te[3] x 2	62.66(3)	62.55(3)	62.78(3)
Te[3] - Te[2] - Te[3] x 2	90.39(4)	88.87(4)	91.93(4)
Te[3] - Te[2] - Te[3] x 4	89.95(3)	89.70(3)	90.22(3)
Te[3] - Te[2] - Te[3] x 4	178.77(4)	177.82(4)	179.85(2)
Te[3] - Te[2] - Te[3] x 2	89.69(4)	87.73(4)	91.68(4)
Y - Te[3] - Y x 2	81.22(3)	81.11(4)	81.33(4)
Y - Te[3] - Te[2] x 2	62.43(3)	61.57(3)	63.32(3)
Y - Te[3] - Te[2] x 4	117.44(3)	116.95(3)	117.92(3)
Y - Te[3] - Te[2] x 2	62.84(3)	62.33(3)	63.35(3)
Te[2] - Te[3] - Te[2] x 2	89.69(4)	87.99(4)	91.42(4)
Te[2] - Te[3] - Te[2] x 4	89.96(3)	89.70(4)	90.22(4)
Te[2] - Te[3] - Te[2] x 4	178.85(4)	177.93(4)	179.905(19)
Te[2] - Te[3] - Te[2] x 2	90.40(4)	88.75(4)	92.05(4)

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Chapter 3

Reactions of Rare-Earth Metals (RE) and Tellurium: Temperature Dependence of the Distortions of the Tellurium Net of RETe_3

Divergence in the Behavior of the Charge Density Wave in RETe_3 (RE = Rare-Earth Element) with Temperature and RE Element”, Malliakas, C. D.; Kanatzidis, M. G. *J. Am. Chem. Soc.* **2006**, *128*, 12612-12613. American Chemical Society (ACS) is gratefully acknowledged for the permission to include this reprint in the Thesis.

3.1. Introduction

Incommensurability in modulated systems is often linked to high-transition-temperature superconductivity¹ and density wave materials.² Incommensurate (IC) to commensurate (C) or near-incommensurate (NIC) transitions may give rise to interesting and often unexplained anomalies in physical properties.³ Charge density wave (CDW) states can be created through a Fermi surface nesting effect and the creation of a new ground state with broken translational symmetry. A band gap opens at the Fermi level and an overall energy lowering is achieved compensating the potentially energetically unfavorable incommensurate transition.

A wide variety of physical characterization techniques have been used to probe and study CDW transitions. Temperature dependent transport, magnetic and thermal properties are some of the typical methods applied.⁴ Since the CDW distortion affects the Fermi surfaces, angle-resolved photoemission spectroscopy (ARPES) has proven to be a useful characterization method for this class of materials.⁵ A direct observation of the electronic band structure near the Fermi surface (obtained through ARPES) gives information of the nature of the CDW state. In some two-dimensional systems, however, this distortion leads only to a pseudo gap keeping the RETe_3 system in the metallic state.⁶ Therefore, structural transitions correlated with these electron band changes can be difficult to examine.

Temperature dependent X-ray scattering studies of incommensurate two dimensional systems remain but a few⁷ and include 2H-NbSe_2 and 2H-TaSe_2 ,^{8,9} NbSe_3 ⁹ and 1T-TaS_2 .¹⁰ In all cases the systems tend to “lock-in” in a more thermodynamically stable commensurate state as the temperature decreases. In other words,

incommensurability (δ) defined as the departure from the commensurate state tends to zero with falling temperature (incommensurability is defined as $\delta = |q_C - q_{IC}|$ where q_C and q_{IC} are the modulation vectors of the commensurate and incommensurate phases respectively). A phenomenological Landau theory developed by McMillan¹¹ can describe the incommensurate to commensurate transitions and explain the instabilities in transport properties etc.

Here we report the temperature dependence of the incommensurate CDW state of RETe₃ (RE = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, and Tm). The results are unexpected in that the CDW modulation dependence as a function of decreasing RE radius and decreasing temperature follows opposite trends, even though both factors cause a unit cell contraction.

The solution of CDW structures of RETe₃ at 300 K was described in the second chapter using superspace crystallographic techniques.¹² The modulations originate from distortion in the ideal square Te net with a q-vector along the *c*-axis of the so-called subcell. Although the RETe₃ exhibit Fermi surface nesting^{4,6}, transport and magnetic properties in the range of 1.8-300 K show no indication of an incommensurate to commensurate transition. Temperature dependent X-ray diffraction experiments on the isostructural LaSeTe₂, showed no temperature dependence of its q-vector.¹³

3.2. Experimental Section

3.2.1. Reagents

The following reagents were used as obtained. All rare-earth metals, 99.9% pure, fillings from ingot, Chinese Rare Earth Information Center, Inner Mongolia, China;

Tellurium shots, 99.9% pure, Tellurex Corporation, Traverse City, MI; Rubidium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Lithium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Lithium Iodide, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Potassium Iodide, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; N, N – Dimethylformamide (DMF), ACS reagent grade, Spectrum Chemicals, New Brunswick, NJ; Diethyl ether anhydrous, ACS reagent grade, Columbus Chemical Industries, Columbus, WI.

3.2.2. Synthesis

$RETe_3$ ($RE = La, Ce, Pr, Nd, Sm, Gd, Tb$ and Dy) – All manipulations were carried out under dry nitrogen atmosphere in a Vacuum Atmospheres Dri-Lab glovebox. Stoichiometric amounts of rare earth (~ 0.3 g) and tellurium (~ 0.82 g) were loaded into quartz tubes under nitrogen together with a double amount (~2 g) of halide flux (0.42:0.58 molar mixtures of RbCl and LiCl). The tubes were sealed under vacuum ($<10^{-4}$ torr) and heated to 650 °C at 12 hours for 6 days. The tubes were then cooled down to room temperature at a rate of 4 °C·min⁻¹. The halide flux was dissolved in water and the crystals were washed with acetone and dried under nitrogen environment. The morphology of the crystals is that of thin plates with a brown (copper-like) color. Electron microprobe energy dispersive spectroscopy (EDS) was performed on several crystals of the compound and confirmed the 1:3 ratio of the rare earth to tellurium and the absence of other elements of the flux. Compounds found to be X-ray pure and moisture sensitive after exposure to air for a few days.

RETe₃ (*RE* = *Ho*, *Er*, *Tm* and *Y*) – In the case of the heavier rare earths the RbCl/LiCl halide flux reacts with the elements producing Rb_xRE_yTe_z compounds. Instead, an eutectic halide of LiI and KI (0.37:0.63 molar mixtures) was used to synthesize the target RETe₃ binaries. Similarly, stoichiometric amounts of rare earth (~ 0.3 g) and tellurium (~ 0.82 g) were loaded into quartz tubes under nitrogen together with a double amount (~ 2 g) of the halide flux. The tubes were sealed under vacuum (<10⁻⁴ torr) and heated to 650 °C at 12 hours for 6 days. The tubes were then cooled down to room temperature at a rate of 4 °C·min⁻¹. The halide flux was dissolved in DMF since the crystals found to be extremely moisture sensitive (surface becomes black after a few seconds of exposure to water / moisture) and the crystals were washed with ether and dried under nitrogen environment. The morphology of the crystals is that of thin plates with a brown (copper-like) color. Electron microprobe energy dispersive spectroscopy (EDS) was performed on several crystals of the compound and confirmed the 1:3 ratio of the rare earth to tellurium and the absence of other elements of the flux. Compounds found to be X-ray pure.

3.2.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – All the temperature dependent measurements were performed on the same single crystal for each RETe₃ compound (RE = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er and Tm). Single crystals were quenched from room temperature to 100 K. The heating rate for warming ramps was ~200 K/h. Typical acquisition time was 12-24 h. Intensity data were collected on a STOE IPDS II diffractometer equipped with a graphite monochromatized Mo radiation ($\lambda = 0.71073\text{\AA}$) and an Image Plate (IP) detector. The data were collected with an ω -scan technique from 0-180° and an arbitrary ϕ -angle. Data reduction was performed with the X-Area package.¹⁴ The length determination and refinement of the q-vectors was performed with the Peaklist 1.06 software part of the X-Area suite using a least square refinement algorithm. An analytical absorption correction was performed (X-Shape within X-Area) and all structures were refined with JANA2000 software.¹⁵ Direct methods of SHELXTL software¹⁶ were used to find the atomic positions in the subcell.

Satellite reflections of first order were observed and used for the refinement. A single modulation wave for positional parameters was used. Only the symmetry allowed Fourier terms were refined. The pseudo-tetragonal character of the crystal system allows the plates to stack and twin in a merohedral fashion. Therefore high electronic densities were observed in different positions from the calculated ones for some of the RETe₃ members. By applying a twin law of a rotation of 90° along *b*-axis

$$\begin{bmatrix} a' \\ b' \\ c' \end{bmatrix} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \text{ the R factors for all the reflections } (R_1/wR_2) \text{ in the refinement}$$

significantly dropped (for the case of the NdTe₃ subcell from 11.97/28.90 to 2.62/5.83).

Detailed crystallographic table reports (bond distances and angles) for each individual

RETe₃ analogue and temperature can be found in tables 3.1-3.95. Temperature was controlled by an Oxford Cryostream 700 Plus cryostat.

Temperature Dependent Transmission Electron Microscopy of HoTe₃ – Selected area electron diffraction (SAED) studies at variable temperatures were carried out on a JEOL 2010F (Japan Electron Optics Laboratories) 200 kV field emission TEM at the Center for Advanced Microscopy of Michigan State University. A thin plate crystal of HoTe₃ was polished and ion-milled in order to be thin enough for TEM study. The crystal was mounted on a copper aperture grid. Temperature dependent (250-325 K) selected area electron diffraction (SAED) patterns for HoTe₃ are shown in Figure 3.20. A GATAN liquid nitrogen automatically controlled low temperature stage was used for the temperature dependent TEM study.

3.3. Results and Discussion

Subcell Description of RETe₃ – The average structure of RETe₃ adopts the space group Cmc₂m. It consists of puckered double layers of (RETe) that are sandwiched by the planar nets of Te making a RETe₃ slab. The slabs then stack along the *b*-axis creating van der Waals gaps. The formula can be more expressly written as (RETe)⁺(Te₂)⁻, Figure 3.1A. The RE atom is in a monocapped tetragonal antiprism of Te atoms, Figure 3.1B. The apparent Te-Te distances in the square net are 3.1034(6) Å (for CeTe₃), Figure 3.1C.

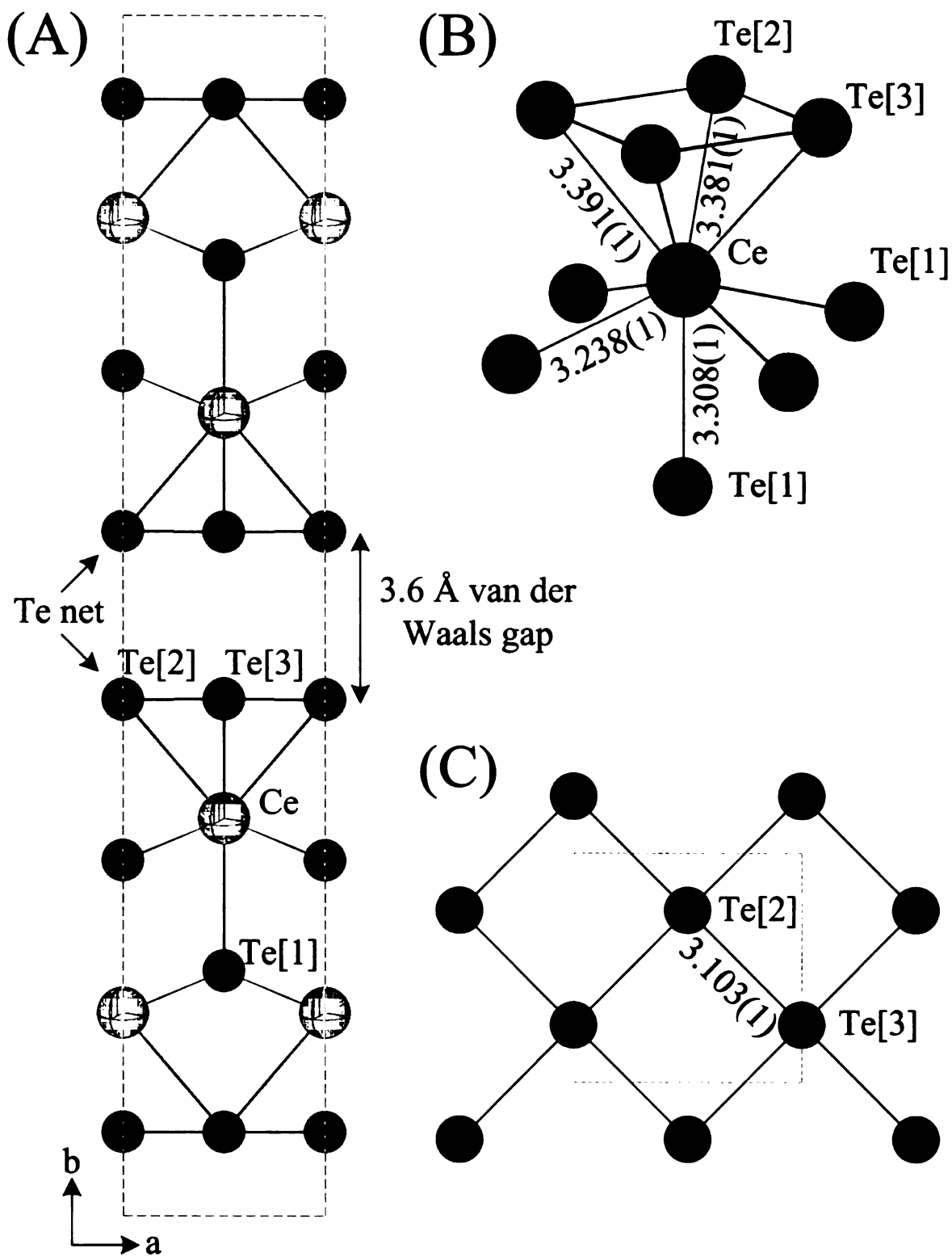


Figure 3.1. (A) Undistorted structure of CeTe_3 . (B) Coordination geometry and environment of Ce. (C) Ideal square net of Te atoms in the CeTe_3 subcell.

Supercell Description of RETe₃ Based on a Modulation q-vector – All crystallographic refinements at variable temperatures converged successfully by using the average structure of NdTe₃ as a starting model. The RETe₃ series adopt the C2cm(00 γ)000 superspace group. A general characteristic is that the direction of the q-vector is always along the c^* axis. Despite the pseudo-tetragonal symmetry there is no bidirectionality at all. Often the presence of twin domains, which is common for these systems, can produce an apparent second q-vector normal to the real one. This artifact can be easily detected from the high residual electron density peaks of the refined subcell. The q-vector as a function of RE for a given temperature increases from La to Tm, Figure 1B. At 100 K, all analogs possess a CDW with q values varying from 0.2719(3) to 0.3028(4) for La and Tm respectively. At 300 K, the CDW for the three heaviest RE (Ho, Er and Tm) disappears judging from the vanishing of the q-vector. At 500 K, only La, Ce and Pr still have a modulation q-vector. Nd has a q-vector of 0.2874(4) at 470 K and for Sm is 0.2936(4) at 400 K. Interestingly, evidence of a lock-in transition to a low index commensurate state at low temperatures (100 K), according to McMillan¹², was not observed as all q-vector values tend to stabilize to an incommensurate state. For a given temperature the CDW state seems to fade with decreasing RE element radius. For example Ho, Er and Tm do not exhibit a CDW state at all at room temperature. This CDW suppression can be attributed to “chemical pressure” where the Te net is squeezed by the decreasing unit cell size caused by the shrinking RE atoms. Indeed it is known that pressure can suppress the CDW state and in some cases can turn on a superconducting state.¹⁷

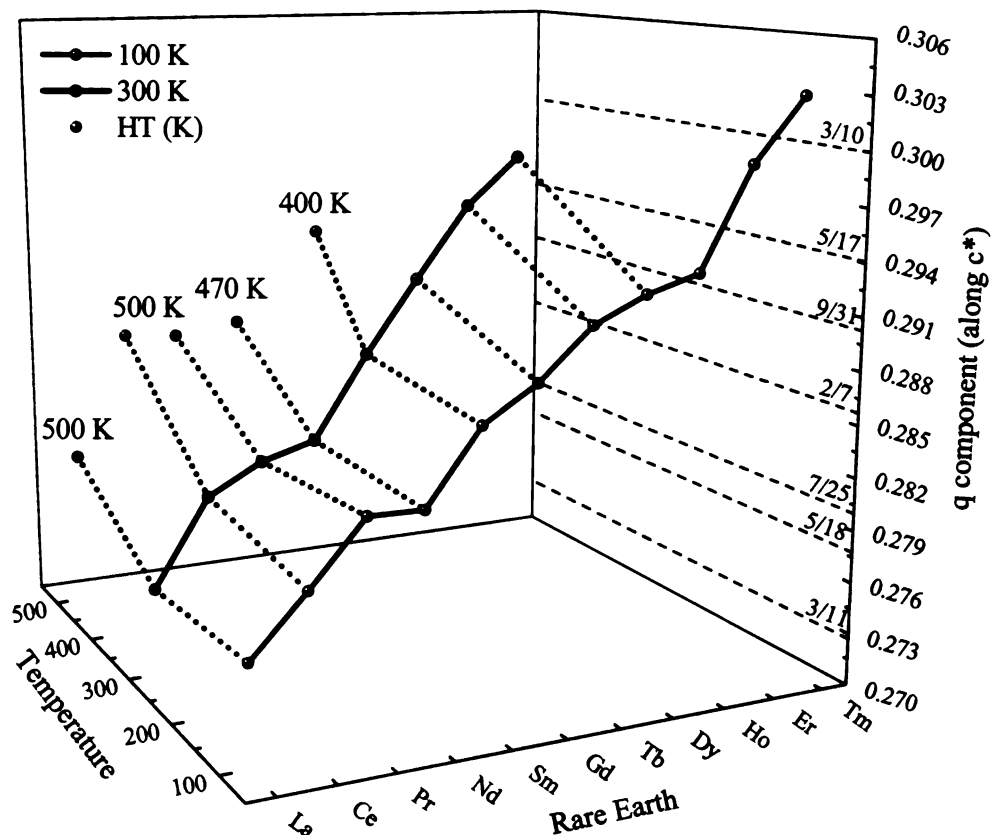


Figure 3.2. q-vector dependence as a function of RE element and temperature. Parallel dashed lines notate some possible low index commensurate approximants.

The systematic change of q-vector with RE element can be naively explained by considering the broadening of frontier orbital bands near the Fermi level with decreasing unit cell volume (i.e. increased orbital overlap) resulting in a change in the nesting vector.⁵ Because temperature variation causes similar changes in the cell volume it is reasonable to expect the same trend in the change of q-vector as the one observed with RE variation. Surprisingly, our experiments show the q-vector for all RETe_3 as a function of temperature follows the opposite trend, Figure 3.2. For the lighter but larger RE elements (Ce-Sm) the change of q-vector from 100 to 300 K is negligible but it is significant between 300 and 500 K. Specifically, for CeTe_3 the q-vector drops from 0.2867(5) at 500 K to 0.2801(3) at 300 K and for PrTe_3 from 0.2864(4) to 0.2818(5). For

Nd and Sm the q-vector vanishes at 500 K. The same irregular trend is more apparent from 300 K to 100 K for the other RE (RE = Gd, Tb, Dy, Ho, Er and Tm) analogues. A possible reason for this behavior is that volume shrinkage associated with a temperature decrease induces a charge redistribution followed with a Te-Te bond length change due to the flexibility of telluride to exhibit a wide range of Te-Te bonds. Although both parameters cause similar changes in the cell volume, the reason for the divergent trends observed for RE and temperature variation is not clear. This suggests that subtle changes in RE-Te bonding across the series play a key role that cannot be accounted for by cell volume changes alone.

Detailed examination of the distorted Te net in SmTe_3 at four different temperatures is shown in Figure 3.3. At 100 K the minimum Te-Te distance in the net is 2.9189(18) Å and the maximum 3.185(2) Å. By arbitrarily taking 3.002 Å to be the Te-Te bonding threshold, the net can be conveniently viewed as a sequence of trimers and tetramers, Figure 3.3A. At 300 K, the minimum and maximum Te-Te distance is 2.955(2) Å and 3.162(3) Å and the Te pattern looks almost identical with the one at low temperature showing, to a large extent, the same sequence of trimers-to-tetramers at a threshold of 3.018 Å but up to a point, Figure 3.3B. The two Te nets begin to differ after a certain number of unit subcells (see from right to left). The distribution of Te-Te bonds has changed and the connectivity of the oligomers now results in a different sequence. Tetramers become trimers and single Te atoms resulting in more trimers in the net. Increasing the temperature to 400 K, the contrast between minimum and maximum Te-Te distance becomes even smaller at 3.011(3) Å and 3.113(3) Å and more apparent changes are observed in the sequence of oligomers. Moreover, the difference between the Te-Te

distances within and between the chains also diminishes and interactions develop between chains, see Figure 3.3C. Bonding interactions between the oligomers is also verified by the observed metallic character of the system.¹⁸ Finally, at 500 K the CDW vanishes to yield a perfect square net of Te atoms and the structure degenerates to the ideal sub-cell Cmc₂m, Figure 3.3D. Similar changes occur in the Te nets of all RETe₃ members with increasing temperature.

Comparison of the structure refinement of CeTe₃ including satellite reflections of second order in respect with the refinement containing only first order reflections – In order to verify if the extremely weak satellite reflections of second order, detected by electron diffraction (Figure 2.3A) and high energy X-rays (Figure 4b in reference 19), effect the structure refinement and bond distributions, we used an even longer exposure time on CeTe₃ at 100 K to detect the second order satellite reflections.

Comparing the statistics of Te-Te bond lengths in the net,

Table 3.14 and Table 3.19, we can conclude that the introduction of second order satellite reflections in the structure refinement does not change the result in the bond distribution considering the calculated error bars. Specifically, the minimum Te-Te bond in the distorted net for the case of taking in account only first order satellite reflections is 2.925(2) Å with an average of 3.079(3) Å and for the case with second order satellite reflections the minimum bonding length is 2.917(4) Å with an average of 3.089(5) Å. The same conclusion can be drawn from the experimental Fourier maps of the two cases in Figure 3.19A-B. In both cases the experimental electronic density of Te atoms in the net can be seen and described (modeled) as a single sinusoidal wave.

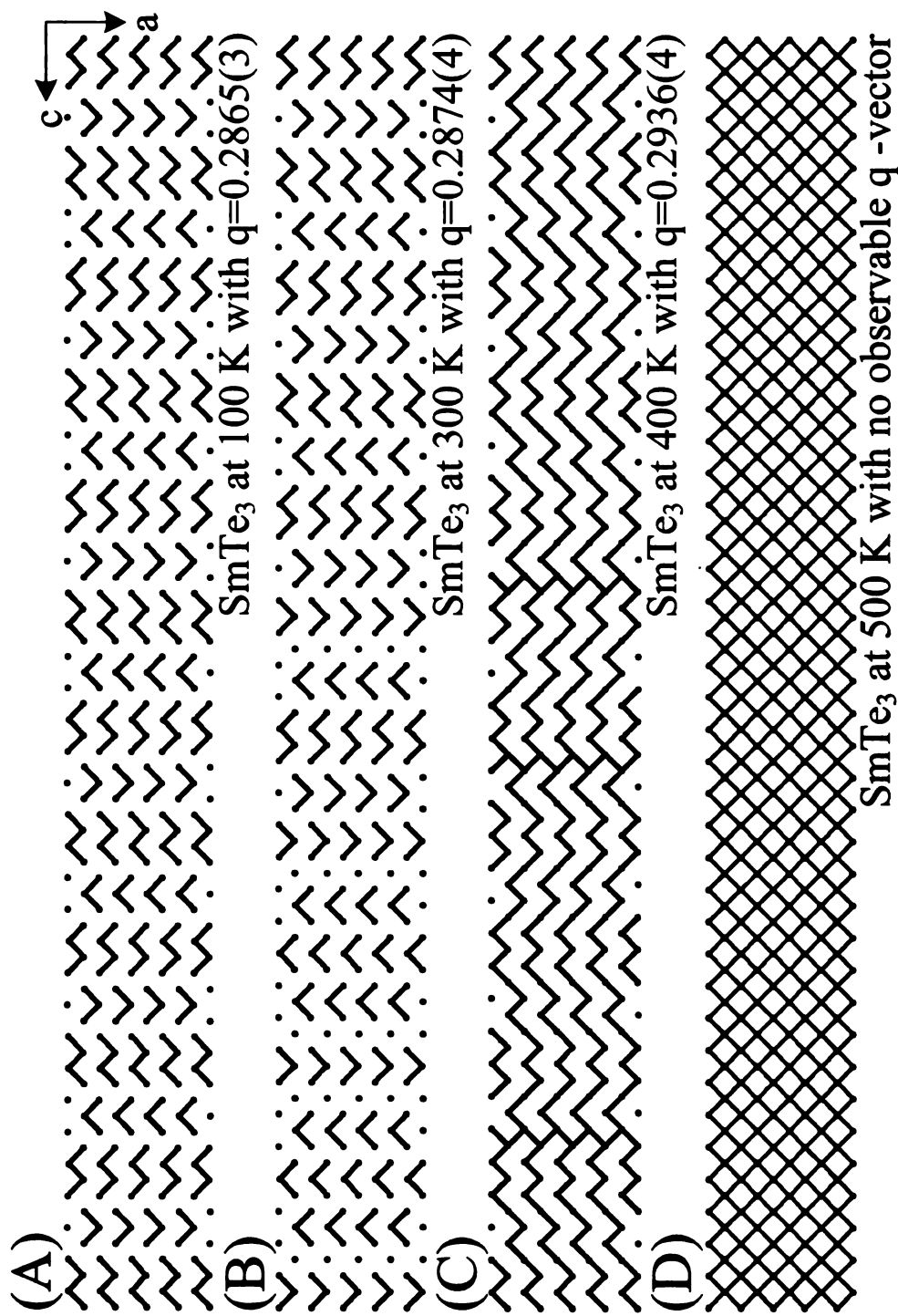


Figure 3.3. Evolution of the CDW in the Te net of SmTe_3 with temperature. (A) the Te net of SmTe_3 at 100 K. V- and N-shaped oligomers are shown using a bonding threshold of 3.002 Å. (B) Te net at 300 K at a threshold of 3.018 Å (C) Te net at 400 K, minimum threshold of 3.042 Å and maximum at 3.063 Å. Intra- and inter-chain interactions begin to be more comparable. (D) Perfect net due to vanishing of the CDW at 500 K at a threshold of 3.070.

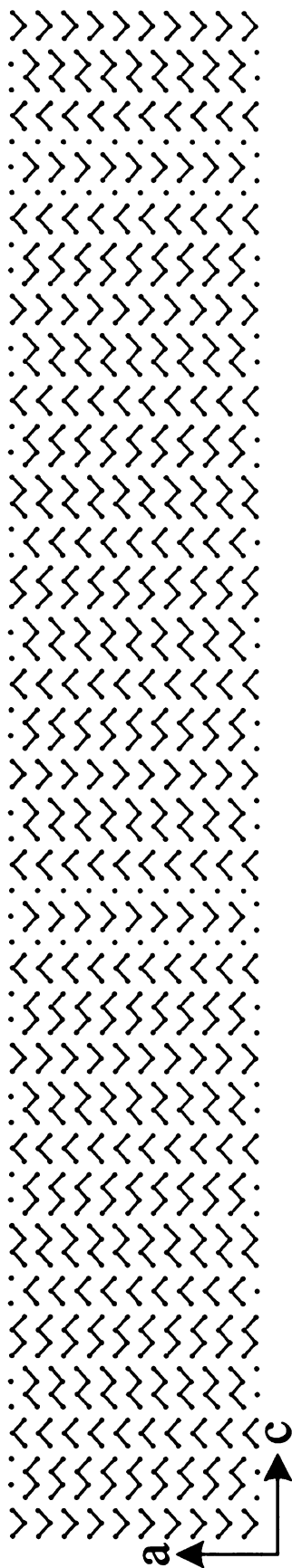


Figure 3.4. LaTe3 at 100 K with $q=0.2719(4)$ and 3.034 Å bonding threshold.

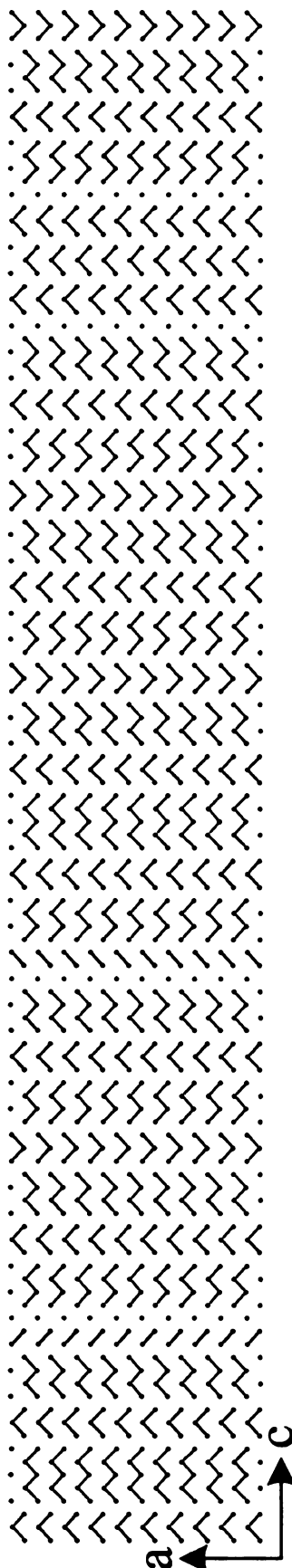


Figure 3.5. LaTe3 at 500 K with $q=0.2793(4)$ and 3.065 Å bonding threshold.

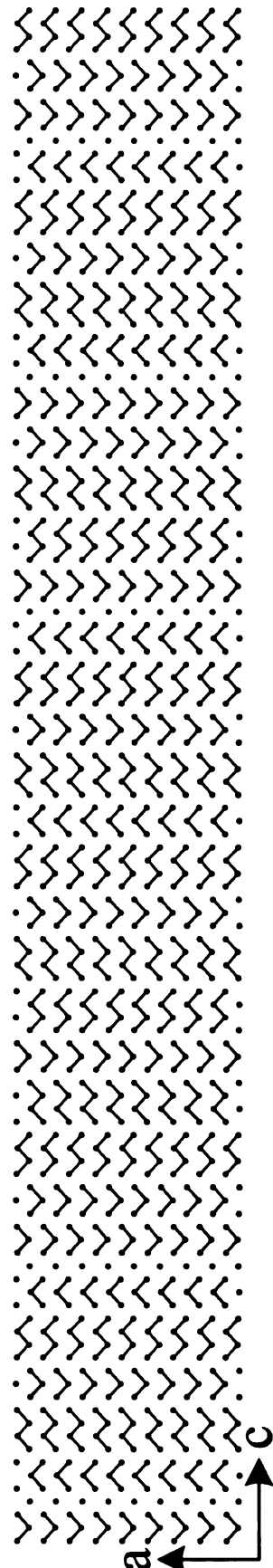


Figure 3.6. CeTe3 at 100 K with $q=0.2790(3)$ and 3.015 Å bonding threshold.

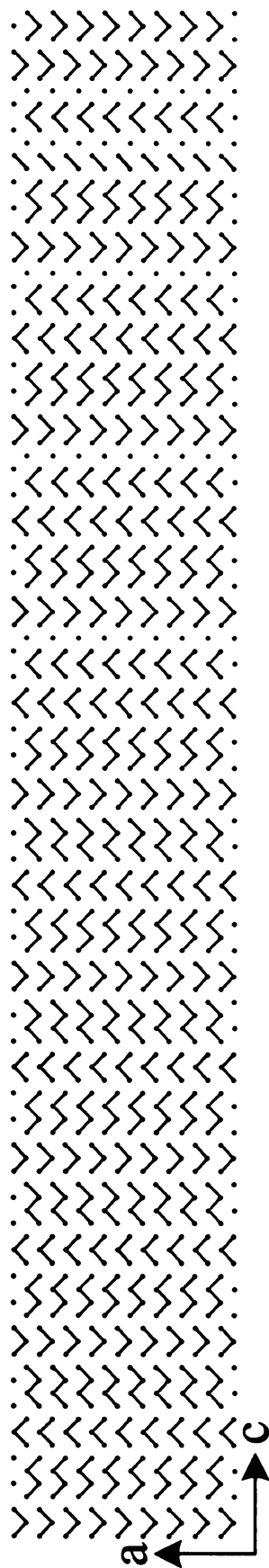


Figure 3.7. CeTe₃ at 500 K with $q=0.2867(5)$ and 3.066 Å bonding threshold.

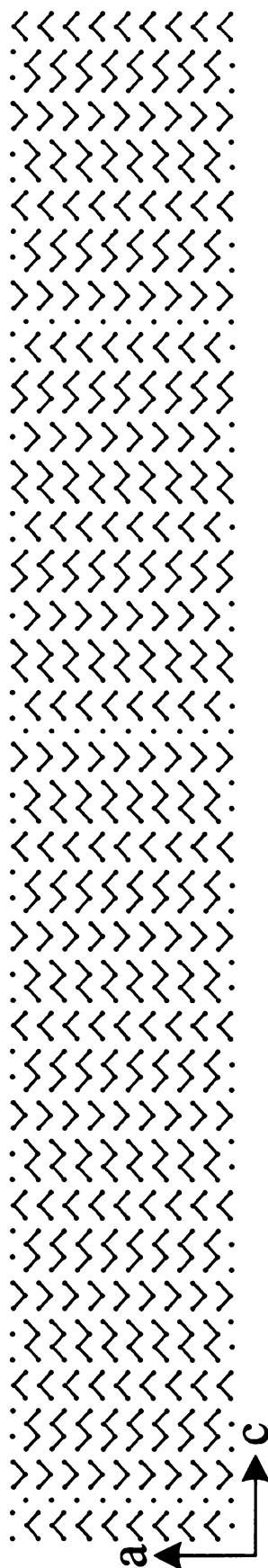


Figure 3.8. PrTe₃ at 100 K with $q=0.2825(5)$ and 3.015 Å bonding threshold.

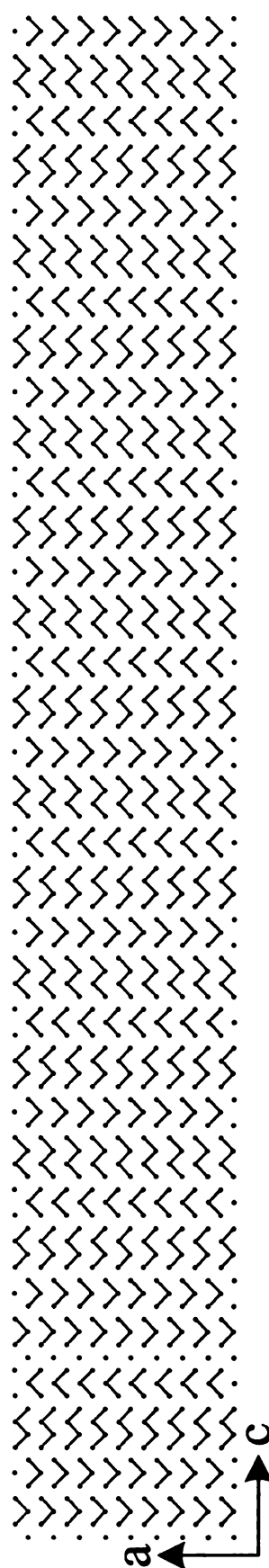


Figure 3.9. PrTe₃ at 500 K with $q=0.2864(5)$ and 3.057 Å bonding threshold.

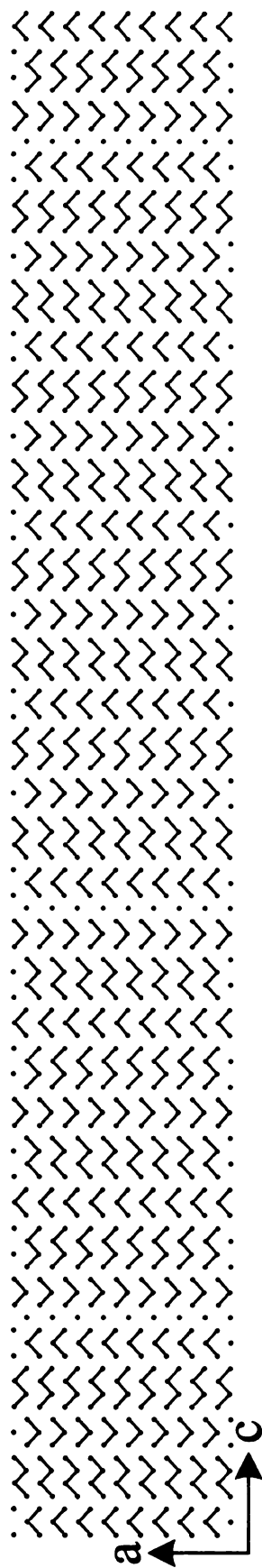


Figure 3.10. NdTe₃ at 100 K with $q=0.2824(4)$ and 3.007 Å bonding threshold.

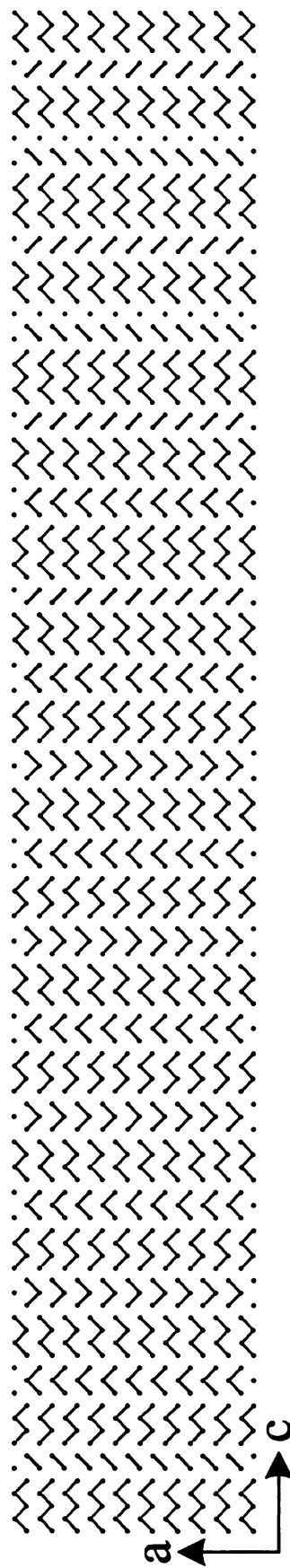


Figure 3.11. NdTe₃ at 470 K with $q=0.2874(4)$ and 3.043 Å bonding threshold.

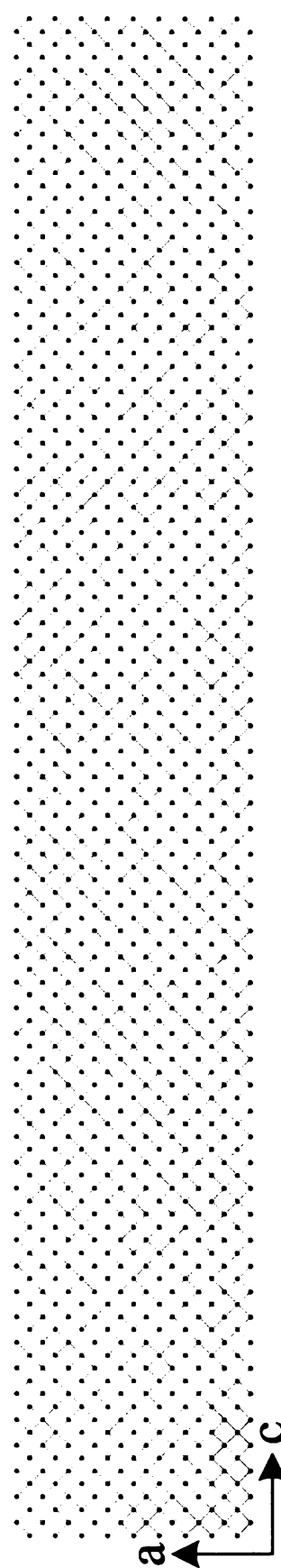


Figure 3.12. NdTe₃ at 500 K with no observable q -vector and 3.098 Å bonding threshold.

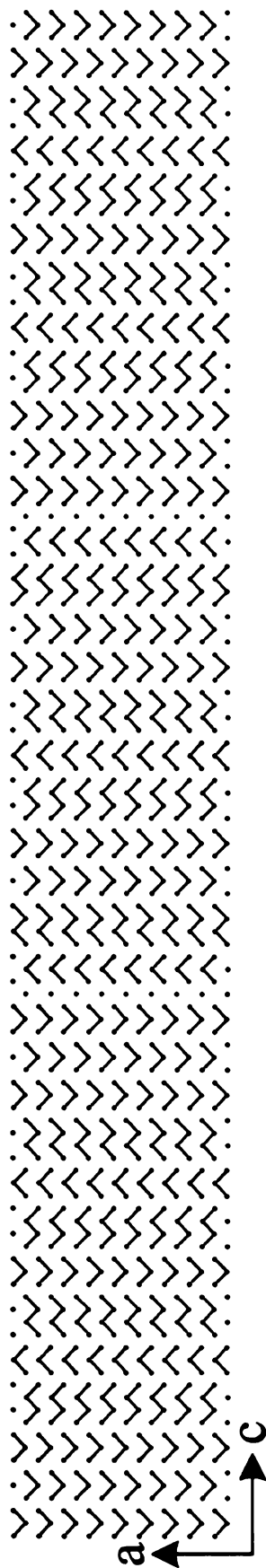


Figure 3.13. GdTe₃ at 100 K with $q=0.2884(3)$ and 2.993 Å bonding threshold.

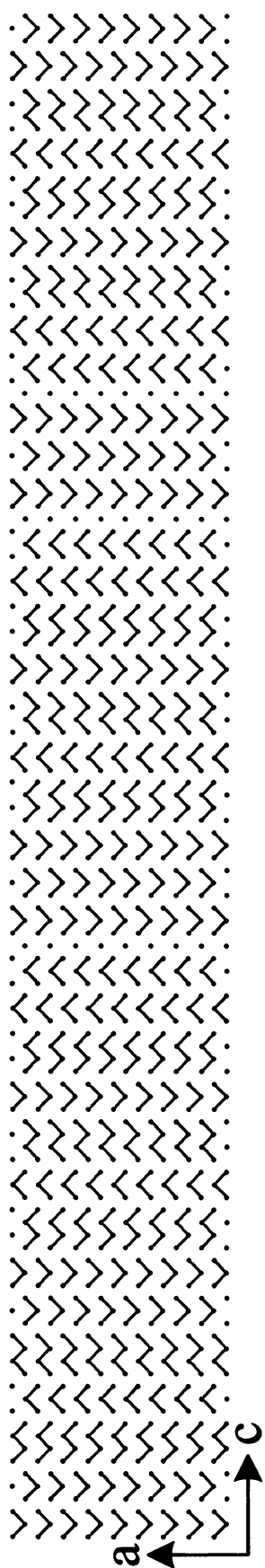


Figure 3.14. TbTe₃ at 100 K with $q=0.2912(5)$ and 2.995 Å bonding threshold.

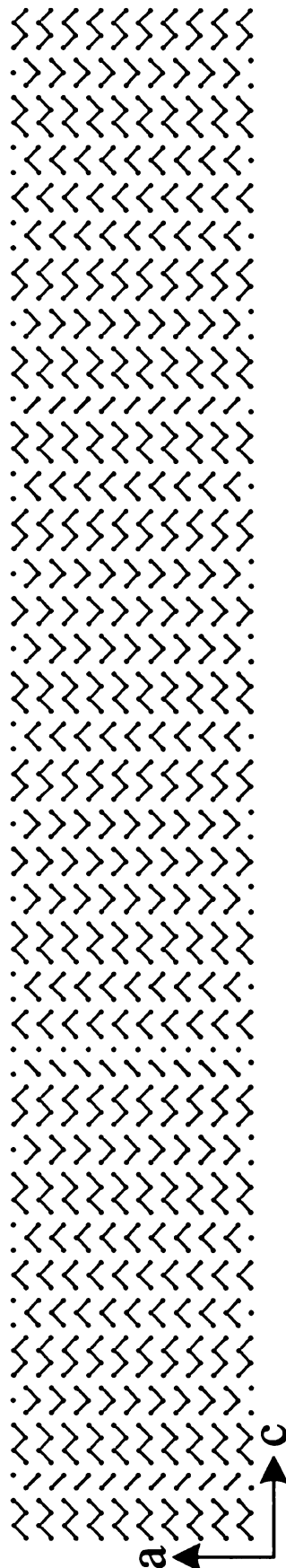


Figure 3.15. DyTe₃ at 100 K with $q=0.2926(3)$ and 2.993 Å bonding threshold.

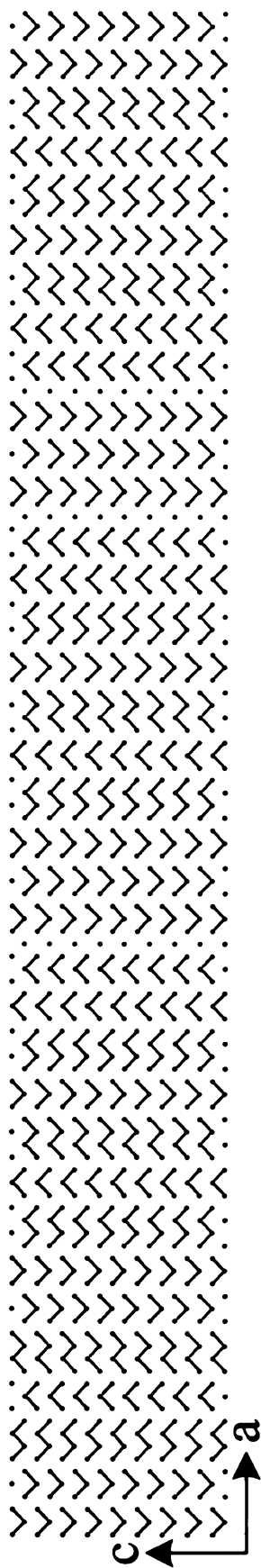


Figure 3.16. HoTe₃ at 100 K with $q=0.2935(3)$ and 2.992 Å bonding threshold.

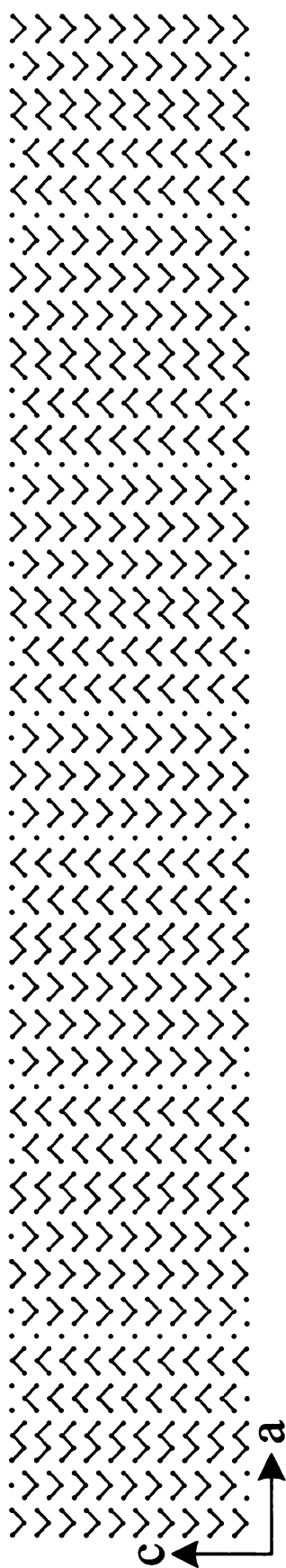


Figure 3.17. ErTe₃ at 100 K with $q=0.2992(4)$ and 2.988 Å bonding threshold.

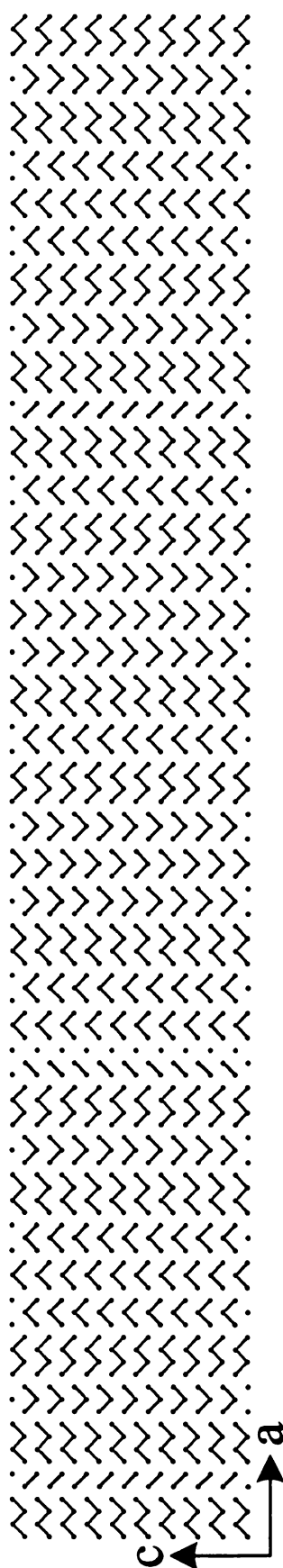


Figure 3.18. TmTe₃ at 100 K with $q=0.3028(4)$ and 2.980 Å bonding threshold.

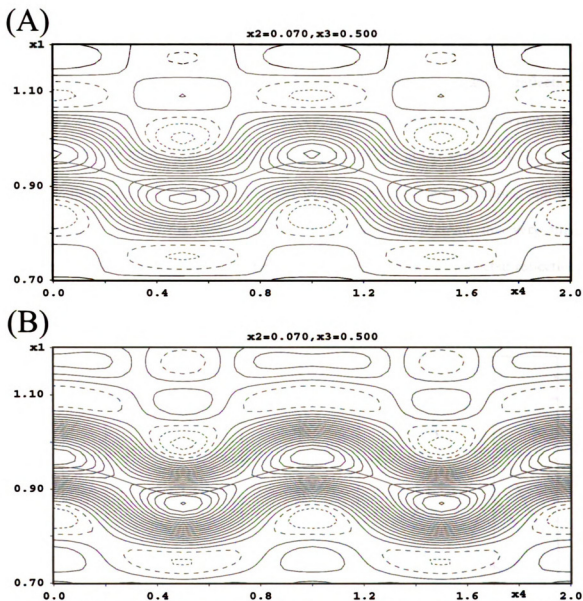


Figure 3.19. Experimental Fourier map of CeTe_3 at 100 K plotted along the modulation direction (t). The central line represents the calculated (fitted) position of $\text{Te}[2]$ (A) Fourier map with the first order satellite reflections. One contour line per $0.2 \text{ e}\text{\AA}^{-3}$. Positive (solid line) cutoff $2.67 \text{ e}\text{\AA}^{-3}$ and negative (dashed line) cutoff $-0.46 \text{ e}\text{\AA}^{-3}$. (B) Fourier map including both first and second order satellite reflections. One contour line per $1 \text{ e}\text{\AA}^{-3}$. Positive cutoff $28.08 \text{ e}\text{\AA}^{-3}$ and negative cutoff $-2.41 \text{ e}\text{\AA}^{-3}$.

Electron Transmission Microscopy of HoTe_3 – Temperature dependent selected area electron diffraction study was performed on HoTe_3 in order to verify the disappearance of the satellite supercell reflections above the CDW transition temperature

(T_{CDW}), Figure 3.20. The modulation q -vector (dotted lines) disappears at the temperature of 300 K and above. The breaking of translational symmetry still exists since the (100) reflection at zero position violates the $Cmcm$ subcell symmetry. There are 25 reflections (18 above 2σ) out of 2024 that violate the $Cmcm$ symmetry based on single crystal x-ray diffraction data at 300K. These violations belong to the $h0l$ group with $l = 1, 3, 5$. The subcell reflections are overexposed, in order to detect the supercell reflections, and also twinning is in most of the cases present. Taking these into account, this very small fraction of violated reflections (in respect with the total number of collected reflections including satellites) was not considered important in order to reduce the symmetry.

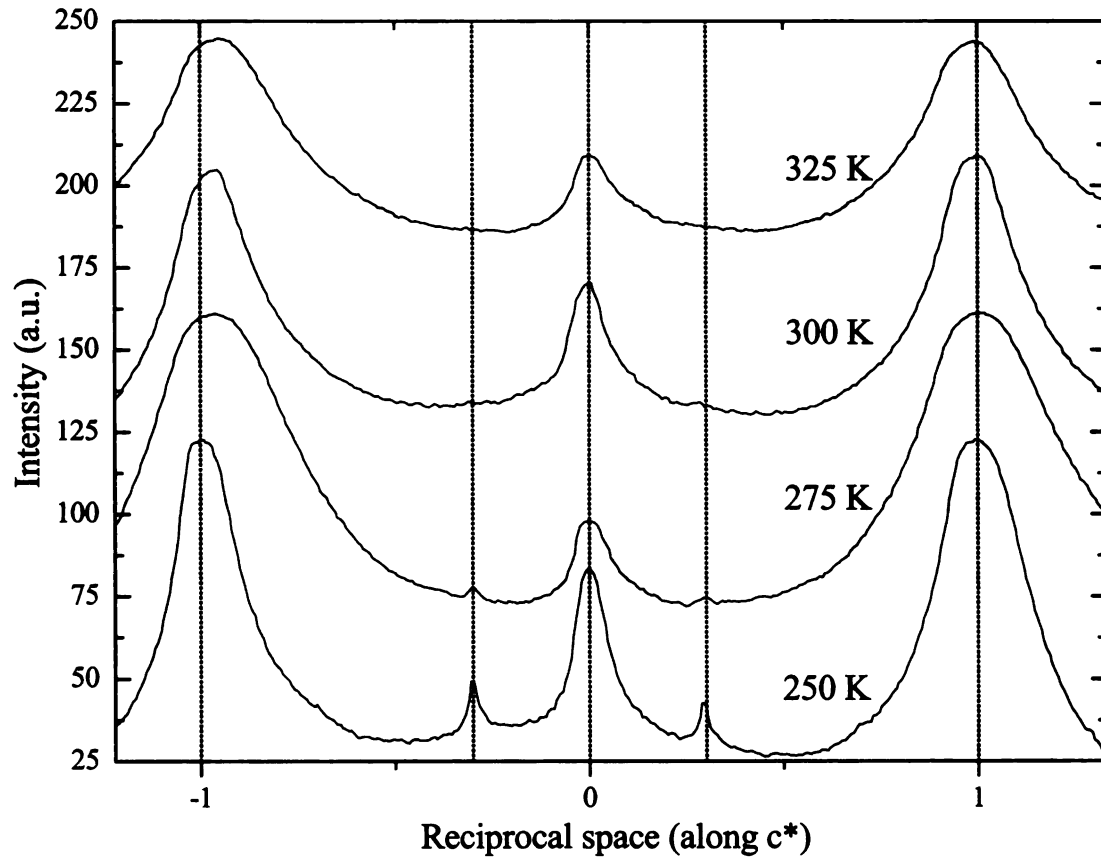


Figure 3.20. Intensity scan along the c^* -axis of the temperature dependent (250-325 K) SAED patterns of the (10l) family of reflection for $HoTe_3$.

3.4. Conclusions

The electronic configuration of the RE atom appears to play a subtle but important role in the CDW of the RETe_3 series, probably through varying involvement of f- and d-orbitals at different temperatures. Unfortunately, at this stage we have no theoretical explanation for this behavior since ab-initio calculations cannot handle temperature variations, nor can they treat easily open f-shell systems. In addition algorithms that can calculate band structures of “aperiodic” systems are not available. The combination of ab-initio and modeling studies however can contribute to the understanding of the role of the f-electrons.

The experimental data reported here regarding the CDW distortions reveal unique behavior among CDW systems and underscores the incomplete level of current understanding of CDW physics.¹⁹ The temperature dependence of the modulated structures of RETe_3 compounds is anomalous. A change in cell volume with RE element has an opposite effect from comparable changes in volume caused by temperature.²⁰ The evolution of CDW across the RETe_3 series and with temperature is so subtle that no other characterization technique, such as ARPES, scanning probe, and transmission electron microscopy can probe them with the required precision. Only the excellent statistics of hundreds of satellite reflections provided by single crystal scattering are able to determine these fine differences.

Table 3.1. Crystal data and structure refinement for LaTe₃ at 100 K.

Empirical formula	LaTe ₃
Formula weight	521.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3779(10) Å, α = 90° b = 26.149(5) Å, β = 90° c = 4.3968(8) Å, γ = 90°
q-vector(1)	0.2757(4)c*
Volume	503.34(17) Å ³
Z	4
Density (calculated)	6.882 g/cm ³
Absorption coefficient	25.306 mm ⁻¹
F(000)	852
Crystal size	0.10 x 0.06 x 0.01 mm ³
Theta range for data collection	2.01 to 29.16°
Index ranges	-6 ≤ h ≤ 5, -35 ≤ k ≤ 30, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	7144 (2378 main + 4766 satellites)
Independent reflections	2099 (749 main + 1350 satellites) [R _{int} = 0.1189]
Completeness to θ = 29.16°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2099 / 0 / 38
Goodness-of-fit on F ²	1.78
Final R indices [I > 2σ(I)]	R _{obs} = 0.0589, wR _{obs} = 0.1356
R indices (all data)	R _{all} = 0.0940, wR _{all} = 0.1429
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0510, wR _{obs} = 0.1282
R main indices (all data)	R _{all} = 0.0546, wR _{all} = 0.1289
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1135, wR _{obs} = 0.1831
R 1 st order satellites (all data)	R _{all} = 0.2698, wR _{all} = 0.2146
Extinction coefficient	0.00034(4)
T _{min} and T _{max} coefficients	0.1189 and 0.9333
Largest diff. peak and hole	4.77 and -2.78 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.2. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for LaTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
La	0	9249	1686(1)	2549	24(1)
	sin, 1	0	0	8(8)	
	cos, 1	59(2)	0(1)	0	
Te[1]	0	9202(12)	2959(1)	2549	24(1)
	sin, 1	0	0	-8(9)	
	cos, 1	8(2)	1(2)	0	
Te[2]	0	9154(15)	689(1)	7549	25(1)
	sin, 1	0	0	-46(10)	
	cos, 1	-325(5)	-17(1)	0	
Te[3]	0	9198(13)	4306(1)	7549	25(1)
	sin, 1	0	0	-11(10)	
	cos, 1	236(4)	1(2)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LaTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	16(1)	38(1)	17(1)	1(1)	0	0
Te[1]	15(1)	39(1)	17(1)	1(2)	0	0
Te[2]	19(1)	38(1)	18(1)	4(1)	0	0
Te[3]	19(1)	38(1)	18(1)	-1(2)	0	0

Table 3.4. Bond lengths distributions [$\text{\AA}$] for LaTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[1]	3.329(3)	3.326(6)	3.331(6)
La - Te[1] x 4	3.238(4)	3.224(4)	3.252(4)
La - Te[2] x 2	3.413(3)	3.375(3)	3.452(3)
La - Te[3] x 2	3.395(5)	3.347(6)	3.444(6)
Te[2] - Te[3] x 2	3.090(7)	2.929(6)	3.256(7)
Te[2] - Te[3] x 2	3.119(7)	2.969(6)	3.272(7)

Table 3.5. Bond angles distributions [°] for LaTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - La - Te[1] x 8	73.34(9)	73.14(9)	73.54(9)
Te[1] - La - Te[2] x 2	139.82(10)	139.31(7)	140.29(7)
Te[1] - La - Te[3] x 2	139.87(12)	139.25(13)	140.49(13)
Te[1] - La - Te[1] x 8	85.52(11)	84.94(11)	86.12(11)
Te[1] - La - Te[1] x 4	146.66(9)	146.65(10)	146.69(8)
Te[1] - La - Te[2] x 4	77.15(11)	75.64(12)	78.71(12)
Te[1] - La - Te[2] x 4	130.76(13)	127.94(13)	133.63(13)
Te[1] - La - Te[3] x 4	77.50(10)	77.00(10)	78.01(10)
Te[1] - La - Te[3] x 4	130.92(11)	130.31(11)	131.51(11)
Te[2] - La - Te[2] x 2	80.26(9)	79.20(11)	81.22(11)
Te[2] - La - Te[3] x 4	53.97(12)	51.05(12)	56.99(13)
Te[3] - La - Te[3] x 2	80.29(12)	80.24(14)	80.31(11)
La - Te[1] - La x 8	106.66(11)	106.31(11)	107.00(11)
La - Te[1] - La x 8	85.50(13)	85.12(14)	85.86(14)
La - Te[1] - La x 4	146.67(10)	146.51(4)	146.82(4)
La - Te[2] - La x 2	80.22(8)	79.28(10)	81.06(10)
La - Te[2] - Te[3] x 4	62.68(8)	62.30(8)	62.91(8)
La - Te[2] - Te[3] x 4	117.31(15)	114.71(17)	119.75(16)
Te[3] - Te[2] - Te[3] x 4	90.9(2)	85.6(2)	96.4(2)
Te[3] - Te[2] - Te[3] x 4	89.60(14)	89.17(14)	90.16(17)
Te[3] - Te[2] - Te[3] x 4	176.3(2)	173.7(2)	179.78(18)
La - Te[3] - La x 2	80.29(5)	80.24(10)	80.31(3)
La - Te[3] - Te[2] x 4	63.04(11)	61.47(11)	64.65(12)
La - Te[3] - Te[2] x 4	117.06(10)	116.74(10)	117.29(10)
Te[2] - Te[3] - Te[2] x 8	89.9(2)	84.49(19)	95.4(2)
Te[2] - Te[3] - Te[2] x 4	176.6(2)	174.2(2)	179.67(7)

Table 3.6. Crystal data and structure refinement for LaTe₃ at 500 K.

Empirical formula	LaTe ₃
Formula weight	521.7
Temperature	500.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.4070(8) Å, α = 90° b = 26.313(4) Å, β = 90° c = 4.4203(7) Å, γ = 90°
q-vector(1)	0.27930c*
Volume	512.59(14) Å ³
Z	4
Density (calculated)	6.7581 g/cm ³
Absorption coefficient	24.849 mm ⁻¹
F(000)	852
Crystal size	0.10 x 0.06 x 0.01 mm ³
Theta range for data collection	2.01 to 29.30°
Index ranges	-6 ≤ h ≤ 6, -35 ≤ k ≤ 32, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	7196 (2374 main + 4822 satellites)
Independent reflections	2127 (758 main + 1369 satellites) [R _{int} = 0.0758]
Completeness to θ = 29.30°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2127 / 0 / 38
Goodness-of-fit on F ²	1.57
Final R indices [I > 2σ(I)]	R _{obs} = 0.0457, wR _{obs} = 0.1114
R indices (all data)	R _{all} = 0.0782, wR _{all} = 0.1203
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0332, wR _{obs} = 0.0879
R main indices (all data)	R _{all} = 0.0357, wR _{all} = 0.0888
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1357, wR _{obs} = 0.2046
R 1 st order satellites (all data)	R _{all} = 0.2866, wR _{all} = 0.2348
Extinction coefficient	0.00058(7)
T _{min} and T _{max} coefficients	0.1189 and 0.9333
Largest diff. peak and hole	3.05 and -2.42 e.Å ⁻³
$R = \frac{\sum F_o - F_c }{\sum F_o }, wR = \left\{ \frac{\sum [w(F_o ^2 - F_c ^2)^2]}{\sum [w(F_o ^4)]} \right\}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.7. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for LaTe_3 at 500 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
La	0	9349	1689(1)	2549	16(1)
	sin, 1	0	0	3(4)	
	cos, 1	47(2)	0(1)	0	
Te[1]	0	9279(5)	2960(1)	2549	16(1)
	sin, 1	0	0	19(5)	
	cos, 1	2(2)	4(1)	0	
Te[2]	0	9216(7)	694(1)	7549	23(1)
	sin, 1	0	0	-70(6)	
	cos, 1	-261(4)	-2(1)	0	
Te[3]	0	9294(6)	4302(1)	7549	23(1)
	sin, 1	0	0	-21(6)	
	cos, 1	209(4)	-9(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LaTe_3 at 500 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	14(1)	18(1)	14(1)	1(1)	0	0
Te[1]	15(1)	18(1)	15(1)	2(1)	0	0
Te[2]	24(1)	23(1)	21(1)	2(1)	0	0
Te[3]	24(1)	21(1)	23(1)	-2(1)	0	0

Table 3.9. Bond lengths distributions [$\text{\AA}$] for LaTe_3 at 500 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[1]	3.345(2)	3.336(4)	3.354(4)
La - Te[1] x 2	3.261(2)	3.244(2)	3.277(2)
La - Te[1] x 2	3.248(2)	3.2361(19)	3.2605(19)
La - Te[2] x 2	3.427(2)	3.4048(19)	3.4474(18)
La - Te[3] x 2	3.416(3)	3.353(4)	3.480(4)
Te[2] - Te[3] x 2	3.097(3)	2.956(3)	3.243(3)
Te[2] - Te[3] x 2	3.148(3)	3.026(3)	3.272(3)

Table 3.10. Bond angles distributions [°] for LaTe₃ at 500 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - La - Te[1] x 8	73.45(4)	73.26(4)	73.65(4)
Te[1] - La - Te[2] x 2	139.79(5)	139.44(4)	140.15(4)
Te[1] - La - Te[3] x 2	139.63(6)	139.30(6)	139.95(6)
Te[1] - La - Te[1] x 6	85.35(5)	85.13(5)	85.56(6)
Te[1] - La - Te[1] x 4	147.06(6)	146.77(9)	147.34(9)
Te[1] - La - Te[2] x 2	76.78(6)	75.23(7)	78.37(7)
Te[1] - La - Te[2] x 2	130.24(6)	128.09(6)	132.41(6)
Te[1] - La - Te[3] x 4	130.84(7)	130.33(6)	131.33(6)
Te[1] - La - Te[1] x 2	85.76(5)	85.07(5)	86.43(6)
Te[1] - La - Te[2] x 2	77.62(6)	76.22(6)	78.99(6)
Te[1] - La - Te[2] x 2	131.55(7)	129.47(6)	133.60(6)
Te[2] - La - Te[2] x 2	80.35(5)	79.56(7)	81.07(7)
Te[2] - La - Te[3] x 2	53.81(6)	51.63(7)	56.04(7)
Te[2] - La - Te[3] x 2	54.80(6)	52.70(7)	56.91(7)
Te[3] - La - Te[3] x 2	80.38(6)	79.87(8)	80.86(8)
La - Te[1] - La x 8	106.61(6)	106.48(5)	106.74(5)
La - Te[1] - La x 8	85.23(4)	85.06(5)	85.40(5)
La - Te[1] - La x 4	147.06(6)	146.69(9)	147.43(9)
La - Te[2] - La x 2	80.32(5)	80.11(7)	80.46(7)
La - Te[2] - Te[3] x 2	62.88(5)	62.59(4)	63.18(4)
La - Te[2] - Te[3] x 2	117.74(8)	115.31(10)	120.08(10)
La - Te[2] - Te[3] x 2	62.37(5)	61.47(4)	63.29(4)
La - Te[2] - Te[3] x 2	116.32(8)	113.00(10)	119.64(10)
Te[3] - Te[2] - Te[3] x 2	91.19(10)	86.84(10)	95.66(12)
Te[3] - Te[2] - Te[3] x 6	89.72(7)	89.09(8)	90.42(9)
Te[3] - Te[2] - Te[3] x 4	176.99(11)	174.44(11)	179.85(10)
La - Te[3] - La x 2	80.38(4)	79.87(7)	80.86(7)
La - Te[3] - Te[2] x 2	62.84(6)	61.31(6)	64.40(6)
La - Te[3] - Te[2] x 4	116.95(6)	116.52(6)	117.49(6)
La - Te[3] - Te[2] x 2	63.31(6)	61.30(6)	65.36(6)
Te[2] - Te[3] - Te[2] x 6	89.37(10)	84.57(10)	94.30(11)
Te[2] - Te[3] - Te[2] x 4	177.11(11)	174.59(11)	179.89(9)
Te[2] - Te[3] - Te[2] x 2	91.18(10)	87.48(10)	94.98(11)

Table 3.11. Crystal data and structure refinement for CeTe₃ at 100 K.

Empirical formula	CeTe ₃
Formula weight	522.9
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3566(6) Å, α = 90° b = 25.920(3) Å, β = 90° c = 4.3722(5) Å, γ = 90°
q-vector(1)	0.2790(3)c*
Volume	493.73(10) Å ³
Z	4
Density (calculated)	7.0326 g/cm ³
Absorption coefficient	26.473 mm ⁻¹
F(000)	856
Crystal size	0.79 x 0.34 x 0.01 mm ³
Theta range for data collection	2.03 to 29.24°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 5, -1 ≤ m ≤ 1
Reflections collected	6832 (2147 main + 4685 satellites)
Independent reflections	1923 (659 main + 1264 satellites) [R _{int} = 0.0266]
Completeness to θ = 29.24°	94%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1923 / 0 / 38
Goodness-of-fit on F ²	1.91
Final R indices [I > 2σ(I)]	R _{obs} = 0.0293, wR _{obs} = 0.0844
R indices (all data)	R _{all} = 0.0454, wR _{all} = 0.1183
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0239, wR _{obs} = 0.0814
R main indices (all data)	R _{all} = 0.0248, wR _{all} = 0.1251
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0528, wR _{obs} = 0.0905
R 1 st order satellites (all data)	R _{all} = 0.1206, wR _{all} = 0.1017
Extinction coefficient	0.00010(8)
T _{min} and T _{max} coefficients	0.0722 and 0.7368
Largest diff. peak and hole	3.43 and -2.89 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.12. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for CeTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Ce	0	9249	1688(1)	2549	3(1)
	sin, 1	0	0	6(4)	
	cos, 1	-66(1)	0(1)	0	
Te[1]	0	9199(5)	2958(1)	2549	4(1)
	sin, 1	0	0	43(5)	
	cos, 1	-11(1)	7(1)	0	
Te[2]	0	9209(6)	696(1)	7549	5(1)
	sin, 1	0	0	-11(5)	
	cos, 1	307(2)	1(1)	0	
Te[3]	0	9242(5)	4301(1)	7549	5(1)
	sin, 1	0	0	14(5)	
	cos, 1	-249(2)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.13. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	3(1)	4(1)	2(1)	-1(1)	0	0
Te[1]	2(1)	4(1)	5(1)	2(1)	0	0
Te[2]	3(1)	6(1)	6(1)	-3(1)	0	0
Te[3]	2(1)	5(1)	7(1)	3(1)	0	0

Table 3.14. Bond lengths distributions [$\text{\AA}$] for CeTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[1]	3.2904(13)	3.270(2)	3.310(2)
Ce - Te[1] x 4	3.2202(19)	3.2069(16)	3.2336(17)
Ce - Te[2] x 2	3.3765(17)	3.3698(18)	3.3807(16)
Ce - Te[3]	3.3527(17)	3.300(2)	3.405(2)
Ce - Te[3]	3.3754(17)	3.326(2)	3.427(2)
Te[2] - Te[3] x 2	3.079(3)	2.925(2)	3.235(3)
Te[2] - Te[3] x 2	3.097(3)	2.945(2)	3.255(3)

Table 3.15. Bond angles distributions [°] for CeTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Ce - Te[1] x 8	73.43(4)	72.81(4)	74.04(4)
Te[1] - Ce - Te[2] x 2	139.58(5)	139.37(6)	139.80(7)
Te[1] - Ce - Te[3]	139.87(5)	139.27(5)	140.49(5)
Te[1] - Ce - Te[3]	139.43(5)	138.81(5)	140.06(5)
Te[1] - Ce - Te[1] x 4	85.52(5)	84.46(5)	86.57(5)
Te[1] - Ce - Te[1] x 4	85.14(6)	84.74(6)	85.56(6)
Te[1] - Ce - Te[1] x 4	146.86(4)	146.38(5)	147.33(5)
Te[1] - Ce - Te[2] x 4	77.20(5)	75.76(5)	78.62(5)
Te[1] - Ce - Te[2] x 4	131.13(5)	128.42(5)	133.80(5)
Te[1] - Ce - Te[3] x 2	77.41(4)	76.76(4)	78.09(4)
Te[1] - Ce - Te[3] x 4	131.04(5)	130.17(5)	131.93(5)
Te[1] - Ce - Te[3] x 2	77.09(4)	76.67(4)	77.52(4)
Te[2] - Ce - Te[2] x 2	80.75(4)	80.64(5)	80.82(4)
Te[2] - Ce - Te[3] x 4	54.47(5)	51.85(5)	57.06(5)
Te[3] - Ce - Te[3] x 2	80.70(4)	80.67(5)	80.72(4)
Ce - Te[1] - Ce x 8	106.57(5)	105.85(4)	107.32(4)
Ce - Te[1] - Ce x 4	85.54(6)	85.45(6)	85.62(6)
Ce - Te[1] - Ce x 4	85.14(4)	84.74(5)	85.56(5)
Ce - Te[1] - Ce x 4	146.87(4)	146.21(6)	147.51(6)
Ce - Te[2] - Ce x 2	80.70(4)	80.55(5)	80.78(4)
Ce - Te[2] - Te[3] x 2	62.36(4)	61.57(3)	63.17(4)
Ce - Te[2] - Te[3] x 4	117.21(7)	113.88(7)	120.49(8)
Ce - Te[2] - Te[3] x 2	62.66(4)	61.95(4)	63.31(4)
Te[3] - Te[2] - Te[3] x 2	90.71(9)	85.57(8)	96.09(10)
Te[3] - Te[2] - Te[3] x 6	89.65(6)	89.43(6)	90.06(7)
Te[3] - Te[2] - Te[3] x 4	176.58(9)	174.24(9)	179.72(3)
Ce - Te[3] - Ce x 2	80.70(3)	80.67(5)	80.720(13)
Ce - Te[3] - Te[2] x 2	62.73(4)	60.77(4)	64.75(5)
Ce - Te[3] - Te[2] x 4	117.30(5)	116.34(5)	118.13(4)
Ce - Te[3] - Te[2] x 2	63.19(4)	61.09(4)	65.39(5)
Te[2] - Te[3] - Te[2] x 6	89.99(8)	85.08(8)	95.03(9)
Te[2] - Te[3] - Te[2] x 4	176.73(9)	174.50(8)	179.73(3)
Te[2] - Te[3] - Te[2] x 2	90.71(8)	85.57(8)	96.05(9)

Table 3.16. Crystal data and structure refinement for CeTe₃ at 100 K (2nd order satellites)

Empirical formula	CeTe ₃
Formula weight	522.9
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3566(6) Å, α = 90° b = 25.920(3) Å, β = 90° c = 4.3722(5) Å, γ = 90°
q-vector(1)	0.2790(3)c*
Volume	493.73(10) Å ³
Z	4
Density (calculated)	7.0326 g/cm ³
Absorption coefficient	26.473 mm ⁻¹
F(000)	856
Crystal size	0.79 x 0.34 x 0.01 mm ³
Theta range for data collection	2.03 to 29.24°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 35, -5 ≤ l ≤ 5, -2 ≤ m ≤ 2
Reflections collected	9106 (2147 main + 6959 satellites)
Independent reflections	2769 (659 main + 2110 satellites) [R _{int} = 0.0335]
Completeness to θ = 29.24°	94%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2769 / 0 / 73
Goodness-of-fit on F ²	1.70
Final R indices [I > 2σ(I)]	R _{obs} = 0.0372, wR _{obs} = 0.0910
R indices (all data)	R _{all} = 0.0637, wR _{all} = 0.1239
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0354, wR _{obs} = 0.0983
R main indices (all data)	R _{all} = 0.0363, wR _{all} = 0.1354
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0350, wR _{obs} = 0.0663
R 1 st order satellites (all data)	R _{all} = 0.0924, wR _{all} = 0.0773
Final R 2 nd order satellites [I > 2σ(I)]	R _{obs} = 0.1520, wR _{obs} = 0.2182
R 2 nd order satellites (all data)	R _{all} = 0.3933, wR _{all} = 0.3471
T _{min} and T _{max} coefficients	0.0722 and 0.7368
Largest diff. peak and hole	5.10 and -3.39 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.17. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for CeTe_3 at 100 K with e.s.d.'s in parentheses (2nd order satellites).

Label	Wave	x	y	z	U_{eq}^*
Ce	0	9249	1688(1)	2549	3(1)
	sin, 1	0	0	0(3)	
	cos, 1	-64(1)	0(1)	0	
	sin, 2	0	0	2(4)	
	cos, 2	1(3)	1(1)	0	
Te[1]	0	9179(5)	2958(1)	2549	4(1)
	sin, 1	0	0	-5(4)	
	cos, 1	-11(1)	-1(1)	0	
	sin, 2	0	0	9(5)	
	cos, 2	-5(3)	0(1)	0	
Te[2]	0	9209(8)	696(1)	7549	6(1)
	sin, 1	0	0	-10(4)	
	cos, 1	292(2)	1(1)	0	
	sin, 2	0	0	-38(8)	
	cos, 2	-19(8)	1(1)	0	
Te[3]	0	9196(6)	4301(1)	7549	6(1)
	sin, 1	0	0	54(4)	
	cos, 1	-242(2)	5(1)	0	
	sin, 2	0	0	-12(8)	
	cos, 2	16(7)	6(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.18. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 at 100 K with e.s.d.'s in parentheses (2nd order satellites).

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	5(1)	3(1)	2(1)	-1(1)	0	0
Te[1]	4(1)	4(1)	6(1)	-4(1)	0	0
Te[2]	5(1)	5(1)	7(1)	-1(1)	0	0
Te[3]	5(1)	4(1)	8(1)	2(1)	0	0

Table 3.19. Bond lengths distributions [Å] for CeTe₃ at 100 K with e.s.d.'s in parentheses (2nd order satellites).

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[1]	3.2917(18)	3.288(3)	3.2941(15)
Ce - Te[1] x 2	3.226(3)	3.207(2)	3.245(3)
Ce - Te[1] x 2	3.213(3)	3.199(3)	3.231(3)
Ce - Te[2] x 2	3.377(3)	3.365(4)	3.386(3)
Ce - Te[3] x 2	3.366(3)	3.316(4)	3.433(4)
Te[2] - Te[3] x 4	3.093(5)	2.920(4)	3.235(5)

Table 3.20. Bond angles distributions [°] for CeTe₃ at 100 K with e.s.d.'s in parentheses (2nd order satellites).

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Ce - Te[1] x 8	73.38(5)	73.17(5)	73.58(5)
Te[1] - Ce - Te[2] x 2	139.59(10)	139.27(9)	139.85(8)
Te[1] - Ce - Te[3] x 2	139.47(6)	139.11(5)	140.19(8)
Te[1] - Ce - Te[1] x 8	85.34(7)	84.96(8)	85.97(8)
Te[1] - Ce - Te[1] x 4	146.91(5)	146.77(4)	147.06(8)
Te[1] - Ce - Te[2] x 4	77.21(8)	75.40(9)	78.84(8)
Te[1] - Ce - Te[2] x 4	131.03(8)	128.42(7)	133.35(7)
Te[1] - Ce - Te[3] x 4	77.13(8)	76.66(8)	77.79(8)
Te[1] - Ce - Te[3] x 4	130.96(10)	130.23(10)	131.75(11)
Te[2] - Ce - Te[2] x 2	80.73(9)	80.15(11)	81.27(9)
Te[2] - Ce - Te[3] x 4	54.61(10)	51.71(10)	57.02(11)
Te[3] - Ce - Te[3] x 2	80.70(6)	80.05(9)	81.12(7)
Ce - Te[1] - Ce x 8	85.74(7)	85.50(8)	86.12(8)
Ce - Te[1] - Ce x 4	146.91(6)	146.75(4)	147.08(4)
Ce - Te[2] - Ce x 2	80.69(6)	80.64(8)	80.77(8)
Ce - Te[2] - Te[3] x 4	117.06(10)	114.19(13)	120.22(12)
Te[3] - Te[2] - Te[3] x 8	90.17(15)	85.68(16)	94.99(19)
Te[3] - Te[2] - Te[3] x 4	176.69(16)	174.74(16)	179.74(9)
Ce - Te[3] - Te[2] x 4	63.02(8)	60.95(8)	64.56(7)
Ce - Te[3] - Te[2] x 4	117.29(9)	116.62(9)	117.76(9)
Te[2] - Te[3] - Te[2] x 4	90.50(14)	85.17(16)	94.82(18)
Te[2] - Te[3] - Te[2] x 4	89.65(13)	88.60(12)	90.19(15)
Te[2] - Te[3] - Te[2] x 4	176.72(15)	175.00(17)	179.22(7)

Table 3.21. Crystal data and structure refinement for CeTe₃ at 500 K.

Empirical formula	CeTe ₃
Formula weight	522.9
Temperature	500.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3837(11) Å, α = 90° b = 26.050(7) Å, β = 90° c = 4.4033(9) Å, γ = 90°
q-vector(1)	0.2867(5)c*
Volume	502.8(2) Å ³
Z	4
Density (calculated)	6.905 g/cm ³
Absorption coefficient	25.993 mm ⁻¹
F(000)	856
Crystal size	0.79 x 0.34 x 0.01 mm ³
Theta range for data collection	2.05 to 29.28°
Index ranges	-6<=h<=6, -35<=k<=35, -6<=l<=5, -1<=m<=1
Reflections collected	7142 (2348 main + 4794 satellites)
Independent reflections	2092 (739 main + 1353 satellites) [R _{int} = 0.0656]
Completeness to θ = 29.28°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2092 / 0 / 38
Goodness-of-fit on F ²	1.36
Final R indices [I>2σ(I)]	R _{obs} = 0.0394, wR _{obs} = 0.0965
R indices (all data)	R _{all} = 0.0759, wR _{all} = 0.1052
Final R main indices [I>2σ(I)]	R _{obs} = 0.0320, wR _{obs} = 0.0833
R main indices (all data)	R _{all} = 0.0342, wR _{all} = 0.0839
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1364, wR _{obs} = 0.1895
R 1 st order satellites (all data)	R _{all} = 0.3646, wR _{all} = 0.2345
Extinction coefficient	0.00034(4)
T _{min} and T _{max} coefficients	0.0722 and 0.7368
Largest diff. peak and hole	1.60 and -2.07 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o $, $wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.22. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for CeTe_3 at 500 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Ce	0	9249	1690(1)	2549	22(1)
	sin, 1	0	0	28(5)	
	cos, 1	34(1)	8(1)	0	
Te[1]	0	9202(8)	2959(1)	2549	22(1)
	sin, 1	0	0	0(5)	
	cos, 1	0(1)	0(1)	0	
Te[2]	0	9210(12)	699(1)	7549	29(1)
	sin, 1	0	0	12(6)	
	cos, 1	-175(3)	-1(1)	0	
Te[3]	0	9176(10)	4299(1)	7549	29(1)
	sin, 1	0	0	16(6)	
	cos, 1	133(3)	-2(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.23. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for CeTe_3 at 500 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	18(1)	30(1)	19(1)	-1(1)	0	0
Te[1]	18(1)	30(1)	19(1)	1(1)	0	0
Te[2]	26(1)	34(1)	27(1)	-1(1)	0	0
Te[3]	25(1)	35(1)	28(1)	-5(1)	0	0

Table 3.24. Bond lengths distributions [$\text{\AA}$] for CeTe_3 at 500 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[1]	3.3051(18)	3.285(3)	3.325(3)
Ce - Te[1] x 4	3.238(3)	3.229(3)	3.247(3)
Ce - Te[2] x 2	3.395(2)	3.374(2)	3.416(2)
Ce - Te[3]	3.390(3)	3.374(4)	3.408(4)
Ce - Te[3]	3.377(3)	3.338(4)	3.416(4)
Te[2] - Te[3] x 2	3.118(5)	3.037(5)	3.201(5)
Te[2] - Te[3] x 2	3.097(5)	3.008(5)	3.187(5)

Table 3.25. Bond angles distributions [°] for CeTe₃ at 500 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Ce - Te[1] x 8	73.63(6)	73.37(6)	73.88(6)
Te[1] - Ce - Te[2] x 2	139.54(6)	139.20(7)	139.91(7)
Te[1] - Ce - Te[3] x 2	139.51(9)	139.05(9)	139.96(9)
Te[1] - Ce - Te[1] x 4	85.69(7)	85.56(7)	85.81(7)
Te[1] - Ce - Te[1] x 4	85.20(8)	84.88(8)	85.53(8)
Te[1] - Ce - Te[1] x 4	147.25(5)	146.50(7)	147.98(7)
Te[1] - Ce - Te[2] x 4	76.95(8)	75.71(8)	78.22(8)
Te[1] - Ce - Te[2] x 4	131.04(10)	129.31(10)	132.79(10)
Te[1] - Ce - Te[3] x 4	76.99(7)	76.93(6)	77.05(6)
Te[1] - Ce - Te[3] x 4	130.73(7)	130.51(8)	130.95(8)
Te[2] - Ce - Te[2] x 2	80.89(5)	80.49(6)	81.26(6)
Te[2] - Ce - Te[3] x 4	54.70(9)	53.11(9)	56.34(9)
Te[3] - Ce - Te[3] x 2	80.74(9)	80.43(10)	81.06(10)
Ce - Te[1] - Ce x 8	106.37(7)	106.28(6)	106.46(6)
Ce - Te[1] - Ce x 4	85.67(9)	85.08(9)	86.24(9)
Ce - Te[1] - Ce x 4	85.20(4)	84.88(6)	85.53(6)
Ce - Te[1] - Ce x 4	147.24(5)	146.69(8)	147.79(8)
Ce - Te[2] - Ce x 2	80.87(5)	80.77(7)	80.95(7)
Ce - Te[2] - Te[3] x 4	62.57(6)	62.25(6)	62.87(6)
Ce - Te[2] - Te[3] x 4	117.12(12)	115.27(13)	118.93(13)
Te[3] - Te[2] - Te[3] x 8	89.91(17)	86.86(16)	93.01(18)
Te[3] - Te[2] - Te[3] x 4	178.09(17)	176.66(17)	179.77(5)
Ce - Te[3] - Ce x 2	80.75(4)	80.43(6)	81.06(6)
Ce - Te[3] - Te[2] x 4	63.08(8)	62.24(8)	63.95(8)
Ce - Te[3] - Te[2] x 4	117.27(7)	116.77(6)	117.75(6)
Te[2] - Te[3] - Te[2] x 4	90.69(16)	88.04(16)	93.39(17)
Te[2] - Te[3] - Te[2] x 4	89.70(12)	89.53(11)	89.81(13)
Te[2] - Te[3] - Te[2] x 4	178.20(16)	176.84(16)	179.78(5)

Table 3.26. Crystal data and structure refinement for PrTe₃ at 100 K.

Empirical formula	PrTe ₃
Formula weight	523.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3475(9) Å, α = 90° b = 25.800(5) Å, β = 90° c = 4.3548(9) Å, γ = 90°
q-vector(1)	0.2825(5)c*
Volume	488.46(17) Å ³
Z	4
Density (calculated)	7.119 g/cm ³
Absorption coefficient	27.177 mm ⁻¹
F(000)	860
Crystal size	0.32 x 0.31 x 0.02 mm ³
Theta range for data collection	2.05 to 29.13°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6121 (1756 main + 4365 satellites)
Independent reflections	1944 (640 main + 1304 satellites) [R _{int} = 0.0293]
Completeness to θ = 29.13°	97%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1944 / 0 / 37
Goodness-of-fit on F ²	1.42
Final R indices [I > 2σ(I)]	R _{obs} = 0.0284, wR _{obs} = 0.0830
R indices (all data)	R _{all} = 0.0440, wR _{all} = 0.0900
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0226, wR _{obs} = 0.0769
R main indices (all data)	R _{all} = 0.0232, wR _{all} = 0.0771
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0534, wR _{obs} = 0.0952
R 1 st order satellites (all data)	R _{all} = 0.1201, wR _{all} = 0.1135
Extinction coefficient	0.00184(7)
T _{min} and T _{max} coefficients	0.0091 and 0.5931
Largest diff. peak and hole	2.09 and -1.80 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.27. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for PrTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Pr	0	9000	1690(1)	2549	1(1)
	sin, 1	0	0	-5(2)	
	cos, 1	-61(1)	0(1)	0	
Te[1]	0	8972(3)	2957(1)	2549	1(1)
	sin, 1	0	0	15(3)	
	cos, 1	-9(1)	5(1)	0	
Te[2]	0	9045(4)	699(1)	7549	2(1)
	sin, 1	0	0	-3(3)	
	cos, 1	278(1)	0(1)	0	
Te[3]	0	9018(3)	4298(1)	7549	2(1)
	sin, 1	0	0	-7(3)	
	cos, 1	-227(1)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.28. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr	2(1)	1(1)	1(1)	1(1)	0	0
Te[1]	2(1)	1(1)	1(1)	2(1)	0	0
Te[2]	2(1)	3(1)	2(1)	-4(1)	0	0
Te[3]	3(1)	3(1)	2(1)	-2(1)	0	0

Table 3.29. Bond lengths distributions [$\text{\AA}$] for PrTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Pr - Te[1]	3.2692(10)	3.2566(16)	3.2817(16)
Pr - Te[1] x 2	3.2173(12)	3.2009(11)	3.2340(11)
Pr - Te[1] x 2	3.2010(12)	3.1816(13)	3.2201(13)
Pr - Te[2] x 2	3.3591(10)	3.3568(10)	3.3609(11)
Pr - Te[3]	3.3457(12)	3.2956(16)	3.3953(16)
Pr - Te[3]	3.3552(12)	3.3117(16)	3.4000(16)
Te[2] - Te[3] x 2	3.0873(18)	2.9489(16)	3.2272(18)
Te[2] - Te[3] x 2	3.0694(18)	2.9306(16)	3.2131(18)

Table 3.30. Bond angles distributions [°] for PrTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Pr - Te[1] x 8	73.38(3)	72.91(3)	73.84(3)
Te[1] - Pr - Te[2] x 2	139.53(3)	139.35(3)	139.72(4)
Te[1] - Pr - Te[3] x 2	139.44(3)	138.94(4)	139.95(4)
Te[1] - Pr - Te[1] x 6	85.19(3)	84.43(3)	85.94(3)
Te[1] - Pr - Te[1] x 4	146.97(3)	146.59(4)	147.33(4)
Te[1] - Pr - Te[2] x 2	77.36(3)	75.92(3)	78.77(3)
Te[1] - Pr - Te[2] x 2	131.19(4)	128.82(4)	133.54(4)
Te[1] - Pr - Te[3] x 4	77.07(3)	76.48(3)	77.68(3)
Te[1] - Pr - Te[3] x 2	131.07(3)	130.34(3)	131.81(3)
Te[1] - Pr - Te[1] x 2	85.72(3)	85.41(3)	86.05(3)
Te[1] - Pr - Te[2] x 2	76.80(3)	75.02(3)	78.60(3)
Te[1] - Pr - Te[2] x 2	130.84(4)	128.51(4)	133.18(4)
Te[1] - Pr - Te[3] x 2	130.88(3)	130.53(3)	131.22(3)
Te[2] - Pr - Te[2] x 2	80.86(3)	80.75(3)	80.91(2)
Te[2] - Pr - Te[3] x 2	54.84(4)	52.53(4)	57.13(4)
Te[2] - Pr - Te[3] x 2	54.39(4)	52.05(4)	56.81(4)
Te[3] - Pr - Te[3] x 2	80.89(3)	80.80(4)	80.96(4)
Pr - Te[1] - Pr x 8	106.70(3)	106.10(3)	107.31(3)
Pr - Te[1] - Pr x 8	85.28(2)	85.035(19)	85.518(19)
Pr - Te[1] - Pr x 4	146.97(3)	146.47(4)	147.47(4)
Pr - Te[2] - Pr x 2	80.81(2)	80.70(3)	80.872(18)
Pr - Te[2] - Te[3] x 4	62.34(2)	61.72(2)	62.97(2)
Pr - Te[2] - Te[3] x 2	116.85(5)	113.73(5)	119.94(5)
Pr - Te[2] - Te[3] x 2	117.54(5)	114.42(5)	120.63(5)
Te[3] - Te[2] - Te[3] x 6	89.90(6)	85.12(6)	94.87(7)
Te[3] - Te[2] - Te[3] x 4	176.91(6)	174.85(6)	179.74(3)
Te[3] - Te[2] - Te[3] x 2	90.53(6)	85.81(6)	95.40(7)
Pr - Te[3] - Pr x 2	80.895(19)	80.80(3)	80.96(3)
Pr - Te[3] - Te[2] x 4	62.88(3)	61.04(3)	64.75(3)
Pr - Te[3] - Te[2] x 4	117.48(3)	116.57(3)	118.29(3)
Te[2] - Te[3] - Te[2] x 2	90.53(5)	85.96(5)	95.21(6)
Te[2] - Te[3] - Te[2] x 6	89.78(5)	89.64(4)	89.95(5)
Te[2] - Te[3] - Te[2] x 4	177.04(6)	175.07(6)	179.72(3)

Table 3.31. Crystal data and structure refinement for PrTe₃ at 500 K.

Empirical formula	PrTe ₃
Formula weight	523.7
Temperature	500.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3630(9) Å, α = 90° b = 26.026(7) Å, β = 90° c = 4.3721(8) Å, γ = 90°
q-vector(1)	0.2864(4)c*
Volume	496.46(18) Å ³
Z	4
Density (calculated)	7.004 g/cm ³
Absorption coefficient	26.739 mm ⁻¹
F(000)	860
Crystal size	0.32 x 0.31 x 0.02 mm ³
Theta range for data collection	2.05 to 29.22°
Index ranges	-5<=h<=6, -34<=k<=35, -6<=l<=6, -1<=m<=1
Reflections collected	6592 (2029 main + 4563 satellites)
Independent reflections	2024 (693 main + 1331 satellites) [R _{int} = 0.0408]
Completeness to θ = 29.22°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2024 / 0 / 38
Goodness-of-fit on F ²	1.29
Final R indices [I>2σ(I)]	R _{obs} = 0.0299, wR _{obs} = 0.0828
R indices (all data)	R _{all} = 0.0607, wR _{all} = 0.0940
Final R main indices [I>2σ(I)]	R _{obs} = 0.0226, wR _{obs} = 0.0626
R main indices (all data)	R _{all} = 0.0232, wR _{all} = 0.0629
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1260, wR _{obs} = 0.1731
R 1 st order satellites (all data)	R _{all} = 0.3513, wR _{all} = 0.2157
Extinction coefficient	0.00158(7)
T _{min} and T _{max} coefficients	0.0091 and 0.5931
Largest diff. peak and hole	2.07 and -2.71 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.32. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for PrTe_3 at 500 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Pr	0	9000	1692(1)	2549	12(1)
	sin, 1	0	0	7(4)	
	cos, 1	27(1)	0(1)	0	
Te[1]	0	9024(3)	2957(1)	2549	12(1)
	sin, 1	0	0	-24(4)	
	cos, 1	-5(1)	0(1)	0	
Te[2]	0	8951(4)	702(1)	7549	18(1)
	sin, 1	0	0	6(6)	
	cos, 1	-133(2)	0(1)	0	
Te[3]	0	8971(3)	4296(1)	7549	18(1)
	sin, 1	0	0	-7(6)	
	cos, 1	113(2)	8(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.33. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for PrTe_3 at 500 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pr	11(1)	14(1)	11(1)	-1(1)	0	0
Te[1]	11(1)	14(1)	10(1)	-1(1)	0	0
Te[2]	19(1)	18(1)	18(1)	4(1)	0	0
Te[3]	18(1)	18(1)	18(1)	0(1)	0	0

Table 3.34. Bond lengths distributions [$\text{\AA}$] for PrTe_3 at 500 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Pr - Te[1]	3.2923(12)	3.292(2)	3.292(2)
Pr - Te[1] x 2	3.2134(15)	3.2043(14)	3.2224(14)
Pr - Te[1] x 2	3.2275(15)	3.2125(15)	3.2427(15)
Pr - Te[2] x 2	3.3790(16)	3.3783(17)	3.3800(14)
Pr - Te[3]	3.3806(13)	3.3720(18)	3.3897(18)
Pr - Te[3]	3.3645(13)	3.3244(18)	3.4040(18)
Te[2] - Te[3] x 2	3.082(2)	3.0144(17)	3.1515(18)
Te[2] - Te[3] x 2	3.095(2)	3.0271(17)	3.1637(18)

Table 3.35. Bond angles distributions [°] for PrTe₃ at 500 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Pr - Te[1] x 6	73.62(3)	73.38(3)	73.86(3)
Te[1] - Pr - Te[1] x 2	73.44(3)	73.27(3)	73.61(3)
Te[1] - Pr - Te[2] x 2	139.67(5)	139.40(7)	139.94(7)
Te[1] - Pr - Te[3] x 2	139.72(3)	139.25(3)	140.17(3)
Te[1] - Pr - Te[1] x 8	85.28(4)	85.00(5)	85.56(5)
Te[1] - Pr - Te[1] x 4	147.06(3)	146.93(5)	147.18(5)
Te[1] - Pr - Te[2] x 2	76.82(4)	76.06(5)	77.60(5)
Te[1] - Pr - Te[2] x 2	130.72(4)	129.61(4)	131.84(4)
Te[1] - Pr - Te[3] x 4	77.16(4)	76.76(4)	77.55(4)
Te[1] - Pr - Te[3] x 4	130.75(6)	130.41(5)	131.09(5)
Te[1] - Pr - Te[2] x 2	77.40(4)	76.65(4)	78.14(4)
Te[1] - Pr - Te[2] x 2	131.17(4)	130.09(4)	132.24(4)
Te[2] - Pr - Te[2] x 2	80.64(5)	80.54(5)	80.71(5)
Te[2] - Pr - Te[3] x 4	54.25(5)	53.02(5)	55.51(5)
Te[3] - Pr - Te[3] x 2	80.61(3)	80.16(4)	81.05(4)
Pr - Te[1] - Pr x 8	106.31(4)	105.95(3)	106.66(3)
Pr - Te[1] - Pr x 6	85.27(4)	85.00(4)	85.53(4)
Pr - Te[1] - Pr x 4	147.06(4)	146.97(3)	147.15(3)
Pr - Te[1] - Pr x 2	85.73(4)	85.56(4)	85.91(4)
Pr - Te[2] - Pr x 2	80.62(3)	80.53(4)	80.70(4)
Pr - Te[2] - Te[3] x 4	62.90(4)	62.39(3)	63.38(3)
Pr - Te[2] - Te[3] x 2	117.54(5)	115.77(5)	119.31(6)
Pr - Te[2] - Te[3] x 2	116.83(5)	115.58(6)	118.07(6)
Te[3] - Te[2] - Te[3] x 2	90.38(7)	88.12(7)	92.67(7)
Te[3] - Te[2] - Te[3] x 6	89.85(6)	89.75(8)	90.01(8)
Te[3] - Te[2] - Te[3] x 4	178.45(7)	177.41(7)	179.82(3)
Pr - Te[3] - Pr x 2	80.61(2)	80.16(4)	81.05(4)
Pr - Te[3] - Te[2] x 4	62.93(4)	61.84(3)	64.05(4)
Pr - Te[3] - Te[2] x 2	117.08(5)	116.26(4)	117.88(4)
Pr - Te[3] - Te[2] x 2	117.41(5)	116.95(5)	117.88(5)
Te[2] - Te[3] - Te[2] x 6	89.91(6)	87.75(6)	92.11(7)
Te[2] - Te[3] - Te[2] x 4	178.45(7)	177.43(7)	179.81(3)
Te[2] - Te[3] - Te[2] x 2	90.38(6)	88.08(6)	92.70(7)

Table 3.36. Crystal data and structure refinement for NdTe₃ at 100 K.

Empirical formula	NdTe ₃
Formula weight	527
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3316(7) Å, α = 90° b = 25.705(5) Å, β = 90° c = 4.3419(7) Å, γ = 90°
q-vector(1)	0.2824(4)c*
Volume	483.44(15) Å ³
Z	4
Density (calculated)	7.239 g/cm ³
Absorption coefficient	28.271 mm ⁻¹
F(000)	864
Crystal size	0.34 x 0.23 x 0.01 mm ³
Theta range for data collection	2.06 to 29.18°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 5, -1 ≤ m ≤ 1
Reflections collected	6601 (2051 main + 4550 satellites)
Independent reflections	1988 (692 main + 1296 satellites) [R _{int} = 0.0259]
Completeness to θ = 29.18°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1988 / 0 / 38
Goodness-of-fit on F ²	1.40
Final R indices [I > 2σ(I)]	R _{obs} = 0.0221, wR _{obs} = 0.0818
R indices (all data)	R _{all} = 0.0375, wR _{all} = 0.0884
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0165, wR _{obs} = 0.0804
R main indices (all data)	R _{all} = 0.0172, wR _{all} = 0.0820
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0530, wR _{obs} = 0.0857
R 1 st order satellites (all data)	R _{all} = 0.1296, wR _{all} = 0.1044
Extinction coefficient	0.00095(5)
T _{min} and T _{max} coefficients	0.0151 and 0.6913
Largest diff. peak and hole	1.59 and -2.02 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.37. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for NdTe₃ at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Nd	0	9249	1690(1)	2549	2(1)
	sin, 1	0	0	20(2)	
	cos, 1	-61(1)	5(1)	0	
Te[1]	0	9224(3)	2955(1)	2549	2(1)
	sin, 1	0	0	0(3)	
	cos, 1	-10(1)	0(1)	0	
Te[2]	0	9162(4)	701(1)	7549	3(1)
	sin, 1	0	0	0(3)	
	cos, 1	261(1)	1(1)	0	
Te[3]	0	9182(3)	4296(1)	7549	3(1)
	sin, 1	0	0	-3(3)	
	cos, 1	-217(1)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.38. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Nd	2(1)	2(1)	1(1)	0(1)	0	0
Te[1]	2(1)	2(1)	1(1)	-1(1)	0	0
Te[2]	2(1)	3(1)	2(1)	4(1)	0	0
Te[3]	3(1)	3(1)	2(1)	1(1)	0	0

Table 3.39. Bond lengths distributions [$\text{\AA}$] for NdTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Nd - Te[1]	3.2513(10)	3.2401(18)	3.2629(18)
Nd - Te[1] x 2	3.1917(12)	3.1706(12)	3.2132(12)
Nd - Te[1] x 2	3.2062(12)	3.1929(11)	3.2192(11)
Nd - Te[2] x 2	3.3446(11)	3.3365(12)	3.3547(12)
Nd - Te[3]	3.3413(13)	3.2869(17)	3.3951(17)
Nd - Te[3]	3.3303(13)	3.2973(17)	3.3645(17)
Te[2] - Te[3] x 2	3.0627(17)	2.9321(15)	3.1947(16)
Te[2] - Te[3] x 2	3.0732(17)	2.9427(15)	3.2082(16)

Table 3.40. Bond angles distributions [°] for NdTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Nd - Te[1] x 8	73.56(3)	73.14(3)	73.96(3)
Te[1] - Nd - Te[2] x 2	139.47(3)	139.20(4)	139.81(3)
Te[1] - Nd - Te[3] x 2	139.59(3)	139.27(4)	139.94(4)
Te[1] - Nd - Te[1] x 8	85.22(3)	85.01(4)	85.44(4)
Te[1] - Nd - Te[1] x 4	146.92(3)	146.49(4)	147.34(4)
Te[1] - Nd - Te[2] x 2	76.83(3)	75.49(3)	78.14(3)
Te[1] - Nd - Te[2] x 2	130.94(4)	128.85(3)	133.00(3)
Te[1] - Nd - Te[3] x 4	77.13(3)	76.63(3)	77.65(3)
Te[1] - Nd - Te[3] x 2	130.90(3)	130.12(3)	131.67(3)
Te[1] - Nd - Te[2] x 2	77.26(3)	75.56(3)	78.99(3)
Te[1] - Nd - Te[2] x 2	131.22(4)	128.82(3)	133.63(3)
Te[1] - Nd - Te[3] x 2	131.10(3)	130.72(3)	131.47(3)
Te[2] - Nd - Te[2] x 2	80.99(3)	80.71(3)	81.18(3)
Te[2] - Nd - Te[3] x 2	54.53(3)	52.48(3)	56.56(3)
Te[2] - Nd - Te[3] x 2	54.82(3)	52.47(3)	57.25(3)
Te[3] - Nd - Te[3] x 2	80.97(3)	80.65(4)	81.26(4)
Nd - Te[1] - Nd x 8	106.71(3)	106.54(3)	106.87(3)
Nd - Te[1] - Nd x 8	85.24(4)	85.21(4)	85.27(4)
Nd - Te[1] - Nd x 4	146.92(3)	146.56(4)	147.28(4)
Nd - Te[2] - Nd x 2	80.95(3)	80.86(4)	80.999(19)
Nd - Te[2] - Te[3] x 4	62.67(2)	62.03(2)	63.32(2)
Nd - Te[2] - Te[3] x 2	117.54(4)	114.65(5)	120.41(5)
Nd - Te[2] - Te[3] x 2	116.99(4)	113.96(5)	119.97(5)
Te[3] - Te[2] - Te[3] x 2	90.46(5)	85.93(5)	95.16(6)
Te[3] - Te[2] - Te[3] x 6	89.76(4)	89.61(3)	89.90(5)
Te[3] - Te[2] - Te[3] x 4	177.10(6)	175.20(6)	179.79(2)
Nd - Te[3] - Nd x 2	80.97(2)	80.65(4)	81.26(4)
Nd - Te[3] - Te[2] x 4	62.84(3)	60.99(3)	64.71(3)
Nd - Te[3] - Te[2] x 2	117.22(3)	116.31(3)	118.06(3)
Nd - Te[3] - Te[2] x 2	117.45(3)	116.54(3)	118.27(3)
Te[2] - Te[3] - Te[2] x 6	90.03(5)	85.71(5)	94.44(6)
Te[2] - Te[3] - Te[2] x 4	177.21(6)	175.38(5)	179.79(3)
Te[2] - Te[3] - Te[2] x 2	90.46(5)	86.13(5)	94.93(6)

Table 3.41. Crystal data and structure refinement for NdTe₃ at 470 K.

Empirical formula	NdTe ₃
Formula weight	527
Temperature	470.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3562(7) Å, α = 90° b = 25.860(6) Å, β = 90° c = 4.3582(7) Å, γ = 90°
q-vector(1)	0.2874(4)c*
Volume	490.95(15) Å ³
Z	4
Density (calculated)	7.128 g/cm ³
Absorption coefficient	27.838 mm ⁻¹
F(000)	864
Crystal size	0.34 x 0.23 x 0.01 mm ³
Theta range for data collection	2.07 to 29.23°
Index ranges	-5 ≤ h ≤ 5, -35 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6816 (2155 main + 4661 satellites)
Independent reflections	2030 (706 main + 1324 satellites) [R _{int} = 0.0549]
Completeness to θ = 29.23°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2030 / 0 / 38
Goodness-of-fit on F ²	1.24
Final R indices [I > 2σ(I)]	R _{obs} = 0.0290, wR _{obs} = 0.0827
R indices (all data)	R _{all} = 0.0517, wR _{all} = 0.0900
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0257, wR _{obs} = 0.0754
R main indices (all data)	R _{all} = 0.0261, wR _{all} = 0.0756
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0953, wR _{obs} = 0.1650
R 1 st order satellites (all data)	R _{all} = 0.3134, wR _{all} = 0.2196
Extinction coefficient	0.00058(5)
T _{min} and T _{max} coefficients	0.0151 and 0.6913
Largest diff. peak and hole	1.42 and -1.61 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.42. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for NdTe_3 at 470 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Nd	0	9249	1693(1)	2549	15(1)
	sin, 1	0	0	3(2)	
	cos, 1	21(1)	0(1)	0	
Te[1]	0	9214(3)	2956(1)	2549	15(1)
	sin, 1	0	0	-3(2)	
	cos, 1	-1(1)	1(1)	0	
Te[2]	0	9192(3)	704(1)	7549	20(1)
	sin, 1	0	0	3(3)	
	cos, 1	-111(2)	6(1)	0	
Te[3]	0	9137(3)	4295(1)	7549	20(1)
	sin, 1	0	0	22(3)	
	cos, 1	84(2)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.43. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe_3 at 470 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Nd	14(1)	18(1)	13(1)	0(1)	0	0
Te[1]	14(1)	17(1)	13(1)	-1(1)	0	0
Te[2]	21(1)	22(1)	18(1)	3(1)	0	0
Te[3]	19(1)	22(1)	19(1)	-2(1)	0	0

Table 3.44. Bond lengths distributions [$\text{\AA}$] for NdTe_3 at 470 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Nd - Te[1]	3.2663(11)	3.2653(19)	3.2673(19)
Nd - Te[1] x 2	3.2081(11)	3.2027(11)	3.2134(11)
Nd - Te[1] x 2	3.2164(11)	3.2086(11)	3.2244(11)
Nd - Te[2] x 2	3.3588(11)	3.3492(12)	3.3689(12)
Nd - Te[3]	3.3742(13)	3.3582(18)	3.3905(18)
Nd - Te[3]	3.3387(12)	3.3193(18)	3.3579(18)
Te[2] - Te[3] x 2	3.0980(16)	3.0476(15)	3.1497(16)
Te[2] - Te[3] x 2	3.0646(16)	3.0066(15)	3.1224(16)

Table 3.45. Bond angles distributions [°] for NdTe₃ at 470 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Nd - Te[1] x 8	73.62(2)	73.56(3)	73.68(3)
Te[1] - Nd - Te[2] x 2	139.54(3)	139.34(3)	139.74(3)
Te[1] - Nd - Te[3] x 2	139.29(3)	139.09(3)	139.50(3)
Te[1] - Nd - Te[1] x 8	85.57(3)	85.35(3)	85.80(3)
Te[1] - Nd - Te[1] x 4	147.13(3)	147.07(4)	147.19(4)
Te[1] - Nd - Te[2] x 4	76.94(3)	76.16(3)	77.73(3)
Te[1] - Nd - Te[2] x 4	130.96(3)	130.10(3)	131.82(3)
Te[1] - Nd - Te[3] x 2	76.81(3)	76.64(3)	76.98(3)
Te[1] - Nd - Te[3] x 2	130.75(3)	130.55(3)	130.95(3)
Te[1] - Nd - Te[3] x 2	131.13(3)	130.88(3)	131.37(3)
Te[1] - Nd - Te[3] x 2	77.21(3)	77.01(2)	77.42(2)
Te[2] - Nd - Te[2] x 2	80.91(3)	80.70(3)	81.10(3)
Te[2] - Nd - Te[3] x 4	54.79(3)	54.02(3)	55.57(3)
Te[3] - Nd - Te[3] x 2	80.92(3)	80.88(4)	80.96(4)
Nd - Te[1] - Nd x 4	106.34(3)	106.22(3)	106.45(3)
Nd - Te[1] - Nd x 4	106.53(3)	106.35(3)	106.72(3)
Nd - Te[1] - Nd x 6	85.30(3)	85.11(4)	85.48(4)
Nd - Te[1] - Nd x 4	147.13(3)	147.03(4)	147.23(4)
Nd - Te[1] - Nd x 2	85.57(3)	85.48(4)	85.67(4)
Nd - Te[2] - Nd x 2	80.90(3)	80.57(4)	81.22(4)
Nd - Te[2] - Te[3] x 4	62.86(2)	62.50(2)	63.20(2)
Nd - Te[2] - Te[3] x 4	117.17(4)	115.56(5)	118.78(5)
Te[3] - Te[2] - Te[3] x 6	89.95(4)	89.73(3)	90.19(4)
Te[3] - Te[2] - Te[3] x 4	178.69(5)	177.41(5)	180
Te[3] - Te[2] - Te[3] x 2	90.68(5)	89.00(5)	92.38(6)
Nd - Te[3] - Nd x 2	80.92(2)	80.88(3)	80.96(3)
Nd - Te[3] - Te[2] x 2	63.11(3)	62.17(3)	64.08(3)
Nd - Te[3] - Te[2] x 4	117.27(3)	116.54(3)	118.00(3)
Nd - Te[3] - Te[2] x 2	62.35(3)	61.83(3)	62.87(3)
Te[2] - Te[3] - Te[2] x 2	90.68(5)	88.95(5)	92.43(5)
Te[2] - Te[3] - Te[2] x 4	89.95(4)	89.73(4)	90.19(4)
Te[2] - Te[3] - Te[2] x 4	178.78(5)	177.56(5)	180
Te[2] - Te[3] - Te[2] x 2	89.42(5)	87.67(5)	91.18(5)

Table 3.46. Crystal data and structure refinement for NdTe₃ at 500 K.

Empirical formula	NdTe ₃
Formula weight	527
Temperature	500.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 4.402(3) Å, α = 90° b = 25.72(2) Å, β = 90° c = 4.360(3) Å, γ = 90°
Volume	493.6(6) Å ³
Z	4
Density (calculated)	7.089 g/cm ³
Absorption coefficient	27.687 mm ⁻¹
F(000)	864
Crystal size	0.34 x 0.23 x 0.01 mm ³
Theta range for data collection	3.17 to 29.03°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 5
Reflections collected	2187
Independent reflections	388 [R _{int} = 0.0476]
Completeness to θ = 29.03°	94%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	388 / 0 / 18
Goodness-of-fit on F ²	1.67
Final R indices [I > 2σ(I)]	R _{obs} = 0.0243, wR _{obs} = 0.0740
R indices (all data)	R _{all} = 0.0249, wR _{all} = 0.0741
Extinction coefficient	0.076(9)
Largest diff. peak and hole	1.65 and -1.60 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w = 1/(σ ² (I) + 0.0016I ²)	

Table 3.47. Atomic coordinates (x10⁴) and equivalent isotropic displacement parameters (Å²x10³) for NdTe₃ at 500 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U _{eq} [*]
Nd	5000	3307(1)	2549	1	12(1)
Te[1]	5000	2045(1)	2549	1	12(1)
Te[2]	0	4294(1)	2549	1	18(1)

Table 3.47. (Cont'd) Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ at 500 K with e.s.d.'s in parentheses.

Te[3]	5000	4295(1)	7549	1	18(1)
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*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.48. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for NdTe₃ at 500 K with e.s.d.'s in parentheses.

Label	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Nd	11(1)	14(1)	11(1)	0	0	0
Te[1]	11(1)	13(1)	11(1)	0	0	0
Te[2]	18(1)	18(1)	18(1)	0	0	0
Te[3]	18(1)	19(1)	17(1)	0	0	0

Table 3.49. Bond distances [$\text{\AA}$] for NdTe₃ at 500 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Nd - Te[1]	3.2468(7)	Nd - Te[2] x 2	3.3599(6)
Nd - Te[1] x 4	3.2271(2)	Nd - Te[3] x 2	3.3475(6)

Table 3.50. Bond angles [$^\circ$] for NdTe₃ at 500 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[1] - Nd - Te[1] x 8	73.712(13)	Nd - Te[1] - Nd x 4	85.997(6)
Te[1] - Nd - Te[2] x 2	139.077(9)	Nd - Te[1] - Nd x 4	147.42(2)
Te[1] - Nd - Te[1] x 4	84.979(6)	Nd - Te[2] - Te[3] x 4	62.294(12)
Te[1] - Nd - Te[1] x 4	85.997(6)	Nd - Te[2] - Te[3] x 4	117.767(17)
Te[1] - Nd - Te[1] x 4	147.42(2)	Te[3] - Te[2] - Te[3] x 4	89.449
Te[1] - Nd - Te[2] x 4	76.420(10)	Te[3] - Te[2] - Te[3] x 4	90.551
Te[1] - Nd - Te[2] x 4	131.197(12)	Te[3] - Te[2] - Te[3] x 4	180
Te[1] - Nd - Te[3] x 4	76.881(10)	Nd - Te[3] - Nd x 2	81.259(16)
Te[1] - Nd - Te[3] x 4	130.745(12)	Nd - Te[3] - Te[2] x 4	62.697(12)
Te[2] - Nd - Te[2] x 2	81.846(14)	Nd - Te[3] - Te[2] x 4	117.243(17)
Te[2] - Nd - Te[3] x 4	55.009(9)	Te[2] - Te[3] - Te[2] x 4	89.449
Te[3] - Nd - Te[3] x 2	81.259(14)	Te[2] - Te[3] - Te[2] x 4	90.551
Nd - Te[1] - Nd x 8	106.288(13)	Te[2] - Te[3] - Te[2] x 4	180

Table 3.51. Crystal data and structure refinement for SmTe₃ at 100 K.

Empirical formula	SmTe ₃
Formula weight	533.2
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3055(6) Å, α = 90° b = 25.553(5) Å, β = 90° c = 4.3247(6) Å, γ = 90°
q-vector(1)	0.2865(3)c*
Volume	475.80(13) Å ³
Z	4
Density (calculated)	7.440 g/cm ³
Absorption coefficient	30.134 mm ⁻¹
F(000)	872
Crystal size	0.17 x 0.11 x 0.01 mm ³
Theta range for data collection	3.18 to 31.90°
Index ranges	-5<=h<=6, -37<=k<=37, -6<=l<=6, -1<=m<=1
Reflections collected	8234 (2535 main + 5699 satellites)
Independent reflections	2408 (826 main + 1582 satellites) [R _{int} = 0.0292]
Completeness to θ = 31.90°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2408 / 0 / 37
Goodness-of-fit on F ²	2.05
Final R indices [I>2σ(I)]	R _{obs} = 0.0312, wR _{obs} = 0.1257
R indices (all data)	R _{all} = 0.0505, wR _{all} = 0.1373
Final R main indices [I>2σ(I)]	R _{obs} = 0.0178, wR _{obs} = 0.0750
R main indices (all data)	R _{all} = 0.0180, wR _{all} = 0.0751
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1064, wR _{obs} = 0.2307
R 1 st order satellites (all data)	R _{all} = 0.1960, wR _{all} = 0.2590
Extinction coefficient	0.00097(7)
T _{min} and T _{max} coefficients	0.0501 and 0.6404
Largest diff. peak and hole	4.30 and -4.05 e.Å ⁻³

$$R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|, wR = \{ \Sigma [w(|F_o|^2 - |F_c|^2)^2] / \Sigma [w(|F_o|^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$$

Table 3.52. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for SmTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Sm	0	9449	1693(1)	2549	2(1)
	sin, 1	0	0	16(4)	
	cos, 1	57(1)	6(1)	0	
Te[1]	0	9425(4)	2952(1)	2549	2(1)
	sin, 1	0	0	-7(4)	
	cos, 1	5(1)	0(1)	0	
Te[2]	0	9413(4)	706(1)	7549	3(1)
	sin, 1	0	0	14(5)	
	cos, 1	-218(2)	0(1)	0	
Te[3]	0	4348(4)	708(1)	2549	3(1)
	sin, 1	0	0	5(4)	
	cos, 1	196(2)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.53. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SmTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	2(1)	2(1)	2(1)	0(1)	0	0
Te[1]	3(1)	2(1)	2(1)	-1(1)	0	0
Te[2]	4(1)	3(1)	3(1)	2(1)	0	0
Te[3]	2(1)	3(1)	3(1)	1(1)	0	0

Table 3.54. Bond lengths distributions [$\text{\AA}$] for SmTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm - Te[1]	3.2195(12)	3.204(2)	3.235(2)
Sm - Te[1] x 2	3.1762(15)	3.1653(12)	3.1870(12)
Sm - Te[1] x 2	3.1903(15)	3.1676(15)	3.2132(15)
Sm - Te[2] x 2	3.3220(14)	3.3075(13)	3.3369(13)
Sm - Te[3]	3.3260(15)	3.300(2)	3.353(2)
Sm - Te[3]	3.2975(15)	3.246(2)	3.349(2)
Te[2] - Te[3] x 2	3.072(2)	2.9619(18)	3.185(2)
Te[2] - Te[3] x 2	3.033(2)	2.9189(18)	3.1483(19)

Table 3.55. Bond angles distributions [°] for SmTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Sm - Te[1] x 8	73.54(3)	73.42(3)	73.65(3)
Te[1] - Sm - Te[2] x 2	139.35(4)	139.14(5)	139.61(5)
Te[1] - Sm - Te[3] x 2	139.36(4)	138.79(4)	139.92(4)
Te[1] - Sm - Te[1] x 2	85.81(4)	85.38(4)	86.25(4)
Te[1] - Sm - Te[1] x 6	85.11(4)	84.83(4)	85.38(4)
Te[1] - Sm - Te[1] x 4	146.89(3)	146.36(4)	147.41(5)
Te[1] - Sm - Te[2] x 4	76.96(4)	75.52(4)	78.43(4)
Te[1] - Sm - Te[2] x 2	131.38(4)	129.24(4)	133.55(4)
Te[1] - Sm - Te[3] x 4	77.00(4)	76.77(3)	77.24(3)
Te[1] - Sm - Te[3] x 2	130.83(5)	130.57(4)	131.08(4)
Te[1] - Sm - Te[2] x 2	130.99(4)	129.28(4)	132.67(4)
Te[1] - Sm - Te[3] x 2	131.18(5)	130.44(4)	131.92(4)
Te[2] - Sm - Te[2] x 2	81.25(4)	81.01(4)	81.44(4)
Te[2] - Sm - Te[3] x 2	55.03(4)	52.98(4)	57.14(4)
Te[2] - Sm - Te[3] x 2	54.55(4)	52.82(4)	56.26(4)
Te[3] - Sm - Te[3] x 2	81.08(4)	80.72(5)	81.44(5)
Sm - Te[1] - Sm x 8	106.39(4)	106.24(4)	106.53(4)
Sm - Te[1] - Sm x 6	85.11(3)	84.83(4)	85.38(4)
Sm - Te[1] - Sm x 4	146.89(4)	146.48(5)	147.29(5)
Sm - Te[1] - Sm x 2	85.82(4)	85.75(5)	85.88(5)
Sm - Te[2] - Sm x 2	81.23(3)	81.13(5)	81.28(3)
Sm - Te[2] - Te[3] x 4	62.53(3)	61.97(3)	63.07(3)
Sm - Te[2] - Te[3] x 4	117.13(5)	114.60(6)	119.64(6)
Te[3] - Te[2] - Te[3] x 6	89.60(6)	85.76(6)	93.53(7)
Te[3] - Te[2] - Te[3] x 4	177.49(7)	175.36(7)	179.85(3)
Te[3] - Te[2] - Te[3] x 2	91.08(7)	87.24(6)	95.04(7)
Sm - Te[3] - Sm x 2	81.08(2)	80.72(4)	81.44(4)
Sm - Te[3] - Te[2] x 2	63.15(4)	61.76(4)	64.61(4)
Sm - Te[3] - Te[2] x 4	117.34(4)	116.54(4)	118.08(4)
Sm - Te[3] - Te[2] x 2	62.43(4)	60.77(4)	64.10(4)
Te[2] - Te[3] - Te[2] x 2	91.05(7)	87.41(7)	94.85(7)
Te[2] - Te[3] - Te[2] x 6	89.66(5)	89.53(4)	89.84(6)
Te[2] - Te[3] - Te[2] x 4	177.52(7)	175.45(7)	179.85(3)

Table 3.56. Crystal data and structure refinement for SmTe₃ at 400 K.

Empirical formula	SmTe ₃
Formula weight	533.2
Temperature	400.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.3269(6) Å, α = 90° b = 25.691(4) Å, β = 90° c = 4.3341(7) Å, γ = 90°
q-vector(1)	0.2936(4)c*
Volume	481.80(13) Å ³
Z	4
Density (calculated)	7.348 g/cm ³
Absorption coefficient	29.759 mm ⁻¹
F(000)	872
Crystal size	0.17 x 0.11 x 0.01 mm ³
Theta range for data collection	2.10 to 29.18°
Index ranges	-5<=h<=5, -34<=k<=34, -6<=l<=6, -1<=m<=1
Reflections collected	6728 (2117 main + 4611 satellites)
Independent reflections	1929 (668 main + 1261 satellites) [R _{int} = 0.1036]
Completeness to θ = 29.18°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1929 / 0 / 38
Goodness-of-fit on F ²	1.45
Final R indices [I>2σ(I)]	R _{obs} = 0.0472, wR _{obs} = 0.1046
R indices (all data)	R _{all} = 0.0827, wR _{all} = 0.1119
Final R main indices [I>2σ(I)]	R _{obs} = 0.0444, wR _{obs} = 0.1022
R main indices (all data)	R _{all} = 0.0453, wR _{all} = 0.1025
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1443, wR _{obs} = 0.1844
R 1 st order satellites (all data)	R _{all} = 0.4709, wR _{all} = 0.3091
Extinction coefficient	0.00023(6)
T _{min} and T _{max} coefficients	0.0501 and 0.6404
Largest diff. peak and hole	3.32 and -2.61 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.57. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for SmTe_3 at 400 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Sm	0	9249	1695(1)	2549	10(1)
	sin, 1	0	0	28(5)	
	cos, 1	19(1)	6(1)	0	
Te[1]	0	9209(5)	2953(1)	2549	9(1)
	sin, 1	0	0	10(6)	
	cos, 1	0(2)	-1(1)	0	
Te[2]	0	9195(7)	708(1)	7549	14(1)
	sin, 1	0	0	1(6)	
	cos, 1	-87(3)	0(1)	0	
Te[3]	0	9228(6)	4291(1)	7549	14(1)
	sin, 1	0	0	-3(6)	
	cos, 1	61(3)	-1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.58. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SmTe_3 at 400 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	10(1)	11(1)	8(1)	1(1)	0	0
Te[1]	9(1)	10(1)	8(1)	-2(1)	0	0
Te[2]	15(1)	15(1)	12(1)	10(1)	0	0
Te[3]	14(1)	15(1)	12(1)	1(1)	0	0

Table 3.59. Bond lengths distributions [$\text{\AA}$] for SmTe_3 at 400 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm - Te[1]	3.2321(15)	3.215(3)	3.249(3)
Sm - Te[1] x 2	3.191(2)	3.182(2)	3.198(2)
Sm - Te[1] x 2	3.195(2)	3.186(2)	3.205(2)
Sm - Te[2] x 2	3.3349(19)	3.3210(19)	3.3487(19)
Sm - Te[3]	3.323(2)	3.320(3)	3.326(3)
Sm - Te[3]	3.339(2)	3.318(3)	3.360(3)
Te[2] - Te[3] x 2	3.052(3)	3.012(3)	3.093(3)
Te[2] - Te[3] x 2	3.073(3)	3.032(3)	3.113(3)

Table 3.60. Bond angles distributions [°] for SmTe₃ at 400 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Sm - Te[1] x 8	73.58(4)	73.38(4)	73.77(4)
Te[1] - Sm - Te[2] x 2	139.46(6)	139.14(7)	139.80(7)
Te[1] - Sm - Te[3]	139.72(5)	139.49(6)	139.95(6)
Te[1] - Sm - Te[3]	139.27(5)	139.23(6)	139.31(6)
Te[1] - Sm - Te[1] x 8	85.57(6)	85.53(6)	85.61(6)
Te[1] - Sm - Te[1] x 4	147.09(5)	146.60(6)	147.58(6)
Te[1] - Sm - Te[2] x 4	76.91(6)	76.21(6)	77.62(6)
Te[1] - Sm - Te[2] x 4	131.02(6)	130.11(6)	131.95(6)
Te[1] - Sm - Te[3] x 4	77.16(5)	77.05(5)	77.28(5)
Te[1] - Sm - Te[3] x 4	131.00(6)	130.69(7)	131.32(7)
Te[2] - Sm - Te[2] x 2	81.06(5)	80.74(6)	81.38(6)
Te[2] - Sm - Te[3] x 4	54.56(6)	53.68(6)	55.47(6)
Te[3] - Sm - Te[3] x 2	81.00(5)	80.74(7)	81.27(7)
Sm - Te[1] - Sm x 8	106.39(5)	106.32(6)	106.47(6)
Sm - Te[1] - Sm x 8	85.41(6)	84.97(7)	85.83(7)
Sm - Te[1] - Sm x 4	147.09(5)	146.78(7)	147.40(7)
Sm - Te[2] - Sm x 2	81.06(5)	81.00(6)	81.11(6)
Sm - Te[2] - Te[3] x 4	62.52(5)	62.34(4)	62.69(4)
Sm - Te[2] - Te[3] x 4	117.48(8)	116.54(9)	118.41(9)
Te[3] - Te[2] - Te[3] x 2	90.49(10)	89.10(10)	91.89(11)
Te[3] - Te[2] - Te[3] x 6	89.89(8)	89.86(7)	89.94(9)
Te[3] - Te[2] - Te[3] x 4	179.07(11)	178.20(10)	180
Sm - Te[3] - Sm x 2	81.00(3)	80.74(6)	81.27(6)
Sm - Te[3] - Te[2] x 2	62.52(5)	62.17(5)	62.87(6)
Sm - Te[3] - Te[2] x 4	117.33(6)	117.10(6)	117.56(6)
Sm - Te[3] - Te[2] x 2	62.91(5)	62.19(5)	63.63(5)
Te[2] - Te[3] - Te[2] x 6	89.73(10)	88.45(10)	91.01(10)
Te[2] - Te[3] - Te[2] x 4	179.14(10)	178.32(10)	180
Te[2] - Te[3] - Te[2] x 2	90.49(10)	89.18(10)	91.80(10)

Table 3.61. Crystal data and structure refinement for SmTe₃ at 500 K.

Empirical formula	SmTe ₃
Formula weight	533.2
Temperature	500.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 4.3343(13) Å, α = 90° b = 25.674(10) Å, β = 90° c = 4.3470(15) Å, γ = 90°
Volume	483.7(3) Å ³
Z	4
Density (calculated)	7.318 g/cm ³
Absorption coefficient	29.639 mm ⁻¹
F(000)	872
Crystal size	0.17 x 0.11 x 0.01 mm ³
Theta range for data collection	4.77 to 29.15°
Index ranges	-5 ≤ h ≤ 5, -21 ≤ k ≤ 34, -5 ≤ l ≤ 5
Reflections collected	1043
Independent reflections	374 [R _{int} = 0.0423]
Completeness to θ = 29.15°	91%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	374 / 0 / 18
Goodness-of-fit on F ²	1.55
Final R indices [I > 2σ(I)]	R _{obs} = 0.0269, wR _{obs} = 0.0698
R indices (all data)	R _{all} = 0.0281, wR _{all} = 0.0701
Extinction coefficient	0.097(9)
Largest diff. peak and hole	1.24 and -1.56 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w = 1/(σ ² (I) + 0.0016I ²)	

Table 3.62. Atomic coordinates (x10⁴) and equivalent isotropic displacement parameters (Å²x10³) for SmTe₃ at 500 K with e.s.d.'s in parentheses.

Label	x	y	z	Occupancy	U _{eq} [*]
Sm	0	1696(1)	2549	1	13(1)
Te[1]	0	2953(1)	2549	1	12(1)
Te[2]	0	4290(1)	7549	1	18(1)

Table 3.62. (Cont'd) Atomic coordinates (x104) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SmTe_3 at 500 K with e.s.d.'s in parentheses.

Te[3]	0	709(1)	7549	1	18(1)
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* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.63. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SmTe_3 at 500 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm	11(1)	15(1)	13(1)	0	0	0
Te[1]	10(1)	14(1)	12(1)	0	0	0
Te[2]	17(1)	19(1)	18(1)	0	0	0
Te[3]	16(1)	19(1)	18(1)	0	0	0

Table 3.64. Bond distances [$\text{\AA}$] for SmTe_3 at 500 K with e.s.d.'s in parentheses.

Label	Distances	Label	Distances
Sm - Te[1]	3.2281(8)	Sm - Te[2] x 2	3.3322(7)
Sm - Te[1] x 4	3.1988(2)	Sm - Te[3] x 2	3.3376(7)

Table 3.65. Bond angles [$^\circ$] for SmTe_3 at 500 K with e.s.d.'s in parentheses.

Label	Angles	Label	Angles
Te[1] - Sm - Te[1] x 8	73.644(14)	Sm - Te[1] - Sm x 4	85.297(7)
Te[1] - Sm - Te[2] x 2	139.430(10)	Sm - Te[1] - Sm x 4	147.29(2)
Te[1] - Sm - Te[1] x 4	85.607(6)	Sm - Te[2] - Te[3] x 4	62.691(13)
Te[1] - Sm - Te[1] x 4	85.297(6)	Sm - Te[2] - Te[3] x 4	117.36(2)
Te[1] - Sm - Te[1] x 4	147.29(2)	Te[3] - Te[2] - Te[3] x 4	90.168
Te[1] - Sm - Te[2] x 4	76.896(12)	Te[3] - Te[2] - Te[3] x 4	89.832
Te[1] - Sm - Te[2] x 4	130.884(13)	Te[3] - Te[2] - Te[3] x 4	180
Te[1] - Sm - Te[3] x 4	76.774(12)	Sm - Te[3] - Sm x 2	81.267(18)
Te[1] - Sm - Te[3] x 4	131.010(13)	Sm - Te[3] - Te[2] x 4	62.511(14)
Te[2] - Sm - Te[2] x 2	81.140(16)	Sm - Te[3] - Te[2] x 4	117.43(2)
Te[2] - Sm - Te[3] x 4	54.798(10)	Te[2] - Te[3] - Te[2] x 4	90.168
Te[3] - Sm - Te[3] x 2	81.267(16)	Te[2] - Te[3] - Te[2] x 4	89.832
Sm - Te[1] - Sm x 8	106.356(14)	Te[2] - Te[3] - Te[2] x 4	180

Table 3.66. Crystal data and structure refinement for GdTe₃ at 100 K.

Empirical formula	GdTe ₃
Formula weight	540
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2954(4) Å, α = 90° b = 25.443(2) Å, β = 90° c = 4.3097(5) Å, γ = 90°
q-vector(1)	0.2884(3)c*
Volume	470.99(8) Å ³
Z	4
Density (calculated)	7.6135 g/cm ³
Absorption coefficient	32.065 mm ⁻¹
F(000)	880
Crystal size	0.11 x 0.10 x 0.01 mm ³
Theta range for data collection	2.10 to 29.11°
Index ranges	-5<=h<=5, -34<=k<=34, -6<=l<=6, -1<=m<=1
Reflections collected	6775 (2206 main + 4569 satellites)
Independent reflections	1906 (667 main + 1239 satellites) [R _{int} = 0.0963]
Completeness to θ = 29.11°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1906 / 0 / 39
Goodness-of-fit on F ²	1.68
Final R indices [I>2σ(I)]	R _{obs} = 0.0438, wR _{obs} = 0.1102
R indices (all data)	R _{all} = 0.0618, wR _{all} = 0.1147
Final R main indices [I>2σ(I)]	R _{obs} = 0.0407, wR _{obs} = 0.1087
R main indices (all data)	R _{all} = 0.0409, wR _{all} = 0.1089
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.0695, wR _{obs} = 0.1180
R 1 st order satellites (all data)	R _{all} = 0.1897, wR _{all} = 0.1416
Extinction coefficient	0.00031(5)
T _{min} and T _{max} coefficients	0.0590 and 0.8188
Largest diff. peak and hole	3.14 and -3.36 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.67. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for GdTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Gd	0	9449	1694(1)	2549	5(1)
	sin, 1	0	0	18(4)	
	cos, 1	58(1)	5(1)	0	
Te[1]	0	9397(5)	2948(1)	2549	5(1)
	sin, 1	0	0	6(5)	
	cos, 1	7(1)	0(1)	0	
Te[2]	0	9320(5)	709(1)	7549	6(1)
	sin, 1	0	0	-3(5)	
	cos, 1	-217(3)	-1(1)	0	
Te[3]	0	4396(5)	710(1)	2549	6(1)
	sin, 1	0	0	-12(6)	
	cos, 1	191(3)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.68. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for GdTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd	5(1)	10(1)	1(1)	1(1)	0	0
Te[1]	4(1)	10(1)	1(1)	0(1)	0	0
Te[2]	6(1)	12(1)	1(1)	2(1)	0	0
Te[3]	6(1)	12(1)	2(1)	2(1)	0	0

Table 3.69. Bond lengths distributions [$\text{\AA}$] for GdTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Gd - Te[1]	3.1901(18)	3.176(3)	3.205(3)
Gd - Te[1] x 4	3.1765(19)	3.1628(17)	3.1901(17)
Gd - Te[2] x 2	3.3068(19)	3.293(2)	3.322(2)
Gd - Te[3] x 2	3.300(2)	3.271(3)	3.329(3)
Te[2] - Te[3] x 2	3.020(3)	2.909(2)	3.134(3)
Te[2] - Te[3] x 2	3.067(3)	2.958(2)	3.178(3)

Table 3.70. Bond angles distributions [°] for GdTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Gd - Te[1] x 8	73.34(4)	73.27(4)	73.42(4)
Te[1] - Gd - Te[2] x 2	139.28(5)	139.06(5)	139.56(5)
Te[1] - Gd - Te[3] x 2	139.34(5)	138.86(5)	139.81(6)
Te[1] - Gd - Te[1] x 8	85.43(5)	85.09(5)	85.79(5)
Te[1] - Gd - Te[1] x 4	146.71(5)	146.26(7)	147.15(7)
Te[1] - Gd - Te[2] x 2	76.57(5)	75.18(6)	77.99(6)
Te[1] - Gd - Te[2] x 2	130.71(5)	128.59(5)	132.85(5)
Te[1] - Gd - Te[3] x 4	77.10(5)	76.85(4)	77.34(4)
Te[1] - Gd - Te[3] x 4	131.13(6)	130.79(6)	131.45(6)
Te[1] - Gd - Te[2] x 2	77.40(5)	76.23(6)	78.55(6)
Te[1] - Gd - Te[2] x 2	131.82(5)	130.07(5)	133.53(5)
Te[2] - Gd - Te[2] x 2	81.36(5)	80.93(6)	81.74(6)
Te[2] - Gd - Te[3] x 2	54.39(6)	52.33(6)	56.52(6)
Te[2] - Gd - Te[3] x 2	55.34(6)	53.67(6)	57.00(6)
Te[3] - Gd - Te[3] x 2	81.23(5)	80.99(7)	81.46(7)
Gd - Te[1] - Gd x 8	106.67(5)	106.49(6)	106.85(6)
Gd - Te[1] - Gd x 8	85.51(6)	85.00(6)	86.01(6)
Gd - Te[1] - Gd x 4	146.71(6)	146.39(7)	147.03(7)
Gd - Te[2] - Gd x 2	81.34(5)	81.18(7)	81.45(7)
Gd - Te[2] - Te[3] x 2	62.67(4)	62.19(4)	63.12(4)
Gd - Te[2] - Te[3] x 2	118.14(7)	115.78(8)	120.46(9)
Gd - Te[2] - Te[3] x 2	62.18(4)	61.58(4)	62.78(4)
Gd - Te[2] - Te[3] x 2	116.75(7)	114.11(8)	119.38(9)
Te[3] - Te[2] - Te[3] x 2	91.15(9)	87.41(8)	94.99(9)
Te[3] - Te[2] - Te[3] x 6	89.73(7)	89.63(6)	89.88(8)
Te[3] - Te[2] - Te[3] x 4	177.50(9)	175.28(9)	180
Gd - Te[3] - Gd x 2	81.23(4)	80.99(7)	81.46(7)
Gd - Te[3] - Te[2] x 2	62.48(5)	61.21(5)	63.81(5)
Gd - Te[3] - Te[2] x 4	117.12(6)	116.50(6)	117.68(6)
Gd - Te[3] - Te[2] x 2	62.94(5)	61.21(5)	64.67(5)
Te[2] - Te[3] - Te[2] x 6	89.37(8)	85.75(8)	93.14(9)
Te[2] - Te[3] - Te[2] x 4	177.54(9)	175.40(9)	180
Te[2] - Te[3] - Te[2] x 2	91.18(8)	87.44(8)	94.94(9)

Table 3.71. Crystal data and structure refinement for TbTe₃ at 100 K.

Empirical formula	TbTe ₃
Formula weight	541.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2801(7) Å, α = 90° b = 25.307(5) Å, β = 90° c = 4.3052(9) Å, γ = 90°
q-vector(1)	0.2912(5)c*
Volume	466.32(16) Å ³
Z	4
Density (calculated)	7.714 g/cm ³
Absorption coefficient	33.429 mm ⁻¹
F(000)	884
Crystal size	0.28 x 0.20 x 0.03 mm ³
Theta range for data collection	2.11 to 29.22°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6506 (2079 main + 4427 satellites)
Independent reflections	1871 (651 main + 1220 satellites) [R _{int} = 0.0311]
Completeness to θ = 29.22°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1871 / 0 / 38
Goodness-of-fit on F ²	1.65
Final R indices [I > 2σ(I)]	R _{obs} = 0.0270, wR _{obs} = 0.1045
R indices (all data)	R _{all} = 0.0412, wR _{all} = 0.1084
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0248, wR _{obs} = 0.1086
R main indices (all data)	R _{all} = 0.0248, wR _{all} = 0.1086
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0471, wR _{obs} = 0.0821
R 1 st order satellites (all data)	R _{all} = 0.1516, wR _{all} = 0.1076
Extinction coefficient	0.00066(5)
T _{min} and T _{max} coefficients	0.0286 and 0.3198
Largest diff. peak and hole	2.56 and -2.74 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.72. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for TbTe₃ at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Tb	0	9249	1696(1)	2549	2(1)
	sin, 1	0	0	-1(3)	
	cos, 1	48(1)	1(1)	0	
Te[1]	0	9161(3)	2947(1)	2549	2(1)
	sin, 1	0	0	-2(3)	
	cos, 1	5(1)	0(1)	0	
Te[2]	0	9250(3)	712(1)	7549	3(1)
	sin, 1	0	0	-5(4)	
	cos, 1	-179(2)	7(1)	0	
Te[3]	0	9234(4)	4286(1)	7549	4(1)
	sin, 1	0	0	22(4)	
	cos, 1	156(2)	-1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.73. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TbTe₃ at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tb	2(1)	4(1)	2(1)	1(1)	0	0
Te[1]	2(1)	4(1)	1(1)	0(1)	0	0
Te[2]	3(1)	6(1)	1(1)	-5(1)	0	0
Te[3]	3(1)	6(1)	3(1)	-3(1)	0	0

Table 3.74. Bond lengths distributions [$\text{\AA}$] for TbTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Tb - Te[1]	3.1638(12)	3.162(2)	3.166(2)
Tb - Te[1] x 2	3.1785(12)	3.1661(12)	3.1906(12)
Tb - Te[1] x 2	3.1555(12)	3.1417(12)	3.1695(12)
Tb - Te[2] x 2	3.2928(12)	3.2794(13)	3.3076(13)
Tb - Te[3]	3.2711(14)	3.2415(19)	3.3014(19)
Tb - Te[3]	3.2908(14)	3.2606(19)	3.3206(19)
Te[2] - Te[3] x 2	3.0404(18)	2.9533(16)	3.1301(17)
Te[2] - Te[3] x 2	3.0317(18)	2.9387(16)	3.1251(17)

Table 3.75. Bond angles distributions [°] for TbTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Tb - Te[1] x 8	73.27(3)	73.14(3)	73.41(3)
Te[1] - Tb - Te[2] x 2	139.15(3)	138.94(4)	139.35(5)
Te[1] - Tb - Te[3] x 2	139.18(3)	138.90(4)	139.46(4)
Te[1] - Tb - Te[1] x 2	85.26(3)	84.83(3)	85.69(3)
Te[1] - Tb - Te[1] x 4	85.02(4)	85.00(3)	85.05(3)
Te[1] - Tb - Te[1] x 4	146.85(3)	146.79(4)	146.91(4)
Te[1] - Tb - Te[2] x 2	77.08(3)	75.88(3)	78.30(4)
Te[1] - Tb - Te[2] x 2	131.46(3)	129.93(3)	133.00(3)
Te[1] - Tb - Te[3] x 4	77.01(3)	76.74(4)	77.28(4)
Te[1] - Tb - Te[3] x 2	131.24(4)	130.87(4)	131.60(4)
Te[1] - Tb - Te[1] x 2	86.03(3)	85.58(3)	86.47(3)
Te[1] - Tb - Te[2] x 2	76.49(3)	75.58(3)	77.38(4)
Te[1] - Tb - Te[2] x 2	131.17(4)	129.52(3)	132.81(3)
Te[1] - Tb - Te[3] x 2	130.90(4)	130.48(4)	131.31(4)
Te[2] - Tb - Te[2] x 2	81.67(3)	81.45(4)	81.83(4)
Te[2] - Tb - Te[3] x 2	54.85(4)	53.11(4)	56.57(4)
Te[3] - Tb - Te[3] x 2	81.42(4)	81.41(5)	81.43(3)
Tb - Te[1] - Tb x 8	106.85(3)	106.59(4)	107.10(4)
Tb - Te[1] - Tb x 2	86.03(4)	85.79(4)	86.26(4)
Tb - Te[1] - Tb x 4	146.85(4)	146.73(2)	146.98(2)
Tb - Te[1] - Tb x 2	85.26(4)	85.03(4)	85.49(4)
Tb - Te[2] - Tb x 2	81.65(3)	81.22(4)	82.04(4)
Tb - Te[2] - Te[3] x 2	117.22(4)	114.72(5)	119.72(5)
Tb - Te[2] - Te[3] x 2	117.89(4)	116.27(5)	119.46(5)
Te[3] - Te[2] - Te[3] x 4	90.21(6)	86.91(5)	93.56(6)
Te[3] - Te[2] - Te[3] x 4	89.61(5)	89.36(4)	89.94(5)
Te[3] - Te[2] - Te[3] x 4	177.96(6)	176.57(6)	179.92(4)
Tb - Te[3] - Tb x 2	81.42(2)	81.41(4)	81.428(12)
Tb - Te[3] - Te[2] x 2	117.57(4)	116.53(3)	118.61(3)
Tb - Te[3] - Te[2] x 2	117.26(4)	116.96(4)	117.53(4)
Te[2] - Te[3] - Te[2] x 4	90.56(6)	87.51(6)	93.68(6)
Te[2] - Te[3] - Te[2] x 4	89.61(4)	89.36(5)	89.94(5)
Te[2] - Te[3] - Te[2] x 4	178.05(6)	176.74(6)	179.87(4)

Table 3.76. Crystal data and structure refinement for DyTe₃ at 100 K.

Empirical formula	DyTe ₃
Formula weight	545.3
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2831(6) Å, α = 90° b = 25.250(5) Å, β = 90° c = 4.2887(6) Å, γ = 90°
q-vector(1)	0.2926(3)c*
Volume	463.81(13) Å ³
Z	4
Density (calculated)	7.807 g/cm ³
Absorption coefficient	34.443 mm ⁻¹
F(000)	888
Crystal size	0.23 x 0.15 x 0.03 mm ³
Theta range for data collection	2.12 to 29.01°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	5891 (1567 main + 4324 satellites)
Independent reflections	1819 (577 main + 1242 satellites) [R _{int} = 0.0397]
Completeness to θ = 29.01°	95 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1819 / 0 / 37
Goodness-of-fit on F ²	1.92
Final R indices [I > 2σ(I)]	R _{obs} = 0.0360, wR _{obs} = 0.1202
R indices (all data)	R _{all} = 0.0522, wR _{all} = 0.1273
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0278, wR _{obs} = 0.1145
R main indices (all data)	R _{all} = 0.0278, wR _{all} = 0.1145
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0856, wR _{obs} = 0.1389
R 1 st order satellites (all data)	R _{all} = 0.1706, wR _{all} = 0.1652
Extinction coefficient	0.00164(14)
T _{min} and T _{max} coefficients	0.0234 and 0.3079
Largest diff. peak and hole	3.33 and -4.82 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.77. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for DyTe₃ at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U _{eq} *
Dy	0	9449	1698(1)	2549	2(1)
	sin, 1	0	0	4(3)	
	cos, 1	46(1)	3(1)	0	
Te[1]	0	9374(3)	2946(1)	2549	1(1)
	sin, 1	0	0	0(3)	
	cos, 1	4(1)	-1(1)	0	
Te[2]	0	9439(4)	714(1)	7549	3(1)
	sin, 1	0	0	29(3)	
	cos, 1	-164(2)	-2(1)	0	
Te[3]	0	4420(4)	715(1)	2549	3(1)
	sin, 1	0	0	-2(3)	
	cos, 1	147(2)	0(1)	0	

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.78. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DyTe₃ at 100 K with e.s.d.'s in parentheses.

Label	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Dy	3(1)	1(1)	2(1)	1(1)	0	0
Te[1]	2(1)	2(1)	1(1)	-1(1)	0	0
Te[2]	3(1)	4(1)	1(1)	-5(1)	0	0
Te[3]	4(1)	3(1)	3(1)	2(1)	0	0

Table 3.79. Bond lengths distributions [$\text{\AA}$] for DyTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Dy - Te[1] x 3	3.1513(12)	3.142(2)	3.160(2)
Dy - Te[1] x 2	3.1686(12)	3.1577(12)	3.1794(12)
Dy - Te[2] x 2	3.2818(13)	3.2674(13)	3.2960(13)
Dy - Te[3]	3.2718(14)	3.2497(19)	3.2945(19)
Dy - Te[3]	3.2835(14)	3.2496(19)	3.3170(19)
Te[2] - Te[3] x 2	3.0366(18)	2.9560(16)	3.1192(17)
Te[2] - Te[3] x 2	3.0260(18)	2.9379(16)	3.1139(17)

Table 3.80. Bond angles distributions [°] for DyTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Dy - Te[1] x 8	73.38(3)	73.31(3)	73.45(3)
Te[1] - Dy - Te[2] x 2	139.18(3)	139.09(4)	139.28(4)
Te[1] - Dy - Te[3] x 2	139.12(3)	138.79(4)	139.45(4)
Te[1] - Dy - Te[1] x 6	85.18(3)	84.82(3)	85.55(3)
Te[1] - Dy - Te[1] x 4	146.97(4)	146.75(5)	147.18(5)
Te[1] - Dy - Te[2] x 2	77.04(3)	76.04(3)	78.05(3)
Te[1] - Dy - Te[2] x 2	131.32(4)	129.73(3)	132.93(3)
Te[1] - Dy - Te[3] x 4	76.83(3)	76.63(3)	77.04(3)
Te[1] - Dy - Te[3] x 4	131.24(4)	131.02(4)	131.47(4)
Te[1] - Dy - Te[1] x 2	85.69(3)	85.21(3)	86.17(3)
Te[1] - Dy - Te[2] x 2	76.58(3)	75.59(4)	77.55(4)
Te[1] - Dy - Te[2] x 2	131.04(4)	129.66(4)	132.40(4)
Te[2] - Dy - Te[2] x 2	81.62(3)	81.57(4)	81.64(3)
Te[2] - Dy - Te[3] x 2	55.20(4)	53.67(4)	56.77(4)
Te[2] - Dy - Te[3] x 2	54.89(4)	53.54(4)	56.23(4)
Te[3] - Dy - Te[3] x 2	81.59(4)	81.42(5)	81.76(5)
Dy - Te[1] - Dy x 8	106.70(3)	106.48(4)	106.91(4)
Dy - Te[1] - Dy x 8	85.29(3)	85.21(4)	85.38(4)
Dy - Te[1] - Dy x 4	146.97(4)	146.82(3)	147.12(3)
Dy - Te[2] - Dy x 2	81.60(3)	81.41(5)	81.76(5)
Dy - Te[2] - Te[3] x 2	62.22(3)	61.77(3)	62.69(3)
Dy - Te[2] - Te[3] x 2	117.21(5)	115.43(6)	118.96(6)
Dy - Te[2] - Te[3] x 2	62.58(3)	62.16(3)	62.98(3)
Dy - Te[2] - Te[3] x 2	117.79(5)	115.75(6)	119.84(6)
Te[3] - Te[2] - Te[3] x 6	89.91(6)	87.06(5)	92.80(6)
Te[3] - Te[2] - Te[3] x 4	178.13(6)	176.86(6)	179.91(4)
Te[3] - Te[2] - Te[3] x 2	90.33(6)	87.43(6)	93.30(6)
Dy - Te[3] - Dy x 2	81.59(2)	81.42(4)	81.76(4)
Dy - Te[3] - Te[2] x 4	62.53(3)	61.58(3)	63.52(3)
Dy - Te[3] - Te[2] x 4	117.63(4)	117.11(4)	118.13(4)
Te[2] - Te[3] - Te[2] x 2	90.31(6)	87.80(6)	92.93(6)
Te[2] - Te[3] - Te[2] x 6	89.88(4)	89.56(4)	90.27(4)
Te[2] - Te[3] - Te[2] x 4	178.18(6)	176.94(6)	179.91(4)

Table 3.81. Crystal data and structure refinement for HoTe₃ at 100 K.

Empirical formula	HoTe ₃
Formula weight	547.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2723(8) Å, α = 90° b = 25.203(4) Å, β = 90° c = 4.2855(6) Å, γ = 90°
q-vector(1)	0.2935(3)c*
Volume	461.45(13) Å ³
Z	4
Density (calculated)	7.882 g/cm ³
Absorption coefficient	35.61 mm ⁻¹
F(000)	892
Crystal size	0.24 x 0.20 x 0.04 mm ³
Theta range for data collection	2.13 to 29.31°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -5 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6536 (2103 main + 4433 satellites)
Independent reflections	1932 (683 main + 1249 satellites) [R _{int} = 0.0391]
Completeness to θ = 29.31°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1932 / 0 / 38
Goodness-of-fit on F ²	1.58
Final R indices [I > 2σ(I)]	R _{obs} = 0.0353, wR _{obs} = 0.1027
R indices (all data)	R _{all} = 0.0501, wR _{all} = 0.1063
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0327, wR _{obs} = 0.1004
R main indices (all data)	R _{all} = 0.0327, wR _{all} = 0.1004
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0684, wR _{obs} = 0.1159
R 1 st order satellites (all data)	R _{all} = 0.1976, wR _{all} = 0.1365
Extinction coefficient	0.00025(3)
T _{min} and T _{max} coefficients	0.0095 and 0.2425
Largest diff. peak and hole	3.47 and -3.36 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.82. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for HoTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Ho	0	9249	1699(1)	2549	9(1)
	sin, 1	0	0	2(3)	
	cos, 1	43(1)	4(1)	0	
Te[1]	0	9168(4)	2945(1)	2549	9(1)
	sin, 1	0	0	-8(4)	
	cos, 1	5(1)	-1(1)	0	
Te[2]	0	9232(4)	715(1)	7549	10(1)
	sin, 1	0	0	17(4)	
	cos, 1	-147(1)	1(1)	0	
Te[3]	0	9221(5)	4284(1)	7549	10(1)
	sin, 1	0	0	4(4)	
	cos, 1	131(1)	0(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.83. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for HoTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ho	9(1)	10(1)	8(1)	2(1)	0	0
Te[1]	9(1)	10(1)	8(1)	-1(1)	0	0
Te[2]	10(1)	12(1)	8(1)	-4(1)	0	0
Te[3]	10(1)	11(1)	9(1)	0(1)	0	0

Table 3.84. Bond lengths distributions [$\text{\AA}$] for HoTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ho - Te[1]	3.1404(13)	3.129(2)	3.152(2)
Ho - Te[1] x 2	3.1651(15)	3.1576(13)	3.1725(13)
Ho - Te[1] x 2	3.1465(15)	3.1304(15)	3.1628(15)
Ho - Te[2] x 2	3.2781(15)	3.2674(14)	3.2880(14)
Ho - Te[3]	3.2659(17)	3.249(2)	3.283(2)
Ho - Te[3]	3.2779(17)	3.246(2)	3.310(2)
Te[2] - Te[3] x 2	3.029(2)	2.9574(19)	3.103(2)
Te[2] - Te[3] x 2	3.023(2)	2.9453(19)	3.101(2)

Table 3.85. Bond angles distributions [°] for HoTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Ho - Te[1] x 4	73.36(3)	73.27(3)	73.45(3)
Te[1] - Ho - Te[1] x 4	73.61(3)	73.33(3)	73.90(3)
Te[1] - Ho - Te[2] x 2	139.16(4)	139.10(6)	139.24(6)
Te[1] - Ho - Te[3] x 2	139.11(4)	138.79(4)	139.43(4)
Te[1] - Ho - Te[1] x 6	85.22(4)	84.84(4)	85.61(4)
Te[1] - Ho - Te[1] x 4	146.97(4)	146.71(5)	147.22(5)
Te[1] - Ho - Te[2] x 2	76.97(4)	76.04(4)	77.92(4)
Te[1] - Ho - Te[2] x 4	131.28(4)	129.82(4)	132.76(4)
Te[1] - Ho - Te[3] x 4	76.86(4)	76.70(4)	77.03(4)
Te[1] - Ho - Te[3] x 4	131.21(5)	131.03(4)	131.38(4)
Te[1] - Ho - Te[1] x 2	85.84(4)	85.45(4)	86.23(4)
Te[1] - Ho - Te[2] x 2	76.57(4)	75.74(4)	77.39(4)
Te[2] - Ho - Te[2] x 2	81.65(4)	81.62(4)	81.67(3)
Te[2] - Ho - Te[3] x 4	55.14(4)	53.81(4)	56.51(4)
Te[3] - Ho - Te[3] x 2	81.52(4)	81.29(5)	81.74(5)
Ho - Te[1] - Ho x 4	106.74(4)	106.56(4)	106.91(4)
Ho - Te[1] - Ho x 4	106.28(4)	105.96(4)	106.61(4)
Ho - Te[1] - Ho x 2	85.84(4)	85.58(5)	86.09(5)
Ho - Te[1] - Ho x 6	85.20(3)	85.04(4)	85.37(4)
Ho - Te[1] - Ho x 4	146.97(4)	146.81(4)	147.13(4)
Ho - Te[2] - Ho x 2	81.64(4)	81.59(5)	81.67(3)
Ho - Te[2] - Te[3] x 2	62.22(3)	61.78(3)	62.65(3)
Ho - Te[2] - Te[3] x 2	117.32(5)	115.56(6)	119.07(6)
Ho - Te[2] - Te[3] x 2	62.53(3)	62.22(3)	62.83(3)
Ho - Te[2] - Te[3] x 2	117.77(5)	116.11(6)	119.41(6)
Te[3] - Te[2] - Te[3] x 8	90.09(6)	87.48(6)	92.73(7)
Te[3] - Te[2] - Te[3] x 4	178.35(7)	177.27(7)	180
Ho - Te[3] - Ho x 2	81.52(3)	81.29(5)	81.74(5)
Ho - Te[3] - Te[2] x 4	62.55(4)	61.59(4)	63.55(4)
Ho - Te[3] - Te[2] x 4	117.56(4)	116.93(4)	118.17(4)
Te[2] - Te[3] - Te[2] x 4	90.34(7)	87.99(7)	92.74(7)
Te[2] - Te[3] - Te[2] x 4	89.79(5)	89.62(4)	89.97(5)
Te[2] - Te[3] - Te[2] x 4	178.40(7)	177.34(7)	179.92(4)

Table 3.86. Crystal data and structure refinement for ErTe₃ at 100 K.

Empirical formula	ErTe ₃
Formula weight	550.1
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2641(8) Å, α = 90° b = 25.164(6) Å, β = 90° c = 4.2791(8) Å, γ = 90°
q-vector(1)	0.2992(4)c*
Volume	459.15(17) Å ³
Z	4
Density (calculated)	7.955 g/cm ³
Absorption coefficient	36.874 mm ⁻¹
F(000)	896
Crystal size	0.50 x 0.32 x 0.03 mm ³
Theta range for data collection	3.23 to 31.78°
Index ranges	-6<=h<=6, -36<=k<=36, -6<=l<=6, -1<=m<=1
Reflections collected	7636 (2391 main + 5245 satellites)
Independent reflections	2342 (811 main + 1531 satellites) [R _{int} = 0.0402]
Completeness to θ = 31.78°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2342 / 0 / 37
Goodness-of-fit on F ²	1.49
Final R indices [I>2σ(I)]	R _{obs} = 0.0307, wR _{obs} = 0.1018
R indices (all data)	R _{all} = 0.0628, wR _{all} = 0.1101
Final R main indices [I>2σ(I)]	R _{obs} = 0.0255, wR _{obs} = 0.0995
R main indices (all data)	R _{all} = 0.0262, wR _{all} = 0.1001
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.0957, wR _{obs} = 0.1248
R 1 st order satellites (all data)	R _{all} = 0.3169, wR _{all} = 0.1888
Extinction coefficient	0.00045(5)
T _{min} and T _{max} coefficients	0.0215 and 0.6350
Largest diff. peak and hole	3.43 and -3.74 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.87. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for ErTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Er	0	9000	1700(1)	2549	4(1)
	sin, 1	0	0	-17(5)	
	cos, 1	40(1)	6(1)	0	
Te[1]	0	8970(3)	2944(1)	2549	4(1)
	sin, 1	0	0	7(7)	
	cos, 1	5(1)	1(1)	0	
Te[2]	0	9025(3)	717(1)	7549	5(1)
	sin, 1	0	0	15(8)	
	cos, 1	-136(2)	1(1)	0	
Te[3]	0	9031(4)	4283(1)	7549	5(1)
	sin, 1	0	0	-3(7)	
	cos, 1	119(2)	1(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.88. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ErTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Er	4(1)	5(1)	4(1)	-1(1)	0	0
Te[1]	2(1)	5(1)	4(1)	1(1)	0	0
Te[2]	4(1)	7(1)	5(1)	0(1)	0	0
Te[3]	4(1)	6(1)	5(1)	3(1)	0	0

Table 3.89. Bond lengths distributions [$\text{\AA}$] for ErTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Er - Te[1]	3.1293(14)	3.117(3)	3.142(3)
Er - Te[1] x 2	3.1591(18)	3.148(2)	3.170(2)
Er - Te[1] x 2	3.1415(18)	3.1270(12)	3.1563(13)
Er - Te[2] x 2	3.272(2)	3.255(2)	3.288(2)
Er - Te[3]	3.2568(16)	3.247(2)	3.267(2)
Er - Te[3]	3.2744(16)	3.240(2)	3.309(2)
Te[2] - Te[3] x 4	3.019(3)	2.9522(18)	3.0865(19)

Table 3.90. Bond angles distributions [°] for ErTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Er - Te[1] x 6	73.38(4)	73.18(3)	73.57(3)
Te[1] - Er - Te[1] x 2	73.62(4)	73.17(3)	74.06(3)
Te[1] - Er - Te[2] x 2	139.15(7)	138.82(9)	139.47(10)
Te[1] - Er - Te[3] x 2	139.18(4)	138.82(4)	139.55(4)
Te[1] - Er - Te[1] x 6	85.26(5)	85.12(5)	85.40(5)
Te[1] - Er - Te[1] x 4	146.99(4)	146.41(5)	147.56(5)
Te[1] - Er - Te[2] x 2	76.90(5)	76.02(5)	77.80(5)
Te[1] - Er - Te[2] x 4	131.25(4)	129.83(4)	132.69(4)
Te[1] - Er - Te[3] x 4	76.91(5)	76.83(5)	76.99(5)
Te[1] - Er - Te[3] x 4	131.22(7)	131.06(8)	131.38(8)
Te[1] - Er - Te[1] x 2	85.85(5)	85.27(5)	86.43(5)
Te[1] - Er - Te[2] x 2	76.59(5)	75.77(6)	77.39(6)
Te[2] - Er - Te[2] x 2	81.69(6)	81.50(6)	81.85(6)
Te[2] - Er - Te[3] x 4	55.07(6)	53.77(5)	56.42(5)
Te[3] - Er - Te[3] x 2	81.52(4)	81.15(5)	81.89(5)
Er - Te[1] - Er x 4	106.72(5)	106.40(6)	107.04(6)
Er - Te[1] - Er x 4	106.29(5)	105.72(4)	106.86(4)
Er - Te[1] - Er x 2	85.85(5)	85.71(5)	85.98(5)
Er - Te[1] - Er x 6	85.18(5)	84.95(4)	85.42(4)
Er - Te[1] - Er x 4	146.99(5)	146.64(7)	147.34(7)
Er - Te[2] - Er x 2	81.68(5)	81.35(6)	81.98(6)
Er - Te[2] - Te[3] x 2	62.20(4)	61.71(4)	62.69(4)
Er - Te[2] - Te[3] x 4	117.44(5)	115.93(7)	118.94(7)
Er - Te[2] - Te[3] x 2	62.53(4)	62.33(4)	62.73(4)
Te[3] - Te[2] - Te[3] x 4	90.31(7)	87.99(7)	92.66(7)
Te[3] - Te[2] - Te[3] x 4	89.77(7)	89.59(10)	90
Te[3] - Te[2] - Te[3] x 4	178.49(9)	177.55(7)	180
Er - Te[3] - Er x 2	81.52(3)	81.15(5)	81.89(5)
Er - Te[3] - Te[2] x 4	62.46(5)	61.59(4)	63.36(4)
Er - Te[3] - Te[2] x 4	117.54(6)	116.89(5)	118.17(5)
Te[2] - Te[3] - Te[2] x 8	90.15(8)	88.03(8)	92.32(8)
Te[2] - Te[3] - Te[2] x 4	178.55(9)	177.64(8)	180

Table 3.91. Crystal data and structure refinement for TmTe₃ at 100 K.

Empirical formula	TmTe ₃
Formula weight	551.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2617(6) Å, α = 90° b = 25.092(4) Å, β = 90° c = 4.2714(8) Å, γ = 90°
q-vector(1)	0.3026(4)c*
Volume	456.76(13) Å ³
Z	4
Density (calculated)	8.021 g/cm ³
Absorption coefficient	38.081 mm ⁻¹
F(000)	900
Crystal size	0.43 x 0.40 x 0.04 mm ³
Theta range for data collection	2.17 to 29.28°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	7724 (2478 main + 5246 satellites)
Independent reflections	1837 (643 main + 1194 satellites) [R _{int} = 0.0786]
Completeness to θ = 29.28°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1837 / 0 / 38
Goodness-of-fit on F ²	2.35
Final R indices [I > 2σ(I)]	R _{obs} = 0.0455, wR _{obs} = 0.1313
R indices (all data)	R _{all} = 0.0681, wR _{all} = 0.1712
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0433, wR _{obs} = 0.1314
R main indices (all data)	R _{all} = 0.0448, wR _{all} = 0.1704
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0903, wR _{obs} = 0.1280
R 1 st order satellites (all data)	R _{all} = 0.3036, wR _{all} = 0.1859
Extinction coefficient	0.00039(5)
T _{min} and T _{max} coefficients	0.0045 and 0.1643
Largest diff. peak and hole	4.24 and -5.04 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{\Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)]\}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.92. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for TmTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Tm	0	9000	1703(1)	2549	7(1)
	sin, 1	0	0	22(6)	
	cos, 1	35(2)	6(1)	0	
Te[1]	0	9085(6)	2942(1)	2549	6(1)
	sin, 1	0	0	-2(8)	
	cos, 1	2(3)	2(2)	0	
Te[2]	0	9019(6)	717(1)	7549	8(1)
	sin, 1	0	0	5(9)	
	cos, 1	-120(5)	1(2)	0	
Te[3]	0	8982(9)	4282(1)	7549	8(1)
	sin, 1	0	0	5(9)	
	cos, 1	111(5)	0(2)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.93. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TmTe_3 at 100 K with e.s.d.'s in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tm	6(1)	11(1)	6(1)	-2(1)	0	0
Te[1]	4(1)	10(1)	5(1)	0(1)	0	0
Te[2]	5(1)	13(1)	5(1)	-2(1)	0	0
Te[3]	6(1)	13(1)	6(1)	-4(1)	0	0

Table 3.94. Bond lengths distributions [$\text{\AA}$] for TmTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Tm - Te[1]	3.107(3)	3.096(5)	3.119(5)
Tm - Te[1] x 2	3.121(3)	3.114(2)	3.128(2)
Tm - Te[1] x 2	3.171(3)	3.154(3)	3.187(3)
Tm - Te[2] x 2	3.269(3)	3.258(3)	3.281(3)
Tm - Te[3]	3.268(3)	3.259(5)	3.278(5)
Tm - Te[3]	3.259(3)	3.226(5)	3.291(5)
Te[2] - Te[3] x 2	3.028(4)	2.968(4)	3.089(4)
Te[2] - Te[3] x 2	3.007(4)	2.944(4)	3.069(4)

Table 3.95. Bond angles distributions [°] for TmTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Tm - Te[1] x 4	73.88(6)	73.70(6)	74.06(6)
Te[1] - Tm - Te[1] x 4	73.20(6)	72.77(6)	73.63(6)
Te[1] - Tm - Te[2] x 2	139.19(8)	138.85(9)	139.55(9)
Te[1] - Tm - Te[3] x 2	139.80(7)	139.45(8)	140.15(8)
Te[1] - Tm - Te[1] x 4	85.27(8)	84.99(8)	85.54(8)
Te[1] - Tm - Te[1] x 4	147.07(7)	146.46(9)	147.67(9)
Te[1] - Tm - Te[2] x 4	76.74(7)	75.76(8)	77.75(8)
Te[1] - Tm - Te[2] x 2	131.67(7)	130.37(7)	132.98(7)
Te[1] - Tm - Te[3] x 2	77.11(8)	77.00(7)	77.21(7)
Te[1] - Tm - Te[3] x 4	130.83(9)	130.56(10)	131.12(10)
Te[1] - Tm - Te[1] x 2	84.70(7)	84.23(7)	85.16(7)
Te[1] - Tm - Te[2] x 2	130.63(7)	129.72(6)	131.54(6)
Te[1] - Tm - Te[3] x 2	76.57(8)	76.24(8)	76.91(8)
Te[2] - Tm - Te[2] x 2	81.59(7)	81.33(8)	81.83(8)
Te[3] - Tm - Te[3] x 2	81.53(9)	81.18(10)	81.89(10)
Tm - Te[1] - Tm x 4	105.85(7)	105.82(8)	105.88(8)
Tm - Te[1] - Tm x 4	107.06(7)	106.60(8)	107.53(8)
Tm - Te[1] - Tm x 2	84.70(7)	84.19(8)	85.19(8)
Tm - Te[1] - Tm x 4	85.27(6)	84.99(8)	85.54(8)
Tm - Te[1] - Tm x 4	147.07(8)	146.56(13)	147.57(13)
Tm - Te[1] - Tm x 2	86.35(8)	86.20(8)	86.50(8)
Tm - Te[2] - Tm x 2	81.58(7)	81.49(10)	81.65(10)
Tm - Te[2] - Te[3] x 4	62.38(6)	62.06(6)	62.68(6)
Tm - Te[2] - Te[3] x 4	117.27(9)	115.78(12)	118.75(12)
Te[3] - Te[2] - Te[3] x 6	89.74(12)	87.61(12)	91.89(13)
Te[3] - Te[2] - Te[3] x 4	178.63(13)	177.46(13)	179.89(6)
Te[3] - Te[2] - Te[3] x 2	90.57(12)	88.51(13)	92.67(13)
Tm - Te[3] - Tm x 2	81.54(5)	81.18(9)	81.89(10)
Tm - Te[3] - Te[2] x 4	62.77(8)	62.02(8)	63.53(8)
Tm - Te[3] - Te[2] x 4	117.56(8)	117.07(8)	118.03(8)
Te[2] - Te[3] - Te[2] x 2	90.57(13)	88.56(14)	92.62(14)
Te[2] - Te[3] - Te[2] x 6	89.84(10)	89.78(8)	89.88(9)
Te[2] - Te[3] - Te[2] x 4	178.66(14)	177.50(14)	179.88(7)

Table 3.96. Crystal data and structure refinement for YTe₃ at 100 K.

Empirical formula	YTe ₃
Formula weight	471.7
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	C2cm(00γ)000
Unit cell dimensions	a = 4.2840(7) Å, α = 90° b = 25.312(4) Å, β = 90° c = 4.2932(9) Å, γ = 90°
q-vector(1)	0.2907(5)c*
Volume	465.54(15) Å ³
Z	4
Density (calculated)	6.728 g/cm ³
Absorption coefficient	31.041 mm ⁻¹
F(000)	780
Crystal size	0.29 x 0.27 x 0.02 mm ³
Theta range for data collection	1.61 to 29.25°
Index ranges	-5 ≤ h ≤ 5, -34 ≤ k ≤ 34, -6 ≤ l ≤ 6, -1 ≤ m ≤ 1
Reflections collected	6556 (2138 main + 4418 satellites)
Independent reflections	1937 (682 main + 1255 satellites) [R _{int} = 0.0558]
Completeness to θ = 29.25°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1937 / 0 / 39
Goodness-of-fit on F ²	1.53
Final R indices [I > 2σ(I)]	R _{obs} = 0.0365, wR _{obs} = 0.0976
R indices (all data)	R _{all} = 0.0545, wR _{all} = 0.1020
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0321, wR _{obs} = 0.0860
R main indices (all data)	R _{all} = 0.0326, wR _{all} = 0.0862
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0704, wR _{obs} = 0.1303
R 1 st order satellites (all data)	R _{all} = 0.1868, wR _{all} = 0.1441
Extinction coefficient	0.00060(8)
T _{min} and T _{max} coefficients	0.0410 and 0.7092
Largest diff. peak and hole	1.93 and -2.27 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 3.97. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for YTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	x	y	z	U_{eq}^*
Y	0	9043(4)	1700(1)	2549	10(1)
	sin, 1	0	0	5(7)	
	cos, 1	-49(1)	0(1)	0	
Te[1]	0	9000	2946(1)	2549	9(1)
	sin, 1	0	0	5(5)	
	cos, 1	-7(1)	-1(1)	0	
Te[2]	0	8993(3)	712(1)	7549	10(1)
	sin, 1	0	0	-15(6)	
	cos, 1	181(2)	0(1)	0	
Te[3]	0	3985(3)	714(1)	2549	10(1)
	sin, 1	0	0	-7(6)	
	cos, 1	-165(2)	6(1)	0	

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3.98. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for YTe_3 at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Y	0	7(1)	15(1)	8(1)	5(1)	0	0
Te[1]	0	7(1)	14(1)	7(1)	-2(1)	0	0
Te[2]	0	9(1)	14(1)	6(1)	-1(1)	0	0
Te[3]	0	9(1)	15(1)	7(1)	1(1)	0	0

Table 3.99. Bond lengths distributions [$\text{\AA}$] for YTe_3 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Y - Te[1]	3.1555(17)	3.152(3)	3.159(3)
Y - Te[1] x 2	3.174(2)	3.1626(18)	3.1867(18)
Y - Te[1] x 2	3.150(2)	3.1352(17)	3.1641(17)
Y - Te[2] x 2	3.296(2)	3.290(2)	3.299(2)
Y - Te[3]	3.306(2)	3.284(3)	3.327(3)
Y - Te[3]	3.272(2)	3.230(3)	3.316(3)
Te[2] - Te[3] x 2	3.036(2)	2.9453(15)	3.1276(15)
Te[2] - Te[3] x 2	3.030(2)	2.9349(15)	3.1282(15)

Table 3.100. Bond angles distributions [°] for YTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Y - Te[1] x 4	73.37(4)	73.20(5)	73.53(5)
Te[1] - Y - Te[1] x 4	73.71(4)	73.54(5)	73.87(5)
Te[1] - Y - Te[2] x 2	139.32(7)	139.21(4)	139.45(6)
Te[1] - Y - Te[3]	138.70(6)	138.23(7)	139.18(7)
Te[1] - Y - Te[3]	140.03(6)	139.86(7)	140.20(7)
Te[1] - Y - Te[1] x 6	85.10(5)	84.61(6)	85.57(6)
Te[1] - Y - Te[1] x 4	147.08(6)	147.06(4)	147.10(3)
Te[1] - Y - Te[2] x 2	76.66(5)	75.56(5)	77.74(5)
Te[1] - Y - Te[2] x 2	130.56(6)	128.94(6)	132.16(6)
Te[1] - Y - Te[3] x 2	76.52(5)	76.14(5)	76.92(5)
Te[1] - Y - Te[3] x 4	130.95(7)	130.62(7)	131.28(6)
Te[1] - Y - Te[1] x 2	85.93(5)	85.53(6)	86.33(6)
Te[1] - Y - Te[2] x 2	77.06(5)	76.00(5)	78.14(5)
Te[1] - Y - Te[2] x 2	131.61(6)	130.00(6)	133.24(6)
Te[1] - Y - Te[3] x 2	77.34(6)	77.15(5)	77.53(5)
Te[2] - Y - Te[2] x 2	81.31(5)	81.15(7)	81.42(7)
Te[3] - Y - Te[3] x 2	81.27(4)	80.95(7)	81.57(7)
Y - Te[1] - Y x 4	106.76(5)	106.51(4)	107.01(4)
Y - Te[1] - Y x 4	106.16(4)	105.86(4)	106.45(4)
Y - Te[1] - Y x 2	85.93(6)	85.73(6)	86.13(6)
Y - Te[1] - Y x 6	85.28(6)	85.23(5)	85.33(5)
Y - Te[1] - Y x 4	147.08(5)	146.95(3)	147.21(3)
Y - Te[2] - Y x 2	81.29(5)	81.20(6)	81.34(5)
Y - Te[2] - Te[3] x 2	117.67(5)	115.43(6)	119.90(6)
Y - Te[2] - Te[3] x 2	117.12(5)	115.15(6)	119.06(6)
Te[3] - Te[2] - Te[3] x 8	90.08(6)	86.84(6)	93.41(6)
Te[3] - Te[2] - Te[3] x 4	177.93(7)	176.65(6)	179.86(4)
Y - Te[3] - Y x 2	81.27(4)	80.95(6)	81.57(6)
Y - Te[3] - Te[2] x 4	117.25(5)	116.31(4)	118.13(4)
Y - Te[3] - Te[2] x 2	62.45(4)	61.30(4)	63.64(4)
Te[2] - Te[3] - Te[2] x 4	90.29(6)	87.27(6)	93.32(6)
Te[2] - Te[3] - Te[2] x 4	89.82(6)	89.65(4)	89.98(6)
Te[2] - Te[3] - Te[2] x 4	177.94(7)	176.68(6)	179.86(6)

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Chapter 4

Effect of the Three Dimensional Character on the Charge Density Waves of the Square Nets of Tellurium of AMRETe₄ (A = K, Na; M = Cu, Ag; RE = La, Ce)

“Charge Density Waves in the Square Nets of Tellurium of AMRETe₄ (A = K, Na; M = Cu, Ag; RE = La, Ce)”, Malliakas, C. D.; Kanatzidis, M. G. *J. Am. Chem. Soc.* **2007**, *129*, 10675-10677. American Chemical Society (ACS) is gratefully acknowledged for the permission to include this reprint in the Thesis.

4.1. Introduction

Charge density waves (CDWs) are cooperative states that arise from the coupling of phonons and free electrons in quasi-one- and two-dimensional metals. The modulation of the electron density due to this coupling creates a new broken symmetry ground state with a lower total free energy through a Peierls distortion. CDW formation is believed to be driven by Fermi surface instabilities mainly caused by nesting effects in the electronic band structure. Sometimes instabilities on the Fermi surface favor another cooperative state, i.e. superconductivity.¹ Understanding the mechanism of CDW destabilization and the competition between CDW states and superconductivity is of fundamental importance.

Several chemical tuning parameters can be employed to manipulate the CDW state. For example, it is of significant interest to be able to suppress a CDW and access a superconducting state. Theoretically, the CDW modulation is a function of the Fermi level and the nesting properties of the Fermi surface.² Doping (Ta and Ti doped NbSe₃)³, intercalation of atoms (In_xNb₃Se₄)⁴ and amine molecules (1T-TaS₂EDA_{0.25})⁵ have been widely used. This type of tuning involves electron transfer and alters the electron count on the CDW which changes the modulation because it changes the energy of the Fermi level. This does not allow the study of the CDW state in a situation where structural changes are decoupled from changes in electron count. To observe such a decoupling, isoelectronic tuning is needed to change the character of Fermi surface nesting but not the electron count of the CDW. The family of AMRETe₄ (A = K, Na; M = Cu, Ag; RE = La, Ce) compounds⁶ may represent such a case.

The structure of AMRETe₄ can be seen as an intergrowth of electronically neutral RETe₃⁷ and ACuTe⁸ slabs in 1:1 ratio. The layered structure of RETe₃ is essentially intercalated with slabs of ACuTe. Because of this the RETe₃ layers in AMRETe₄ are significantly separated compared to those in RETe₃, as shown in Figure 4.1. As the RETe₃ phases have CDWs,⁹ AMRETe₄ too have CDWs. Because the alternating layers are neutral, no electron transfer between them is necessary and the ACuTe layer does not alter the electron count in the adjacent layers of RETe₃. The insertion of the ACuTe layer does however disrupt the van der Waals interactions that are present in the structure of the binaries RETe₃. Here we report the details of the CDW in AMRETe₄ and compare them to those of the parent RETe₃ compounds.

We find that the CDW in AMRETe₄, which originates from a distortion of the Te nets in the RETe₃ slab in these compounds, is still present but, surprisingly, the modulation q-vectors are significantly different from the ones found in the RETe₃ series.¹⁰ The q-vector changes from $\sim 2/7$ in the binary phases to $\sim 1/3$ in the quaternary modifying the character of the CDW. If the CDW q-vector were strictly governed by the electronic structure of the RETe₃ itself no significant changes would be expected by separating the RETe₃ slabs.

The insertion of the ACuTe layers into the van der Waals gaps of the RETe₃ structure separates the RETe₃ slabs, Figure 4.1. The inter-slab interactions in RETe₃ should be diminished so that a quasi three-dimensional system becomes more two-dimensional in character. This opens the possibility that the changes in the CDW of AMRETe₄ arise from the enhanced two-dimensionality of the RETe₃ layer.¹¹ This would imply that the van der Waals interface between adjacent Te square nets in RETe₃ is

important in affecting the Fermi surface nesting. The AMRETe₄ compound could present a rare example that illustrates the effect of dimensionality on the CDW distortion without changing the electron count.

4.2. Experimental Section

4.2.1. Reagents

The following reagents were used as obtained. Potassium metal, Spectrum Chemicals Mfg. Corp., Gardena, CA; Sodium metal, Spectrum Chemicals Mfg. Corp., Gardena, CA; Lanthanum metal, 40 mesh, Cerac, Milwaukee, WI; Cerium metal, ~ 1 mm turnings, Cerac, Milwaukee, WI; Copper metal, 40 mesh, Cerac, Milwaukee, WI; Tellurium chunks, Tellurex Corp, Traverse City, MI; N, N – Dimethylformamide (DMF), ACS reagent grade, Spectrum Chemicals, New Brunswick, NJ; Diethyl ether anhydrous, ACS reagent grade, Columbus Chemical Industries, Columbus, WI.

Alkali Metal Telluride, A₂Te (A = K, Na) – 5.836 g (0.15 mol) K (or 3.448 g of Na) was sliced in small pieces (~ 3 mm) in a N₂ filled glovebox and combined with 9.523 g (0.075 mol) Te in a 1000 mL single neck round bottom flask. A Teflon coated magnetic stir bar was added in the flask as well. The flask was connected to a glass adapter with a stopcock joint and removed from the glovebox. The flask and adapter were then connected to a dry condenser apparatus and chilled to -78 C using a dry ice/acetone bath. Approximately 800 mL of pure NH₃ were condensed, under N₂ atmosphere, onto the reagents, yielding a purple solution. The solution was kept under stirring and maintained at -78 C for up to 16 hours. The dry ice/acetone mixture was removed and the NH₃ was allowed to evaporate off as the flask warmed up to room temperature under a constant

flow of N₂ for ~ 6 hours. The resulting powder (brown color for K₂Te and white-gray for Na₂Te) was evacuated on a Schlenk line for ~ 4 hours and taken into a N₂ filled glovebox. The product was ground to a fine powder with a mortar and pestle and placed into a screw-capped vial in the glovebox.

4.2.2. Synthesis

AMRETe₄ (*A*=K, Na; *M* = Cu, Ag; *RE* = La, Ce) – $A_{1-x}M_{1+x}RETe_4$ was synthesized from a mixture of A₂Te (*A* = K, Na; 0.500 mmol), *M* (*M* = Cu, Ag; 0.125 mmol), *RE* (*RE* = La, Ce; 0.125 mmol), and Te (2.0 mmol) that was sealed under vacuum in a quartz tube and heated to 700 °C for 5 days. The tube was then cooled to 300 °C at a rate of 4 °C/h, followed by quenching to room temperature at a rate of 10 °C/h. The excess A₂Te_y flux was washed off with N,N-dimethylformamide under nitrogen to reveal very thin red-brown plate-shaped crystals.

4.2.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – All temperature dependent measurements were performed on the same single crystal for each AMRETe₄ compound. Single crystals were quenched from room temperature to 100 K. The heating rate for warming ramps was

~200 K/h. Typical acquisition time was around 24 h. Detailed crystallographic table reports for each individual AMRETe₄ analogue and temperature can be found in tables 4.4 - 4.53. Intensity data were collected on a STOE IPDS II diffractometer equipped with a graphite monochromatized Mo radiation ($\lambda = 0.71073 \text{ \AA}$) and an Image Plate (IP) detector. The data were collected with an ω -scan technique from 0-180° and an arbitrary ϕ -angle. Data reduction was performed with the X-Area package.¹² The length determination and refinement of the q-vectors was performed with the Peaklist 1.06 software part of the X-Area suite using a least square refinement algorithm. An analytical absorption correction was performed (X-Shape within X-Area) and all structures were refined with JANA2000 software.¹³ Direct methods of SHELXTL software¹⁴ were used to find the atomic positions in the subcell.

Satellite reflections of first order were observed and used for the refinement. A single modulation wave for positional and temperature parameters was used. Only the symmetry allowed Fourier terms were refined. In more details, the sinusoidal coefficients in all the directions for positional (x, y and z) and thermal parameters (U_{11} , U_{22} , U_{33} , U_{12} , U_{13} and U_{23}) were freely refined and the corresponding cosine coefficients values were induced by symmetry.

Some of the quaternary analogues had twin domains that could be described with a twin law of 90 degrees rotation along the *c*-axis $[0 \ -1 \ 0 \ 1 \ 0 \ 0 \ 0 \ 1]$. Several centrosymmetric superspace groups were tested yielding R-values for the satellites to more than 50%. Temperature was controlled by an Oxford Cryostream 700 Plus cryostat.

Charge transport measurements - Electrical resistivity and thermopower data were measured as a function of temperature for single crystals of KCuLaTe₄. Electrical

contact for the resistivity measurement was made using silver paint and Cu wire directly on to the crystal surface. Measurements were made for arbitrary current directions in the ab-plane using a standard four point contact geometry (AC) in a Quantum Design Physical Property Measurement System (PPMS). Electrical contact for the thermopower measurement was made using gold paint on an alumina stage of a SB-100 Seebeck Measurement MMR System.

Infrared (IR) Spectroscopy – Optical diffuse reflectance measurements were performed on single crystals of all AMRETe₄ members at room temperature. The spectra were recorded in the Mid-IR region (6000 – 400 cm⁻¹) with a Nicolet 6700 FT-IR Spectrometer equipped with a diffuse reflectance collector from Spectra-Tech Inc.

4.3. Results and Discussion

Subcell Description of AMRETe₄ (A=K, Na; M = Cu, Ag; RE = La, Ce) – The AMRETe₄ adopt a layered structure composed of two types of layers, the semiconductive [NaCuTe] and metallic [RETe₃], Figure 4.1. Each component is known to exist as an independent compound.^{7,8} The [RETe₃] layer adopts the NdTe₃ structure type and has an anti-PbO type [RETe]⁺ sublayer sandwiched between two square Te nets. The [CuTe]⁻ layer can be described as an ideal anti-PbO structure type, made up of ribbon tetrahedral [CuTe₄] units that share edges in two dimensions. The neutral [NaCuTe] and [RETe₃] slabs alternate in a 1:1 ratio and stack along the *c*-axis separated by van der Waals gaps to build the structure. Since both slabs have no net charge the average electron count in the Te atoms of the net of the [RETe₃] sublayer remains -0.5 e⁻. No electron transfer is necessary between the [NaCuTe] and [RETe₃] slabs. A more descriptive formula of the

structure can be $\text{Na}^+[\text{CuTe}]^-\text{[RETe]}^+[\text{Te}_2]^-$. The single crystal structure refinement indicated that in some members of the family there is some interchange between the alkali atoms and monovalent M atoms in their crystallographic sites in the form $\text{A}_{1-x}\text{M}_x\text{RETe}_4$. In most of the quaternary series the alkali metal site is mixed-occupied with the coinage metal (except the K/Cu combination). The similar atomic radii and same square antiprismatic site environment of these atoms can facilitate such disorder.

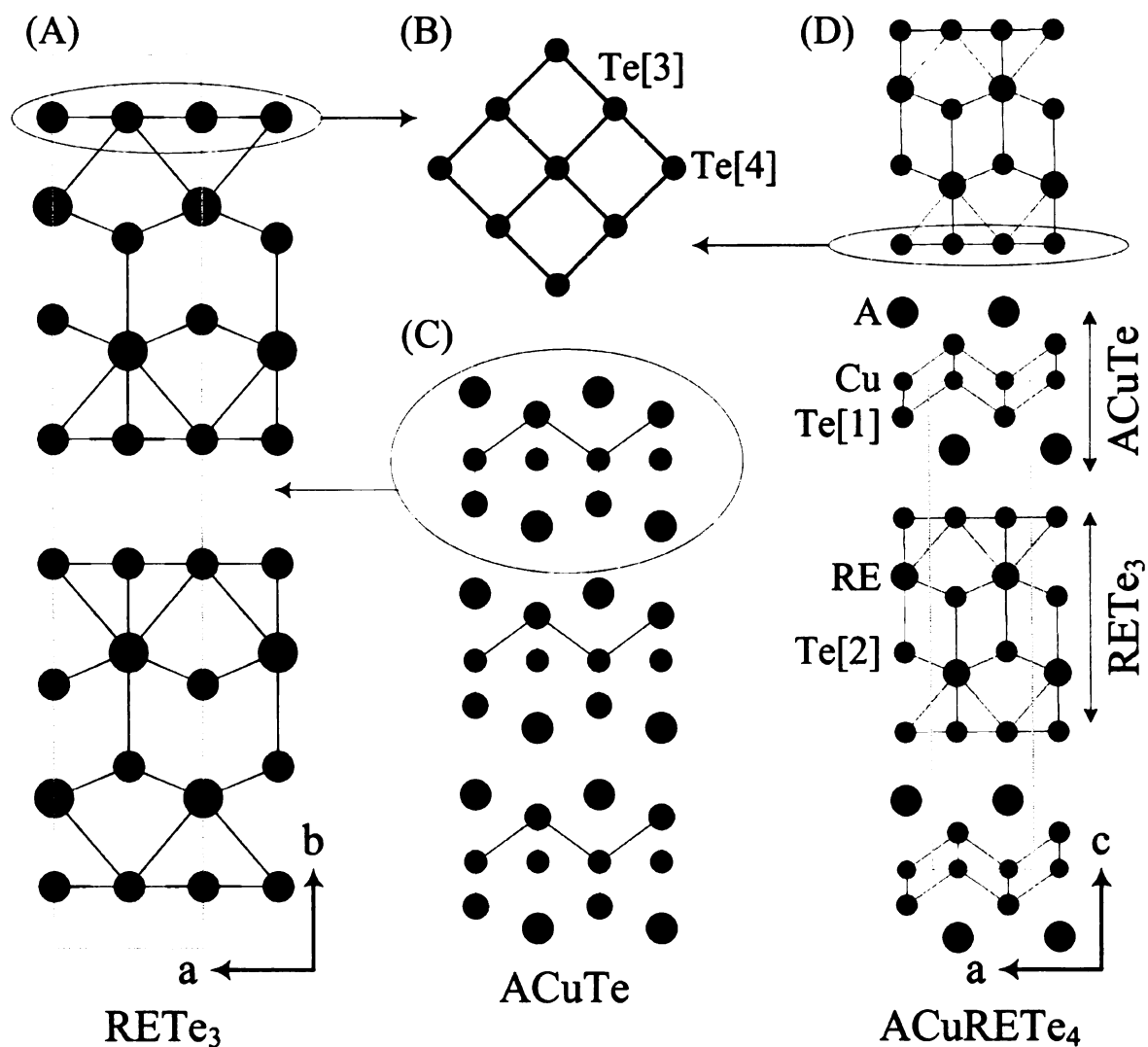


Figure 4.1. (A) The layered structure of RETe_3 (NdTe_3 -type). The van der Waals gap is indicated by the arrow. (B) The undistorted square net of Te atoms in RETe_3 and AMRETe_4 . (C) The electronically neutral ACuTe layer which when inserted in the structure of RETe_3 gives AMRETe_4 . (D) The structure of AMRETe_4 (A = K, Na; M = Cu, Ag; RE = La, Ce).

Supercell Description of AMRETe₄ (A=K, Na; M = Cu, Ag; RE = La, Ce) – The CDW in all A_{1-x}M_{1+x}RETe₄ analogs gives rise to modulated incommensurate superstructures. The application of superspace crystallographic techniques was necessary to solve their structure. Although the undistorted (no CDW) subcell structure has a tetragonal symmetry (Table 4.3), the modulation q-vector is always along the *b*-axis giving orthorhombic symmetry. The distortion is located in the planar Te nets of the RETe₃ slabs. The [CuTe] layer also contains a square Te net. However, it is not distorted as the formal charge on each Te atom in this layer is 2- and Te-Te interatomic distances greater than 4.4 Å. Most of the A_{1-x}M_{1+x}RETe₄ (A = K, Na; M = Cu, Ag; RE = La, Ce) analogs adopt the P2₁2₁2(0β1/2)0s0 superspace group, except for NaMCeTe₄ (M = Ag and Cu) which adopts P2₁2₁2(0β0)0s0 and KAgRETe₄ (RE = La, Ce) which adopts the lower symmetry Pm(0β1/2)0 superspace group.

The q-vector varies from 0.3361(6) in KAgCeTe₄ to 0.3861(5) in KCuLaTe₄, at 100 K. The difference in the cell constants along the plane of the Te net between these quaternary phases and the corresponding RETe₃ binaries is negligible (~2 %). Surprisingly, however, the difference in q-vectors between quaternary (0.3550(8) for KCuCeTe₄) and binary (0.2790(3) for CeTe₃) compounds is large ~30 %. A 2 % change in the lattice constant cannot account for the large change in q-vector. A difference of ~2 % in the cell parameters the binary RETe₃ results in no more than 6 % change in the q-vector since a 2 % decrease in the *c*-axis of CeTe₃ (q = 0.2790(3)) gives a cell constant comparable with the cell of HoTe₃ (q = 0.2935(3)) at 100 K. Given that the RETe₃ layers in the quaternary and binary compounds are isoelectronic, the large change in the CDW

character could arise from the alteration occurring in interlayer coupling between adjacent Te nets of RETe_3 slabs upon insertion of the AMTe layer.

The new CDW modulations found in the quaternary compounds features Te_x oligomers which are different from those observed in the RETe_3 (RE = La and Ce) series. The majority of oligomers in the binary RETe_3 compounds are tetramers and trimers and occasionally single Te atoms and W-shaped pentamers.¹⁵ In contrast, every Te pattern within the $\text{A}_{1-x}\text{M}_{1+x}\text{RETe}_4$ series is unique with a different sequence of oligomers along the modulation direction. Interestingly, tetramers were not found in most of the quaternary phases. Instead, a sequence of trimers and pentamers with one linear Te atom and occasionally monomers and dimers is observed for the compounds that have a q-vector in the range of 0.36(1), Figures 4.2 - 4.5, 4.7, 4.9. For the two cases that the q-vector deviates significantly from this range the Te patterns start to contain tetramers similar to those found in the binaries. Specifically, the majority of oligomers in the Te net of KCuLaTe_4 (q-vector of 0.3861(5)) consists of dimers and occasionally trimers, tetramers and single Te atoms, Figure 4.6. For KAgCeTe_4 (q-vector of 0.3861(5)) the net is mainly composed by trimers and a smaller fraction of dimers and tetramers, Figure 4.9. The bond length distribution between Te atoms in the nets of $\text{A}_{1-x}\text{M}_{1+x}\text{RETe}_4$ is comparable with that in the RETe_3 binaries, Table 4.2.

The q-vector increases as the cell volume decreases, for example from 0.3361(6) in KAgCeTe_4 to 0.3861(5) in KCuLaTe_4 , at 100 K. The same trend exists in the RETe_3 series.¹⁵ The temperature dependence of the q-vector between 100 K and 300 K seems negligible.

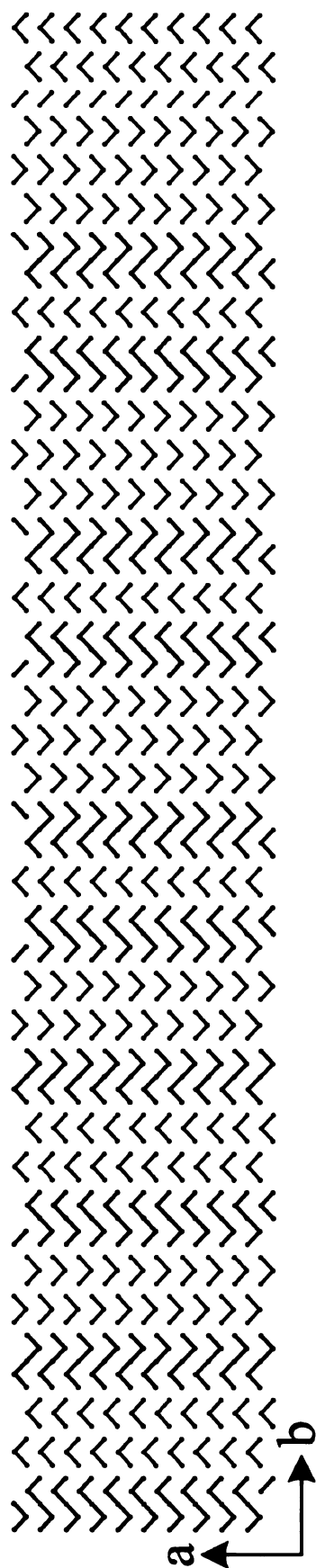


Figure 4.2. $\text{Na}_{0.61(2)}\text{Cu}_{1.39(2)}\text{LaTe}_4$ at 100 K with $q = 0.3632(8)b^* + 1/2c^*$ and $3.075 \text{ \AA}$ threshold.

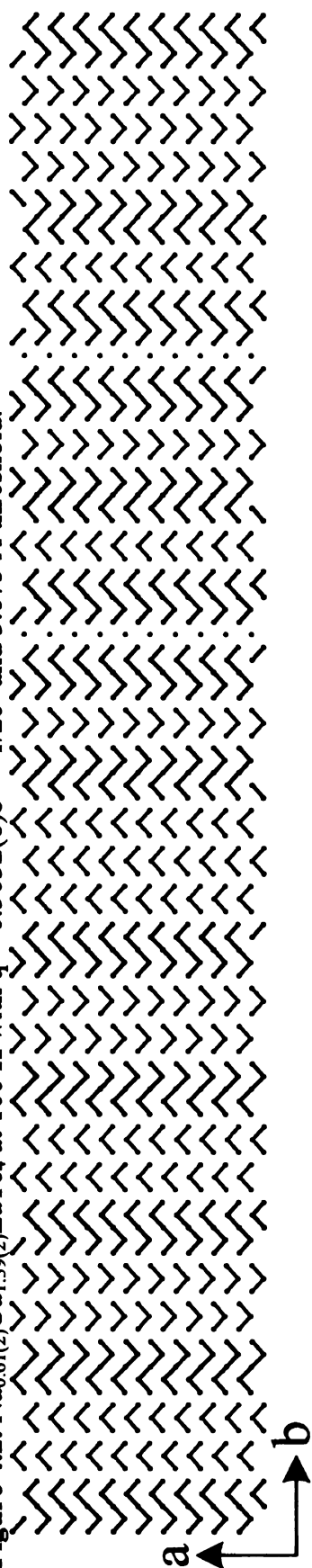


Figure 4.3. $\text{Na}_{0.75(2)}\text{Cu}_{1.25(2)}\text{CeTe}_4$ at 100 K with $q = 0.3621(7)b^* + 3.035 \text{ \AA}$ threshold.

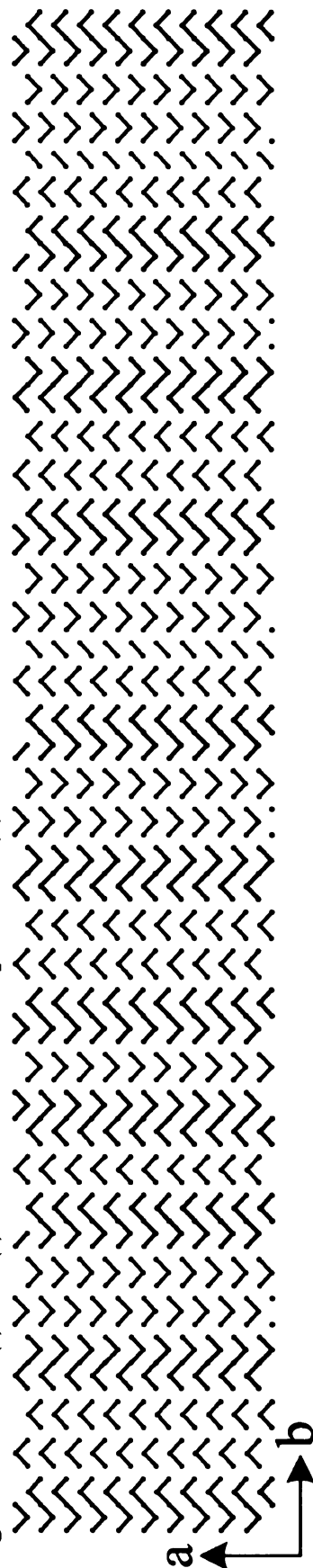


Figure 4.4. $\text{Na}_{0.72(1)}\text{Ag}_{1.28(1)}\text{LaTe}_4$ at 100 K with $q = 0.3660(8)b^* + 1/2c^*$ and $3.097 \text{ \AA}$ threshold.

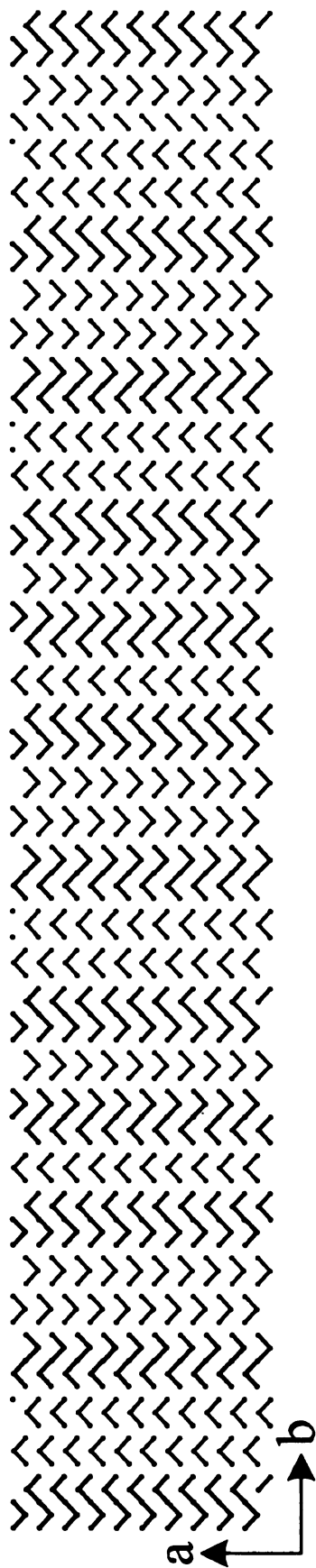


Figure 4.5. $\text{Na}_{0.79(1)}\text{Ag}_{1.21(1)}\text{CeTe}_4$ at 100 K with $q = 0.3681(8)b^* + 3.070 \text{ \AA}$ threshold.

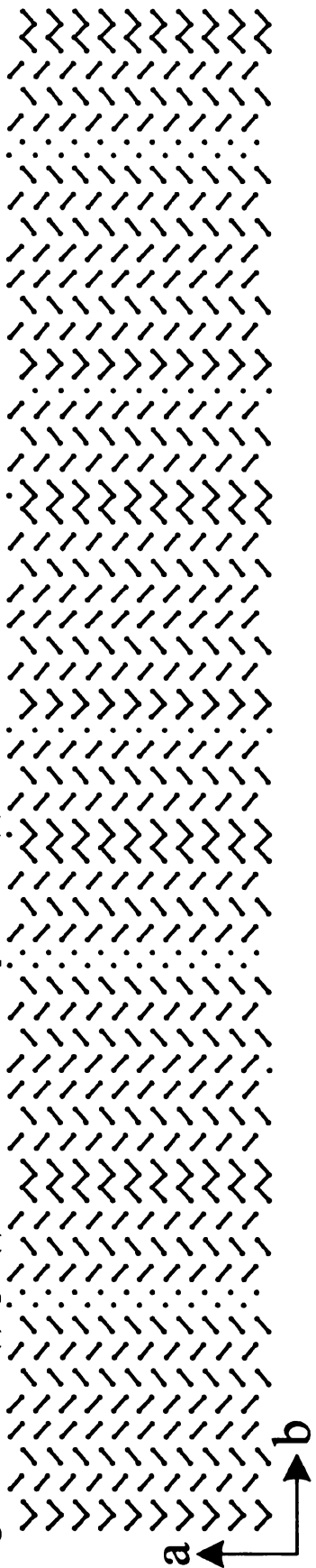


Figure 4.6. KCuLaTe_4 at 100 K with $q = 0.3861(5)b^* + 1/2c^* + 3.109 \text{ \AA}$ threshold.

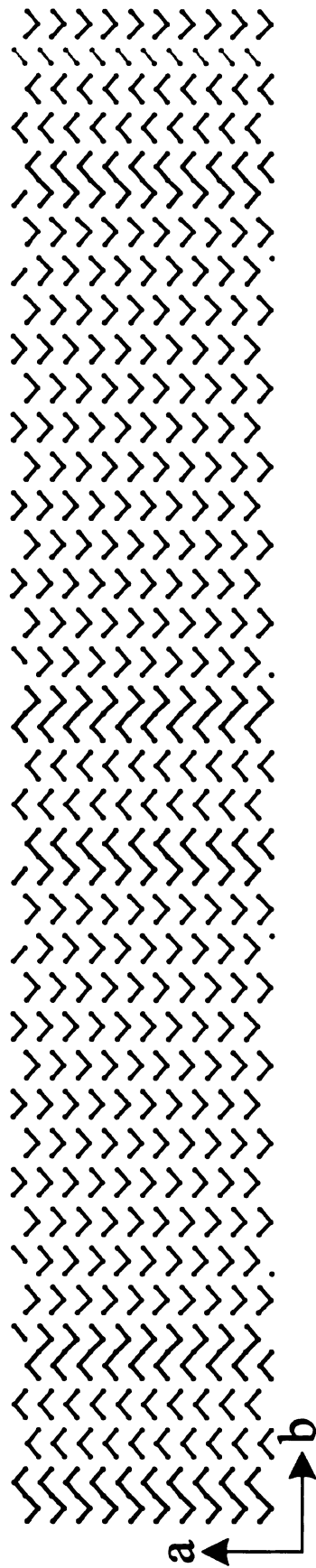


Figure 4.7. $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 100 K with $q = 0.3466(7)b^* + 1/2c^*$ and 3.062 Å threshold.

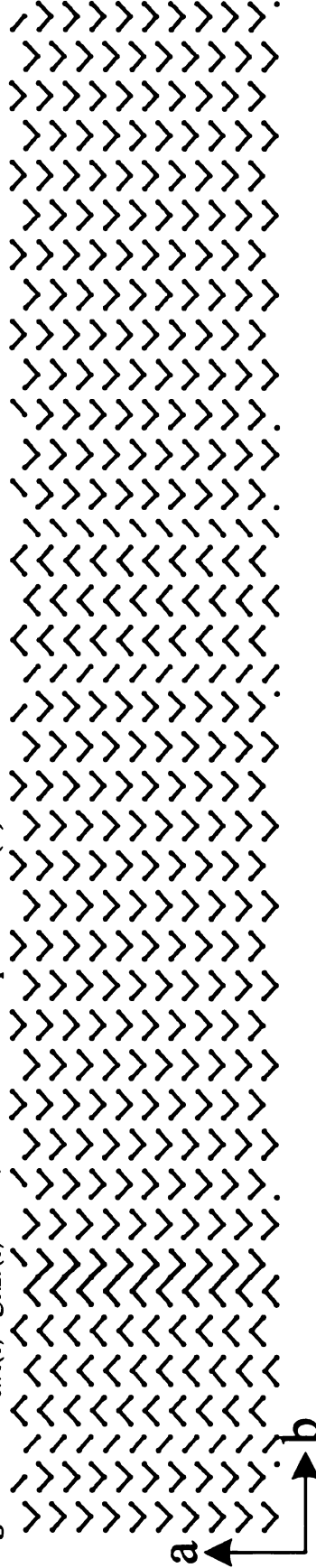


Figure 4.8. $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 300 K with $q = 0.3450(7)b^* + 1/2c^*$ and 3.100 Å threshold.

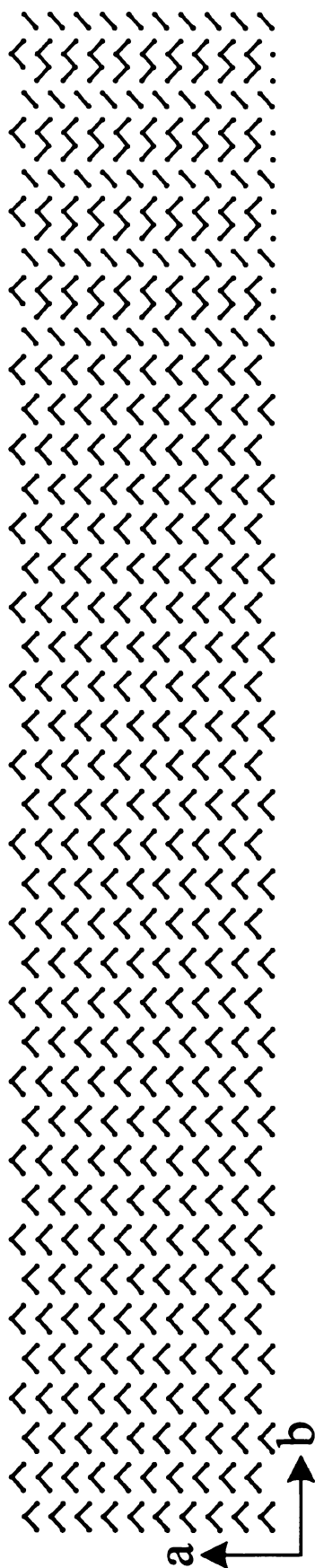


Figure 4.9. KAgCeTe₄ at 100 K with $q = 0.3361(6)b^* + 1/2c^*$ and 3.080 Å threshold.

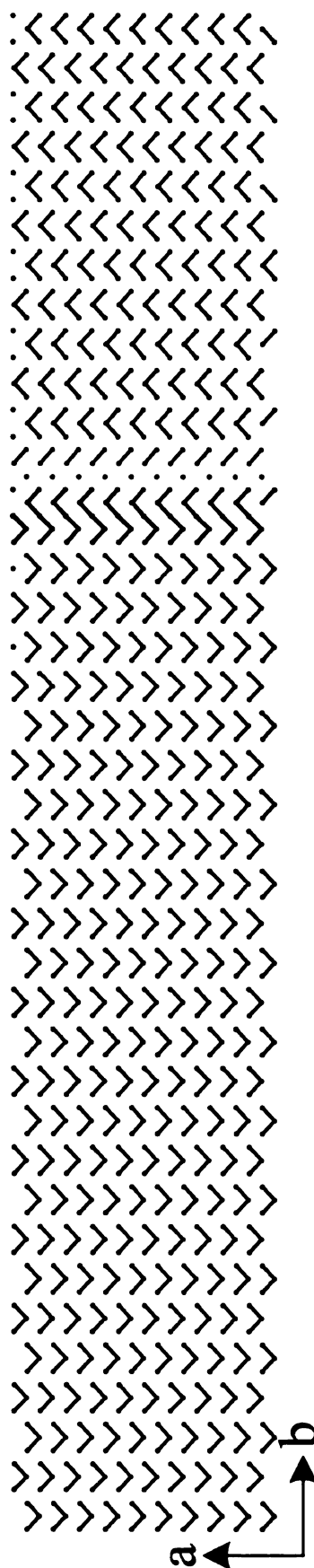


Figure 4.10. KAgCeTe₄ at 300 K with $q = 0.3381(8)b^* + 1/2c^*$ and 3.096 Å threshold.

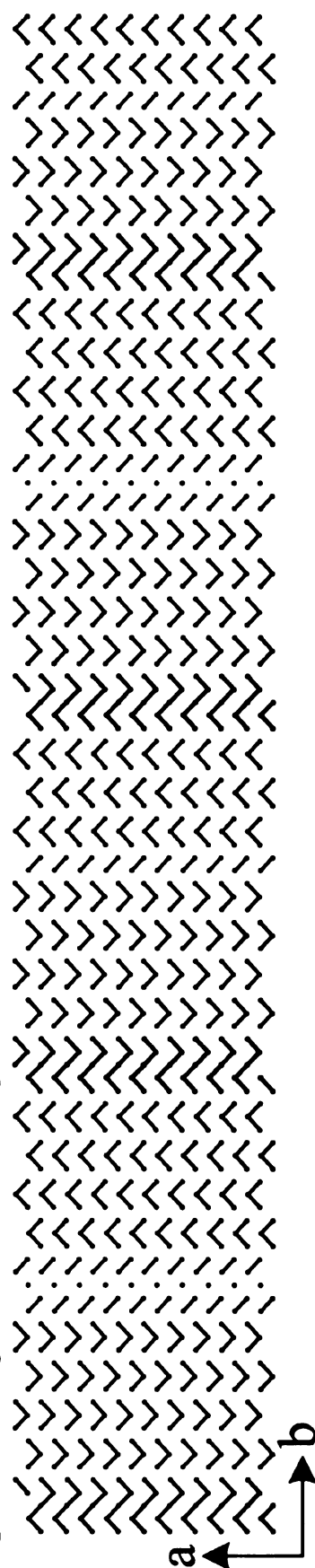


Figure 4.11. KCuCeTe₄ at 100 K with $q = 0.3550(8)b^* + 1/2c^*$ and 3.055 Å threshold.

Disorder and purity of $A_{1-x}M_{1+x}RETe_4$ - All $A_{1-x}M_{1+x}RETe_4$ ($A = K, Na$; $M = Cu, Ag$; $RE = La, Ce$) compounds were synthesized from an excess of reactive A_xTe_y flux. Similar ionic radii and coordination geometry of A and M (except the K/Cu combination) created disorder on the A crystallographic site and a fraction of M was found to occupy site A as well. Therefore, the occupational fraction x couldn't be controlled by these experimental conditions. Nevertheless, different x values will not affect the electron count on the Te net of the $[RETe_3]$ layer of the quaternaries and the CDW modulation. Different concentrations of M though may change the number of carriers and resistivity but not the metallic character of the materials.

The major phase from the flux reactions was the target quaternary compound. Minor impurities were indexed as $RETe_3$ binaries (and ARE_3Te_8 and $A_2M_5RE_2Te_9$ in some other cases). Figure 4.12 shows a representative powder x-ray diffraction pattern of the as synthesized $NaAgCeTe_4$ phase in comparison with the calculated powder patterns of the quaternary and $CeTe_3$ phases respectively.

Since crystal morphology and color of quaternary and binary phases were identical, Energy dispersive spectroscopy (EDS) was performed on the single crystals used for transport measurements. The analysis verified the presence of all four elements in the crystals.

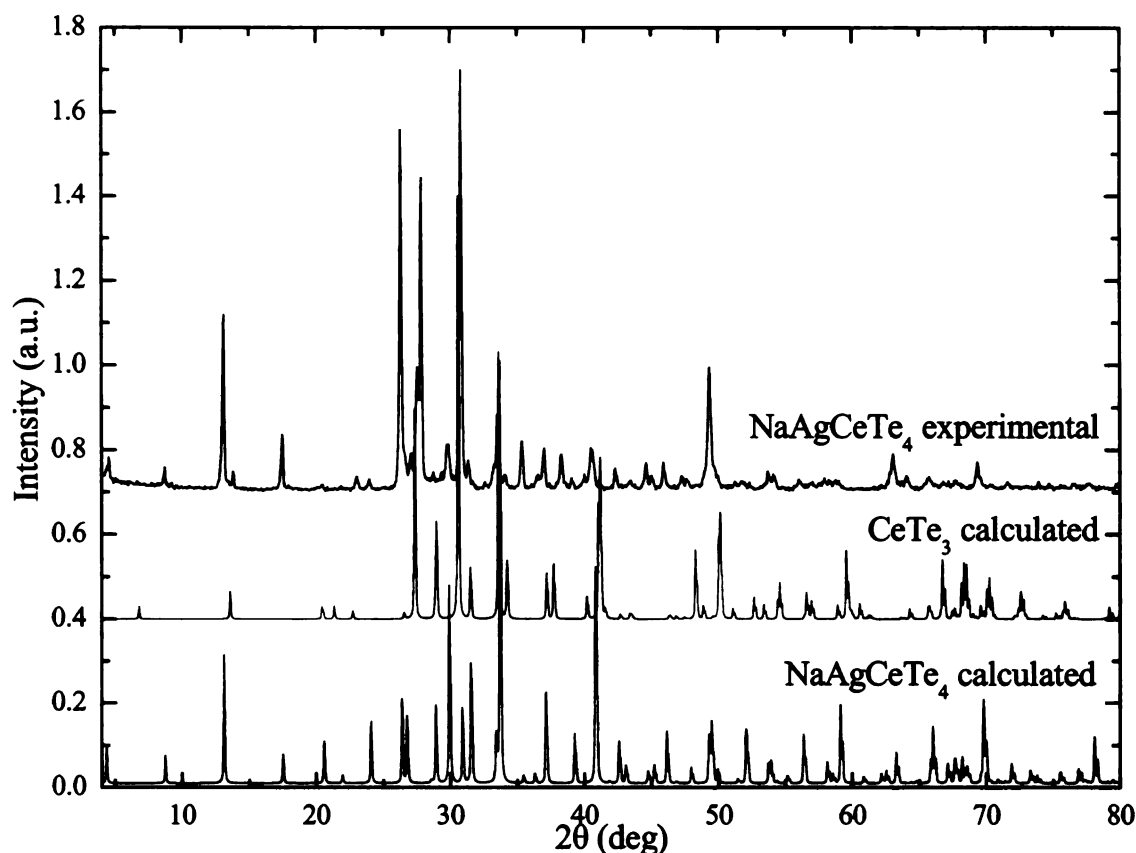


Figure 4.12. Comparison of the experimental X-ray powder pattern of NaAgCeTe_4 with the calculated powder patterns of the quaternary and CeTe_3 .

Band structure calculation of KCuLaTe_4 – The calculations were performed using the self-consistent full-potential linearized augmented plane wave method (LAPW)¹⁶ and the generalized gradient approximation (GGA)¹⁷ for the exchange and correlation potential. The experimental cell constants (Table 4.29) and atomic coordinates (Table 4.1) from the crystal structure refinement of KCuLaTe_4 in Pmmn were used. Directions in the Brillouin zone (BZ) of Pmmn space group are shown in Figure 4.15.¹⁸ Interatomic forces were minimized within 0.1 mRy/bohr using a reverse-communication trust-region quasi-Newton method from the Port library.¹⁹ Scalar relativistic corrections were included and a spin-orbit interaction was incorporated using a second variational procedure.²⁰ The values of the atomic radii were taken to be: 2.7 a.u. for K atom, 2.4 a.u.

for Cu atom, 2.7 a.u. for La atom and 2.5 a.u. for Te atoms, where a.u. is the atomic unit (0.529 Å). Convergence of the self-consistent iterations was performed for 30 k points inside the irreducible BZ to within 0.0001 Ry with a cutoff of -6.0 Ry between the valence and the core states. The calculations were performed using WIEN2K program.²¹

Electronic band structure calculations performed on the undistorted structure of KCuLaTe₄ confirm that the Fermi surface topology favors the formation of a nesting vector (q-vector) along the b* direction with a value of ~0.33, Figure 4.16.²² The Fermi surface topology is similar to the one for LaTe₃ (Figure 2.23) that forms a nesting vector of 0.28(2). The difference is the presence of three extra bands, mainly Cu d and Te p in character from the [KCuTe] layer, that are crossing the Fermi surface and they are located outside the nesting region of the p bands of the Te net of [RETe₃] (see Figure 4.14 and Figure 4.16).

Table 4.1. Atomic coordinates for KCuLaTe₄ in Pmmn used for the DFT calculation.

Label	x	y	z
La	0.25	0.25	0.393210
Te[1]	0.25	0.75	0.263449
Te[2]	0.25	0.75	0.736298
Te[3]	0.25	0.25	0.078509
Te[4]	0.25	0.25	0.561304
K	0.25	0.75	0.000283
Cu	0.25	0.25	0.873042

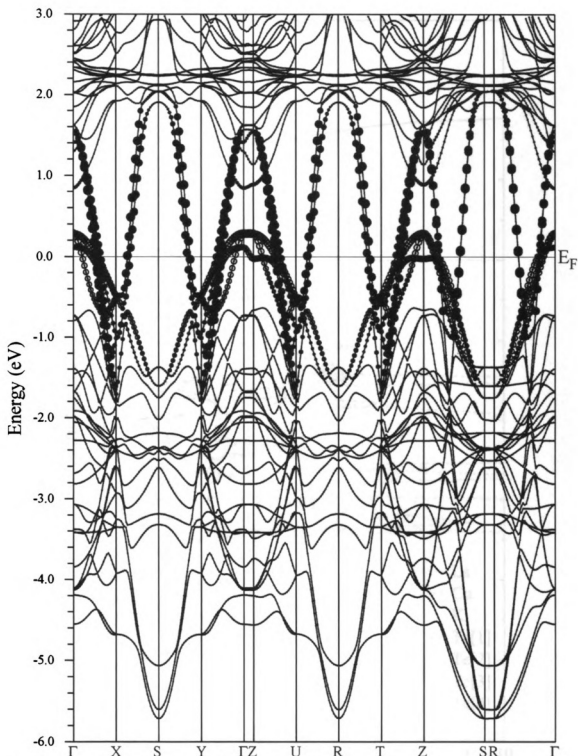


Figure 4.13. Band structure of KCuLaTe_4 near the Fermi level. Cu d and Te[3] p bands from the [KCuTe] layer are drawn in open circles. Te[1] and Te[2] p bands from the distorted planar net are drawn in closed circles. The contribution of each orbital is proportional to the breadth of the circles tracing out the band. Only the bands that cross the Fermi surface are drawn in circles for clarity.

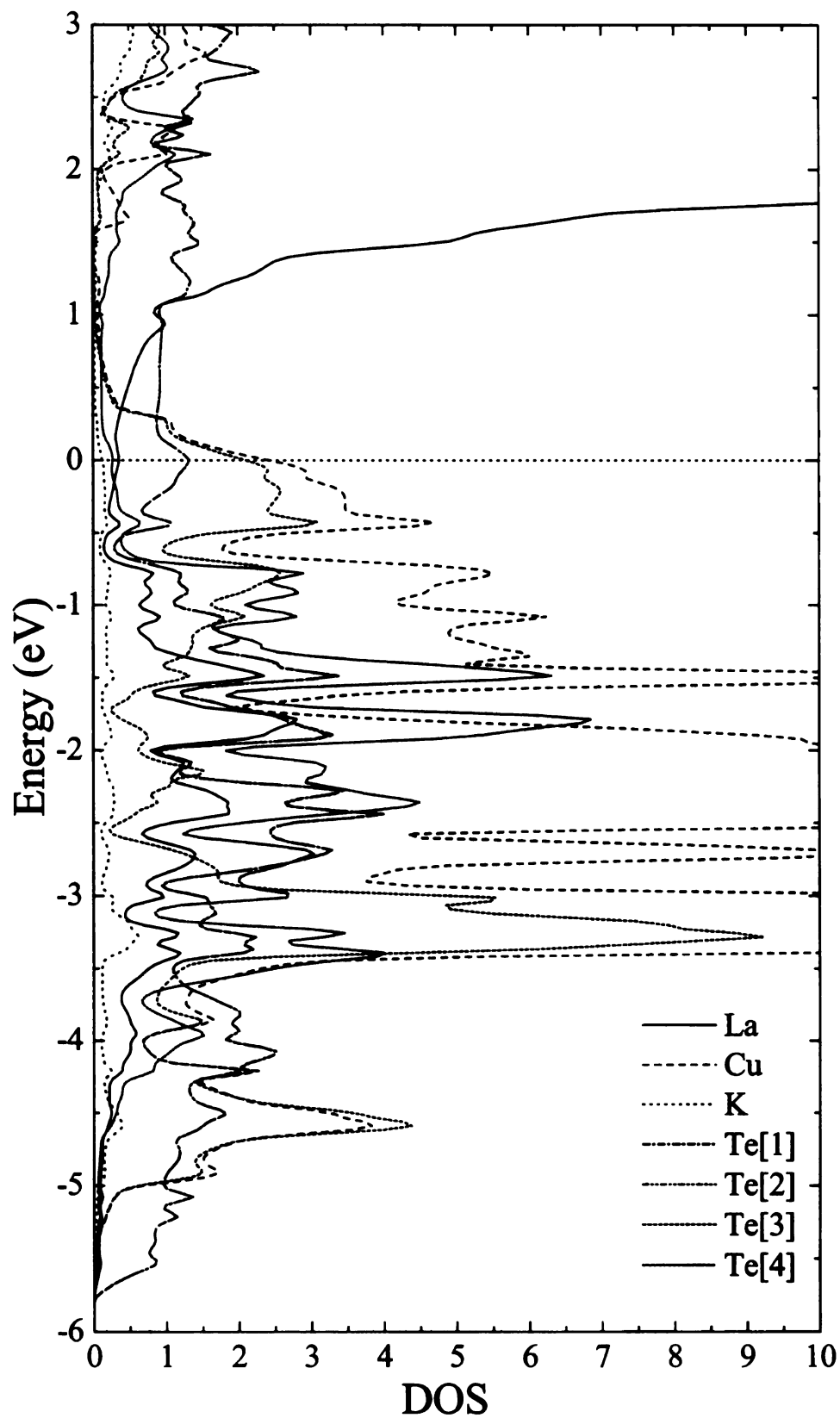


Figure 4.14. Total density of states (DOS) of KCuLaTe_4 near the Fermi level. Te[1] and Te[2] are the tellurium atoms in the $[\text{RETe}_3]$ net, Te[3] is in the $[\text{CuTe}]$ layer and Te[4] is in the $[\text{RETe}_3]$ slab.

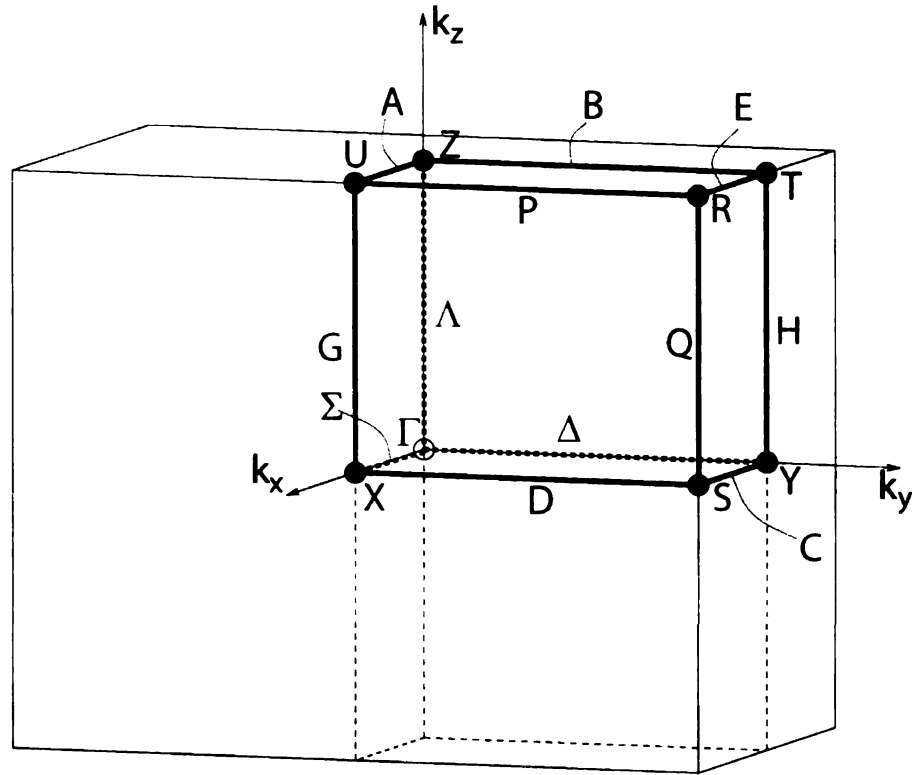


Figure 4.15. Brillouin zone of Pmmn space group.

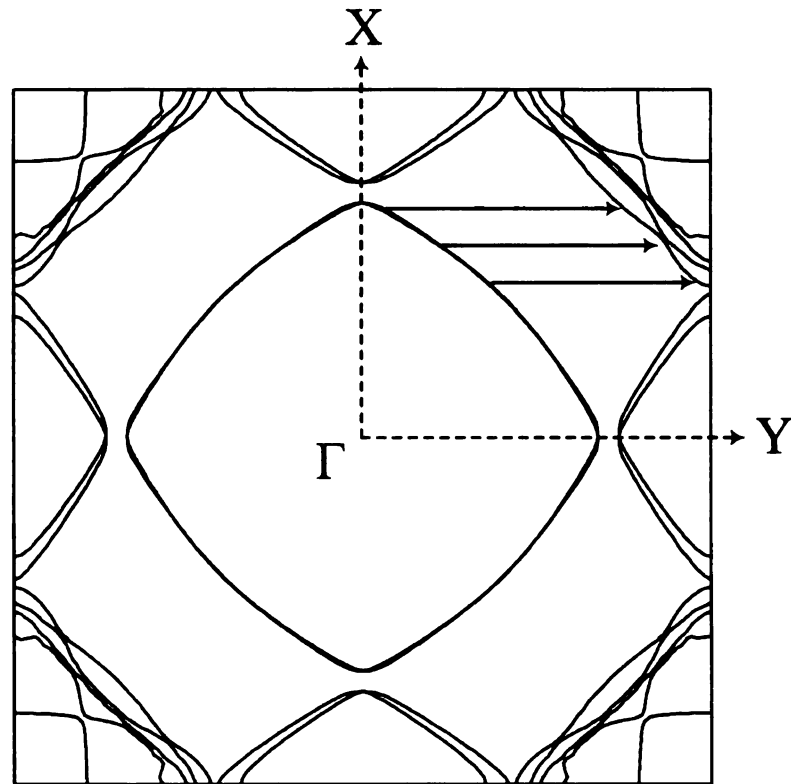


Figure 4.16. Fermi surface topology of KCuLaTe_4 . Possible nesting vectors (q -vectors) with an average length of $0.33(2)$ along the b^* -axis (Y point) are drawn in arrows.

Charge transport measurements - Generally, the formation of CDWs leads to the appearance of energy gaps at the Fermi level (E_f). In the case of RETe_3 however near E_f there is an energy gap associated with the CDW distortion of the Te net but some electronic states still remain at E_f because of bands associated with other parts of the structure. Thus, the CDW distortions do not create a fully gapped Fermi surface.²³ This situation creates a poor metal character for RETe_3 and this is confirmed by electrical resistivity measurements.²⁴ The situation in KCuLaTe_4 is similar as indicated by the temperature dependent resistivity data shown in Figure 4.17. The thermopower varies between +35 to +55 $\mu\text{V/K}$ in the range of 300-550 K. These are relatively small values and are consistent with metallic p-type character for the material, Figure 4.18.

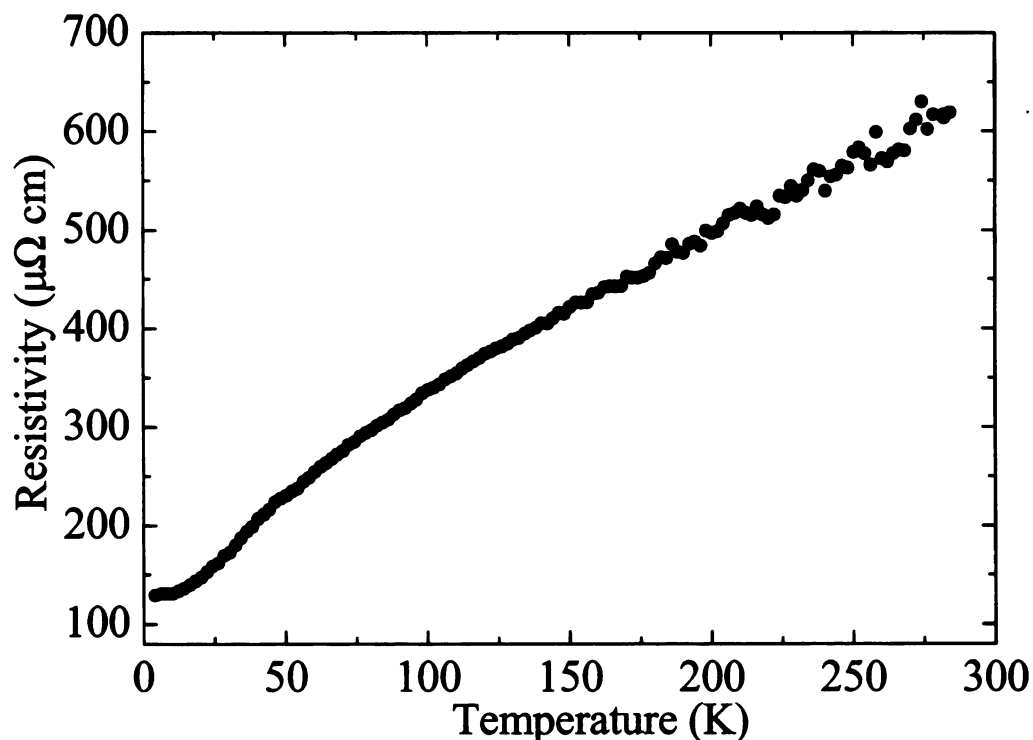


Figure 4.17. Temperature dependent resistivity of KCuLaTe_4 single crystal.

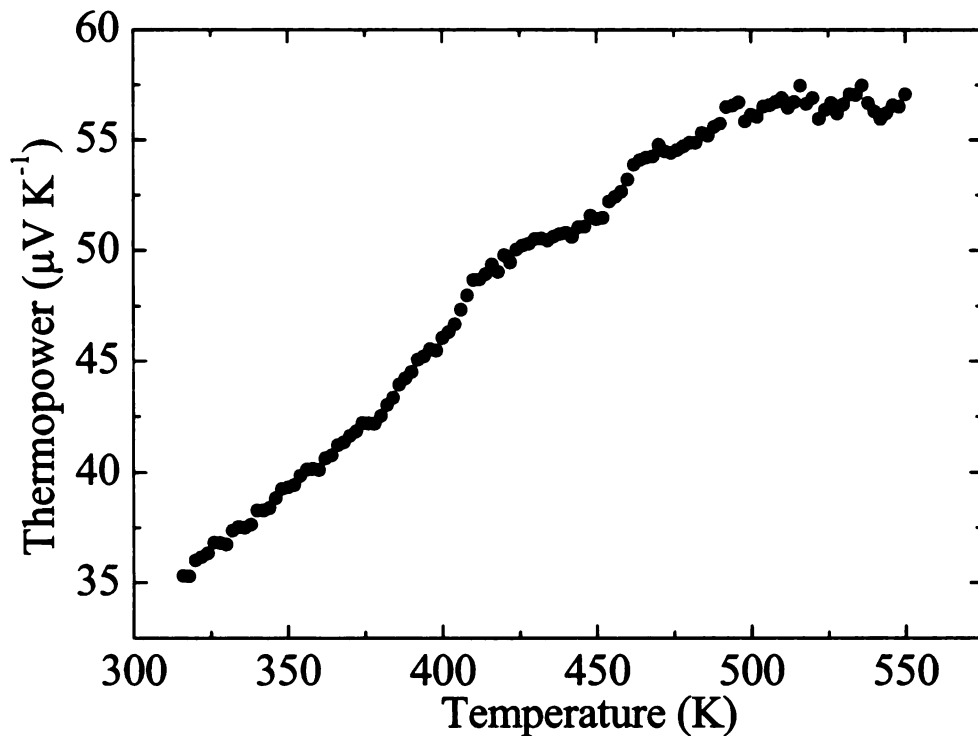


Figure 4.18. Dependence of thermopower with temperature of KCuLaTe_4 single crystal.

Infrared (IR) Spectroscopy – Despite the poor metal character of AMRETe_4 , there are spectroscopically observed electronic transitions which can be assigned to the CDW energy gap of the Te-net. The energy values are between 0.25(2) eV for $\text{Na}_{0.60}\text{Cu}_{1.40}\text{LaTe}_4$ and 0.33(2) eV for KCuCeTe_4 at room temperature as measured by infrared diffuse reflectance spectroscopy, Table 4.2. A representative plot of the apparent energy gap is shown in Figure 4.19.

Table 4.2. Comparison of the minimum and maximum distances of Te-Te within the net (X-ray diffraction at 100K) and room temperature energy gap values of all $A_{1-x}M_xRETe_4$ ($A = K, Na$; $M = Cu, Ag$; $RE = La, Ce$) quaternary compounds with the binary $RETe_3$ analogs.

Compound	Minimum distance (Å)	Maximum distance (Å)	Energy gap (eV)
CeTe ₃	2.925(2)	3.255(3)	0.27(2)
LaTe ₃	2.929(6)	3.272(7)	0.25(2)
Na _{0.60(2)} Cu _{1.40(2)} LaTe ₄	2.999(4)	3.260(4)	0.25(2)
Na _{0.78(1)} Cu _{1.22(1)} CeTe ₄	2.975(3)	3.241(2)	0.27(2)
Na _{0.70(1)} Ag _{1.30(1)} LaTe ₄	3.037(4)	3.273(3)	0.27(2)
Na _{0.78(1)} Ag _{1.22(1)} CeTe ₄	2.985(3)	3.264(3)	0.28(2)
KCuCeTe ₄	2.972(2)	3.275(2)	0.33(2)
KCuLaTe ₄	2.910(4)	3.392(4)	0.30(2)
K _{0.71(2)} Ag _{1.29(2)} LaTe ₄	2.929(4)	3.447(4)	0.28(2)
KAgCeTe ₄	2.896(9)	3.406(9)	0.30(2)

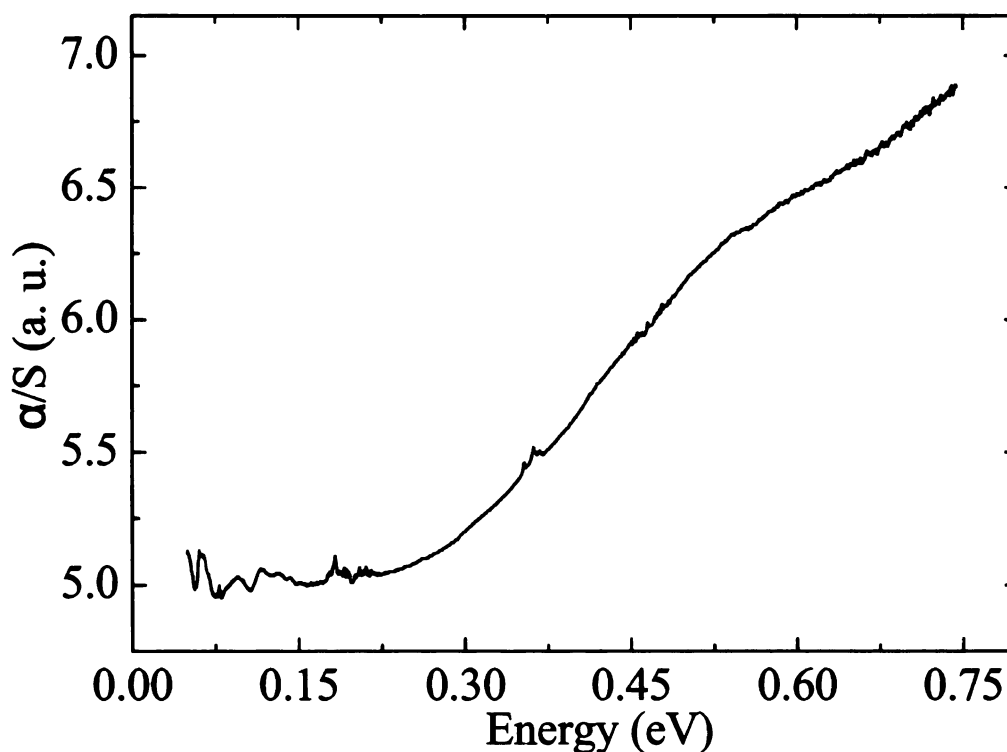


Figure 4.19. Typical room temperature infrared absorption spectrum of $Na_{0.78}Cu_{1.22}CeTe_4$ showing energy gap at around 0.27 eV.

4.4. Conclusions

The AMRETe₄ together with the RETe₃ are excellent model systems for fundamental studies of CDW distortions because their structures are simple and exhibit a wave modulation along a single axis direction. The results reported here suggest that interactions along the third, cross-plane dimension in the quasi-two dimensional systems of AMRETe₄ and RETe₃ play an important role on defining the CDW modulations.²⁵ The van der Waals gaps in RETe₃ influence band dispersion which alters the Fermi surface nesting thereby changing the CDW character. In this regard the van der Waals gaps in RETe₃ are not simple “innocent” spacers. Thus, we would expect the application of pressure to strongly influence these gaps and greatly affect and even suppress the CDW.

Table 4.3. Crystal data and structure refinement for undistorted (no CDW) KCuCeTe₄.

Empirical formula	KCuCeTe ₄
Formula weight	753.16
Temperature	100.0(3) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P4/nmm
Unit cell dimensions	a = 4.4142(6) Å, α = 90.00° b = 4.4142(6) Å, β = 90.00° c = 21.086(4) Å, γ = 90.00°
Volume	410.86(11) Å ³
Z	2
Density (calculated)	6.088 g/cm ³
Absorption coefficient	22.378 mm ⁻¹
F(000)	628
Crystal size	0.15 x 0.10 x 0.01 mm ³
Theta range for data collection	4.72 to 29.06°
Index ranges	-5 ≤ h ≤ 6, -5 ≤ k ≤ 5, -28 ≤ l ≤ 28
Reflections collected	2548
Independent reflections	379 [R _{int} = 0.0831]
Completeness to θ = 29.06°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	379 / 0 / 20
Goodness-of-fit on F ²	1.097
Final R indices [>2σ(I)]	R _{obs} = 0.0274, wR _{obs} = 0.0600
R indices (all data)	R _{all} = 0.0294, wR _{all} = 0.0610
Extinction coefficient	0.0031(6)
Largest diff. peak and hole	2.534 and -1.773 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and}$ $w = 1 / [\sigma^2(F_o^2) + (0.0199P)^2 + 6.3438P] \text{ where } P = (F_o^2 + 2F_c^2) / 3$	

Table 4.4. Crystal data and structure refinement for KAgCeTe₄ at 100 K.

Empirical formula	KAgCeTe ₄
Formula weight	797.5
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.4445(9) Å, α = 90° b = 4.4800(8) Å, β = 90° c = 21.398(4) Å, γ = 90°
q-vector	0.3358(10)b* + 1/2c*
Volume	426.07(14) Å ³
Z	2
Density (calculated)	6.214 g/cm ³
Absorption coefficient	21.391 mm ⁻¹
F(000)	664
Crystal size	0.40 x 0.06 x 0.01 mm ³
Theta range for data collection	1.59 to 29.30°
Index ranges	-6<=h<=6, -6<=k<=5, -29<=l<=29, -1<=m<=1
Reflections collected	9881 (2694 main + 7187 satellites)
Independent reflections	5312 (1698 main + 3614 satellites) [R _{int} = 0.1072]
Completeness to θ = 29.30°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5312 / 0 / 193
Goodness-of-fit on F ²	2.50
Final R indices [I>2σ(I)]	R _{obs} = 0.0916, wR _{obs} = 0.2164
R indices (all data)	R _{all} = 0.1461, wR _{all} = 0.2260
Final R main indices [I>2σ(I)]	R _{obs} = 0.0824, wR _{obs} = 0.2104
R main indices (all data)	R _{all} = 0.0923, wR _{all} = 0.2142
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1411, wR _{obs} = 0.2498
R 1 st order satellites (all data)	R _{all} = 0.3183, wR _{all} = 0.2855
Extinction coefficient	0.00085(8)
T _{min} and T _{max} coefficients	0.1676 and 0.9143
Largest diff. peak and hole	8.25 and -7.74 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w=1/(σ ² (I)+0.0016I ²)	

Table 4.5. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce[1]	0	0	5000	4010	1	22(1)
	sin, 1	-89(8)	-3(4)	2(2)		
	cos, 1	-28(3)	8(11)	1(1)		
Ce[2]	0	5013(5)	0	5934(1)	1	15(1)
	sin, 1	101(8)	-2(3)	1(2)		
	cos, 1	-31(2)	-8(10)	0(1)		
Te[1]	0	5250(9)	0	9169(2)	1	27(1)
	sin, 1	-13(3)	-12(12)	0(1)		
	cos, 1	49(10)	-3(3)	-1(3)		
Te[2]	0	272(9)	5000	783(3)	1	32(1)
	sin, 1	1(2)	5(13)	0(1)		
	cos, 1	3(9)	-1(3)	1(3)		
Te[3]	0	5016(10)	0	4406(3)	1	21(1)
	sin, 1	-10(9)	3(2)	-3(3)		
	cos, 1	-2(2)	-13(12)	0(1)		
Te[4]	0	10022(10)	5000	5529(2)	1	15(1)
	sin, 1	-40(10)	1(2)	2(3)		
	cos, 1	7(2)	5(12)	0(1)		
Te[5]	0	5144(11)	5000	2833(2)	1	25(1)
	sin, 1	-216(11)	44(12)	-5(3)		
	cos, 1	-175(9)	-55(15)	-4(2)		
Te[6]	0	113(12)	0	2826(2)	1	27(1)
	sin, 1	217(12)	-38(13)	-1(3)		
	cos, 1	177(10)	47(15)	-1(2)		
Te[7]	0	5117(13)	5000	7112(3)	1	24(1)
	sin, 1	-386(9)	-42(12)	1(3)		
	cos, 1	301(7)	-54(16)	-1(2)		
Te[8]	0	159(12)	0	7111(3)	1	21(1)
	sin, 1	297(8)	78(11)	-7(3)		
	cos, 1	-232(7)	100(14)	5(2)		

Table 4.5. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

K[1]	0	5325(20)	0	1441(6)	1	24(3)
	sin, 1	50(13)	-15(40)	10(4)		
	cos, 1	105(30)	11(17)	21(8)		
K[2]	0	345(20)	5000	8454(5)	1	24(3)
	sin, 1	15(20)	55(40)	8(4)		
	cos, 1	-5(40)	35(20)	-15(8)		
Ag[1]	0	322(13)	0	9967(3)	1	32(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Ag[2]	0	5306(12)	5000	9961(3)	1	30(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.6. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce[1]	0	27(1)	23(2)	16(1)	0	-3(1)	0
	sin, 1	-1(2)	-2(3)	2(2)	-1(1)	0(2)	0(1)
	cos, 1	0(1)	0(1)	1(1)	3(1)	0(1)	1(2)
Ce[2]	0	5(1)	6(1)	35(1)	0	-1(1)	0
	sin, 1	2(2)	1(2)	-4(3)	1(1)	1(2)	0(1)
	cos, 1	0(1)	0(1)	1(1)	2(1)	0(1)	0(2)
Te[1]	0	25(2)	25(2)	31(2)	0	0(1)	0
	sin, 1	0(1)	1(1)	-1(1)	-4(2)	0(1)	0(2)
	cos, 1	-1(2)	-3(3)	3(3)	-1(1)	-1(2)	0(1)
Te[2]	0	27(2)	28(2)	41(2)	0	-5(1)	0
	sin, 1	0(1)	0(1)	1(1)	2(2)	0(1)	0(3)
	cos, 1	2(2)	-1(3)	3(4)	-1(1)	-2(2)	0(1)
Te[3]	0	16(1)	17(2)	31(2)	0	-1(1)	0
	sin, 1	1(2)	2(3)	-6(3)	0(1)	-1(2)	1(1)
	cos, 1	0(1)	0(1)	-1(1)	-1(1)	0(1)	-3(2)

Table 4.6. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

Te[4]	0	16(1)	13(2)	18(1)	0	-3(1)	0
	sin, 1	-1(2)	-1(3)	4(3)	0(1)	-1(2)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	-2(2)	0(1)	-1(2)
Te[5]	0	44(2)	22(2)	9(1)	0	-3(1)	0
	sin, 1	8(3)	0(3)	-10(2)	-4(2)	-2(2)	4(2)
	cos, 1	6(2)	0(3)	-8(2)	5(2)	-2(2)	-4(2)
Te[6]	0	47(2)	27(2)	6(1)	0	-4(1)	0
	sin, 1	-6(3)	-3(4)	-1(2)	-8(2)	-4(2)	4(2)
	cos, 1	-5(2)	-2(3)	-1(2)	10(2)	-3(2)	-4(2)
Te[7]	0	9(1)	13(2)	49(2)	0	-1(1)	0
	sin, 1	8(2)	1(3)	-1(3)	-3(1)	-2(2)	1(2)
	cos, 1	-6(2)	0(2)	1(2)	-4(2)	2(2)	2(3)
Te[8]	0	10(1)	11(2)	44(2)	0	-2(1)	0
	sin, 1	-4(2)	0(3)	8(3)	5(1)	1(2)	0(2)
	cos, 1	3(2)	0(2)	-6(2)	7(2)	-1(2)	0(2)
K[1]	0	15(4)	18(6)	39(7)	0	3(3)	0
	sin, 1	-1(2)	3(4)	-12(5)	-1(4)	1(2)	-2(7)
	cos, 1	-3(5)	5(8)	-24(10)	0(2)	2(5)	1(3)
K[2]	0	30(5)	30(6)	10(4)	0	2(3)	0
	sin, 1	-4(4)	-7(5)	9(4)	12(6)	0(3)	0(7)
	cos, 1	8(8)	12(10)	-18(7)	7(3)	0(6)	0(4)
Ag[1]	0	35(2)	31(3)	30(2)	0	-1(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Ag[2]	0	29(2)	27(2)	34(2)	0	1(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0

Table 4.7. Bond lengths distributions [$\text{\AA}$] for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce[1] - Te[3] x 4	3.263(6)	3.237(6)	3.288(6)
Ce[1] - Te[4]	3.252(7)	3.250(9)	3.254(9)
Ce[1] - Te[5]	3.318(7)	3.250(8)	3.385(8)
Ce[1] - Te[5]	3.402(7)	3.361(8)	3.444(8)
Ce[1] - Te[6] x 2	3.383(7)	3.368(7)	3.395(7)
Ce[2] - Te[3]	3.268(8)	3.260(10)	3.276(10)
Ce[2] - Te[4] x 4	3.270(6)	3.230(5)	3.308(5)
Ce[2] - Te[7] x 2	3.377(8)	3.356(9)	3.392(8)
Ce[2] - Te[8]	3.316(8)	3.223(9)	3.412(9)
Ce[2] - Te[8]	3.404(8)	3.338(9)	3.469(9)
Te[1] - K[2] x 2	3.481(17)	3.443(17)	3.520(17)
Te[1] - Ag[1]	2.776(8)	2.758(9)	2.796(9)
Te[1] - Ag[1]	2.827(8)	2.810(9)	2.844(9)
Te[1] - Ag[2] x 2	2.808(6)	2.804(7)	2.813(7)
Te[2] - K[1] x 4	3.442(15)	3.428(15)	3.455(15)
Te[2] - Ag[1] x 2	2.840(7)	2.839(7)	2.842(7)
Te[2] - Ag[2]	2.823(8)	2.821(9)	2.825(9)
Te[2] - Ag[2]	2.846(8)	2.846(9)	2.846(9)
Te[5] - Te[6] x 3	3.166(9)	3.014(9)	3.322(9)
Te[5] - Te[6]	3.147(9)	2.992(9)	3.305(9)
Te[7] - Te[8] x 2	3.145(9)	2.896(9)	3.402(9)
Te[7] - Te[8] x 2	3.176(9)	2.949(9)	3.406(9)
Te[7] - K[2]	3.573(19)	3.47(2)	3.68(2)
Ag[1] - Ag[2] x 4	3.160(6)	3.160(6)	3.160(6)

Table 4.8. Bond angles distributions [$^\circ$] for KAgCeTe_4 at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[3] - Ce[1] - Te[3] x 2	86.73(13)	85.64(14)	87.81(14)
Te[3] - Ce[1] - Te[3] x 4	85.70(14)	85.50(16)	85.91(16)
Te[3] - Ce[1] - Te[3] x 4	149.9(2)	149.6(2)	150.2(2)
Te[3] - Ce[1] - Te[4] x 4	75.04(16)	74.71(16)	75.37(16)

Table 4.8. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Ce[1] - Te[5] x 2	75.87(17)	75.40(15)	76.36(16)
Te[3] - Ce[1] - Te[5] x 2	130.46(18)	129.39(17)	131.52(17)
Te[3] - Ce[1] - Te[6] x 2	75.55(17)	73.81(17)	77.24(17)
Te[3] - Ce[1] - Te[6] x 2	131.26(19)	128.77(16)	133.73(17)
Te[3] - Ce[1] - Te[3] x 2	86.39(12)	85.72(14)	87.07(14)
Te[3] - Ce[1] - Te[5] x 2	129.82(18)	129.13(18)	130.48(18)
Te[3] - Ce[1] - Te[5] x 2	74.60(16)	74.04(17)	75.15(17)
Te[3] - Ce[1] - Te[6] x 2	74.36(17)	72.67(18)	76.09(18)
Te[3] - Ce[1] - Te[6] x 2	129.61(18)	126.92(17)	132.30(17)
Te[4] - Ce[1] - Te[5]	139.58(18)	139.1(2)	140.0(2)
Te[4] - Ce[1] - Te[5]	137.61(17)	136.8(2)	138.4(2)
Te[4] - Ce[1] - Te[6] x 2	138.46(17)	138.12(13)	138.83(16)
Te[5] - Ce[1] - Te[5] x 2	82.80(19)	82.4(2)	83.2(2)
Te[5] - Ce[1] - Te[6] x 2	56.04(17)	53.41(17)	58.63(17)
Te[5] - Ce[1] - Te[6] x 2	55.63(17)	53.11(17)	58.20(17)
Te[6] - Ce[1] - Te[6] x 2	82.97(17)	82.12(18)	83.72(18)
Te[3] - Ce[2] - Te[4] x 4	74.67(17)	74.19(17)	75.17(18)
Te[3] - Ce[2] - Te[7] x 2	138.25(17)	137.96(14)	138.77(16)
Te[3] - Ce[2] - Te[8]	139.46(19)	139.0(2)	139.9(2)
Te[3] - Ce[2] - Te[8]	137.74(19)	136.9(2)	138.6(2)
Te[4] - Ce[2] - Te[4] x 4	86.50(14)	85.21(14)	87.83(15)
Te[4] - Ce[2] - Te[4] x 4	85.56(14)	85.48(14)	85.66(14)
Te[4] - Ce[2] - Te[4] x 4	149.3(2)	149.2(2)	149.46(19)
Te[4] - Ce[2] - Te[7] x 2	75.61(17)	72.76(18)	78.48(18)
Te[4] - Ce[2] - Te[7] x 2	131.41(19)	127.50(19)	135.3(2)
Te[4] - Ce[2] - Te[8] x 2	76.10(17)	75.07(15)	77.11(16)
Te[4] - Ce[2] - Te[8] x 2	130.69(17)	129.26(16)	132.09(16)
Te[4] - Ce[2] - Te[7] x 2	74.56(17)	71.87(18)	77.22(18)
Te[4] - Ce[2] - Te[7] x 2	129.99(19)	125.88(19)	134.0(2)
Te[4] - Ce[2] - Te[8] x 2	129.98(17)	128.59(18)	131.37(18)
Te[4] - Ce[2] - Te[8] x 2	74.85(16)	73.91(17)	75.82(17)
Te[7] - Ce[2] - Te[7] x 2	83.3(2)	82.4(2)	83.9(2)
Te[7] - Ce[2] - Te[8] x 4	56.02(17)	51.65(16)	60.46(17)
Te[8] - Ce[2] - Te[8] x 2	82.8(2)	82.4(2)	83.1(2)

Table 4.8. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 100 K with e.s.d.'s in parentheses.

K[2] - Te[1] - K[2] x 2	80.1(4)	80.1(4)	80.1(4)
K[2] - Te[1] - K[2] x 2	78.6(4)	78.0(4)	79.2(4)
K[2] - Te[1] - K[2] x 2	128.2(4)	128.0(4)	128.4(4)
K[2] - Te[1] - Ag[1] x 2	77.1(3)	76.6(3)	77.5(3)
K[2] - Te[1] - Ag[1] x 2	139.9(3)	139.3(3)	140.5(3)
K[2] - Te[1] - Ag[2] x 2	76.0(3)	75.3(3)	76.7(3)
K[2] - Te[1] - Ag[2] x 2	141.6(3)	141.1(3)	142.1(3)
Ag[1] - Te[1] - Ag[1] x 2	105.0(3)	104.9(3)	105.0(3)
Ag[1] - Te[1] - Ag[2] x 2	68.68(18)	68.39(19)	68.96(19)
Ag[1] - Te[1] - Ag[2] x 2	68.22(18)	67.99(19)	68.4(2)
Ag[2] - Te[1] - Ag[2] x 2	105.8(3)	105.8(3)	105.9(3)
K[1] - Te[2] - K[1] x 4	81.2(4)	81.1(4)	81.3(4)
K[1] - Te[2] - K[1] x 4	80.0(3)	79.4(3)	80.7(3)
K[1] - Te[2] - K[1] x 4	131.9(5)	131.0(5)	132.8(5)
K[1] - Te[2] - Ag[1] x 4	75.1(3)	74.7(3)	75.6(3)
K[1] - Te[2] - Ag[1] x 2	140.4(3)	139.3(3)	141.4(3)
K[1] - Te[2] - Ag[2] x 2	75.8(3)	74.7(3)	77.0(3)
K[1] - Te[2] - Ag[2] x 4	139.1(3)	138.9(3)	139.3(3)
K[1] - Te[2] - Ag[1] x 2	138.9(3)	138.7(3)	139.2(3)
K[1] - Te[2] - Ag[2] x 2	75.1(3)	75.0(3)	75.1(3)
Ag[1] - Te[2] - Ag[1] x 2	104.1(3)	104.1(3)	104.2(3)
Ag[1] - Te[2] - Ag[2] x 2	67.84(19)	67.80(19)	67.88(19)
Ag[1] - Te[2] - Ag[2] x 2	67.29(19)	67.26(18)	67.31(18)
Ag[2] - Te[2] - Ag[2] x 2	103.3(3)	103.2(3)	103.3(3)
Ce[1] - Te[3] - Ce[1] x 2	86.39(15)	86.02(17)	86.77(17)
Ce[1] - Te[3] - Ce[1] x 4	85.70(12)	85.50(13)	85.91(13)
Ce[1] - Te[3] - Ce[1] x 4	149.9(3)	149.5(3)	150.2(3)
Ce[1] - Te[3] - Ce[2] x 4	105.02(17)	104.50(16)	105.53(16)
Ce[1] - Te[3] - Ce[1] x 2	86.73(15)	86.37(17)	87.07(17)
Ce[1] - Te[4] - Ce[2] x 4	105.19(18)	104.93(18)	105.45(18)
Ce[2] - Te[4] - Ce[2] x 4	86.35(15)	85.32(17)	87.37(17)
Ce[2] - Te[4] - Ce[2] x 4	85.56(12)	85.48(13)	85.66(12)
Ce[2] - Te[4] - Ce[2] x 4	149.3(2)	149.1(2)	149.6(2)
Ce[1] - Te[5] - Ce[1] x 2	82.80(18)	82.42(18)	83.16(18)

Table 4.8. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 100 K with e.s.d.'s in parentheses.

Ce[1] - Te[5] - Te[6] x 2	61.91(18)	60.12(17)	63.72(19)
Ce[1] - Te[5] - Te[6] x 2	118.3(2)	117.7(2)	118.8(2)
Ce[1] - Te[5] - Te[6] x 2	117.5(2)	115.9(2)	119.1(2)
Ce[1] - Te[5] - Te[6] x 2	63.06(19)	60.83(18)	65.4(2)
Te[6] - Te[5] - Te[6] x 2	90.2(2)	86.1(2)	94.4(3)
Te[6] - Te[5] - Te[6] x 4	89.4(2)	88.3(2)	90.9(2)
Te[6] - Te[5] - Te[6] x 4	176.8(3)	174.7(3)	179.6(3)
Te[6] - Te[5] - Te[6] x 2	90.9(2)	85.6(2)	96.4(3)
Ce[1] - Te[6] - Ce[1] x 2	82.92(17)	82.59(17)	83.16(18)
Ce[1] - Te[6] - Te[5] x 2	60.90(18)	59.77(18)	62.17(18)
Ce[1] - Te[6] - Te[5] x 2	117.2(2)	114.2(2)	120.3(3)
Ce[1] - Te[6] - Te[5] x 2	62.47(18)	61.67(17)	63.17(18)
Ce[1] - Te[6] - Te[5] x 2	118.4(2)	115.0(2)	121.7(3)
Ce[1] - Te[6] - K[1] x 2	126.8(3)	124.2(3)	129.3(3)
Te[5] - Te[6] - Te[5] x 2	90.9(2)	86.9(2)	95.1(3)
Te[5] - Te[6] - Te[5] x 4	89.4(2)	88.3(2)	90.9(2)
Te[5] - Te[6] - Te[5] x 4	176.8(3)	174.6(3)	179.5(3)
Te[5] - Te[6] - K[1] x 2	66.1(3)	64.0(3)	68.2(3)
Te[5] - Te[6] - Te[5] x 2	90.3(2)	84.8(2)	95.8(3)
Te[5] - Te[6] - K[1] x 2	114.5(3)	113.9(3)	115.0(3)
Ce[2] - Te[7] - Ce[2] x 2	83.1(2)	82.9(2)	83.3(2)
Ce[2] - Te[7] - Te[8] x 2	60.9(2)	59.20(18)	62.9(2)
Ce[2] - Te[7] - Te[8] x 2	117.6(3)	112.7(3)	122.3(3)
Ce[2] - Te[7] - Te[8] x 2	62.5(2)	61.22(19)	63.5(2)
Ce[2] - Te[7] - Te[8] x 2	118.5(3)	112.7(3)	124.3(3)
Ce[2] - Te[7] - K[2] x 4	126.3(4)	121.3(3)	131.1(4)
Te[8] - Te[7] - Te[8] x 2	91.3(2)	84.9(2)	98.0(3)
Te[8] - Te[7] - Te[8] x 4	89.2(2)	87.6(2)	91.5(2)
Te[8] - Te[7] - Te[8] x 4	174.9(3)	171.5(3)	180
Te[8] - Te[7] - K[2] x 2	65.5(3)	61.7(3)	69.3(4)
Te[8] - Te[7] - K[2] x 2	116.0(4)	114.3(4)	117.9(4)
Te[8] - Te[7] - Te[8] x 2	90.2(2)	81.5(2)	99.4(3)
Te[8] - Te[7] - K[2] x 2	114.6(4)	114.1(4)	114.9(4)
Te[8] - Te[7] - K[2] x 2	63.7(3)	60.2(3)	67.4(4)

Table 4.8. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 100 K with e.s.d.'s in parentheses.

K[2] - Te[7] - K[2]	75.3(4)	74.4(4)	76.0(4)
Ce[2] - Te[8] - Ce[2] x 2	82.8(2)	82.4(2)	83.1(2)
Ce[2] - Te[8] - Te[7] x 2	61.7(2)	59.14(18)	64.4(2)
Ce[2] - Te[8] - Te[7] x 2	118.0(3)	117.1(3)	118.7(3)
Ce[2] - Te[8] - K[2] x 2	126.7(3)	123.6(3)	129.9(3)
Ce[2] - Te[8] - Te[7] x 2	117.3(3)	114.3(3)	120.1(3)
Ce[2] - Te[8] - Te[7] x 2	63.0(2)	59.51(18)	66.7(2)
Ce[2] - Te[8] - K[2] x 2	125.8(3)	122.2(3)	129.4(3)
Te[7] - Te[8] - Te[7] x 2	90.2(2)	84.0(2)	96.8(3)
Te[7] - Te[8] - Te[7] x 4	89.2(2)	87.6(2)	91.5(2)
Te[7] - Te[8] - Te[7] x 4	175.2(3)	172.3(3)	179.8(3)
Te[7] - Te[8] - K[2] x 2	65.1(3)	63.0(3)	67.4(3)
Te[7] - Te[8] - K[2] x 2	116.7(4)	112.4(3)	121.1(4)
Te[7] - Te[8] - Te[7] x 2	91.3(2)	83.5(2)	99.2(3)
Te[7] - Te[8] - K[2] x 2	62.9(3)	62.5(3)	63.4(3)
Te[7] - Te[8] - K[2] x 2	114.9(4)	111.4(3)	118.3(4)
Te[2] - K[1] - Te[2] x 6	80.4(3)	79.0(4)	81.9(4)
Te[2] - K[1] - Te[2] x 4	131.9(6)	130.4(6)	133.3(7)
Te[2] - K[1] - Te[6] x 2	135.0(5)	133.7(4)	136.3(4)
Te[2] - K[1] - Te[2] x 2	81.2(4)	80.8(4)	81.6(4)
Te[2] - K[1] - Te[6] x 2	87.7(3)	87.5(3)	87.9(3)
Te[1] - K[2] - Te[1] x 2	78.6(3)	78.0(3)	79.2(3)
Te[1] - K[2] - Te[1] x 2	128.2(5)	127.1(5)	129.3(5)
Te[1] - K[2] - Te[1] x 2	80.1(4)	79.3(4)	80.9(4)
Te[1] - K[2] - Te[7] x 2	137.4(5)	136.2(5)	138.5(5)
Te[1] - K[2] - Te[7] x 2	89.0(4)	86.7(4)	91.3(5)
Te[1] - K[2] - Te[8] x 2	88.0(4)	86.9(4)	89.1(4)
Te[1] - K[2] - Te[8] x 2	139.1(5)	136.3(4)	142.0(5)
Te[7] - K[2] - Te[7]	75.3(4)	74.4(4)	76.0(4)
Te[7] - K[2] - Te[8] x 2	51.6(3)	47.9(3)	55.4(3)
Te[1] - Ag[1] - Te[1] x 2	105.0(3)	104.9(3)	105.0(3)
Te[1] - Ag[1] - Te[2] x 2	111.40(19)	111.23(18)	111.58(19)
Te[1] - Ag[1] - Ag[2] x 2	55.60(16)	55.42(16)	55.79(16)
Te[1] - Ag[1] - Ag[2] x 4	123.93(19)	123.74(19)	124.11(19)

Table 4.8. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Ag[1] - Te[2] x 2	112.58(19)	112.40(18)	112.76(18)
Te[1] - Ag[1] - Ag[2] x 2	56.14(16)	55.97(16)	56.30(16)
Te[2] - Ag[1] - Te[2] x 2	104.1(3)	104.1(3)	104.1(3)
Te[2] - Ag[1] - Ag[2] x 2	55.81(16)	55.78(16)	55.85(16)
Te[2] - Ag[1] - Ag[2] x 2	123.8(2)	123.8(2)	123.8(2)
Te[2] - Ag[1] - Ag[2] x 2	56.44(16)	56.43(16)	56.46(16)
Te[2] - Ag[1] - Ag[2] x 2	124.7(3)	124.6(3)	124.7(3)
Ag[2] - Ag[1] - Ag[2] x 2	90.27(18)	90.27(18)	90.27(18)
Ag[2] - Ag[1] - Ag[2] x 4	89.54(10)	89.54(10)	89.54(10)
Ag[2] - Ag[1] - Ag[2] x 4	179.5(3)	179.5(3)	179.5(3)
Ag[2] - Ag[1] - Ag[2] x 2	90.64(18)	90.64(18)	90.64(18)
Te[1] - Ag[2] - Te[1] x 2	105.8(3)	105.7(3)	106.0(3)
Te[1] - Ag[2] - Te[2] x 2	111.5(2)	111.0(2)	111.9(2)
Te[1] - Ag[2] - Te[2] x 2	112.5(2)	112.2(2)	112.8(2)
Te[1] - Ag[2] - Ag[1] x 2	55.18(16)	54.78(17)	55.60(17)
Te[1] - Ag[2] - Ag[1] x 2	124.3(2)	123.9(3)	124.7(3)
Te[1] - Ag[2] - Ag[1] x 2	56.18(16)	55.80(17)	56.55(17)
Te[1] - Ag[2] - Ag[1] x 2	125.0(2)	124.6(3)	125.4(3)
Te[2] - Ag[2] - Te[2] x 2	103.3(3)	103.2(3)	103.3(3)
Te[2] - Ag[2] - Ag[1] x 4	56.27(16)	56.23(18)	56.31(18)
Te[2] - Ag[2] - Ag[1] x 4	123.5(2)	123.5(2)	123.5(2)
Ag[1] - Ag[2] - Ag[1] x 2	90.64(17)	90.64(17)	90.64(17)
Ag[1] - Ag[2] - Ag[1] x 4	89.54(10)	89.54(10)	89.54(10)
Ag[1] - Ag[2] - Ag[1] x 4	179.5(3)	179.5(3)	179.5(3)
Ag[1] - Ag[2] - Ag[1] x 2	90.27(17)	90.27(17)	90.27(17)

Table 4.9. Crystal data and structure refinement for KAgCeTe₄ at 300 K.

Empirical formula	KAgCeTe ₄
Formula weight	797.5
Temperature	300.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	$a = 4.4657(9) \text{ Å}, \alpha = 90^\circ$ $b = 4.4927(8) \text{ Å}, \beta = 90^\circ$ $c = 21.525(4) \text{ Å}, \gamma = 90^\circ$
q-vector	$0.3381(8)b^* + 1/2c^*$
Volume	$431.85(14) \text{ Å}^3$
Z	2
Density (calculated)	6.131 g/cm^3
Absorption coefficient	21.104 mm^{-1}
F(000)	664
Crystal size	$0.37 \times 0.15 \times 0.04 \text{ mm}^3$
Theta range for data collection	1.89 to 29.24°
Index ranges	$-6 \leq h \leq 6, -6 \leq k \leq 5, -29 \leq l \leq 29, -1 \leq m \leq 1$
Reflections collected	9810 (2577 main + 7233 satellites)
Independent reflections	5326 (1657 main + 3669 satellites) [$R_{\text{int}} = 0.0890$]
Completeness to $\theta = 29.24^\circ$	96%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5326 / 0 / 193
Goodness-of-fit on F^2	2.13
Final R indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0800, wR_{\text{obs}} = 0.1818$
R indices (all data)	$R_{\text{all}} = 0.1367, wR_{\text{all}} = 0.1943$
Final R main indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0715, wR_{\text{obs}} = 0.1767$
R main indices (all data)	$R_{\text{all}} = 0.0818, wR_{\text{all}} = 0.1821$
Final R 1 st order satellites [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.1239, wR_{\text{obs}} = 0.2077$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.3094, wR_{\text{all}} = 0.2507$
Extinction coefficient	$0.00081(8)$
T _{min} and T _{max} coefficients	0.0271 and 0.1176
Largest diff. peak and hole	7.55 and -4.17 e.Å^{-3}
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.10. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KAgCeTe_4 at 300 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce[1]	0	0	5000	4010	1	23(1)
	sin, 1	-98(6)	2(3)	3(2)		
	cos, 1	-32(2)	-7(9)	1(1)		
Ce[2]	0	5004(4)	0	5924(1)	1	21(1)
	sin, 1	75(7)	-2(3)	4(2)		
	cos, 1	-22(2)	-7(8)	-1(1)		
Te[1]	0	5214(9)	0	9168(3)	1	37(1)
	sin, 1	-11(2)	-7(11)	0(1)		
	cos, 1	43(8)	-2(3)	-2(3)		
Te[2]	0	229(9)	5000	774(3)	1	40(1)
	sin, 1	4(2)	2(11)	0(1)		
	cos, 1	14(8)	0(3)	1(3)		
Te[3]	0	5015(9)	0	4412(2)	1	23(1)
	sin, 1	17(7)	0(2)	1(2)		
	cos, 1	3(1)	-1(9)	0(1)		
Te[4]	0	10014(9)	5000	5529(2)	1	20(1)
	sin, 1	6(8)	0(2)	0(2)		
	cos, 1	-1(1)	-3(10)	0(1)		
Te[5]	0	5118(10)	5000	2839(2)	1	30(1)
	sin, 1	-206(8)	42(10)	-6(2)		
	cos, 1	-167(7)	-52(12)	-5(2)		
Te[6]	0	110(11)	0	2837(2)	1	31(1)
	sin, 1	196(8)	-35(10)	-1(2)		
	cos, 1	158(7)	43(12)	-1(2)		
Te[7]	0	5100(12)	5000	7108(3)	1	28(1)
	sin, 1	-409(7)	-49(11)	-6(2)		
	cos, 1	319(6)	-63(14)	5(2)		
Te[8]	0	133(11)	0	7101(3)	1	28(1)
	sin, 1	298(7)	67(10)	-11(2)		
	cos, 1	-231(6)	86(13)	9(2)		

Table 4.10. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KAgCeTe_4 at 300 K with e.s.d.'s in parentheses.

K[1]	0	5255(20)	0	1458(7)	1	37(4)
	sin, 1	-24(11)	25(30)	6(4)		
	cos, 1	-45(20)	-12(16)	12(7)		
K[2]	0	275(30)	5000	8462(6)	1	35(3)
	sin, 1	-118(19)	15(40)	4(4)		
	cos, 1	235(40)	15(20)	-8(7)		
Ag[1]	0	286(12)	0	9963(3)	1	46(2)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Ag[2]	0	5275(12)	5000	9954(3)	1	42(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.11. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KAgCeTe_4 at 300 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce[1]	0	25(1)	20(2)	24(1)	0	-1(1)	0
	sin, 1	-1(1)	-1(2)	4(2)	0(1)	1(1)	0(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	0(1)	1(2)
Ce[2]	0	14(1)	12(1)	36(1)	0	0(1)	0
	sin, 1	0(1)	0(2)	-3(2)	0(1)	3(1)	1(1)
	cos, 1	0(1)	0(1)	1(1)	-1(1)	-1(1)	2(2)
Te[1]	0	31(1)	30(2)	49(2)	0	5(1)	0
	sin, 1	1(1)	0(1)	-1(1)	-2(2)	0(1)	0(2)
	cos, 1	-2(2)	-1(3)	4(3)	0(1)	-1(2)	0(1)
Te[2]	0	36(2)	35(2)	49(2)	0	-3(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(2)	0(1)	0(2)
	cos, 1	0(2)	1(3)	2(3)	0(1)	-2(2)	0(1)
Te[3]	0	19(1)	20(2)	31(2)	0	1(1)	0
	sin, 1	-1(1)	1(2)	-2(2)	0(1)	-2(2)	0(1)
	cos, 1	0(1)	0(1)	0(1)	-1(1)	0(1)	-1(2)

Table 4.11. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KAgCeTe_4 at 300 K with e.s.d.'s in parentheses.

Te[4]	0	20(1)	12(2)	28(2)	0	-1(1)	0
	sin, 1	2(1)	0(2)	4(2)	0(1)	1(2)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	1(1)	0(1)	-1(2)
Te[5]	0	41(2)	30(2)	20(1)	0	1(1)	0
	sin, 1	7(2)	5(3)	-5(2)	1(1)	1(2)	3(1)
	cos, 1	6(2)	4(2)	-4(2)	-1(2)	1(1)	-4(2)
Te[6]	0	46(2)	29(2)	17(1)	0	-1(1)	0
	sin, 1	-5(2)	3(3)	3(2)	-5(1)	2(2)	3(1)
	cos, 1	-4(2)	3(2)	2(2)	7(2)	1(1)	-4(2)
Te[7]	0	17(1)	19(2)	49(2)	0	-1(1)	0
	sin, 1	5(2)	-4(2)	7(3)	-6(1)	-5(2)	3(2)
	cos, 1	-4(1)	3(2)	-5(2)	-8(2)	4(1)	4(2)
Te[8]	0	25(1)	14(2)	44(2)	0	-2(1)	0
	sin, 1	-6(2)	-4(2)	12(3)	2(1)	2(2)	4(1)
	cos, 1	4(2)	3(2)	-9(2)	3(1)	-2(1)	5(2)
K[1]	0	26(5)	29(6)	57(7)	0	-3(4)	0
	sin, 1	3(2)	-4(4)	-5(5)	3(4)	-2(2)	0(7)
	cos, 1	7(5)	-8(8)	-10(9)	-2(2)	-4(5)	0(3)
K[2]	0	43(6)	41(8)	22(4)	0	10(4)	0
	sin, 1	10(4)	9(5)	-1(4)	-2(6)	6(3)	-2(6)
	cos, 1	-19(8)	-17(10)	2(7)	-1(3)	-12(6)	-1(3)
Ag[1]	0	45(2)	47(3)	47(2)	0	6(2)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Ag[2]	0	40(2)	36(3)	52(3)	0	-2(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0

Table 4.12. Bond lengths distributions [Å] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce[1] - Te[3] x 4	3.279(5)	3.244(5)	3.314(5)
Ce[1] - Te[4]	3.270(6)	3.265(8)	3.276(8)
Ce[1] - Te[5]	3.332(6)	3.267(7)	3.398(7)
Ce[1] - Te[5]	3.402(6)	3.372(7)	3.433(7)
Ce[1] - Te[6] x 2	3.381(6)	3.364(6)	3.396(6)
Ce[2] - Te[3]	3.254(7)	3.247(8)	3.261(8)
Ce[2] - Te[4] x 4	3.276(5)	3.250(5)	3.302(5)
Ce[2] - Te[7] x 2	3.403(7)	3.378(7)	3.427(7)
Ce[2] - Te[8]	3.339(7)	3.224(8)	3.458(8)
Ce[2] - Te[8]	3.418(7)	3.359(8)	3.478(7)
Te[1] - K[2] x 4	3.497(17)	3.436(17)	3.559(17)
Te[1] - Ag[1]	2.788(8)	2.770(9)	2.806(9)
Te[1] - Ag[1]	2.839(8)	2.826(9)	2.853(9)
Te[1] - Ag[2] x 2	2.813(7)	2.809(7)	2.816(7)
Te[2] - K[1] x 4	3.487(15)	3.455(15)	3.518(15)
Te[2] - Ag[1] x 2	2.845(7)	2.844(7)	2.845(7)
Te[2] - Ag[2]	2.830(8)	2.824(9)	2.836(9)
Te[2] - Ag[2]	2.862(8)	2.858(9)	2.867(9)
Te[5] - Te[6] x 4	3.170(8)	3.029(8)	3.316(8)
Te[7] - Te[8] x 2	3.160(8)	2.907(8)	3.422(8)
Te[7] - Te[8] x 2	3.185(8)	2.946(8)	3.427(8)
Ag[1] - Ag[2] x 4	3.171(5)	3.171(5)	3.171(5)

Table 4.13. Bond angles distributions [°] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[3] - Ce[1] - Te[3] x 4	86.50(10)	85.33(11)	87.67(12)
Te[3] - Ce[1] - Te[3] x 4	85.69(12)	85.60(13)	85.79(13)
Te[3] - Ce[1] - Te[3] x 4	149.43(18)	149.24(18)	149.59(17)
Te[3] - Ce[1] - Te[4] x 4	74.78(13)	74.24(13)	75.31(13)
Te[3] - Ce[1] - Te[5] x 2	75.85(14)	75.40(14)	76.28(14)
Te[3] - Ce[1] - Te[5] x 4	130.66(14)	129.74(14)	131.57(14)

Table 4.13. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

Te[3] - Ce[1] - Te[6] x 2	75.62(14)	74.00(14)	77.21(14)
Te[3] - Ce[1] - Te[6] x 2	131.47(15)	129.15(14)	133.77(14)
Te[3] - Ce[1] - Te[5] x 2	74.78(14)	74.35(15)	75.21(14)
Te[3] - Ce[1] - Te[6] x 2	74.47(14)	72.95(15)	76.02(15)
Te[3] - Ce[1] - Te[6] x 2	129.85(15)	127.17(14)	132.52(14)
Te[4] - Ce[1] - Te[5]	139.25(15)	139.07(17)	139.44(16)
Te[4] - Ce[1] - Te[5]	137.69(14)	137.38(16)	138.00(16)
Te[4] - Ce[1] - Te[6] x 2	138.27(13)	137.91(12)	138.71(14)
Te[5] - Ce[1] - Te[5] x 2	83.06(15)	82.56(16)	83.55(16)
Te[5] - Ce[1] - Te[6] x 4	56.30(14)	53.91(14)	58.64(14)
Te[6] - Ce[1] - Te[6] x 2	83.32(14)	82.49(15)	84.06(15)
Te[3] - Ce[2] - Te[4] x 4	75.04(15)	74.66(15)	75.42(15)
Te[3] - Ce[2] - Te[7] x 2	138.51(14)	137.96(13)	139.10(12)
Te[3] - Ce[2] - Te[8]	139.47(16)	138.69(18)	140.30(18)
Te[3] - Ce[2] - Te[8]	137.81(16)	136.22(18)	139.48(18)
Te[4] - Ce[2] - Te[4] x 4	86.57(12)	85.78(12)	87.38(13)
Te[4] - Ce[2] - Te[4] x 4	85.83(12)	85.71(12)	85.95(12)
Te[4] - Ce[2] - Te[4] x 4	149.98(19)	149.7(2)	150.3(2)
Te[4] - Ce[2] - Te[7] x 2	75.48(15)	72.39(16)	78.61(16)
Te[4] - Ce[2] - Te[7] x 2	130.95(17)	127.19(16)	134.69(17)
Te[4] - Ce[2] - Te[8] x 2	75.76(15)	74.80(14)	76.74(14)
Te[4] - Ce[2] - Te[8] x 4	130.41(15)	128.92(14)	131.86(14)
Te[4] - Ce[2] - Te[7] x 2	74.55(15)	71.81(16)	77.29(16)
Te[4] - Ce[2] - Te[7] x 2	129.67(17)	125.38(16)	133.88(17)
Te[4] - Ce[2] - Te[8] x 2	74.64(14)	73.42(15)	75.89(15)
Te[7] - Ce[2] - Te[7] x 2	82.83(16)	81.43(17)	83.87(17)
Te[7] - Ce[2] - Te[8] x 4	55.85(15)	51.70(14)	60.07(14)
Te[8] - Ce[2] - Te[8] x 2	82.70(17)	81.83(18)	83.49(18)
K[2] - Te[1] - K[2] x 8	80.0(4)	79.3(4)	80.7(4)
K[2] - Te[1] - K[2] x 4	128.7(4)	127.7(4)	129.7(4)
K[2] - Te[1] - Ag[1] x 4	76.6(3)	75.3(3)	78.0(4)
K[2] - Te[1] - Ag[1] x 4	139.9(3)	139.3(3)	140.6(3)
K[2] - Te[1] - Ag[2] x 4	75.8(3)	75.5(3)	76.1(3)
K[2] - Te[1] - Ag[2] x 2	141.4(3)	140.0(3)	142.7(4)

Table 4.13. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

K[2] - Te[1] - Ag[2] x 2	139.6(3)	138.4(3)	140.7(4)
Ag[1] - Te[1] - Ag[1] x 2	105.0(3)	104.9(3)	105.2(3)
Ag[1] - Te[1] - Ag[2] x 4	68.80(19)	68.52(19)	69.07(19)
Ag[2] - Te[1] - Ag[2] x 2	106.0(3)	105.9(3)	106.1(3)
K[1] - Te[2] - K[1] x 8	80.2(3)	80.0(3)	80.4(3)
K[1] - Te[2] - K[1] x 4	130.1(4)	129.8(4)	130.5(4)
K[1] - Te[2] - Ag[1] x 4	75.9(3)	75.5(3)	76.3(3)
K[1] - Te[2] - Ag[1] x 4	140.7(3)	140.5(3)	140.9(3)
K[1] - Te[2] - Ag[2] x 4	76.4(3)	76.3(3)	76.5(3)
K[1] - Te[2] - Ag[2] x 4	139.7(3)	139.3(3)	140.1(3)
Ag[1] - Te[2] - Ag[1] x 2	104.3(3)	104.3(3)	104.4(3)
Ag[1] - Te[2] - Ag[2] x 4	67.95(19)	67.86(19)	68.04(19)
Ag[2] - Te[2] - Ag[2] x 2	103.4(3)	103.3(3)	103.4(3)
Ce[1] - Te[3] - Ce[1] x 8	86.19(12)	85.61(14)	86.78(14)
Ce[1] - Te[3] - Ce[1] x 4	149.4(2)	149.2(2)	149.7(2)
Ce[1] - Te[3] - Ce[2] x 4	105.20(14)	104.91(14)	105.48(14)
Ce[1] - Te[4] - Ce[2] x 4	104.91(15)	104.34(16)	105.48(16)
Ce[2] - Te[4] - Ce[2] x 8	86.39(13)	86.02(14)	86.75(15)
Ce[2] - Te[4] - Ce[2] x 4	150.0(2)	149.8(2)	150.2(2)
Ce[1] - Te[5] - Ce[1] x 2	83.06(15)	82.56(15)	83.55(16)
Ce[1] - Te[5] - Te[6] x 4	61.81(15)	60.17(14)	63.46(16)
Ce[1] - Te[5] - Te[6] x 4	118.3(2)	117.8(2)	118.6(2)
Te[6] - Te[5] - Te[6] x 8	90.4(2)	86.54(19)	94.3(2)
Te[6] - Te[5] - Te[6] x 4	177.0(2)	175.3(2)	179.9(2)
Ce[1] - Te[6] - Ce[1] x 2	83.28(14)	83.11(14)	83.38(14)
Ce[1] - Te[6] - Te[5] x 2	61.06(15)	59.95(15)	62.29(15)
Ce[1] - Te[6] - Te[5] x 2	117.4(2)	114.6(2)	120.2(2)
Ce[1] - Te[6] - Te[5] x 2	62.46(15)	61.61(14)	63.24(15)
Ce[1] - Te[6] - Te[5] x 2	118.7(2)	115.5(2)	121.9(2)
Te[5] - Te[6] - Te[5] x 8	90.5(2)	86.88(19)	94.3(2)
Te[5] - Te[6] - Te[5] x 4	177.1(2)	175.4(2)	179.9(3)
Ce[2] - Te[7] - Ce[2] x 2	82.62(17)	81.86(17)	83.11(17)
Ce[2] - Te[7] - Te[8] x 2	60.99(17)	58.98(16)	63.33(17)
Ce[2] - Te[7] - Te[8] x 4	117.2(2)	111.9(2)	122.5(3)

Table 4.13. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

Ce[2] - Te[7] - Te[8] x 2	62.35(17)	61.07(16)	63.42(18)
Ce[2] - Te[7] - K[2] x 4	126.5(3)	122.4(3)	130.5(3)
Te[8] - Te[7] - Te[8] x 4	91.1(2)	84.24(18)	98.3(2)
Te[8] - Te[7] - Te[8] x 4	89.31(19)	87.77(18)	91.53(19)
Te[8] - Te[7] - Te[8] x 4	174.7(3)	171.3(3)	179.4(3)
Te[8] - Te[7] - K[2] x 4	65.7(3)	62.7(3)	68.7(3)
Te[8] - Te[7] - K[2] x 4	115.9(3)	114.1(4)	117.7(3)
Ce[2] - Te[8] - Ce[2] x 2	82.70(18)	81.83(18)	83.49(18)
Ce[2] - Te[8] - Te[7] x 2	61.97(17)	59.08(15)	65.02(18)
Ce[2] - Te[8] - Te[7] x 4	118.1(2)	117.2(2)	118.8(2)
Ce[2] - Te[8] - K[2] x 4	126.8(3)	122.8(3)	130.8(3)
Ce[2] - Te[8] - Te[7] x 2	63.15(17)	59.68(16)	66.80(19)
Te[7] - Te[8] - Te[7] x 8	90.2(2)	84.00(18)	96.8(2)
Te[7] - Te[8] - Te[7] x 4	175.2(2)	172.2(2)	179.7(3)
Te[7] - Te[8] - K[2] x 4	64.9(3)	63.4(3)	66.8(3)
Te[7] - Te[8] - K[2] x 4	116.0(3)	111.2(3)	120.8(3)
Te[2] - K[1] - Te[2] x 8	79.9(3)	79.7(4)	80.0(4)
Te[2] - K[1] - Te[2] x 4	130.1(6)	129.3(6)	130.9(6)
Te[1] - K[2] - Te[1] x 8	79.1(4)	77.0(4)	81.1(4)
Te[1] - K[2] - Te[1] x 4	128.7(5)	128.1(6)	129.3(6)
Te[1] - K[2] - Te[7] x 4	86.6(4)	86.2(4)	86.8(4)
Te[1] - K[2] - Te[7] x 4	136.6(5)	135.1(5)	138.1(5)
Te[1] - K[2] - Te[8] x 4	86.8(4)	83.9(3)	89.5(3)
Te[1] - K[2] - Te[8] x 4	135.8(5)	131.6(5)	140.0(5)
Te[1] - Ag[1] - Te[1] x 2	105.0(3)	104.9(3)	105.2(3)
Te[1] - Ag[1] - Te[2] x 2	111.26(18)	111.04(18)	111.49(18)
Te[1] - Ag[1] - Ag[2] x 4	55.47(16)	55.31(16)	55.64(16)
Te[1] - Ag[1] - Ag[2] x 4	123.9(2)	123.8(2)	124.1(2)
Te[1] - Ag[1] - Te[2] x 2	112.57(18)	112.35(18)	112.78(18)
Te[2] - Ag[1] - Te[2] x 2	104.3(3)	104.3(3)	104.3(3)
Te[2] - Ag[1] - Ag[2] x 4	55.81(16)	55.68(17)	55.93(17)
Te[2] - Ag[1] - Ag[2] x 4	123.8(3)	123.7(3)	123.9(3)
Ag[2] - Ag[1] - Ag[2] x 8	90.22(17)	90.22(17)	90.22(17)
Ag[2] - Ag[1] - Ag[2] x 4	179.3(3)	179.3(3)	179.3(3)

Table 4.13. (Cont'd) Bond angles distributions [°] for KAgCeTe₄ at 300 K with e.s.d.'s in parentheses.

Te[1] - Ag[2] - Te[1] x 2	106.0(3)	105.9(3)	106.1(3)
Te[1] - Ag[2] - Te[2] x 2	111.30(19)	110.9(2)	111.7(2)
Te[1] - Ag[2] - Te[2] x 2	112.51(19)	112.2(2)	112.8(2)
Te[1] - Ag[2] - Ag[1] x 2	55.23(16)	54.86(17)	55.61(17)
Te[1] - Ag[2] - Ag[1] x 4	124.3(3)	124.0(3)	124.6(3)
Te[1] - Ag[2] - Ag[1] x 2	56.28(16)	55.96(17)	56.59(17)
Te[2] - Ag[2] - Te[2] x 2	103.4(3)	103.3(3)	103.4(3)
Te[2] - Ag[2] - Ag[1] x 4	56.06(17)	56.01(16)	56.12(16)
Te[2] - Ag[2] - Ag[1] x 4	123.5(2)	123.4(2)	123.5(2)
Ag[1] - Ag[2] - Ag[1] x 4	90.47(17)	90.47(17)	90.47(17)
Ag[1] - Ag[2] - Ag[1] x 4	89.65(10)	89.65(10)	89.65(10)
Ag[1] - Ag[2] - Ag[1] x 4	179.3(3)	179.3(3)	179.3(3)

Table 4.14. Crystal data and structure refinement for $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 100 K.

Empirical formula	$\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$
Formula weight	816.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	$\text{Pm}(0\beta 1/2)0$
Unit cell dimensions	$a = 4.4838(5)$ Å, $\alpha = 90^\circ$ $b = 4.5057(6)$ Å, $\beta = 90^\circ$ $c = 20.877(3)$ Å, $\gamma = 90^\circ$
q-vector	$0.3466(7)b^* + 1/2c^*$
Volume	$421.77(10)$ Å ³
Z	2
Density (calculated)	6.4249 g/cm ³
Absorption coefficient	21.716 mm ⁻¹
F(000)	678
Crystal size	$0.09 \times 0.05 \times 0.02$ mm ³
Theta range for data collection	1.64 to 29.28°
Index ranges	$-6 \leq h \leq 6$, $-6 \leq k \leq 6$, $-29 \leq l \leq 29$, $-1 \leq m \leq 1$
Reflections collected	10322 (2681 main + 7641 satellites)
Independent reflections	5856 (1830 main + 4026 satellites) [$R_{\text{int}} = 0.0577$]
Completeness to $\theta = 29.28^\circ$	98%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5856 / 16 / 212
Goodness-of-fit on F^2	1.54
Final R indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0518$, $wR_{\text{obs}} = 0.1207$
R indices (all data)	$R_{\text{all}} = 0.0916$, $wR_{\text{all}} = 0.1306$
Final R main indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0322$, $wR_{\text{obs}} = 0.0869$
R main indices (all data)	$R_{\text{all}} = 0.0344$, $wR_{\text{all}} = 0.0874$
Final R 1 st order satellites [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.1429$, $wR_{\text{obs}} = 0.2551$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.2727$, $wR_{\text{all}} = 0.2883$
Extinction coefficient	$0.00074(7)$
T_{min} and T_{max} coefficients	0.1953 and 0.7151
Largest diff. peak and hole	4.32 and -3.51 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o $, $wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.15. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
La[1]	0	0	5000	4010	1	9(1)
	sin, 1	-1(3)	0(1)	1(1)		
	cos, 1	0(1)	0(3)	0(1)		
La[2]	0	4999(3)	0	6000(1)	1	9(1)
	sin, 1	142(5)	6(1)	4(1)		
	cos, 1	-46(2)	18(4)	-1(1)		
Te[1]	0	5008(4)	0	8996(1)	1	19(1)
	sin, 1	-16(2)	-10(5)	1(1)		
	cos, 1	48(7)	-3(2)	-2(1)		
Te[2]	0	7(3)	5000	722(1)	1	17(1)
	sin, 1	4(1)	-1(4)	0(1)		
	cos, 1	19(4)	0(1)	0(1)		
Te[3]	0	4998(4)	0	4432(1)	1	9(1)
	sin, 1	1(3)	1(1)	2(1)		
	cos, 1	0(1)	-4(3)	0(1)		
Te[4]	0	10000(4)	5000	5592(1)	1	8(1)
	sin, 1	-40(6)	-2(1)	1(1)		
	cos, 1	8(1)	-12(4)	0(1)		
Te[5]	0	5007(4)	5000	2796(1)	1	17(1)
	sin, 1	-19(5)	-2(4)	-2(1)		
	cos, 1	-16(4)	3(5)	-2(1)		
Te[6]	0	3(4)	0	2794(1)	1	20(1)
	sin, 1	28(6)	-15(5)	-1(1)		
	cos, 1	23(5)	18(6)	-1(1)		
Te[7]	0	5011(6)	5000	7224(1)	1	13(1)
	sin, 1	-355(5)	-86(4)	-3(1)		
	cos, 1	298(4)	-102(5)	2(1)		
Te[8]	0	2(5)	0	7220(1)	1	12(1)
	sin, 1	340(4)	91(4)	1(1)		
	cos, 1	-285(4)	108(5)	-1(1)		

Table 4.15. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

K[1]	0	4981(13)	0	1394(3)	1	23(1)
	sin, 1	16(6)	-7(14)	1(2)		
	cos, 1	34(12)	3(6)	2(4)		
K[2]	0	1	5000	8512	0.416(13)	12(1)
	sin, 1	1(5)	44(6)	4(1)		
	cos, 1	-2(10)	22(3)	-7(2)		
Ag[1]	0	15(5)	0	9921(1)	1	20(1)
	sin, 1	-1(1)	-5(8)	0(1)		
	cos, 1	31(8)	0(1)	-3(2)		
Ag[2]	0	5013(5)	5000	9918(1)	1	21(1)
	sin, 1	-1(1)	-18(8)	0(1)		
	cos, 1	31(8)	0(1)	-2(2)		
Ag[3]	0	1(5)	5000	8512(1)	0.584(13)	12(1)
	sin, 1	1(5)	44(6)	4(1)		
	cos, 1	-2(10)	22(3)	-7(2)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.16. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_{0.71(1)}\text{Ag}_{1.29(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La[1]	0	9(1)	9(1)	9(1)	0	0(1)	0
	sin, 1	1(1)	0(1)	-2(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	1(1)	0(1)	0(1)
La[2]	0	7(1)	7(1)	12(1)	0	-1(1)	0
	sin, 1	-3(1)	0(1)	1(1)	1(1)	-1(1)	0(1)
	cos, 1	1(1)	0(1)	0(1)	1(1)	0(1)	1(1)
Te[1]	0	18(1)	21(1)	17(1)	0	-1(1)	0
	sin, 1	1(1)	0(1)	-1(1)	-2(1)	1(1)	1(1)
	cos, 1	-2(1)	0(1)	3(1)	0(1)	-2(1)	0(1)
Te[2]	0	11(1)	11(1)	29(1)	0	-1(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	-2(1)	0(1)	0(1)	0(1)

Table 4.17. Bond lengths distributions [Å] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La[1] - Te[3] x 4	3.2991(19)	3.298(2)	3.300(2)
La[1] - Te[4]	3.304(3)	3.303(4)	3.305(4)
La[1] - Te[5] x 2	3.381(3)	3.368(3)	3.394(3)
La[1] - Te[6] x 2	3.394(3)	3.388(3)	3.401(3)
La[2] - Te[3]	3.272(3)	3.268(4)	3.277(4)
La[2] - Te[4] x 4	3.291(3)	3.234(3)	3.347(3)
La[2] - Te[7] x 2	3.412(3)	3.368(3)	3.446(3)
La[2] - Te[8] x 2	3.394(4)	3.302(4)	3.487(4)
Te[1] - K[2] x 4	3.337(4)	3.307(3)	3.367(3)
Te[1] - Ag[1] x 2	2.957(4)	2.951(6)	2.962(6)
Te[1] - Ag[2] x 2	2.963(4)	2.958(4)	2.968(4)
Te[1] - Ag[3] x 4	3.337(4)	3.307(4)	3.367(4)
Te[2] - K[1] x 2	3.481(7)	3.474(7)	3.488(7)
Te[2] - K[1] x 2	3.466(7)	3.454(7)	3.478(7)
Te[2] - Ag[1] x 2	2.806(3)	2.802(3)	2.809(3)
Te[2] - Ag[2] x 2	2.799(4)	2.797(5)	2.801(5)
Te[5] - Te[6] x 4	3.180(4)	3.158(4)	3.201(4)
Te[7] - Te[8] x 4	3.185(4)	2.930(4)	3.447(4)
Te[7] - K[2] x 2	3.507(4)	3.395(5)	3.624(5)
Te[7] - Ag[3] x 2	3.507(5)	3.395(5)	3.624(5)
Te[8] - K[2] x 2	3.517(4)	3.491(4)	3.539(4)
Te[8] - Ag[3] x 2	3.517(4)	3.491(5)	3.539(4)
Ag[1] - Ag[2] x 4	3.179(4)	3.171(4)	3.187(4)

Table 4.18. Bond angles distributions [°] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[3] - La[1] - Te[3] x 4	86.14(5)	86.08(5)	86.19(5)
Te[3] - La[1] - Te[3] x 4	85.64(5)	85.60(5)	85.68(5)
Te[3] - La[1] - Te[3] x 4	148.98(7)	148.97(9)	148.99(9)
Te[3] - La[1] - Te[4] x 4	74.49(6)	74.27(6)	74.71(6)
Te[3] - La[1] - Te[5] x 4	75.53(6)	75.49(6)	75.58(6)

Table 4.18. (Cont'd). Bond angles distributions [°] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Te[3] - La[1] - Te[5] x 4	130.62(6)	130.50(6)	130.73(6)
Te[3] - La[1] - Te[6] x 4	75.35(6)	75.05(6)	75.65(6)
Te[3] - La[1] - Te[6] x 4	130.80(7)	130.61(6)	130.99(6)
Te[4] - La[1] - Te[5] x 2	138.53(7)	138.18(9)	138.89(9)
Te[4] - La[1] - Te[6] x 2	138.42(6)	138.24(5)	138.59(5)
Te[5] - La[1] - Te[5] x 2	83.01(8)	82.84(8)	83.18(8)
Te[5] - La[1] - Te[6] x 4	55.93(7)	55.74(7)	56.12(7)
Te[6] - La[1] - Te[6] x 2	83.16(7)	82.85(8)	83.48(8)
Te[3] - La[2] - Te[4] x 4	75.00(7)	74.28(8)	75.73(8)
Te[3] - La[2] - Te[7] x 2	138.47(6)	137.58(5)	139.59(6)
Te[3] - La[2] - Te[8] x 2	138.70(9)	138.29(10)	139.15(11)
Te[4] - La[2] - Te[4] x 4	86.44(7)	84.84(7)	88.09(8)
Te[4] - La[2] - Te[4] x 4	85.89(6)	85.59(6)	86.23(6)
Te[4] - La[2] - Te[4] x 4	150.02(10)	149.75(11)	150.27(10)
Te[4] - La[2] - Te[7] x 4	75.02(7)	72.20(7)	77.86(7)
Te[4] - La[2] - Te[7] x 4	130.32(9)	126.51(9)	134.14(10)
Te[4] - La[2] - Te[8] x 4	75.22(7)	74.14(7)	76.26(7)
Te[4] - La[2] - Te[8] x 4	130.10(7)	128.69(7)	131.47(7)
Te[7] - La[2] - Te[7] x 2	82.83(7)	81.04(8)	84.29(8)
Te[7] - La[2] - Te[8] x 4	55.79(7)	51.46(7)	60.17(7)
Te[8] - La[2] - Te[8] x 2	82.62(8)	82.42(9)	82.74(9)
K[2] - Te[1] - K[2] x 4	84.92(9)	84.90(10)	84.95(10)
K[2] - Te[1] - K[2] x 4	84.48(8)	84.00(7)	84.97(7)
K[2] - Te[1] - K[2] x 4	144.73(11)	144.71(12)	144.76(12)
K[2] - Te[1] - Ag[1] x 4	71.84(9)	71.57(9)	72.11(9)
K[2] - Te[1] - Ag[1] x 4	135.03(10)	134.62(11)	135.43(11)
K[2] - Te[1] - Ag[2] x 4	71.57(8)	71.03(9)	72.11(9)
K[2] - Te[1] - Ag[2] x 4	135.27(11)	134.80(13)	135.74(13)
K[2] - Te[1] - Ag[3] x 4	84.92(9)	84.90(10)	84.95(10)
K[2] - Te[1] - Ag[3] x 4	84.48(8)	84.00(8)	84.97(8)
K[2] - Te[1] - Ag[3] x 4	144.73(12)	144.71(13)	144.76(13)
Ag[1] - Te[1] - Ag[1] x 2	98.51(11)	98.47(14)	98.55(14)
Ag[1] - Te[1] - Ag[2] x 4	64.93(8)	64.56(8)	65.30(8)
Ag[1] - Te[1] - Ag[3] x 4	71.84(9)	71.57(8)	72.11(8)

Table 4.18. (Cont'd) Bond angles distributions [°] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Ag[1] - Te[1] - Ag[3] x 4	134.96(9)	134.46(9)	135.45(9)
Ag[2] - Te[1] - Ag[2] x 2	98.99(11)	98.73(12)	99.25(12)
Ag[2] - Te[1] - Ag[3] x 4	71.57(9)	71.03(8)	72.11(9)
Ag[2] - Te[1] - Ag[3] x 4	135.27(12)	134.80(11)	135.74(11)
Ag[3] - Te[1] - Ag[3] x 4	84.92(9)	84.90(10)	84.95(10)
Ag[3] - Te[1] - Ag[3] x 4	84.48(9)	84.00(8)	84.97(8)
Ag[3] - Te[1] - Ag[3] x 4	144.73(12)	144.71(13)	144.76(13)
K[1] - Te[2] - K[1] x 6	80.66(15)	80.52(15)	80.79(15)
K[1] - Te[2] - K[1] x 4	132.40(19)	132.2(2)	132.6(2)
K[1] - Te[2] - Ag[1] x 4	73.81(13)	73.56(13)	74.05(13)
K[1] - Te[2] - Ag[1] x 4	139.51(14)	139.44(15)	139.58(15)
K[1] - Te[2] - Ag[2] x 4	73.96(15)	73.80(16)	74.11(16)
K[1] - Te[2] - Ag[2] x 4	139.42(13)	139.17(14)	139.67(14)
K[1] - Te[2] - K[1] x 2	81.08(15)	80.98(15)	81.17(15)
Ag[1] - Te[2] - Ag[1] x 2	106.83(12)	106.71(13)	106.95(13)
Ag[1] - Te[2] - Ag[2] x 4	69.11(11)	68.98(10)	69.25(10)
Ag[2] - Te[2] - Ag[2] x 2	106.33(12)	106.23(15)	106.44(15)
La[1] - Te[3] - La[1] x 4	86.18(5)	86.13(6)	86.23(6)
La[1] - Te[3] - La[1] x 4	85.64(4)	85.60(4)	85.68(4)
La[1] - Te[3] - La[1] x 4	148.98(8)	148.85(9)	149.11(9)
La[1] - Te[3] - La[2] x 4	105.53(6)	104.62(6)	106.42(6)
La[1] - Te[4] - La[2] x 4	104.98(7)	104.50(7)	105.45(7)
La[2] - Te[4] - La[2] x 4	86.45(7)	85.55(8)	87.33(8)
La[2] - Te[4] - La[2] x 4	85.89(6)	85.59(5)	86.23(5)
La[2] - Te[4] - La[2] x 4	150.03(10)	149.66(8)	150.43(8)
La[1] - Te[5] - La[1] x 2	83.01(7)	82.84(8)	83.18(8)
La[1] - Te[5] - Te[6] x 4	62.18(8)	61.94(8)	62.41(8)
La[1] - Te[5] - Te[6] x 4	117.96(10)	117.82(10)	118.11(10)
Te[6] - Te[5] - Te[6] x 4	90.23(9)	89.99(10)	90.48(10)
Te[6] - Te[5] - Te[6] x 4	89.72(9)	89.47(9)	89.97(9)
Te[6] - Te[5] - Te[6] x 4	179.61(12)	179.36(12)	179.85(12)
La[1] - Te[6] - La[1] x 2	83.16(7)	83.05(7)	83.27(7)
La[1] - Te[6] - Te[5] x 4	61.82(7)	61.52(7)	62.12(7)
La[1] - Te[6] - Te[5] x 4	117.97(11)	117.55(11)	118.40(11)

Table 4.18. (Cont'd) Bond angles distributions [°] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Te[5] - Te[6] - Te[5] x 4	90.32(10)	89.75(10)	90.91(10)
Te[5] - Te[6] - Te[5] x 4	89.72(9)	89.47(9)	89.97(9)
Te[5] - Te[6] - Te[5] x 4	179.55(12)	179.33(12)	179.82(13)
La[2] - Te[7] - La[2] x 2	82.67(7)	82.48(7)	82.80(7)
La[2] - Te[7] - Te[8] x 4	61.77(7)	59.67(7)	64.18(7)
La[2] - Te[7] - Te[8] x 4	117.74(11)	112.73(10)	122.69(11)
La[2] - Te[7] - K[2] x 2	125.01(9)	120.11(9)	129.89(9)
La[2] - Te[7] - K[2] x 2	125.20(9)	120.12(9)	130.42(10)
La[2] - Te[7] - Ag[3] x 3	125.01(10)	120.11(9)	129.89(9)
La[2] - Te[7] - Ag[3]	125.24(10)	120.12(9)	130.42(10)
Te[8] - Te[7] - Te[8] x 4	90.51(10)	84.41(9)	96.92(12)
Te[8] - Te[7] - Te[8] x 4	89.39(8)	87.09(8)	92.48(8)
Te[8] - Te[7] - Te[8] x 4	174.87(12)	171.89(12)	179.83(12)
Te[8] - Te[7] - K[2] x 4	63.29(8)	60.03(8)	66.59(9)
Te[8] - Te[7] - K[2] x 4	116.68(10)	113.93(10)	119.64(10)
Te[8] - Te[7] - Ag[3] x 4	63.29(9)	60.03(8)	66.59(9)
Te[8] - Te[7] - Ag[3] x 4	116.68(10)	113.93(10)	119.64(10)
K[2] - Te[7] - K[2] x 2	79.50(9)	78.91(9)	79.92(9)
K[2] - Te[7] - Ag[3] x 2	79.50(9)	78.91(10)	79.92(10)
Ag[3] - Te[7] - Ag[3] x 2	79.50(10)	78.91(11)	79.92(11)
La[2] - Te[8] - La[2] x 2	82.62(8)	82.42(9)	82.74(9)
La[2] - Te[8] - Te[7] x 4	62.42(8)	59.48(7)	65.56(8)
La[2] - Te[8] - Te[7] x 4	117.71(9)	116.18(10)	118.99(10)
La[2] - Te[8] - K[2] x 4	125.09(9)	121.41(9)	128.85(9)
La[2] - Te[8] - Ag[3] x 4	125.09(9)	121.41(10)	128.85(9)
Te[7] - Te[8] - Te[7] x 4	90.64(10)	84.63(9)	97.10(12)
Te[7] - Te[8] - Te[7] x 4	89.39(9)	87.09(8)	92.48(9)
Te[7] - Te[8] - Te[7] x 4	174.92(12)	171.76(12)	179.71(13)
Te[7] - Te[8] - K[2] x 4	62.71(8)	60.35(7)	65.37(8)
Te[7] - Te[8] - K[2] x 4	116.85(11)	112.53(10)	121.26(11)
Te[7] - Te[8] - Ag[3] x 4	62.71(8)	60.35(8)	65.37(8)
Te[7] - Te[8] - Ag[3] x 4	116.85(11)	112.53(10)	121.26(12)
K[2] - Te[8] - K[2] x 2	79.65(8)	78.97(8)	80.21(8)
K[2] - Te[8] - Ag[3] x 2	79.65(9)	78.97(9)	80.21(9)

Table 4.18. (Cont'd) Bond angles distributions [°] for $K_{0.71(1)}Ag_{1.29(1)}LaTe_4$ at 100 K with e.s.d.'s in parentheses.

Ag[3] - Te[8] - Ag[3] x 2	79.65(9)	78.97(9)	80.21(9)
Te[2] - K[1] - Te[2] x 2	81.07(16)	80.77(18)	81.39(18)
Te[2] - K[1] - Te[2] x 6	80.39(13)	80.32(13)	80.46(13)
Te[2] - K[1] - Te[2] x 4	132.4(3)	132.2(2)	132.6(2)
Te[1] - K[2] - Te[1] x 4	85.06(9)	85.04(10)	85.07(10)
Te[1] - K[2] - Te[1] x 4	84.48(7)	84.00(8)	84.97(8)
Te[1] - K[2] - Te[1] x 4	144.74(12)	144.18(14)	145.29(14)
Te[1] - K[2] - Te[7] x 4	78.70(9)	76.58(8)	80.93(9)
Te[1] - K[2] - Te[7] x 4	131.49(9)	129.34(9)	133.65(9)
Te[1] - K[2] - Te[8] x 4	78.47(8)	75.83(8)	81.09(8)
Te[1] - K[2] - Te[8] x 4	131.72(12)	128.77(10)	134.69(10)
Te[7] - K[2] - Te[7] x 2	79.50(10)	78.91(10)	79.92(11)
Te[7] - K[2] - Te[8] x 4	53.90(8)	49.87(8)	57.85(8)
Te[8] - K[2] - Te[8] x 2	79.80(9)	77.94(10)	81.46(10)
Te[1] - Ag[1] - Te[1] x 2	98.51(11)	98.47(16)	98.55(16)
Te[1] - Ag[1] - Te[2] x 4	112.81(10)	112.70(10)	112.92(10)
Te[1] - Ag[1] - Ag[2] x 4	57.57(8)	57.55(7)	57.59(7)
Te[1] - Ag[1] - Ag[2] x 4	122.22(11)	122.22(10)	122.23(10)
Te[2] - Ag[1] - Te[2] x 2	106.83(12)	106.63(17)	107.03(17)
Te[2] - Ag[1] - Ag[2] x 4	55.34(8)	55.26(7)	55.43(7)
Te[2] - Ag[1] - Ag[2] x 4	124.71(12)	124.31(16)	125.12(16)
Ag[2] - Ag[1] - Ag[2] x 4	90.26(10)	89.88(13)	90.62(13)
Ag[2] - Ag[1] - Ag[2] x 4	89.72(9)	89.54(7)	89.90(7)
Ag[2] - Ag[1] - Ag[2] x 4	179.70(13)	179.57(17)	179.81(13)
Te[1] - Ag[2] - Te[1] x 2	98.99(11)	98.93(15)	99.05(15)
Te[1] - Ag[2] - Te[2] x 4	112.85(11)	112.33(12)	113.39(12)
Te[1] - Ag[2] - Ag[1] x 4	57.44(8)	57.16(9)	57.72(9)
Te[1] - Ag[2] - Ag[1] x 4	122.68(12)	122.37(10)	122.99(10)
Te[2] - Ag[2] - Te[2] x 2	106.34(13)	106.23(17)	106.44(18)
Te[2] - Ag[2] - Ag[1] x 4	55.53(8)	55.27(7)	55.79(7)
Te[2] - Ag[2] - Ag[1] x 4	124.30(11)	123.94(12)	124.68(12)
Ag[1] - Ag[2] - Ag[1] x 4	90.31(10)	90.07(12)	90.55(13)
Ag[1] - Ag[2] - Ag[1] x 4	89.72(9)	89.54(11)	89.90(11)
Ag[1] - Ag[2] - Ag[1] x 4	179.69(13)	179.64(14)	179.77(12)

Table 4.19. Crystal data and structure refinement for KCuCeTe₄ at 100K.

Empirical formula	KCuCeTe ₄
Formula weight	753.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β1/2)0s0
Unit cell dimensions	a = 4.4065(6) Å, α = 90° b = 4.4220(6) Å, β = 90° c = 21.086(3) Å, γ = 90°
q-vector	0.3550(8)b* + 1/2c*
Volume	410.87(10) Å ³
Z	2
Density (calculated)	6.0859 g/cm ³
Absorption coefficient	22.421 mm ⁻¹
F(000)	628
Crystal size	0.15 x 0.10 x 0.01 mm ³
Theta range for data collection	1.70 to 29.33°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 6, -29 ≤ l ≤ 29, -1 ≤ m ≤ 1
Reflections collected	9890 (2580 main + 7310 satellites)
Independent reflections	3204 (995 main + 2209 satellites) [R _{int} = 0.0742]
Completeness to θ = 29.33°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3204 / 0 / 101
Goodness-of-fit on F ²	1.58
Final R indices [I > 2σ(I)]	R _{obs} = 0.0493, wR _{obs} = 0.1209
R indices (all data)	R _{all} = 0.0915, wR _{all} = 0.1281
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0421, wR _{obs} = 0.1134
R main indices (all data)	R _{all} = 0.0456, wR _{all} = 0.1144
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0948, wR _{obs} = 0.1539
R 1 st order satellites (all data)	R _{all} = 0.2700, wR _{all} = 0.1820
Extinction coefficient	0.00104(11)
T _{min} and T _{max} coefficients	0.0955 and 0.7759
Largest diff. peak and hole	3.69 and -2.63 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.20. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KCuCeTe_4 at 100K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce	0	0	0	4013(1)	1	13(1)
	sin, 1	22(1)	-7(2)	2(1)		
	cos, 1	-68(1)	22(5)	1(1)		
Te[1]	0	0	0	705(1)	1	16(1)
	sin, 1	-24(2)	-4(6)	0(1)		
	cos, 1	5(1)	1(1)	-1(2)		
Te[2]	0	0	0	5566(1)	1	12(1)
	sin, 1	0(1)	-6(1)	1(2)		
	cos, 1	0(2)	-33(6)	0(1)		
Te[3]	0	0	5000	2813(1)	1	17(1)
	sin, 1	-173(2)	28(4)	-2(2)		
	cos, 1	211(2)	-34(5)	-1(1)		
Te[4]	0	0	5000	7185(1)	1	16(1)
	sin, 1	150(2)	12(4)	3(2)		
	cos, 1	183(2)	15(5)	-2(1)		
K	0	0	0	8590(1)	1	17(1)
	sin, 1	-56(6)	159(19)	8(2)		
	cos, 1	-27(3)	76(9)	-17(5)		
Cu	0	0	5000	-1(1)	1	21(1)
	sin, 1	-32(8)	28(12)	0		
	cos, 1	0	0	-5(3)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.21. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuCeTe_4 at 100K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	0	7(1)	14(1)	17(1)	7(1)	0	0
	sin, 1	-2(1)	-1(1)	1(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	0(1)	0(1)	0(1)	1(1)

Table 4.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuCeTe_4 at 100K with e.s.d.'s in parentheses.

Te[1]	0	9(1)	17(1)	22(1)	4(1)	0	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	1(1)	1(1)
	cos, 1	-1(1)	1(1)	0(2)	0(1)	0(1)	0(1)
Te[2]	0	7(1)	13(1)	17(1)	-7(1)	0	0
	sin, 1	1(1)	1(1)	-3(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	-1(1)	-2(1)
Te[3]	0	13(1)	19(1)	18(1)	12(1)	0	0
	sin, 1	-1(1)	0(1)	0(1)	-2(1)	2(1)	2(1)
	cos, 1	-1(1)	0(1)	0(1)	-2(1)	-2(1)	-3(1)
Te[4]	0	12(1)	19(1)	17(1)	-4(1)	0	0
	sin, 1	-2(1)	1(1)	-3(1)	-1(1)	-1(1)	0(1)
	cos, 1	2(1)	-1(1)	2(1)	1(1)	-1(1)	0(1)
K	0	14(1)	19(2)	20(1)	-9(2)	0	0
	sin, 1	-5(2)	-1(2)	8(2)	0(1)	-1(1)	4(3)
	cos, 1	11(4)	2(4)	-16(4)	1(1)	0(1)	2(2)
Cu	0	17(1)	25(1)	20(1)	-11(2)	0	0
	sin, 1	0	0	0	0	1(1)	-12(2)
	cos, 1	1(3)	2(3)	0(3)	0(2)	0	0

Table 4.22. Bond lengths distributions [$\text{\AA}$] for KCuCeTe_4 at 100K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[2]	3.276(3)	3.272(4)	3.280(4)
Ce - Te[2] x 4	3.2453(19)	3.2329(14)	3.2575(14)
Ce - Te[3] x 2	3.361(3)	3.343(3)	3.381(3)
Ce - Te[4] x 2	3.352(3)	3.303(3)	3.401(3)
Te[1] - K x 4	3.457(6)	3.390(6)	3.525(6)
Te[1] - Cu x 2	2.665(4)	2.655(4)	2.676(4)
Te[1] - Cu x 2	2.657(3)	2.652(3)	2.663(3)
Te[3] - Te[4] x 4	3.123(2)	3.008(3)	3.242(2)
Cu - Cu x 4	3.121(4)	3.103(5)	3.140(5)

Table 4.23. Bond angles distributions [°] for KCuCeTe₄ at 100K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - Ce - Te[2] x 8	74.12(7)	73.99(7)	74.26(7)
Te[2] - Ce - Te[3] x 2	138.80(8)	138.04(9)	139.53(9)
Te[2] - Ce - Te[4] x 2	138.91(5)	138.50(5)	139.32(5)
Te[2] - Ce - Te[2] x 4	85.90(4)	85.09(4)	86.70(4)
Te[2] - Ce - Te[2] x 4	85.52(5)	85.06(6)	85.98(6)
Te[2] - Ce - Te[2] x 4	148.24(10)	147.98(11)	148.53(11)
Te[2] - Ce - Te[3] x 4	75.97(6)	74.82(5)	77.09(5)
Te[2] - Ce - Te[3] x 4	130.85(5)	128.62(6)	133.11(7)
Te[2] - Ce - Te[4] x 4	76.11(5)	75.77(6)	76.46(6)
Te[2] - Ce - Te[4] x 4	130.72(7)	129.92(8)	131.52(8)
Te[3] - Ce - Te[3] x 2	82.34(8)	82.09(9)	82.68(9)
Te[3] - Ce - Te[4] x 4	55.45(5)	53.07(5)	57.81(5)
Te[4] - Ce - Te[4] x 2	82.18(7)	81.91(8)	82.49(8)
K - Te[1] - K x 4	79.49(15)	77.89(17)	81.10(17)
K - Te[1] - K x 4	79.20(13)	77.78(13)	80.62(13)
K - Te[1] - K x 4	129.07(17)	128.58(17)	129.56(16)
K - Te[1] - Cu x 8	73.13(15)	72.30(14)	73.96(14)
K - Te[1] - Cu x 8	140.40(11)	139.71(12)	141.08(12)
Cu - Te[1] - Cu x 4	112.11(13)	111.92(15)	112.29(15)
Cu - Te[1] - Cu x 8	71.81(13)	71.50(13)	72.12(13)
Ce - Te[2] - Ce x 8	105.87(7)	105.74(7)	106.01(7)
Ce - Te[2] - Ce x 4	85.90(4)	85.53(3)	86.27(3)
Ce - Te[2] - Ce x 4	85.52(5)	85.06(5)	85.98(5)
Ce - Te[2] - Ce x 4	148.25(10)	148.11(12)	148.39(12)
Ce - Te[3] - Ce x 2	82.28(8)	81.94(8)	82.71(9)
Ce - Te[3] - Te[4] x 4	62.11(7)	61.50(7)	62.78(7)
Ce - Te[3] - Te[4] x 4	117.75(9)	114.87(8)	120.53(10)
Ce - Te[3] - K x 4	127.09(13)	126.08(12)	127.95(13)
Te[4] - Te[3] - Te[4] x 4	90.34(5)	86.04(5)	94.68(5)
Te[4] - Te[3] - Te[4] x 4	89.69(7)	88.96(7)	90.24(7)
Te[4] - Te[3] - Te[4] x 2	176.85(7)	175.08(7)	179.87(12)
Te[4] - Te[3] - K x 4	65.13(13)	64.44(12)	65.82(13)
Te[4] - Te[3] - K x 4	114.90(15)	113.05(14)	116.61(14)

Table 4.23. (Cont'd) Bond angles distributions [°] for KCuCeTe₄ at 100K with e.s.d.'s in parentheses.

Te[4] - Te[3] - Te[4] x 2	177.62(7)	176.28(7)	179.89(13)
Ce - Te[4] - Ce x 2	82.19(8)	81.91(8)	82.49(8)
Ce - Te[4] - Te[3] x 4	62.45(7)	60.78(7)	64.15(8)
Ce - Te[4] - Te[3] x 4	117.64(10)	116.38(10)	118.85(10)
Te[3] - Te[4] - Te[3] x 4	90.34(5)	86.24(4)	94.45(5)
Te[3] - Te[4] - Te[3] x 4	89.70(7)	88.96(6)	90.24(6)
Te[3] - Te[4] - Te[3] x 2	177.65(8)	176.35(7)	179.89(12)
Te[3] - Te[4] - Te[3] x 2	177.09(7)	175.47(7)	179.88(12)
Te[1] - K - Te[1] x 4	79.51(11)	78.92(10)	80.09(10)
Te[1] - K - Te[1] x 4	79.19(15)	77.78(14)	80.62(15)
Te[1] - K - Te[1] x 4	129.1(2)	127.8(3)	130.4(3)
Te[1] - K - Te[3] x 4	87.95(10)	86.28(11)	89.64(11)
Te[1] - K - Te[3] x 4	136.5(2)	133.6(2)	139.3(2)
Te[1] - Cu - Te[1] x 4	112.10(14)	111.7(2)	112.5(2)
Te[1] - Cu - Te[1] x 8	108.19(11)	107.96(6)	108.42(6)
Te[1] - Cu - Cu x 4	53.98(9)	53.79(7)	54.17(7)
Te[1] - Cu - Cu x 8	125.95(13)	125.74(14)	126.17(14)
Te[1] - Cu - Cu x 4	54.21(9)	54.15(10)	54.28(10)
Cu - Cu - Cu x 4	90.20(11)	89.84(12)	90.56(12)
Cu - Cu - Cu x 4	89.80(13)	89.25(14)	90.35(15)
Cu - Cu - Cu x 4	179.52(16)	179.32(19)	179.9(2)

Table 4.24. Crystal data and structure refinement for KCuCeTe₄ at 300 K.

Empirical formula	KCuCeTe ₄
Formula weight	753.2
Temperature	300.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β1/2)0s0
Unit cell dimensions	a = 4.4229(3) Å, α = 90° b = 4.4371(3) Å, β = 90° c = 21.1976(17) Å, γ = 90°
q-vector	0.3538(4)b* + 1/2c*
Volume	416.00(5) Å ³
Z	2
Density (calculated)	6.0108 g/cm ³
Absorption coefficient	22.145 mm ⁻¹
F(000)	628
Crystal size	0.13 x 0.04 x 0.01 mm ³
Theta range for data collection	1.69 to 29.22°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 5, -29 ≤ l ≤ 29, -1 ≤ m ≤ 1
Reflections collected	10364 (2672 main + 7692 satellites)
Independent reflections	3277 (1048 main + 2229 satellites) [R _{int} = 0.0400]
Completeness to θ = 29.22°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3277 / 0 / 101
Goodness-of-fit on F ²	1.10
Final R indices [I > 2σ(I)]	R _{obs} = 0.0302, wR _{obs} = 0.0717
R indices (all data)	R _{all} = 0.0624, wR _{all} = 0.0832
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0189, wR _{obs} = 0.0506
R main indices (all data)	R _{all} = 0.0211, wR _{all} = 0.0516
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0916, wR _{obs} = 0.1293
R 1 st order satellites (all data)	R _{all} = 0.2258, wR _{all} = 0.1602
Extinction coefficient	0.00017(7)
T _{min} and T _{max} coefficients	0.1274 and 0.8570
Largest diff. peak and hole	1.56 and -1.54 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.25. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KCuCeTe_4 at 300 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce	0	0	0	4018(1)	1	10(1)
	sin, 1	28(1)	-7(1)	0(1)		
	cos, 1	-87(1)	23(4)	0(1)		
Te[1]	0	0	0	705(1)	1	20(1)
	sin, 1	-29(2)	-10(5)	0(1)		
	cos, 1	6(1)	2(1)	-2(1)		
Te[2]	0	0	0	5564(1)	1	10(1)
	sin, 1	0(1)	1(1)	-2(1)		
	cos, 1	1(1)	3(4)	0(1)		
Te[3]	0	0	5000	2822(1)	1	15(1)
	sin, 1	-242(2)	-17(3)	-3(1)		
	cos, 1	297(3)	21(4)	-2(1)		
Te[4]	0	0	5000	7176(1)	1	14(1)
	sin, 1	194(2)	11(3)	3(1)		
	cos, 1	238(2)	14(4)	-2(1)		
K	0	0	0	8580(1)	1	25(1)
	sin, 1	-70(6)	-35(18)	3(2)		
	cos, 1	-33(3)	-17(8)	-6(3)		
Cu	0	0	5000	-1(1)	1	32(1)
	sin, 1	-40(8)	94(14)	0		
	cos, 1	0	0	-16(2)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.26. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuCeTe_4 at 300 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	0	10(1)	8(1)	12(1)	1(1)	0	0
	sin, 1	-2(1)	-2(1)	3(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	1(1)	0(1)	-1(1)	1(1)

Table 4.26. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuCeTe_4 at 300 K with e.s.d.'s in parentheses.

Te[1]	0	18(1)	17(1)	25(1)	8(1)	0	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	1(1)	-1(1)	0(1)	0(1)	0(1)
Te[2]	0	9(1)	9(1)	11(1)	-1(1)	0	0
	sin, 1	0(1)	3(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	-1(1)	0(1)	0(1)	-1(1)	-2(1)
Te[3]	0	18(1)	13(1)	14(1)	4(1)	0	0
	sin, 1	3(1)	-2(1)	-3(1)	-4(1)	2(1)	1(1)
	cos, 1	2(1)	-2(1)	-2(1)	-3(1)	-2(1)	-1(1)
Te[4]	0	18(1)	11(1)	13(1)	2(1)	0	0
	sin, 1	-13(1)	0(1)	2(1)	-3(1)	0(1)	1(1)
	cos, 1	11(1)	0(1)	-2(1)	2(1)	0(1)	1(1)
K	0	28(2)	22(2)	25(1)	-9(3)	0	0
	sin, 1	-5(2)	1(2)	11(2)	0(1)	2(1)	9(3)
	cos, 1	10(3)	-2(3)	-23(3)	0(1)	1(1)	4(1)
Cu	0	34(1)	35(1)	26(1)	-8(2)	0	0
	sin, 1	0	0	0	0	0(1)	-16(2)
	cos, 1	-5(2)	-5(3)	9(3)	2(2)	0	0

Table 4.27. Bond lengths distributions [$\text{\AA}$] for KCuCeTe_4 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[2]	3.2782(18)	3.273(3)	3.284(3)
Ce - Te[2] x 4	3.2557(13)	3.2341(14)	3.2775(14)
Ce - Te[3] x 2	3.371(2)	3.367(2)	3.379(2)
Ce - Te[4] x 2	3.3607(19)	3.2980(17)	3.4241(17)
Te[1] - K x 4	3.480(5)	3.464(5)	3.496(5)
Te[1] - Cu x 2	2.677(4)	2.638(5)	2.714(5)
Te[1] - Cu x 2	2.667(3)	2.649(3)	2.684(3)
Te[3] - Te[4] x 4	3.1340(19)	2.952(2)	3.324(2)
Cu - Cu x 4	3.133(4)	3.081(5)	3.185(5)

Table 4.28. Bond angles distributions [°] for KCuCeTe₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - Ce - Te[2] x 8	74.19(5)	73.82(5)	74.55(5)
Te[2] - Ce - Te[3] x 2	138.74(5)	138.42(7)	139.16(5)
Te[2] - Ce - Te[4] x 2	138.86(3)	138.34(3)	139.39(3)
Te[2] - Ce - Te[2] x 4	85.92(3)	85.03(2)	86.81(2)
Te[2] - Ce - Te[2] x 4	85.57(3)	85.38(4)	85.75(4)
Te[2] - Ce - Te[2] x 4	148.37(6)	148.31(7)	148.46(7)
Te[2] - Ce - Te[3] x 4	75.91(4)	73.69(4)	78.10(4)
Te[2] - Ce - Te[3] x 4	130.79(4)	127.63(4)	133.96(5)
Te[2] - Ce - Te[4] x 4	76.01(4)	75.44(4)	76.62(4)
Te[2] - Ce - Te[4] x 4	130.70(5)	129.75(6)	131.64(5)
Te[3] - Ce - Te[3] x 2	82.42(5)	82.16(6)	82.87(6)
Te[3] - Ce - Te[4] x 4	55.53(4)	52.51(4)	58.56(4)
Te[4] - Ce - Te[4] x 2	82.29(5)	82.15(5)	82.47(5)
K - Te[1] - K x 4	79.21(14)	78.79(15)	79.63(15)
K - Te[1] - K x 4	78.90(11)	78.48(10)	79.33(10)
K - Te[1] - K x 4	128.34(12)	128.26(12)	128.42(12)
K - Te[1] - Cu x 8	73.44(13)	72.72(13)	74.18(13)
K - Te[1] - Cu x 8	140.55(10)	140.35(10)	140.75(10)
Cu - Te[1] - Cu x 4	112.01(13)	111.51(14)	112.49(14)
Cu - Te[1] - Cu x 8	71.79(14)	70.81(13)	72.78(13)
Ce - Te[2] - Ce x 8	105.81(5)	105.41(4)	106.20(4)
Ce - Te[2] - Ce x 4	85.92(2)	85.43(2)	86.40(2)
Ce - Te[2] - Ce x 4	85.57(4)	85.38(3)	85.75(3)
Ce - Te[2] - Ce x 4	148.37(6)	147.89(8)	148.86(8)
Ce - Te[3] - Ce x 2	82.31(6)	81.97(6)	82.81(6)
Ce - Te[3] - Te[4] x 4	62.06(5)	60.78(5)	63.32(5)
Ce - Te[3] - Te[4] x 4	117.73(6)	113.66(6)	121.63(7)
Ce - Te[3] - K x 4	127.14(11)	123.31(11)	130.84(12)
Te[4] - Te[3] - Te[4] x 2	90.43(4)	84.53(4)	96.45(5)
Te[4] - Te[3] - Te[4] x 4	89.62(5)	89.28(5)	90.09(5)
Te[4] - Te[3] - Te[4] x 2	176.32(6)	174.25(6)	179.88(6)
Te[4] - Te[3] - K x 4	65.23(11)	62.52(10)	67.97(11)
Te[4] - Te[3] - K x 4	114.90(12)	114.13(12)	115.80(12)

Table 4.28. (Cont'd) Bond angles distributions [°] for KCuCeTe₄ at 300 K with e.s.d.'s in parentheses.

Te[4] - Te[3] - Te[4] x 2	176.04(6)	173.82(6)	179.88(6)
Te[4] - Te[3] - Te[4] x 2	90.33(4)	84.53(4)	96.45(5)
Ce - Te[4] - Ce x 2	82.29(5)	82.15(5)	82.47(5)
Ce - Te[4] - Te[3] x 4	62.47(5)	60.01(5)	65.00(5)
Ce - Te[4] - Te[3] x 4	117.66(7)	116.26(7)	118.94(7)
Te[3] - Te[4] - Te[3] x 2	90.43(4)	84.97(4)	95.92(4)
Te[3] - Te[4] - Te[3] x 4	89.62(5)	89.28(5)	90.09(6)
Te[3] - Te[4] - Te[3] x 4	176.54(6)	174.58(6)	179.89(7)
Te[3] - Te[4] - Te[3] x 2	90.33(4)	84.97(4)	95.92(4)
Te[1] - K - Te[1] x 4	79.21(8)	78.71(7)	79.70(7)
Te[1] - K - Te[1] x 4	78.90(12)	78.48(15)	79.33(15)
Te[1] - K - Te[1] x 4	128.34(16)	127.91(19)	128.76(19)
Te[1] - K - Te[3] x 4	88.30(8)	87.50(9)	89.12(10)
Te[1] - K - Te[3] x 4	136.78(18)	136.6(2)	136.9(2)
Te[1] - Cu - Te[1] x 4	112.00(14)	110.8(2)	113.3(2)
Te[1] - Cu - Te[1] x 8	108.20(11)	107.43(16)	108.98(16)
Te[1] - Cu - Cu x 4	53.97(10)	53.38(8)	54.55(9)
Te[1] - Cu - Cu x 8	125.87(13)	124.97(13)	126.77(13)
Te[1] - Cu - Cu x 4	54.23(9)	53.78(10)	54.70(10)
Cu - Cu - Cu x 4	90.17(12)	89.17(13)	91.18(13)
Cu - Cu - Cu x 4	89.82(15)	88.01(16)	91.67(17)
Cu - Cu - Cu x 4	178.67(17)	178.2(2)	179.5(2)

Table 4.29. Crystal data and structure refinement for KCuLaTe₄ at 100 K.

Empirical formula	KCuLaTe ₄
Formula weight	752
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β1/2)0s0
Unit cell dimensions	a = 4.4421(4) Å, α = 90° b = 4.4517(4) Å, β = 90° c = 19.7507(18) Å, γ = 90°
q-vector	0.3861(5)b* + 1/2c*
Volume	390.57(6) Å ³
Z	2
Density (calculated)	6.3919 g/cm ³
Absorption coefficient	23.161 mm ⁻¹
F(000)	626
Crystal size	0.28 x 0.10 x 0.03 mm ³
Theta range for data collection	2.34 to 31.85°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 6, -29 ≤ l ≤ 29, -1 ≤ m ≤ 1
Reflections collected	12470 (3519 main + 8951 satellites)
Independent reflections	4003 (1326 main + 2677 satellites) [R _{int} = 0.0814]
Completeness to θ = 31.85°	98%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4003 / 0 / 96
Goodness-of-fit on F ²	2.06
Final R indices [I > 2σ(I)]	R _{obs} = 0.0699, wR _{obs} = 0.1680
R indices (all data)	R _{all} = 0.1105, wR _{all} = 0.1753
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0617, wR _{obs} = 0.1716
R main indices (all data)	R _{all} = 0.0671, wR _{all} = 0.1730
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1131, wR _{obs} = 0.1501
R 1 st order satellites (all data)	R _{all} = 0.2553, wR _{all} = 0.1857
Extinction coefficient	0.00053(14)
T _{min} and T _{max} coefficients	0.0209 and 0.1467
Largest diff. peak and hole	8.05 and -4.48 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.30. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for KCuLaTe_4 at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
La	0	0	0	3932(1)	1	18(1)
	sin, 1	46(1)	9(3)	0(2)		
	cos, 1	-133(3)	-26(9)	0(1)		
Te[1]	0	0	0	781(1)	1	31(1)
	sin, 1	-8(5)	40(13)	8(1)		
	cos, 1	2(1)	-10(3)	31(3)		
Te[2]	0	0	0	5613(1)	1	18(1)
	sin, 1	1(1)	0(2)	1(2)		
	cos, 1	5(3)	1(10)	0(1)		
Te[3]	0	0	5000	2636(1)	1	18(1)
	sin, 1	-309(5)	-27(8)	-1(2)		
	cos, 1	337(5)	30(8)	-1(2)		
Te[4]	0	0	5000	7368(1)	1	23(1)
	sin, 1	280(5)	-17(9)	-2(2)		
	cos, 1	304(5)	-18(9)	2(2)		
K	0	0	0	8729(2)	1	25(2)
	sin, 1	-115(13)	145(40)	-2(3)		
	cos, 1	-49(5)	59(16)	5(8)		
Cu	0	0	5000	15(4)	1	58(2)
	sin, 1	-55(30)	165(30)	0		
	cos, 1	0(1)	-1(1)	0		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.31. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuLaTe_4 at 300 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	0	23(1)	7(1)	25(1)	4(1)	0	0
	sin, 1	-9(2)	-3(2)	6(1)	-1(1)	0(1)	0(1)
	cos, 1	-3(1)	-1(1)	2(1)	0(1)	0(1)	1(1)

Table 4.31. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for KCuLaTe_4 at 300 K with e.s.d.'s in parentheses.

Te[1]	0	34(1)	13(1)	46(1)	-9(1)	0	0
	sin, 1	1(1)	1(1)	-6(1)	-1(1)	2(1)	0(2)
	cos, 1	4(3)	5(2)	-24(2)	-3(1)	-1(1)	0(1)
Te[2]	0	23(1)	6(1)	25(1)	-6(1)	0	0
	sin, 1	-4(2)	-4(2)	5(2)	2(1)	0(1)	0(1)
	cos, 1	1(1)	1(1)	-1(1)	0(1)	0(1)	-1(1)
Te[3]	0	14(1)	18(1)	22(1)	11(1)	0	0
	sin, 1	-1(1)	0(2)	-1(1)	-5(1)	3(1)	-2(1)
	cos, 1	-1(1)	0(2)	-1(1)	-5(1)	-3(1)	2(1)
Te[4]	0	16(1)	22(1)	30(1)	-9(1)	0	0
	sin, 1	1(2)	-4(2)	2(1)	-2(1)	0(1)	-2(1)
	cos, 1	0(1)	3(2)	-2(1)	2(1)	0(1)	-2(2)
K	0	26(3)	16(3)	33(1)	1(2)	0	0
	sin, 1	2(3)	1(3)	-1(3)	1(1)	0(3)	-9(4)
	cos, 1	-4(7)	-2(7)	2(6)	-1(2)	0(1)	-4(2)
Cu	0	101(4)	34(2)	38(1)	-4(7)	0	0
	sin, 1	0	0	0	0	-3(2)	-24(4)
	cos, 1	0	0	0	0	0(1)	0(1)

Table 4.32. Bond lengths distributions [$\text{\AA}$] for KCuLaTe_4 at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[2]	3.320(4)	3.317(5)	3.323(5)
La - Te[2] x 4	3.270(3)	3.221(3)	3.320(3)
La - Te[3] x 2	3.396(5)	3.381(5)	3.417(5)
La - Te[4] x 2	3.396(4)	3.318(4)	3.476(4)
Te[1] - K x 4	3.289(10)	3.186(11)	3.394(11)
Te[1] - Cu x 2	2.693(9)	2.602(12)	2.782(12)
Te[1] - Cu x 2	2.723(9)	2.682(6)	2.763(6)
Te[3] - Te[4] x 4	3.147(4)	2.910(5)	3.392(4)
Te[3] - K x 2	3.494(10)	3.402(9)	3.590(8)
Te[4] - K x 2	3.493(13)	3.451(12)	3.534(12)
K - Cu x 2	3.377(15)	3.333(14)	3.423(14)

Table 4.32. (Cont'd) Bond lengths distributions [Å] for KCuLaTe₄ at 300 K with e.s.d.'s in parentheses.

K - Cu x 2	3.332(12)	3.311(14)	3.354(14)
Cu - Cu x 4	3.146(12)	3.061(14)	3.231(14)

Table 4.33. Bond angles distributions [°] for KCuLaTe₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - La - Te[2] x 8	74.07(10)	73.41(10)	74.71(10)
Te[2] - La - Te[3] x 2	138.88(12)	138.27(14)	139.30(14)
Te[2] - La - Te[4] x 2	139.17(7)	138.75(8)	139.62(8)
Te[2] - La - Te[2] x 4	85.80(6)	84.45(5)	87.17(5)
Te[2] - La - Te[2] x 4	85.56(8)	85.29(9)	85.80(9)
Te[2] - La - Te[2] x 4	148.13(12)	148.09(11)	148.19(14)
Te[2] - La - Te[3] x 4	76.17(9)	73.21(9)	79.09(9)
Te[2] - La - Te[3] x 4	130.78(8)	126.73(9)	134.85(10)
Te[2] - La - Te[4] x 4	76.33(8)	75.81(8)	76.90(9)
Te[2] - La - Te[4] x 4	130.68(12)	129.87(12)	131.47(12)
Te[3] - La - Te[3] x 2	82.08(11)	81.77(10)	82.67(12)
Te[3] - La - Te[4] x 4	55.26(9)	51.72(9)	58.87(8)
Te[4] - La - Te[4] x 2	81.66(10)	81.56(12)	81.84(11)
K - Te[1] - K x 8	85.1(3)	84.0(3)	86.3(3)
K - Te[1] - K x 4	145.8(3)	144.7(3)	147.0(3)
K - Te[1] - Cu x 4	66.8(3)	66.4(3)	67.1(3)
K - Te[1] - Cu x 8	136.4(4)	135.4(4)	137.5(4)
K - Te[1] - Cu x 4	67.6(3)	66.2(3)	69.0(3)
Cu - Te[1] - Cu x 2	111.6(3)	111.0(3)	112.2(4)
Cu - Te[1] - Cu x 8	71.0(3)	69.4(3)	72.7(3)
Cu - Te[1] - Cu x 2	109.3(3)	107.3(3)	111.6(3)
La - Te[2] - La x 8	105.93(10)	105.03(11)	106.83(11)
La - Te[2] - La x 4	85.81(6)	85.26(5)	86.34(5)
La - Te[2] - La x 4	85.55(8)	85.29(6)	85.80(6)
La - Te[2] - La x 4	148.14(12)	147.92(16)	148.36(15)
La - Te[3] - La x 2	81.92(11)	81.73(10)	82.30(11)
La - Te[3] - Te[4] x 4	62.38(11)	60.86(10)	63.80(11)

Table 4.33. (Cont'd) Bond angles distributions [°] for KCuLaTe₄ at 300 K with e.s.d.'s in parentheses.

La - Te[3] - Te[4] x 4	117.84(13)	112.82(12)	122.62(14)
La - Te[3] - K x 4	125.6(2)	121.8(2)	129.2(3)
Te[4] - Te[3] - Te[4] x 4	90.48(10)	83.62(9)	97.45(11)
Te[4] - Te[3] - Te[4] x 4	89.59(12)	88.68(12)	90.11(12)
Te[4] - Te[3] - Te[4] x 2	175.91(14)	173.62(14)	179.79(17)
Te[4] - Te[3] - K x 4	63.2(2)	60.9(2)	65.7(3)
Te[4] - Te[3] - K x 4	116.4(3)	114.7(3)	117.9(3)
Te[4] - Te[3] - Te[4] x 2	175.20(14)	172.51(14)	179.75(17)
K - Te[3] - K x 2	78.90(19)	78.7(2)	79.2(2)
La - Te[4] - La x 2	81.66(11)	81.56(11)	81.84(12)
La - Te[4] - Te[3] x 4	62.45(10)	59.39(10)	65.59(11)
La - Te[4] - Te[3] x 4	117.23(15)	115.86(16)	118.43(15)
La - Te[4] - K x 4	125.61(18)	122.20(17)	128.9(2)
Te[3] - Te[4] - Te[3] x 4	90.47(9)	83.90(9)	97.10(10)
Te[3] - Te[4] - Te[3] x 4	89.58(13)	88.68(12)	90.11(13)
Te[3] - Te[4] - Te[3] x 2	175.47(14)	172.94(14)	179.85(15)
Te[3] - Te[4] - K x 4	63.18(18)	62.13(18)	64.49(18)
Te[3] - Te[4] - K x 4	117.0(2)	112.66(19)	121.1(2)
Te[3] - Te[4] - Te[3] x 2	176.03(14)	173.83(14)	179.85(16)
K - Te[4] - K x 2	79.2(3)	77.6(3)	80.9(3)
Te[1] - K - Te[1] x 8	85.16(17)	83.87(17)	86.45(18)
Te[1] - K - Te[1] x 4	145.7(4)	145.3(5)	146.3(5)
Te[1] - K - Te[3] x 4	78.35(18)	77.91(19)	78.8(2)
Te[1] - K - Te[3] x 4	131.0(4)	129.2(4)	132.8(4)
Te[1] - K - Te[4] x 4	78.1(2)	76.5(3)	79.8(2)
Te[1] - K - Te[4] x 4	131.1(2)	127.2(3)	135.0(3)
Te[1] - K - Cu x 8	48.2(3)	47.0(3)	49.4(3)
Te[1] - K - Cu x 8	103.0(4)	102.8(4)	103.1(4)
Te[3] - K - Te[3] x 2	78.9(3)	78.7(3)	79.2(3)
Te[3] - K - Te[4] x 4	53.56(18)	49.97(15)	57.15(16)
Te[3] - K - Cu x 4	125.5(4)	124.0(4)	127.0(4)
Te[3] - K - Cu x 2	98.7(2)	97.2(3)	100.2(3)
Te[3] - K - Cu x 2	176.7(4)	174.9(4)	178.1(4)
Te[4] - K - Te[4] x 2	79.3(3)	79.0(2)	79.9(3)

Table 4.33. (Cont'd) Bond angles distributions [°] for KCuLaTe₄ at 300 K with e.s.d.'s in parentheses.

Te[4] - K - Cu x 2	99.1(4)	97.5(3)	100.8(3)
Te[4] - K - Cu x 2	176.6(4)	174.5(4)	178.9(4)
Te[4] - K - Cu x 4	125.0(3)	122.7(3)	127.3(3)
Cu - K - Cu x 2	82.4(4)	80.5(4)	84.4(4)
Cu - K - Cu x 8	55.9(3)	54.4(3)	57.5(3)
Cu - K - Cu x 2	83.6(4)	83.4(4)	83.9(4)
Te[1] - Cu - Te[1] x 2	111.6(3)	111.2(3)	111.9(3)
Te[1] - Cu - Te[1] x 10	108.9(3)	107.9(4)	109.9(5)
Te[1] - Cu - K x 4	83.0(3)	82.2(3)	83.8(3)
Te[1] - Cu - K x 2	165.4(4)	164.3(3)	166.5(3)
Te[1] - Cu - K x 4	65.2(3)	63.5(3)	67.1(4)
Te[1] - Cu - Cu x 4	54.9(3)	54.2(2)	55.7(2)
Te[1] - Cu - Cu x 4	126.5(4)	125.6(3)	127.5(3)
Te[1] - Cu - K x 4	64.2(2)	62.0(2)	66.5(2)
Te[1] - Cu - K x 2	166.8(3)	165.9(3)	168.3(3)
Te[1] - Cu - Cu x 4	54.0(3)	53.0(2)	55.1(2)
Te[1] - Cu - Cu x 4	124.4(4)	121.7(4)	127.2(4)
K - Cu - K x 2	82.5(3)	80.8(4)	84.2(4)
K - Cu - K x 8	124.0(4)	121.6(5)	126.5(5)
K - Cu - Cu x 4	61.3(3)	60.1(3)	62.5(3)
K - Cu - Cu x 4	116.9(3)	116.3(3)	117.5(3)
K - Cu - K x 2	83.6(3)	83.4(3)	83.9(3)
K - Cu - Cu x 4	62.8(3)	61.4(4)	64.2(4)
K - Cu - Cu x 4	119.0(4)	116.6(4)	121.3(4)
Cu - Cu - Cu x 8	90.1(4)	88.3(4)	91.8(4)
Cu - Cu - Cu x 4	177.1(4)	176.4(5)	177.9(3)

Table 4.34. Crystal data and structure refinement for Na_{0.78(1)}Ag_{1.22(1)}CeTe₄ at 100 K.

Empirical formula	Na _{0.78(1)} Ag _{1.22(1)} CeTe ₄
Formula weight	800.1
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β0)0s0
Unit cell dimensions	a = 4.4139(7) Å, α = 90° b = 4.4185(8) Å, β = 90° c = 20.245(3) Å, γ = 90°
q-vector	0.3681(8)b*
Volume	394.83(11) Å ³
Z	2
Density (calculated)	6.7275 g/cm ³
Absorption coefficient	23.121 mm ⁻¹
F(000)	664
Crystal size	0.20 x 0.14 x 0.10 mm ³
Theta range for data collection	1.97 to 29.25°
Index ranges	-6<= <i>h</i> <=6, -6<= <i>k</i> <=6, -27<= <i>l</i> <=27, -1<= <i>m</i> <=1
Reflections collected	10679 (3140 main + 7539 satellites)
Independent reflections	3163 (1035 main + 2128 satellites) [R _{int} = 0.0965]
Completeness to θ = 29.25°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3163 / 15 / 101
Goodness-of-fit on F ²	2.09
Final R indices [I>2σ(I)]	R _{obs} = 0.0637, wR _{obs} = 0.1581
R indices (all data)	R _{all} = 0.1018, wR _{all} = 0.1672
Final R main indices [I>2σ(I)]	R _{obs} = 0.0544, wR _{obs} = 0.1529
R main indices (all data)	R _{all} = 0.0590, wR _{all} = 0.1553
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1296, wR _{obs} = 0.1955
R 1 st order satellites (all data)	R _{all} = 0.2961, wR _{all} = 0.2416
Extinction coefficient	0.00103(13)
T _{min} and T _{max} coefficients	0.0621 and 0.1486
Largest diff. peak and hole	4.87 and -3.41 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o $, $wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.35. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.78(1)}\text{Ag}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce	0	0	0	3973(1)	1	15(1)
	sin, 1	61(3)	-7(6)	0		
	cos, 1	0	0	3(2)		
Te[1]	0	0	0	912(1)	1	23(1)
	sin, 1	-6(3)	10(8)	0		
	cos, 1	0	0	2(2)		
Te[2]	0	0	0	5591(1)	1	14(1)
	sin, 1	-4(3)	-3(7)	0		
	cos, 1	0	0	3(2)		
Te[3]	0	0	5000	2722(1)	1	18(1)
	sin, 1	-266(6)	49(7)	0		
	cos, 1	0	0	-1(2)		
Te[4]	0	0	5000	7276(1)	1	19(1)
	sin, 1	221(6)	-5(7)	0		
	cos, 1	0	0	2(2)		
Na	0	0	0	8602	0.781(10)	33(2)
	sin, 1	-47(12)	25(30)	0		
	cos, 1	0	0	-23(8)		
Ag[1]	0	0	5000	0(1)	1	24(1)
	sin, 1	-21(10)	44(10)	0		
	cos, 1	0	0	-4(2)		
Ag[2]	0	0	0	8602(3)	0.219(10)	33(2)
	sin, 1	-47(12)	25(30)	0		
	cos, 1	0	0	-23(8)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.36. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.78(1)}\text{Ag}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	0	10(1)	10(1)	24(1)	-5(1)	0	0
	sin, 1	0	0	0	0	0(1)	1(1)
	cos, 1	-6(1)	-1(1)	0(1)	0(1)	0	0

Table 4.36. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.78(1)}\text{Ag}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Te[1]	0	19(1)	18(1)	31(1)	-7(1)	0	0
	sin, 1	0	0	0	0	0(1)	1(1)
	cos, 1	3(2)	2(2)	0(2)	0(1)	0	0
Te[2]	0	9(1)	9(1)	25(1)	6(1)	0	0
	sin, 1	0	0	0	0	-1(1)	2(1)
	cos, 1	-4(1)	-1(1)	5(2)	0(1)	0	0
Te[3]	0	15(1)	15(1)	25(1)	-6(1)	0	0
	sin, 1	0	0	0	0	2(1)	-4(1)
	cos, 1	1(2)	2(1)	-2(2)	-4(1)	0	0
Te[4]	0	15(1)	16(1)	25(1)	12(1)	0	0
	sin, 1	0	0	0	0	-1(1)	-2(1)
	cos, 1	2(2)	2(1)	1(2)	1(1)	0	0
Na	0	26(2)	25(2)	46(3)	-9(3)	0	0
	sin, 1	0	0	0	0	1(2)	30(5)
	cos, 1	-20(6)	1(5)	-20(8)	-2(3)	0	0
Ag[1]	0	22(1)	23(1)	27(1)	-5(1)	0	0
	sin, 1	0	0	0	0	1(1)	4(2)
	cos, 1	-3(2)	-2(2)	4(2)	2(2)	0	0
Ag[2]	0	26(2)	25(2)	46(3)	-9(3)	0	0
	sin, 1	0	0	0	0	1(2)	30(5)
	cos, 1	-20(6)	1(5)	-20(8)	-2(3)	0	0

Table 4.37. Bond lengths distributions [$\text{\AA}$] for $\text{Na}_{0.78(1)}\text{Ag}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[2]	3.275(3)	3.275(5)	3.2754(13)
Ce - Te[2] x 4	3.246(2)	3.228(2)	3.264(2)
Ce - Te[3] x 2	3.362(3)	3.343(3)	3.383(3)
Ce - Te[4] x 2	3.356(3)	3.309(2)	3.402(2)
Te[1] - Na x 4	3.274(6)	3.247(7)	3.300(7)
Te[1] - Ag[1] x 4	2.879(4)	2.861(4)	2.897(4)
Te[1] - Ag[2] x 4	3.274(6)	3.247(7)	3.300(7)
Te[3] - Te[4] x 4	3.124(2)	3.010(3)	3.241(3)

Table 4.37. (Cont'd) Bond lengths distributions [Å] for Na_{0.78(1)}Ag_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Na x 2	3.472(8)	3.402(4)	3.543(4)
Te[3] - Ag[2] x 2	3.472(9)	3.402(6)	3.543(6)
Te[4] - Na x 2	3.477(9)	3.439(12)	3.517(12)
Te[4] - Ag[2] x 2	3.477(10)	3.439(13)	3.517(13)
Ag[1] - Ag[1] x 4	3.123(4)	3.099(5)	3.147(5)

Table 4.38. Bond angles distributions [°] for Na_{0.78(1)}Ag_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - Ce - Te[2] x 8	74.18(5)	73.82(5)	74.55(5)
Te[2] - Ce - Te[3] x 2	138.86(7)	138.56(7)	139.09(8)
Te[2] - Ce - Te[4] x 2	138.88(5)	138.48(5)	139.29(5)
Te[2] - Ce - Te[2] x 8	85.80(6)	85.18(5)	86.42(5)
Te[2] - Ce - Te[2] x 4	148.37(8)	148.24(12)	148.50(12)
Te[2] - Ce - Te[3] x 4	75.99(7)	74.76(6)	77.20(6)
Te[2] - Ce - Te[3] x 4	130.74(7)	128.71(7)	132.80(7)
Te[2] - Ce - Te[4] x 4	76.01(6)	75.47(7)	76.56(7)
Te[2] - Ce - Te[4] x 4	130.73(9)	129.98(9)	131.47(9)
Te[3] - Ce - Te[3] x 2	82.23(8)	81.93(10)	82.62(9)
Te[3] - Ce - Te[4] x 4	55.43(7)	53.22(7)	57.64(6)
Te[4] - Ce - Te[4] x 2	82.24(7)	82.17(10)	82.33(10)
Na - Te[1] - Na x 8	84.88(19)	84.76(18)	85.01(18)
Na - Te[1] - Na x 4	145.05(19)	144.51(16)	145.58(17)
Na - Te[1] - Ag[1] x 8	71.02(17)	70.4(2)	71.6(2)
Na - Te[1] - Ag[1] x 8	135.27(16)	134.8(2)	135.75(19)
Na - Te[1] - Ag[2] x 8	84.88(19)	84.76(18)	85.01(18)
Na - Te[1] - Ag[2] x 4	145.0(2)	144.51(19)	145.58(19)
Ag[1] - Te[1] - Ag[1] x 4	100.23(12)	99.97(16)	100.48(16)
Ag[1] - Te[1] - Ag[1] x 8	65.69(11)	65.23(10)	66.16(10)
Ag[1] - Te[1] - Ag[2] x 8	71.02(16)	70.40(16)	71.64(16)
Ag[1] - Te[1] - Ag[2] x 8	135.26(14)	134.83(15)	135.70(15)
Ag[2] - Te[1] - Ag[2] x 8	84.9(2)	84.76(18)	85.01(18)
Ag[2] - Te[1] - Ag[2] x 4	145.0(2)	144.5(2)	145.6(2)

Table 4.38. (Cont'd) Bond angles distributions [°] for Na_{0.78(1)}Ag_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Ce - Te[2] - Ce x 8	105.81(6)	105.30(6)	106.33(6)
Ce - Te[2] - Ce x 4	85.80(5)	85.49(5)	86.10(5)
Ce - Te[2] - Ce x 4	85.68(6)	85.65(6)	85.71(6)
Ce - Te[2] - Ce x 4	148.37(9)	148.05(13)	148.69(13)
Ce - Te[3] - Ce x 2	82.17(8)	82.03(11)	82.39(11)
Ce - Te[3] - Te[4] x 4	62.17(5)	61.74(6)	62.63(5)
Ce - Te[3] - Te[4] x 4	117.67(8)	114.78(7)	120.47(7)
Ce - Te[3] - Na x 4	125.55(17)	123.65(17)	127.34(19)
Ce - Te[3] - Ag[2] x 4	125.55(17)	123.65(18)	127.34(19)
Te[4] - Te[3] - Te[4] x 4	90.19(7)	86.14(8)	94.27(9)
Te[4] - Te[3] - Te[4] x 4	89.84(8)	89.25(10)	90.39(9)
Te[4] - Te[3] - Te[4] x 2	177.04(9)	175.39(12)	179.87(8)
Te[4] - Te[3] - Na x 4	63.40(16)	61.85(16)	64.94(17)
Te[4] - Te[3] - Na x 4	116.69(18)	115.77(17)	117.49(17)
Te[4] - Te[3] - Ag[2] x 4	63.40(17)	61.85(16)	64.94(18)
Te[4] - Te[3] - Ag[2] x 4	116.69(18)	115.77(18)	117.49(17)
Te[4] - Te[3] - Te[4] x 2	177.73(9)	176.47(12)	179.91(9)
Na - Te[3] - Na x 2	78.92(14)	78.0(2)	79.9(2)
Na - Te[3] - Ag[2] x 2	78.92(15)	78.0(2)	79.9(2)
Ag[2] - Te[3] - Ag[2] x 2	78.92(16)	78.0(2)	79.9(2)
Ce - Te[4] - Ce x 2	82.24(6)	82.17(11)	82.33(11)
Ce - Te[4] - Te[3] x 4	62.38(6)	60.88(6)	63.95(6)
Ce - Te[4] - Te[3] x 4	117.72(8)	116.75(8)	118.64(9)
Ce - Te[4] - Na x 4	125.53(13)	123.42(14)	127.65(15)
Ce - Te[4] - Ag[2] x 4	125.53(13)	123.42(15)	127.65(15)
Te[3] - Te[4] - Te[3] x 4	90.12(7)	86.39(8)	93.97(9)
Te[3] - Te[4] - Te[3] x 4	89.85(8)	89.25(8)	90.39(7)
Te[3] - Te[4] - Te[3] x 2	177.69(9)	176.40(12)	179.90(7)
Te[3] - Te[4] - Na x 4	63.17(13)	62.37(14)	64.02(14)
Te[3] - Te[4] - Na x 4	116.64(14)	114.13(13)	119.21(13)
Te[3] - Te[4] - Ag[2] x 4	63.17(13)	62.37(14)	64.02(14)
Te[3] - Te[4] - Ag[2] x 4	116.64(15)	114.13(14)	119.21(14)
Te[3] - Te[4] - Te[3] x 2	177.48(9)	176.07(12)	179.91(7)
Na - Te[4] - Na x 2	78.9(2)	78.2(2)	79.6(2)

Table 4.38. (Cont'd) Bond angles distributions [°] for Na_{0.78(1)}Ag_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Na - Te[4] - Ag[2] x 2	78.9(2)	78.2(2)	79.6(2)
Ag[2] - Te[4] - Ag[2] x 2	78.9(2)	78.2(2)	79.6(2)
Te[1] - Na - Te[1] x 8	84.87(13)	84.17(13)	85.59(13)
Te[1] - Na - Te[1] x 4	145.0(3)	143.4(5)	146.7(5)
Te[1] - Na - Te[3] x 4	78.67(13)	77.60(13)	79.77(14)
Te[1] - Na - Te[3] x 4	131.3(3)	129.8(2)	132.8(2)
Te[1] - Na - Te[4] x 4	78.63(16)	77.89(12)	79.38(12)
Te[1] - Na - Te[4] x 4	131.4(2)	128.9(2)	133.8(2)
Te[3] - Na - Te[3] x 2	78.93(18)	78.0(3)	79.9(3)
Te[3] - Na - Te[4] x 4	53.41(14)	52.09(9)	54.78(9)
Te[4] - Na - Te[4] x 2	78.94(19)	78.0(3)	79.9(3)
Te[1] - Ag[1] - Te[1] x 4	100.23(11)	100.06(16)	100.40(16)
Te[1] - Ag[1] - Te[1] x 8	114.30(11)	113.99(17)	114.62(17)
Te[1] - Ag[1] - Ag[1] x 8	57.14(8)	56.97(8)	57.31(8)
Te[1] - Ag[1] - Ag[1] x 8	122.89(12)	122.61(12)	123.19(12)
Ag[1] - Ag[1] - Ag[1] x 8	90.06(12)	89.58(12)	90.54(12)
Ag[1] - Ag[1] - Ag[1] x 4	179.43(15)	179.15(19)	179.88(18)
Te[1] - Ag[2] - Te[1] x 8	84.87(14)	84.17(14)	85.59(14)
Te[1] - Ag[2] - Te[1] x 4	145.0(4)	143.4(6)	146.7(6)
Te[1] - Ag[2] - Te[3] x 4	78.67(13)	77.60(14)	79.77(14)
Te[1] - Ag[2] - Te[3] x 4	131.3(3)	129.8(2)	132.8(2)
Te[1] - Ag[2] - Te[4] x 4	78.63(16)	77.89(12)	79.38(13)
Te[1] - Ag[2] - Te[4] x 4	131.4(2)	128.9(3)	133.8(3)
Te[3] - Ag[2] - Te[3] x 2	78.9(2)	78.0(4)	79.9(4)
Te[3] - Ag[2] - Te[4] x 4	53.41(15)	52.09(11)	54.78(11)
Te[4] - Ag[2] - Te[4] x 2	78.9(2)	78.0(4)	79.9(4)

Table 4.39. Crystal data and structure refinement for Na_{0.70(1)}Ag_{1.30(1)}LaTe₄ at 100 K.

Empirical formula	Na _{0.70(1)} Ag _{1.30(1)} LaTe ₄
Formula weight	805.6
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β1/2)0s0
Unit cell dimensions	a = 4.4415(6) Å, α = 90° b = 4.4467(7) Å, β = 90° c = 20.239(3) Å, γ = 90°
q-vector	0.3660(8)b* + 1/2c*
Volume	399.72(10) Å ³
Z	2
Density (calculated)	6.6914 g/cm ³
Absorption coefficient	22.605 mm ⁻¹
F(000)	667
Crystal size	0.21 x 0.12 x 0.08 mm ³
Theta range for data collection	1.75 to 29.16°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 6, -27 ≤ l ≤ 28, -1 ≤ m ≤ 1
Reflections collected	10043 (2510 main + 7533 satellites)
Independent reflections	3162 (999 main + 2163 satellites) [R _{int} = 0.0987]
Completeness to θ = 29.16°	97%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3162 / 15 / 102
Goodness-of-fit on F ²	2.50
Final R indices [I > 2σ(I)]	R _{obs} = 0.0735, wR _{obs} = 0.1917
R indices (all data)	R _{all} = 0.1139, wR _{all} = 0.2053
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0645, wR _{obs} = 0.1914
R main indices (all data)	R _{all} = 0.0714, wR _{all} = 0.2004
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1369, wR _{obs} = 0.1937
R 1 st order satellites (all data)	R _{all} = 0.3004, wR _{all} = 0.2384
Extinction coefficient	0.00090(15)
T _{min} and T _{max} coefficients	0.0573 and 0.1544
Largest diff. peak and hole	6.32 and -4.74 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 4.40. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.70(1)}\text{Ag}_{1.30(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
La	0	0	0	3962(1)	1	13(1)
	sin, 1	19(1)	2(2)	-5(2)		
	cos, 1	-56(3)	-6(7)	-2(1)		
Te[1]	0	0	0	913(1)	1	18(1)
	sin, 1	-7(3)	1(8)	1(1)		
	cos, 1	2(1)	0(2)	4(2)		
Te[2]	0	0	0	5597(1)	1	13(1)
	sin, 1	0(1)	-2(1)	0(2)		
	cos, 1	-1(3)	-12(7)	0(1)		
Te[3]	0	0	5000	2700(1)	1	19(1)
	sin, 1	-163(4)	14(6)	-1(2)		
	cos, 1	185(5)	-16(7)	-1(2)		
Te[4]	0	0	5000	7299(1)	1	19(1)
	sin, 1	133(4)	12(6)	1(2)		
	cos, 1	151(5)	14(7)	-1(1)		
Na	0	0	0	8615	0.703(12)	32(2)
	sin, 1	-53(11)	-55(20)	7(3)		
	cos, 1	-25(5)	-27(11)	-16(6)		
Ag[1]	0	0	5000	0(1)	1	21(1)
	sin, 1	-33(10)	44(11)	0		
	cos, 1	0	0	1(3)		
Ag[2]	0	0	0	8615(3)	0.297(12)	32(2)
	sin, 1	-53(11)	-55(20)	7(3)		
	cos, 1	-25(5)	-27(11)	-16(6)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.41. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.70(1)}\text{Ag}_{1.30(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	0	11(1)	12(1)	18(1)	-8(1)	0	0
	sin, 1	-1(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	1(1)	-1(1)

Table 4.41. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.70}\text{Ag}_{1.30}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Te[1]	0	17(1)	17(1)	19(1)	-7(1)	0	0
	sin, 1	0(1)	-1(1)	1(1)	0(1)	-1(1)	-2(1)
	cos, 1	-1(1)	-3(2)	4(2)	0(1)	0(1)	1(1)
Te[2]	0	10(1)	11(1)	17(1)	7(1)	0	0
	sin, 1	-1(1)	-3(1)	4(2)	0(1)	0(1)	0(1)
	cos, 1	0(1)	1(1)	-1(1)	0(1)	-1(1)	0(1)
Te[3]	0	19(1)	19(1)	17(1)	-5(1)	0	0
	sin, 1	-3(1)	0(1)	3(1)	-2(1)	2(1)	1(1)
	cos, 1	-3(1)	0(1)	3(1)	-2(1)	-2(1)	-1(1)
Te[4]	0	18(1)	22(1)	17(1)	11(1)	0	0
	sin, 1	1(1)	2(1)	-1(1)	1(1)	0(1)	-2(1)
	cos, 1	-1(1)	-2(1)	1(1)	-1(1)	0(1)	-2(1)
Na	0	37(4)	26(3)	32(3)	-11(3)	0	0
	sin, 1	17(3)	6(2)	8(3)	-4(1)	-1(2)	-28(4)
	cos, 1	-36(6)	-14(5)	-17(6)	10(3)	0(1)	-13(2)
Ag[1]	0	21(1)	22(1)	19(1)	-5(2)	0	0
	sin, 1	0	0	0	0	0(1)	2(2)
	cos, 1	4(2)	-4(2)	5(2)	0(2)	0	0
Ag[2]	0	37(4)	26(3)	32(3)	-11(3)	0	0
	sin, 1	17(3)	6(2)	8(3)	-4(1)	-1(2)	-28(4)
	cos, 1	-36(6)	-14(5)	-17(6)	10(3)	0(1)	-13(2)

Table 4.42. Bond lengths distributions [$\text{\AA}$] for $\text{Na}_{0.70(1)}\text{Ag}_{1.30(1)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[2]	3.309(3)	3.298(5)	3.320(5)
La - Te[2] x 4	3.267(2)	3.248(2)	3.286(2)
La - Te[3] x 2	3.388(4)	3.386(4)	3.391(4)
La - Te[4] x 2	3.382(3)	3.341(3)	3.425(3)
Te[1] - Na x 4	3.284(7)	3.271(6)	3.298(6)
Te[1] - Ag[1] x 4	2.891(4)	2.871(5)	2.911(5)
Te[1] - Ag[2] x 4	3.284(7)	3.271(6)	3.298(6)
Te[3] - Te[4] x 4	3.143(4)	3.037(4)	3.253(4)

Table 4.42. (Cont'd) Bond lengths distributions [Å] for Na_{0.70(1)}Ag_{1.30(1)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Na x 2	3.466(8)	3.407(6)	3.526(6)
Te[3] - Ag[2] x 2	3.466(9)	3.407(8)	3.526(7)
Te[4] - Na x 2	3.472(9)	3.442(9)	3.499(9)
Te[4] - Ag[2] x 2	3.472(10)	3.442(10)	3.499(10)
Ag[1] - Ag[1] x 4	3.142(4)	3.117(5)	3.168(5)

Table 4.43. Bond angles distributions [°] for Na_{0.70(1)}Ag_{1.30(1)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - La - Te[2] x 8	74.14(8)	73.90(9)	74.38(9)
Te[2] - La - Te[3] x 2	138.93(10)	138.68(9)	139.15(8)
Te[2] - La - Te[4] x 2	138.96(6)	138.59(6)	139.34(6)
Te[2] - La - Te[2] x 4	85.78(5)	85.20(4)	86.36(4)
Te[2] - La - Te[2] x 4	85.65(6)	85.45(5)	85.86(5)
Te[2] - La - Te[2] x 4	148.27(11)	147.97(13)	148.59(13)
Te[2] - La - Te[3] x 4	76.08(7)	74.72(7)	77.43(7)
Te[2] - La - Te[3] x 4	130.75(7)	128.92(8)	132.58(8)
Te[2] - La - Te[4] x 4	76.11(7)	75.87(8)	76.35(8)
Te[2] - La - Te[4] x 4	130.73(10)	130.39(10)	131.06(10)
Te[3] - La - Te[3] x 2	82.09(9)	81.70(10)	82.56(10)
Te[3] - La - Te[4] x 4	55.34(7)	53.12(7)	57.56(7)
Te[4] - La - Te[4] x 2	82.07(8)	81.91(10)	82.25(10)
Na - Te[1] - Na x 8	85.22(19)	84.3(2)	86.1(2)
Na - Te[1] - Na x 4	146.2(2)	145.40(19)	146.99(19)
Na - Te[1] - Ag[1] x 8	70.43(18)	69.81(16)	71.06(16)
Na - Te[1] - Ag[1] x 8	134.95(16)	134.41(17)	135.49(17)
Na - Te[1] - Ag[2] x 8	85.22(19)	84.3(2)	86.1(2)
Na - Te[1] - Ag[2] x 4	146.2(2)	145.4(2)	147.0(2)
Ag[1] - Te[1] - Ag[1] x 4	100.56(12)	100.35(14)	100.76(14)
Ag[1] - Te[1] - Ag[1] x 8	65.88(12)	65.48(12)	66.28(12)
Ag[1] - Te[1] - Ag[2] x 8	70.43(17)	69.81(17)	71.06(17)
Ag[1] - Te[1] - Ag[2] x 8	134.95(15)	134.67(14)	135.23(14)
Ag[2] - Te[1] - Ag[2] x 8	85.22(19)	84.3(2)	86.1(2)

Table 4.43. (Cont'd) Bond angles distributions [°] for Na_{0.70(1)}Ag_{1.30(1)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Ag[2] - Te[1] - Ag[2] x 4	146.2(2)	145.4(2)	147.0(2)
La - Te[2] - La x 8	105.86(8)	105.45(9)	106.27(9)
La - Te[2] - La x 4	85.78(5)	85.53(4)	86.03(4)
La - Te[2] - La x 4	85.65(6)	85.45(8)	85.86(8)
La - Te[2] - La x 4	148.28(11)	148.01(14)	148.55(13)
La - Te[3] - La x 2	82.04(9)	81.97(9)	82.17(10)
La - Te[3] - Te[4] x 4	62.24(8)	61.73(8)	62.76(8)
La - Te[3] - Te[4] x 4	117.65(11)	115.00(10)	120.22(11)
La - Te[3] - Na x 4	125.40(17)	123.03(16)	127.72(18)
La - Te[3] - Ag[2] x 4	125.40(17)	123.03(17)	127.72(18)
Te[4] - Te[3] - Te[4] x 4	90.18(8)	86.42(8)	93.96(9)
Te[4] - Te[3] - Te[4] x 4	89.85(10)	89.39(10)	90.15(10)
Te[4] - Te[3] - Te[4] x 2	177.37(11)	175.90(11)	179.89(14)
Te[4] - Te[3] - Na x 4	63.18(17)	61.25(16)	65.11(17)
Te[4] - Te[3] - Na x 4	116.92(18)	116.47(19)	117.36(18)
Te[4] - Te[3] - Ag[2] x 4	63.18(17)	61.25(16)	65.11(17)
Te[4] - Te[3] - Ag[2] x 4	116.92(19)	116.47(19)	117.36(19)
Te[4] - Te[3] - Te[4] x 2	177.79(11)	176.55(11)	179.90(14)
Na - Te[3] - Na x 2	79.67(16)	78.99(17)	80.39(17)
Na - Te[3] - Ag[2] x 2	79.67(17)	78.99(18)	80.39(18)
Ag[2] - Te[3] - Ag[2] x 2	79.67(18)	78.99(18)	80.39(19)
La - Te[4] - La x 2	82.07(9)	81.91(9)	82.25(9)
La - Te[4] - Te[3] x 4	62.44(8)	60.80(8)	64.10(9)
La - Te[4] - Te[3] x 4	117.66(12)	116.63(12)	118.60(12)
La - Te[4] - Na x 4	125.41(14)	123.01(13)	127.76(14)
La - Te[4] - Ag[2] x 4	125.41(14)	123.01(14)	127.76(14)
Te[3] - Te[4] - Te[3] x 4	90.18(8)	86.70(8)	93.64(8)
Te[3] - Te[4] - Te[3] x 4	89.85(10)	89.39(9)	90.15(10)
Te[3] - Te[4] - Te[3] x 2	177.97(11)	176.84(11)	179.92(13)
Te[3] - Te[4] - Na x 4	62.98(13)	62.11(13)	63.82(14)
Te[3] - Te[4] - Na x 4	116.93(15)	114.47(15)	119.34(15)
Te[3] - Te[4] - Ag[2] x 4	62.98(14)	62.11(14)	63.82(14)
Te[3] - Te[4] - Ag[2] x 4	116.93(15)	114.47(15)	119.34(16)
Te[3] - Te[4] - Te[3] x 2	177.58(11)	176.22(11)	179.91(13)

Table 4.43. (Cont'd) Bond angles distributions [°] for Na_{0.70}Ag_{1.30}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Na - Te[4] - Na x 2	79.7(2)	79.3(2)	80.1(2)
Na - Te[4] - Ag[2] x 2	79.7(2)	79.3(2)	80.1(2)
Ag[2] - Te[4] - Ag[2] x 2	79.7(2)	79.3(2)	80.1(2)
Te[1] - Na - Te[1] x 8	85.21(13)	84.56(13)	85.86(13)
Te[1] - Na - Te[1] x 4	146.2(3)	144.9(4)	147.5(4)
Te[1] - Na - Te[3] x 4	77.88(13)	77.43(13)	78.34(14)
Te[1] - Na - Te[3] x 4	131.0(3)	130.4(3)	131.7(3)
Te[1] - Na - Te[4] x 4	77.86(17)	76.4(2)	79.4(2)
Te[1] - Na - Te[4] x 4	131.1(2)	128.7(2)	133.5(2)
Te[3] - Na - Te[3] x 2	79.7(2)	79.0(2)	80.4(2)
Te[3] - Na - Te[4] x 4	53.89(14)	52.33(12)	55.45(12)
Te[4] - Na - Te[4] x 2	79.7(2)	78.8(2)	80.6(3)
Te[1] - Ag[1] - Te[1] x 4	100.56(13)	100.51(18)	100.61(18)
Te[1] - Ag[1] - Te[1] x 8	114.12(11)	114.02(17)	114.22(17)
Te[1] - Ag[1] - Ag[1] x 8	57.03(9)	56.83(9)	57.24(9)
Te[1] - Ag[1] - Ag[1] x 8	122.97(12)	122.72(11)	123.23(11)
Ag[1] - Ag[1] - Ag[1] x 8	90.06(12)	89.56(12)	90.57(12)
Ag[1] - Ag[1] - Ag[1] x 2	179.41(14)	179.07(19)	180
Ag[1] - Ag[1] - Ag[1] x 2	179.69(13)	179.52(19)	180
Te[1] - Ag[2] - Te[1] x 8	85.21(14)	84.56(14)	85.86(14)
Te[1] - Ag[2] - Te[1] x 4	146.2(4)	144.9(4)	147.5(4)
Te[1] - Ag[2] - Te[3] x 4	77.88(14)	77.43(14)	78.34(14)
Te[1] - Ag[2] - Te[3] x 4	131.0(3)	130.4(3)	131.7(3)
Te[1] - Ag[2] - Te[4] x 4	77.86(18)	76.4(2)	79.4(2)
Te[1] - Ag[2] - Te[4] x 4	131.1(2)	128.7(3)	133.5(3)
Te[3] - Ag[2] - Te[3] x 2	79.7(2)	79.0(3)	80.4(3)
Te[3] - Ag[2] - Te[4] x 4	53.89(16)	52.33(14)	55.45(14)
Te[4] - Ag[2] - Te[4] x 2	79.7(2)	78.8(3)	80.6(3)

Table 4.44. Crystal data and structure refinement for Na_{0.78(1)}Cu_{1.22(1)}CeTe₄ at 100 K.

Empirical formula	Na _{0.78(1)} Cu _{1.22(1)} CeTe ₄
Formula weight	747.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β0)0s0
Unit cell dimensions	a = 4.3850(6) Å, α = 90° b = 4.3973(6) Å, β = 90° c = 19.810(3) Å, γ = 90°
q-vector	0.3621(7)b*
Volume	381.99(9) Å ³
Z	2
Density (calculated)	6.4836 g/cm ³
Absorption coefficient	24.212 mm ⁻¹
F(000)	620
Crystal size	0.70 x 0.10 x 0.01 mm ³
Theta range for data collection	1.96 to 29.30°
Index ranges	-6<=h<=6, -6<=k<=5, -27<=l<=27, -1<=m<=1
Reflections collected	9743 (2763 main + 6980 satellites)
Independent reflections	3090 (1028 main + 2062 satellites) [R _{int} = 0.0482]
Completeness to θ = 29.30°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3090 / 15 / 102
Goodness-of-fit on F ²	1.45
Final R indices [I>2σ(I)]	R _{obs} = 0.0454, wR _{obs} = 0.1114
R indices (all data)	R _{all} = 0.0917, wR _{all} = 0.1225
Final R main indices [I>2σ(I)]	R _{obs} = 0.0337, wR _{obs} = 0.0980
R main indices (all data)	R _{all} = 0.0385, wR _{all} = 0.1004
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1237, wR _{obs} = 0.1803
R 1 st order satellites (all data)	R _{all} = 0.3073, wR _{all} = 0.2228
Extinction coefficient	0.00019(4)
T _{min} and T _{max} coefficients	0.0773 and 0.9088
Largest diff. peak and hole	3.30 and -3.56 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w=1/(σ ² (I)+0.0016I ²)	

Table 4.45. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.78(1)}\text{Cu}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Ce	0	0	0	3943(1)	1	9(1)
	sin, 1	61(2)	1(6)	0		
	cos, 1	0	0	-1(1)		
Te[1]	0	0	0	787(1)	1	16(1)
	sin, 1	-14(2)	-31(7)	0		
	cos, 1	0	0	20(2)		
Te[2]	0	0	0	5603(1)	1	9(1)
	sin, 1	0(2)	-2(6)	0		
	cos, 1	0	0	3(2)		
Te[3]	0	0	5000	2663(1)	1	12(1)
	sin, 1	-286(4)	11(7)	0		
	cos, 1	0	0	0(2)		
Te[4]	0	0	5000	7336(1)	1	12(1)
	sin, 1	220(4)	-16(7)	0		
	cos, 1	0	0	1(2)		
Na	0	0	0	8743	0.785(13)	20(1)
	sin, 1	-53(10)	-55(30)	0		
	cos, 1	0	0	5(6)		
Cu[1]	0	0	5000	-1(1)	1	28(1)
	sin, 1	-53(14)	-88(17)	0		
	cos, 1	0	0	8(3)		
Cu[2]	0	0	0	8743(2)	0.215(13)	20(1)
	sin, 1	-53(10)	-55(30)	0		
	cos, 1	0	0	5(6)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.46. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.78(1)}\text{Cu}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ce	0	6(1)	8(1)	13(1)	-3(1)	0	0
	sin, 1	0	0	0	0	0(1)	-2(1)
	cos, 1	-1(1)	0(1)	1(1)	1(1)	0	0

Table 4.46. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.78}\text{Cu}_{1.22}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Te[1]	0	10(1)	13(1)	24(1)	7(1)	0	0
	sin, 1	0	0	0	0	0(1)	2(1)
	cos, 1	8(1)	8(1)	-13(1)	1(1)	0	0
Te[2]	0	6(1)	8(1)	12(1)	6(1)	0	0
	sin, 1	0	0	0	0	0(1)	1(1)
	cos, 1	-1(1)	1(1)	-1(1)	0(1)	0	0
Te[3]	0	11(1)	12(1)	13(1)	-5(1)	0	0
	sin, 1	0	0	0	0	0(1)	-3(1)
	cos, 1	-5(1)	5(1)	1(1)	-2(1)	0	0
Te[4]	0	10(1)	13(1)	13(1)	6(1)	0	0
	sin, 1	0	0	0	0	1(1)	0(1)
	cos, 1	3(1)	-2(1)	1(1)	3(1)	0	0
Na	0	15(2)	23(2)	22(2)	-9(4)	0	0
	sin, 1	0	0	0	0	-4(2)	-17(5)
	cos, 1	-13(5)	8(7)	1(6)	4(2)	0	0
Cu[1]	0	29(1)	34(1)	21(1)	1(3)	0	0
	sin, 1	0	0	0	0	-1(1)	8(3)
	cos, 1	16(3)	-19(3)	2(3)	-2(3)	0	0
Cu[2]	0	15(2)	23(2)	22(2)	-9(4)	0	0
	sin, 1	0	0	0	0	-4(2)	-17(5)
	cos, 1	-13(5)	8(7)	1(6)	4(2)	0	0

Table 4.47. Bond lengths distributions [$\text{\AA}$] for $\text{Na}_{0.78(1)}\text{Cu}_{1.22(1)}\text{CeTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Ce - Te[2]	3.288(2)	3.280(4)	3.296(4)
Ce - Te[2] x 4	3.2327(17)	3.213(2)	3.2524(19)
Ce - Te[3] x 2	3.357(2)	3.356(2)	3.360(2)
Ce - Te[4] x 2	3.3505(19)	3.3049(14)	3.3965(15)
Te[1] - Na x 4	3.242(6)	3.228(4)	3.256(4)
Te[1] - Cu[1] x 4	2.696(5)	2.684(4)	2.707(4)
Te[1] - Cu[2] x 4	3.242(6)	3.228(4)	3.256(4)
Te[3] - Te[4] x 4	3.106(2)	2.975(3)	3.241(2)

Table 4.47. (Cont'd) Bond lengths distributions [Å] for Na_{0.78(1)}Cu_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Na x 2	3.545(6)	3.482(3)	3.610(3)
Te[3] - Cu[2] x 2	3.545(7)	3.482(4)	3.610(4)
Na - Cu[1] x 4	3.321(9)	3.296(11)	3.347(11)
Cu[1] - Cu[1] x 4	3.105(6)	3.056(7)	3.154(7)
Cu[1] - Cu[2] x 4	3.321(10)	3.296(11)	3.347(11)

Table 4.48. Bond angles distributions [°] for Na_{0.78(1)}Cu_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - Ce - Te[2] x 8	73.85(4)	73.50(4)	74.19(4)
Te[2] - Ce - Te[3] x 2	139.03(7)	138.93(5)	139.14(5)
Te[2] - Ce - Te[4] x 2	139.13(4)	138.70(4)	139.58(4)
Te[2] - Ce - Te[2] x 4	85.71(5)	85.12(4)	86.31(4)
Te[2] - Ce - Te[2] x 4	85.41(5)	85.33(4)	85.49(4)
Te[2] - Ce - Te[2] x 4	147.69(6)	147.54(9)	147.85(9)
Te[2] - Ce - Te[3] x 4	76.39(6)	74.82(5)	77.95(5)
Te[2] - Ce - Te[3] x 4	130.96(5)	128.80(5)	133.13(6)
Te[2] - Ce - Te[4] x 4	76.50(5)	75.96(6)	77.06(6)
Te[2] - Ce - Te[4] x 4	130.86(7)	130.16(9)	131.54(9)
Te[3] - Ce - Te[3] x 2	81.89(6)	81.77(7)	82.11(8)
Te[3] - Ce - Te[4] x 4	55.19(5)	52.94(6)	57.44(6)
Te[4] - Ce - Te[4] x 2	81.74(5)	81.64(7)	81.87(7)
Na - Te[1] - Na x 8	85.4(2)	84.4(3)	86.4(3)
Na - Te[1] - Na x 4	146.57(16)	145.34(14)	147.79(14)
Na - Te[1] - Cu[1] x 8	67.25(19)	67.03(19)	67.47(19)
Na - Te[1] - Cu[1] x 8	136.00(17)	135.40(17)	136.60(16)
Na - Te[1] - Cu[2] x 8	85.4(2)	84.4(3)	86.4(3)
Na - Te[1] - Cu[2] x 4	146.57(17)	145.34(15)	147.79(15)
Cu[1] - Te[1] - Cu[1] x 4	109.29(15)	107.32(18)	111.29(17)
Cu[1] - Te[1] - Cu[1] x 8	70.43(17)	69.24(16)	71.62(16)
Cu[1] - Te[1] - Cu[2] x 8	67.25(19)	67.03(18)	67.47(18)
Cu[1] - Te[1] - Cu[2] x 8	136.00(16)	135.81(19)	136.19(19)
Cu[2] - Te[1] - Cu[2] x 8	85.4(2)	84.4(3)	86.4(3)

Table 4.48. (Cont'd) Bond angles distributions [°] for Na_{0.78(1)}Cu_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Cu[2] - Te[1] - Cu[2] x 4	146.57(18)	145.34(16)	147.79(16)
Ce - Te[2] - Ce x 8	106.15(5)	105.75(5)	106.55(5)
Ce - Te[2] - Ce x 4	85.71(5)	85.46(4)	85.96(4)
Ce - Te[2] - Ce x 4	85.41(5)	85.33(4)	85.49(4)
Ce - Te[2] - Ce x 4	147.70(7)	147.32(11)	148.07(11)
Ce - Te[3] - Ce x 2	81.83(6)	81.78(4)	81.90(8)
Ce - Te[3] - Te[4] x 4	62.29(5)	61.62(5)	62.94(5)
Ce - Te[3] - Te[4] x 4	117.63(6)	114.52(5)	120.65(5)
Ce - Te[3] - Na x 4	126.42(19)	123.56(19)	129.2(2)
Ce - Te[3] - Cu[2] x 4	126.4(2)	123.56(19)	129.2(2)
Te[4] - Te[3] - Te[4] x 4	90.30(6)	85.99(6)	94.66(7)
Te[4] - Te[3] - Te[4] x 4	89.73(7)	89.57(7)	90.01(5)
Te[4] - Te[3] - Te[4] x 4	177.20(8)	175.61(10)	180
Te[4] - Te[3] - Na x 4	64.19(19)	61.92(18)	66.5(2)
Te[4] - Te[3] - Na x 4	115.87(19)	115.3(2)	116.53(19)
Te[4] - Te[3] - Cu[2] x 4	64.19(19)	61.92(18)	66.5(2)
Te[4] - Te[3] - Cu[2] x 4	115.9(2)	115.3(2)	116.5(2)
Na - Te[3] - Na x 2	76.39(11)	76.20(15)	76.63(15)
Na - Te[3] - Cu[2] x 2	76.39(11)	76.20(16)	76.63(16)
Cu[2] - Te[3] - Cu[2] x 2	76.39(12)	76.20(16)	76.63(16)
Ce - Te[4] - Ce x 2	81.74(4)	81.64(7)	81.87(7)
Ce - Te[4] - Te[3] x 4	62.53(4)	60.87(5)	64.25(5)
Ce - Te[4] - Te[3] x 4	117.50(7)	116.66(6)	118.30(7)
Ce - Te[4] - Na x 4	126.40(13)	124.47(13)	128.34(15)
Ce - Te[4] - Cu[2] x 4	126.40(13)	124.47(14)	128.34(15)
Te[3] - Te[4] - Te[3] x 4	90.23(6)	86.39(6)	94.19(7)
Te[3] - Te[4] - Te[3] x 4	89.74(7)	89.57(9)	90.01(6)
Te[3] - Te[4] - Te[3] x 2	177.42(8)	175.97(10)	180
Te[3] - Te[4] - Na x 4	63.93(13)	63.55(14)	64.33(14)
Te[3] - Te[4] - Na x 4	115.95(14)	113.64(13)	118.26(14)
Te[3] - Te[4] - Cu[2] x 4	63.93(14)	63.55(14)	64.33(14)
Te[3] - Te[4] - Cu[2] x 4	115.95(14)	113.64(13)	118.26(14)
Te[3] - Te[4] - Te[3] x 2	177.58(8)	176.22(10)	180
Te[1] - Na - Te[1] x 8	85.40(11)	84.88(9)	85.92(9)

Table 4.48. (Cont'd) Bond angles distributions [°] for Na_{0.78(1)}Cu_{1.22(1)}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Na - Te[1] x 4	146.6(2)	146.4(4)	146.7(4)
Te[1] - Na - Te[3] x 4	78.93(12)	78.66(11)	79.17(11)
Te[1] - Na - Te[3] x 4	130.1(3)	129.6(3)	130.6(3)
Te[1] - Na - Te[4] x 4	78.81(17)	76.9(2)	80.7(2)
Te[1] - Na - Te[4] x 4	130.24(16)	128.11(13)	132.34(13)
Te[1] - Na - Cu[1] x 8	48.36(16)	48.01(14)	48.70(14)
Te[1] - Na - Cu[1] x 8	103.5(2)	102.8(2)	104.1(2)
Te[3] - Na - Te[3] x 2	76.39(14)	76.2(3)	76.6(3)
Te[3] - Na - Te[4] x 4	51.90(11)	49.78(8)	54.07(8)
Te[3] - Na - Cu[1] x 4	126.1(2)	125.48(11)	126.69(11)
Te[3] - Na - Cu[1] x 2	100.46(11)	99.16(14)	101.77(15)
Te[3] - Na - Cu[1] x 2	176.7(2)	175.3(2)	177.6(3)
Cu[1] - Na - Cu[1] x 4	82.9(2)	82.1(3)	83.7(3)
Cu[1] - Na - Cu[1] x 8	55.75(18)	54.84(15)	56.66(15)
Te[1] - Cu[1] - Te[1] x 11	109.30(15)	109.0(2)	109.6(2)
Te[1] - Cu[1] - Na x 4	83.9(2)	82.5(2)	85.3(3)
Te[1] - Cu[1] - Na x 4	166.8(3)	165.5(3)	168.1(3)
Te[1] - Cu[1] - Na x 8	64.3(2)	63.6(2)	64.9(2)
Te[1] - Cu[1] - Cu[1] x 8	54.70(12)	53.60(15)	55.77(16)
Te[1] - Cu[1] - Cu[1] x 8	125.24(17)	124.48(19)	125.95(18)
Te[1] - Cu[1] - Cu[2] x 4	83.9(2)	82.5(2)	85.3(3)
Te[1] - Cu[1] - Cu[2] x 4	166.8(3)	165.5(3)	168.1(3)
Te[1] - Cu[1] - Cu[2] x 8	64.3(2)	63.6(2)	64.9(2)
Te[1] - Cu[1] - Te[1]	109.59(14)	107.6(2)	111.5(3)
Na - Cu[1] - Na x 4	82.9(3)	82.0(3)	83.8(3)
Na - Cu[1] - Na x 8	124.3(3)	122.9(3)	125.6(3)
Na - Cu[1] - Cu[1] x 8	62.11(14)	61.25(16)	62.95(16)
Na - Cu[1] - Cu[1] x 8	117.99(17)	117.71(17)	118.26(16)
Na - Cu[1] - Cu[2] x 4	82.9(3)	82.0(3)	83.8(3)
Na - Cu[1] - Cu[2] x 8	124.3(3)	122.9(3)	125.6(3)
Cu[1] - Cu[1] - Cu[1] x 8	90.16(18)	89.18(15)	91.13(14)
Cu[1] - Cu[1] - Cu[1] x 4	179.2(2)	178.9(3)	179.7(2)
Cu[1] - Cu[1] - Cu[2] x 8	62.11(17)	61.25(19)	62.9(2)
Cu[1] - Cu[1] - Cu[2] x 8	118.0(2)	117.54(18)	118.42(18)

Table 4.48. (Cont'd) Bond angles distributions [°] for Na_{0.78}Cu_{1.22}CeTe₄ at 100 K with e.s.d.'s in parentheses.

Cu[2] - Cu[1] - Cu[2] x 4	82.9(3)	82.0(3)	83.8(3)
Cu[2] - Cu[1] - Cu[2] x 8	124.3(3)	122.9(3)	125.6(3)
Te[1] - Cu[2] - Te[1] x 8	85.40(11)	84.88(10)	85.92(10)
Te[1] - Cu[2] - Te[1] x 4	146.6(3)	146.4(5)	146.7(5)
Te[1] - Cu[2] - Te[3] x 4	78.93(12)	78.66(11)	79.17(11)
Te[1] - Cu[2] - Te[3] x 4	130.1(3)	129.6(3)	130.6(3)
Te[1] - Cu[2] - Te[4] x 4	78.81(17)	76.9(2)	80.7(2)
Te[1] - Cu[2] - Te[4] x 4	130.24(18)	128.11(14)	132.34(15)
Te[1] - Cu[2] - Cu[1] x 8	48.36(16)	48.01(14)	48.70(14)
Te[1] - Cu[2] - Cu[1] x 8	103.5(2)	102.8(2)	104.1(2)
Te[3] - Cu[2] - Te[3] x 2	76.39(16)	76.2(3)	76.6(3)
Te[3] - Cu[2] - Te[4] x 4	51.90(12)	49.78(9)	54.07(10)
Te[3] - Cu[2] - Cu[1] x 4	126.1(2)	125.48(11)	126.69(11)
Te[3] - Cu[2] - Cu[1] x 2	100.46(11)	99.16(14)	101.77(15)
Te[3] - Cu[2] - Cu[1] x 2	176.7(2)	175.3(2)	177.6(3)
Cu[1] - Cu[2] - Cu[1] x 4	82.9(2)	82.1(3)	83.7(3)
Cu[1] - Cu[2] - Cu[1] x 8	55.75(19)	54.84(16)	56.66(16)

Table 4.49. Crystal data and structure refinement for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K.

Empirical formula	Na _{0.60(2)} Cu _{1.40(2)} LaTe ₄
Formula weight	752.1
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2(0β1/2)0s0
Unit cell dimensions	a = 4.4178(6) Å, α = 90° b = 4.4257(7) Å, β = 90° c = 19.760(3) Å, γ = 90°
q-vector	0.3632(8)b* + 1/2c*
Volume	386.34(10) Å ³
Z	2
Density (calculated)	6.4628 g/cm ³
Absorption coefficient	23.982 mm ⁻¹
F(000)	624
Crystal size	0.11 x 0.05 x 0.01 mm ³
Theta range for data collection	1.75 to 29.20°
Index ranges	-5 ≤ h ≤ 6, -6 ≤ k ≤ 6, -27 ≤ l ≤ 27, -1 ≤ m ≤ 1
Reflections collected	9695 (2678 main + 7017 satellites)
Independent reflections	3082 (1003 main + 2079 satellites) [R _{int} = 0.0865]
Completeness to θ = 29.20°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3082 / 15 / 102
Goodness-of-fit on F ²	1.99
Final R indices [I > 2σ(I)]	R _{obs} = 0.0699, wR _{obs} = 0.1726
R indices (all data)	R _{all} = 0.1232, wR _{all} = 0.1828
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0615, wR _{obs} = 0.1718
R main indices (all data)	R _{all} = 0.0679, wR _{all} = 0.1741
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1298, wR _{obs} = 0.1833
R 1 st order satellites (all data)	R _{all} = 0.3383, wR _{all} = 0.2699
Extinction coefficient	0.00063(8)
T _{min} and T _{max} coefficients	0.1077 and 0.8402
Largest diff. peak and hole	7.03 and -6.29 e.Å ⁻³

$$R = \sum ||F_o| - |F_c|| / \sum |F_o|, wR = \{ \sum [w(|F_o|^2 - |F_c|^2)^2] / \sum [w(|F_o|^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$$

Table 4.50. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.60(2)}\text{Cu}_{1.40(2)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
La	0	0	0	3931(1)	1	13(1)
	sin, 1	21(2)	-1(2)	0(2)		
	cos, 1	-60(4)	2(7)	0(1)		
Te[1]	0	0	0	781(1)	1	21(1)
	sin, 1	-7(5)	-4(9)	7(1)		
	cos, 1	2(1)	1(2)	29(2)		
Te[2]	0	0	0	5612(1)	1	12(1)
	sin, 1	0(1)	1(2)	1(2)		
	cos, 1	0(4)	7(9)	0(1)		
Te[3]	0	0	5000	2636(1)	1	17(1)
	sin, 1	-185(6)	-11(6)	-1(1)		
	cos, 1	201(6)	12(6)	-1(1)		
Te[4]	0	0	5000	7364(1)	1	17(1)
	sin, 1	140(5)	2(6)	0(1)		
	cos, 1	153(6)	2(7)	0(1)		
Na	0	0	0	8760	0.60(2)	24(1)
	sin, 1	-54(17)	-25(30)	-2(3)		
	cos, 1	-22(7)	-12(12)	6(6)		
Cu[1]	0	0	5000	1(1)	1	34(1)
	sin, 1	-45(30)	-25(20)	0		
	cos, 1	0	0	5(4)		
Cu[2]	0	0	0	8760(2)	0.40(2)	24(1)
	sin, 1	-54(17)	-25(30)	-2(3)		
	cos, 1	-22(7)	-12(12)	6(6)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 4.51. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.60(2)}\text{Cu}_{1.40(2)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Label	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La	0	10(1)	10(1)	18(1)	5(1)	0	0
	sin, 1	-1(2)	-1(1)	0(1)	1(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)

Table 4.51. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.60(2)}\text{Cu}_{1.40(2)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Te[1]	0	14(1)	15(1)	33(1)	-5(1)	0	0
	sin, 1	3(1)	2(1)	-5(1)	0(1)	0(1)	2(2)
	cos, 1	12(2)	9(2)	-18(2)	-1(1)	0(1)	0(1)
Te[2]	0	9(1)	9(1)	18(1)	-8(1)	0	0
	sin, 1	-2(2)	3(2)	3(2)	1(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	0(1)	-1(1)	0(1)
Te[3]	0	16(1)	17(1)	17(1)	8(1)	0	0
	sin, 1	1(2)	0(1)	0(1)	-1(1)	1(1)	0(1)
	cos, 1	1(2)	0(1)	0(1)	-1(1)	-1(1)	0(1)
Te[4]	0	16(1)	19(1)	17(1)	-10(1)	0	0
	sin, 1	1(2)	0(1)	0(1)	-2(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	0(1)	2(1)	0(1)	0(1)
Na	0	25(3)	25(2)	21(2)	-14(5)	0	0
	sin, 1	-3(3)	2(2)	0(2)	-1(1)	2(4)	0(5)
	cos, 1	7(8)	-5(6)	1(5)	2(3)	1(2)	0(2)
Cu[1]	0	38(2)	38(2)	25(1)	3(5)	0	0
	sin, 1	0	0	0	0	0(2)	3(4)
	cos, 1	13(6)	-18(5)	0(4)	3(6)	0	0
Cu[2]	0	25(3)	25(2)	21(2)	-14(5)	0	0
	sin, 1	-3(3)	2(2)	0(2)	-1(1)	2(4)	0(5)
	cos, 1	7(8)	-5(6)	1(5)	2(3)	1(2)	0(2)

Table 4.52. Bond lengths distributions [$\text{\AA}$] for $\text{Na}_{0.60(2)}\text{Cu}_{1.40(2)}\text{LaTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La - Te[2]	3.320(3)	3.319(4)	3.321(4)
La - Te[2] x 4	3.255(3)	3.236(3)	3.273(3)
La - Te[3] x 2	3.385(4)	3.382(4)	3.391(4)
La - Te[4] x 2	3.381(3)	3.339(3)	3.423(3)
Te[1] - Na x 4	3.255(8)	3.233(11)	3.279(10)
Te[1] - Cu[1] x 4	2.698(7)	2.677(8)	2.718(8)
Te[1] - Cu[2] x 4	3.255(8)	3.233(11)	3.279(11)
Te[3] - Te[4] x 4	3.127(4)	2.999(4)	3.260(4)

Table 4.52. (Cont'd) Bond lengths distributions [Å] for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Na x 2	3.533(8)	3.474(7)	3.595(7)
Te[3] - Cu[2] x 2	3.533(9)	3.474(8)	3.595(8)
Na - Cu[1] x 4	3.302(11)	3.287(11)	3.317(11)
Cu[1] - Cu[1] x 4	3.126(10)	3.102(11)	3.151(11)
Cu[1] - Cu[2] x 4	3.302(12)	3.287(12)	3.317(12)

Table 4.53. Bond angles distributions [°] for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[2] - La - Te[2] x 8	73.88(8)	73.63(9)	74.14(9)
Te[2] - La - Te[3] x 2	139.13(9)	139.00(9)	139.23(7)
Te[2] - La - Te[4] x 2	139.21(7)	138.88(8)	139.54(8)
Te[2] - La - Te[2] x 4	85.68(5)	85.06(5)	86.30(5)
Te[2] - La - Te[2] x 4	85.49(6)	85.42(5)	85.56(5)
Te[2] - La - Te[2] x 4	147.76(10)	147.76(11)	147.78(12)
Te[2] - La - Te[3] x 4	76.45(7)	74.81(7)	78.06(8)
Te[2] - La - Te[3] x 4	130.87(8)	128.60(8)	133.16(9)
Te[2] - La - Te[4] x 4	76.51(7)	76.20(7)	76.84(7)
Te[2] - La - Te[4] x 4	130.81(9)	130.33(10)	131.29(10)
Te[3] - La - Te[3] x 2	81.69(8)	81.56(9)	81.92(9)
Te[3] - La - Te[4] x 4	55.08(7)	52.98(7)	57.18(7)
Te[4] - La - Te[4] x 2	81.58(8)	81.57(8)	81.61(9)
Na - Te[1] - Na x 8	85.7(2)	84.8(3)	86.5(3)
Na - Te[1] - Na x 4	147.7(2)	145.9(2)	149.4(2)
Na - Te[1] - Cu[1] x 8	66.5(3)	66.4(3)	66.6(3)
Na - Te[1] - Cu[1] x 8	135.8(3)	134.9(3)	136.6(3)
Na - Te[1] - Cu[2] x 8	85.7(2)	84.8(3)	86.5(3)
Na - Te[1] - Cu[2] x 4	147.7(2)	145.9(2)	149.4(2)
Cu[1] - Te[1] - Cu[1] x 4	110.2(2)	108.0(2)	112.5(2)
Cu[1] - Te[1] - Cu[1] x 8	70.9(3)	70.1(3)	71.6(3)
Cu[1] - Te[1] - Cu[2] x 8	66.5(2)	66.4(2)	66.6(2)
Cu[1] - Te[1] - Cu[2] x 8	135.8(2)	135.2(2)	136.3(2)
Cu[2] - Te[1] - Cu[2] x 8	85.7(2)	84.8(3)	86.5(3)

Table 4.53. (Cont'd) Bond angles distributions [°] for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Cu[2] - Te[1] - Cu[2] x 4	147.7(2)	145.9(2)	149.4(2)
La - Te[2] - La x 8	106.12(9)	105.77(10)	106.46(10)
La - Te[2] - La x 4	85.68(5)	85.42(5)	85.93(5)
La - Te[2] - La x 4	85.48(7)	85.42(9)	85.56(9)
La - Te[2] - La x 4	147.77(10)	147.62(13)	147.92(13)
La - Te[3] - La x 2	81.63(8)	81.58(8)	81.75(9)
La - Te[3] - Te[4] x 4	62.39(8)	61.53(8)	63.22(8)
La - Te[3] - Te[4] x 4	117.56(10)	114.67(10)	120.35(11)
La - Te[3] - Na x 4	126.2(2)	123.4(2)	129.0(2)
La - Te[3] - Cu[2] x 4	126.2(2)	123.4(2)	129.0(2)
Te[4] - Te[3] - Te[4] x 4	90.23(10)	86.12(9)	94.38(10)
Te[4] - Te[3] - Te[4] x 4	89.81(9)	89.56(10)	90.02(9)
Te[4] - Te[3] - Te[4] x 4	177.47(12)	176.04(12)	180
Te[4] - Te[3] - Na x 4	63.9(2)	61.81(19)	65.9(2)
Te[4] - Te[3] - Na x 4	116.2(2)	115.6(2)	116.9(2)
Te[4] - Te[3] - Cu[2] x 4	63.9(2)	61.81(19)	65.9(2)
Te[4] - Te[3] - Cu[2] x 4	116.2(2)	115.6(2)	116.9(2)
Na - Te[3] - Na x 2	77.36(17)	77.09(17)	77.67(17)
Na - Te[3] - Cu[2] x 2	77.36(17)	77.09(18)	77.67(18)
Cu[2] - Te[3] - Cu[2] x 2	77.36(18)	77.09(18)	77.67(18)
La - Te[4] - La x 2	81.58(8)	81.57(8)	81.61(8)
La - Te[4] - Te[3] x 4	62.57(8)	60.89(8)	64.26(9)
La - Te[4] - Te[3] x 4	117.46(11)	116.57(11)	118.29(11)
La - Te[4] - Na x 4	126.21(17)	124.30(16)	128.08(17)
La - Te[4] - Cu[2] x 4	126.21(17)	124.30(16)	128.08(17)
Te[3] - Te[4] - Te[3] x 4	90.23(9)	86.53(9)	93.91(10)
Te[3] - Te[4] - Te[3] x 4	89.80(10)	89.56(10)	90.02(10)
Te[3] - Te[4] - Te[3] x 4	177.62(12)	176.26(12)	180
Te[3] - Te[4] - Na x 4	63.68(16)	63.24(16)	64.16(16)
Te[3] - Te[4] - Na x 4	116.28(17)	114.04(17)	118.44(18)
Te[3] - Te[4] - Cu[2] x 4	63.68(16)	63.24(16)	64.16(16)
Te[3] - Te[4] - Cu[2] x 4	116.28(18)	114.04(17)	118.44(18)
Te[1] - Na - Te[1] x 8	85.66(16)	85.12(18)	86.22(18)
Te[1] - Na - Te[1] x 4	147.7(3)	147.2(4)	148.1(4)

Table 4.53. (Cont'd) Bond angles distributions [°] for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Na - Te[3] x 4	78.06(16)	77.59(15)	78.54(15)
Te[1] - Na - Te[3] x 4	129.9(3)	129.4(3)	130.4(3)
Te[1] - Na - Te[4] x 4	78.0(2)	76.1(2)	79.8(3)
Te[1] - Na - Te[4] x 4	130.0(2)	127.6(2)	132.3(2)
Te[1] - Na - Cu[1] x 8	48.5(3)	48.0(3)	49.1(3)
Te[1] - Na - Cu[1] x 8	104.4(3)	103.7(3)	105.1(3)
Te[3] - Na - Te[3] x 2	77.36(19)	77.1(2)	77.7(2)
Te[3] - Na - Te[4] x 4	52.51(14)	50.42(12)	54.61(12)
Te[3] - Na - Cu[1] x 4	125.4(3)	125.0(3)	125.8(3)
Te[3] - Na - Cu[1] x 2	99.3(2)	98.1(3)	100.4(3)
Te[3] - Na - Cu[1] x 2	176.6(3)	175.4(3)	177.7(3)
Cu[1] - Na - Cu[1] x 4	84.2(3)	84.0(3)	84.3(3)
Cu[1] - Na - Cu[1] x 8	56.6(3)	56.0(2)	57.1(2)
Te[1] - Cu[1] - Te[1] x 4	110.3(2)	109.7(3)	110.8(3)
Te[1] - Cu[1] - Te[1] x 8	109.1(2)	107.7(4)	110.5(4)
Te[1] - Cu[1] - Na x 4	82.8(2)	81.6(3)	84.0(3)
Te[1] - Cu[1] - Na x 4	166.9(3)	165.8(3)	168.0(3)
Te[1] - Cu[1] - Na x 8	64.9(3)	64.7(3)	65.0(3)
Te[1] - Cu[1] - Cu[1] x 8	54.5(2)	53.6(3)	55.4(3)
Te[1] - Cu[1] - Cu[1] x 8	125.5(3)	125.2(4)	125.8(4)
Te[1] - Cu[1] - Cu[2] x 4	82.8(3)	81.6(3)	84.0(3)
Te[1] - Cu[1] - Cu[2] x 4	166.9(3)	165.8(3)	168.0(3)
Te[1] - Cu[1] - Cu[2] x 8	64.9(3)	64.7(3)	65.0(3)
Na - Cu[1] - Na x 4	84.2(3)	83.7(3)	84.6(3)
Na - Cu[1] - Na x 8	123.4(3)	122.7(3)	124.2(3)
Na - Cu[1] - Cu[1] x 8	61.7(2)	61.3(2)	62.0(2)
Na - Cu[1] - Cu[1] x 8	118.3(3)	118.0(3)	118.6(3)
Na - Cu[1] - Cu[2] x 4	84.2(3)	83.7(3)	84.6(3)
Na - Cu[1] - Cu[2] x 8	123.4(3)	122.7(3)	124.2(3)
Cu[1] - Cu[1] - Cu[1] x 8	90.1(3)	89.6(3)	90.6(3)
Cu[1] - Cu[1] - Cu[1] x 4	179.8(3)	179.7(3)	179.9(3)
Cu[1] - Cu[1] - Cu[2] x 8	61.7(2)	61.3(3)	62.0(3)
Cu[1] - Cu[1] - Cu[2] x 8	118.3(3)	117.9(3)	118.7(3)
Cu[2] - Cu[1] - Cu[2] x 4	84.2(3)	83.7(3)	84.6(3)

Table 4.53. (Cont'd) Bond angles distributions [°] for Na_{0.60(2)}Cu_{1.40(2)}LaTe₄ at 100 K with e.s.d.'s in parentheses.

Cu[2] - Cu[1] - Cu[2] x 8	123.4(3)	122.7(3)	124.2(3)
Te[1] - Cu[2] - Te[1] x 8	85.66(17)	85.12(18)	86.22(19)
Te[1] - Cu[2] - Te[1] x 4	147.7(3)	147.2(4)	148.1(4)
Te[1] - Cu[2] - Te[3] x 4	78.06(16)	77.59(15)	78.54(15)
Te[1] - Cu[2] - Te[3] x 4	129.9(3)	129.4(3)	130.4(3)
Te[1] - Cu[2] - Te[4] x 4	78.0(2)	76.1(2)	79.8(3)
Te[1] - Cu[2] - Te[4] x 4	130.0(2)	127.6(2)	132.3(2)
Te[1] - Cu[2] - Cu[1] x 8	48.5(3)	48.0(3)	49.1(3)
Te[1] - Cu[2] - Cu[1] x 8	104.4(3)	103.7(3)	105.1(3)
Te[3] - Cu[2] - Te[3] x 2	77.4(2)	77.1(2)	77.7(2)
Te[3] - Cu[2] - Te[4] x 4	52.51(15)	50.42(12)	54.61(13)
Te[3] - Cu[2] - Cu[1] x 4	125.4(3)	125.0(3)	125.8(3)
Te[3] - Cu[2] - Cu[1] x 2	99.3(2)	98.1(3)	100.4(3)
Te[3] - Cu[2] - Cu[1] x 2	176.6(3)	175.4(3)	177.7(3)
Cu[1] - Cu[2] - Cu[1] x 4	84.2(3)	84.0(3)	84.3(3)
Cu[1] - Cu[2] - Cu[1] x 8	56.6(3)	56.0(2)	57.1(2)

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CHARGE DENSITY WAVES AND STRUCTURAL MODULATIONS
IN POLYTELLURIDE COMPOUNDS

VOLUME II

By

Christos D. Malliakas

A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

Department of Chemistry

2007

Chapter 5

Charge Density Wave Distortions in Square Nets of Tellurium in Layered

Intergrowth Polytelluride Compounds: Sm_2Te_5 and $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$

5.1. Introduction

Low-dimensional systems often exhibit electronic instabilities that can lead to charge density waves (CDWs) or superconductivity. The CDWs have a characteristic frequency q (q -vector) and this vector corresponds to the so-called nesting vector of the Fermi surface (FS). Nesting favors electron-phonon coupling and is believed to be responsible for the formation of the CDW and often overpowers the competing superconductive state. Although the description of the CDW behavior for one-dimensional systems is well established theoretically no proper models have been developed for the two-dimensional cases.¹

Recent studies have focused on the high-temperature CDW family of materials RETe_2 and RETe_3 . (RE = rare earth element) and have shed new insights as to the nature of the phenomenon in these materials.^{2,3,4} However, only recently it was recognized through angle-resolved photoemission spectroscopy (ARPES) studies that LaTe_2 is the first semiconductor that its two-dimensional CDW distortion is Fermi surface nesting driven.⁵ The RETe_3 family has gained more attention the recent years because of its two-dimensional incommensurate CDW modulated states and their effect to the electronic structure. Extensive structural,⁶ spectroscopic⁷ and other physical⁸ studies have revealed unique chemical and physical behavior among the classical CDW systems. However, surprisingly physical and structural characterization studies of the other members of the family RE_2Te_5 remain but a few.⁹

The structure of RE_2Te_5 is essentially a 1:1 combination of the structures of RETe_2 and RETe_3 , Figure 5.5. It contains one square net of Te^{1-} atoms found in the RETe_2 family and two square nets of $\text{Te}^{1/2-}$ atoms present in the RETe_3 compound.

Therefore, RE_2Te_5 is unique in that it possesses simultaneously two individual planar nets of tellurium each with its own average oxidation state of 1- and 1/2- respectively. It is well known that the number of electrons per Te atom controls the type of CDW modulation.¹⁰ Variations in the electron count alter the energy of the Fermi level thus the nesting properties of the Fermi surface (q-vector). CDW modulations from combination of tellurium nets in different oxidation states though have not been reported up to date and their electronic behavior is unknown. Although the CDW RETe_2 and RETe_3 compounds are substructure components of the RE_2Te_5 phase no CDW distortions have been found for the composite structure.⁹

Here, we report for the first time the existence and crystallographic solution of the incommensurate CDW modulations in Sm_2Te_5 . We find that each of the two types of planar Te nets has its own CDW distortion. This is manifested by the existence of two individual q-vectors in the structure. We have verified the two CDW modulations by direct visualization of the distortions with Scanning Tunneling Microscopy (STM). The independent character of the two q-vectors was examined with high temperature single crystal X-ray diffraction experiments going above the CDW transition. Additionally, the SmTe_{2-x} parent substructure was reexamined using the superspace crystallographic approach in order to properly compare its CDW distortions to the ones observed in the composite $\text{Sm}_2\text{Te}_{5-x}$.

Furthermore, two individual q-vectors were found in the recently reported intergrowth $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10-x}$ compound that possesses two $\text{Te}^{1/2-}$ and Te^{1-} nets too.^{10,11} The layered structure is composed by the two substructures of LaTe_3 and $\text{K}_2\text{Ag}_4\text{Te}_4$ ¹² that alternate in a 1:1 ratio and stack along the *c*-axis. One vector is commensurate and

corresponds to the CDW distortion in the $\text{Te}^{1/2-}$ net of LaTe_3 . The second incommensurate q-vector is created from long range ordered vacancies in the Te^{1-} net of the $\text{K}_2\text{Ag}_4\text{Te}_{4-x}$ substructure.

5.2. Experimental Section

5.2.1. Reagents

The following reagents were used as obtained. Potassium metal, analytical reagent, Aldrich Chemical Co., Milwaukee, WI; Lanthanum metal, 40 mesh, Cerac, Milwaukee, WI; Samarium metal, 40 mesh, Cerac, Milwaukee, WI; Tellurium chunks, Tellurex Corp, Traverse City, MI; Rubidium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; Lithium Chloride, 99.8% pure, 20 mesh, Cerac Specialty Inorganics, Milwaukee, WI; N, N – Dimethylformamide (DMF), ACS reagent grade, Spectrum Chemicals, New Brunswick, NJ; Diethyl ether anhydrous, ACS reagent grade, Columbus Chemical Industries, Columbus, WI.

Silver powder – A silver coin (99.9% purity of ~ 31 g) was dissolved in 250 mL of aqua regia (3 parts of concentrated HCl and one part of HNO_3) under stirring. The solution was neutralized with NaBH_4 and the pale gray precipitate was filtered, washed with copious amounts of distilled water, acetone and dried in a vacuum oven.

Potassium Telluride, K_2Te – 5.836 g (0.15 mol) K was sliced in small pieces (~ 3 mm) in a N_2 filled glovebox and combined with 9.523 g (0.075 mol) Te in a 1000 mL single neck round bottom flask. A Teflon coated magnetic stir bar was added in the flask as well. The flask was connected to a glass adapter with a stopcock joint and removed from the glovebox. The flask and adapter were then connected to a dry condenser

apparatus and chilled to -78 °C using a dry ice/acetone bath. Approximately 800 mL of pure NH₃ were condensed, under N₂ atmosphere, onto the reagents, yielding a purple solution. The solution was kept under stirring and maintained at -78 °C for up to 16 hours. The dry ice/acetone mixture was removed and the NH₃ was allowed to evaporate off as the flask warmed up to room temperature under a constant flow of N₂ for ~ 6 hours. The resulting brown colored powder was evacuated on a Schlenk line for ~ 4 hours and taken into a N₂ filled glovebox. The product was ground to a fine powder with a mortar and pestle and placed into a screw-capped vial in the glovebox.

5.2.2. Synthesis

Sm₂Te₅ – All manipulations were carried out under dry nitrogen atmosphere in a Vacuum Atmospheres Dri-Lab glovebox. Stoichiometric amounts of Sm (2 mmol) and Te (5 mmol) were loaded into a quartz tube together with a double amount (~ 2 g) of halide flux (0.42:0.58 molar mixtures of RbCl and LiCl). The tube was sealed under vacuum (<10⁻⁴ torr), heated to 650 °C at 12 hours for 6 days and cooled down to room temperature at a rate of 4 °C min⁻¹. The halide flux was dissolved in water and the crystals were washed with acetone and dried under nitrogen environment. The morphology of the crystals is that of thick plates (Figure 5.1) with a dark copper-like color. The compound found to contain significant SmTe₃ impurities of ~ 50% (PXRD), Figure 5.2.

SmTe₂ – All manipulations were carried out under dry nitrogen atmosphere in a Vacuum Atmospheres Dri-Lab glovebox. Stoichiometric amounts of Sm (1 mmol) and Te (2 mmol) were loaded into a quartz tube together with a double amount (~ 2 g) of halide flux (0.42:0.58 molar mixtures of RbCl and LiCl). The tube was sealed under

vacuum ($<10^{-4}$ torr), heated to 700 °C at 12 hours for 6 days and cooled down to room temperature at a rate of 4 °C min⁻¹. The halide flux was dissolved in water and the crystals were washed with acetone and dried under nitrogen environment. The morphology of the crystals is that of thin black plates. The compound found to be ~ 100 % pure (PXRD).

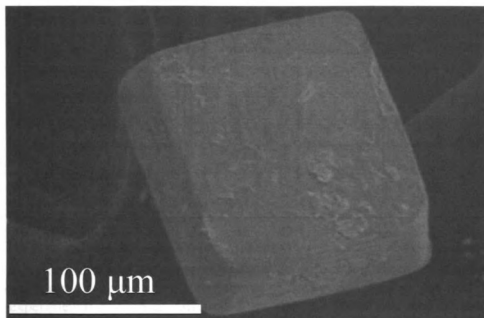


Figure 5.1. SEM image of a thick plate-like Sm₂Te₅ single crystal.

$K_2Ag_4La_2Te_{10-x} - K_2Ag_4La_2Te_{10-x}$ was synthesized from a mixture of 0.247 g K₂Te (1.20 mmol), 0.146 Ag (1.35 mmol), 0.084 g La (0.60 mmol), and 0.612 g Te (4.80 mmol) that was sealed under vacuum in a quartz tube and heated to 800 °C for 5 days. The tube was then cooled to 300 °C at a rate of 4 °C/h, followed by quenching to room temperature at a rate of 10 °C/h. The excess K₂Te_y flux was washed off with N,N-dimethylformamide under nitrogen to reveal very thin red-brown plate-shaped crystals. The compound found to contain KAgLaTe₄ impurities of ~ 30 % (PXRD, Figure 5.4) of the same crystal habit

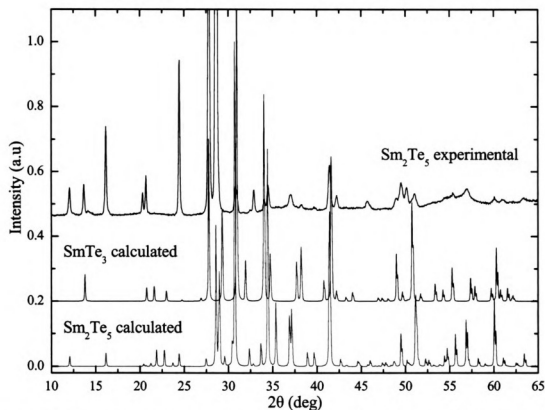


Figure 5.2. Comparison of the experimental powder diffraction pattern of the as prepared Sm_2Te_5 compound with the calculated patterns of SmTe_3 and Sm_2Te_5 . Relative intensity of the experimental pattern is different from the calculated one due to preferential orientation of the plate-like crystals.

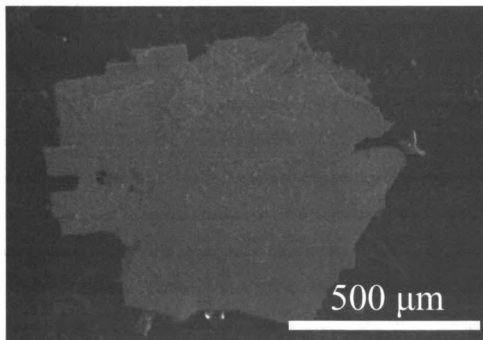


Figure 5.3. SEM image of a plate-like $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ single crystal.

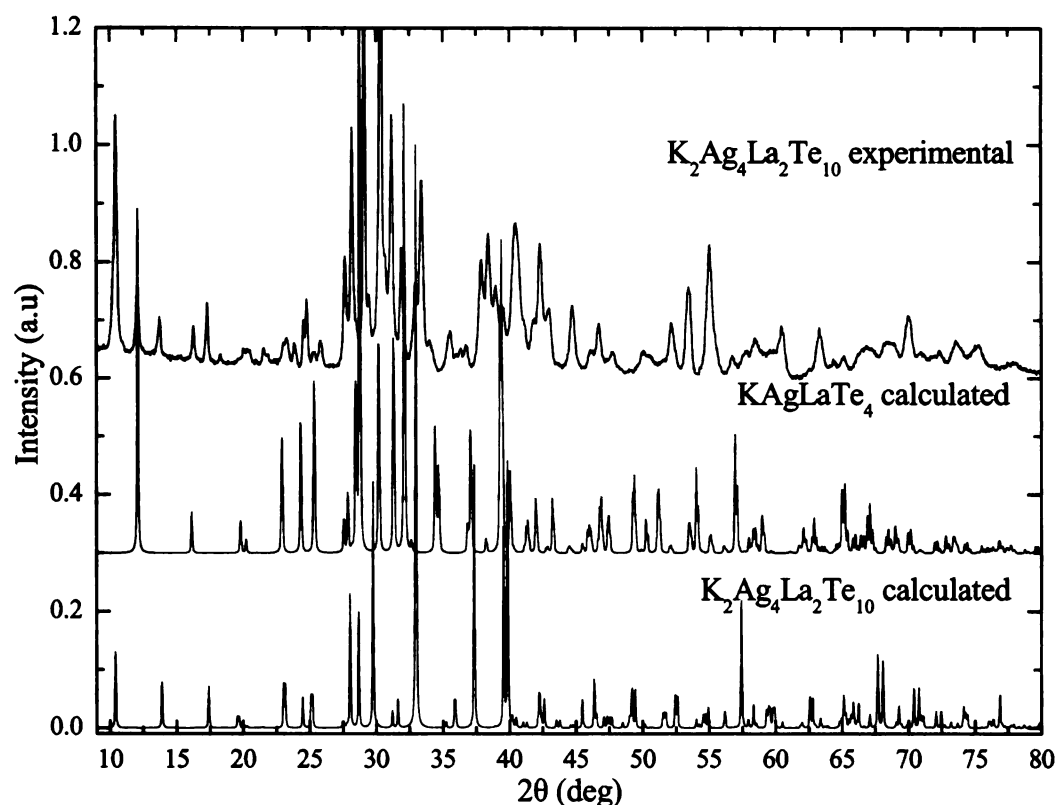


Figure 5.4. Comparison of the experimental powder diffraction pattern of the as prepared $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ compound with the calculated patterns of KAgLaTe_4 and $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$. Relative intensity of the experimental pattern is different from the calculated one due to preferential orientation of the plate-like crystals.

5.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – A STOE IPDS II diffractometer was used to collect intensity data (Mo $K\alpha$ radiation). An analytical absorption correction was

performed, and all structures were refined with JANA2000 software (Petricek, V.; Dusek, M. Institute of Physics; Praha, Czech Republic, 2000). The length determination and refinement of the q -vectors was performed with the Peaklist 1.06 software part of the X-Area 1.39 suite (X-Area, IPDS Software, STOE & Cie GmbH, Darmstadt, 2006) using a least square refinement algorithm.

Satellite reflections of first order for both q -vectors and mixed order reflections ($q_1 + q_2$, $q_1 - q_2$) were observed at 100 K and used for the refinement for Sm_2Te_5 , SmTe_2 and $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$. Four modulation waves (q_1 , q_2 , $q_1 + q_2$, $q_1 - q_2$) for positional, temperature parameters and occupational (for the atoms in the Te^{1-} net) distortions were used. Fourier terms were freely refined. The centrosymmetric P-1 superspace group gave R-values for the satellites to more than 30% for Sm_2Te_5 and $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$. One order of satellite reflections of a single q -vector was observed at 500 K for Sm_2Te_5 . One modulation wave for positional, temperature parameters and occupational distortions was used and the Fourier terms were freely refined.

Since the only acceptable solutions was based on a triclinic cell for Sm_2Te_5 , the original orthorhombic system was transformed to a triclinic cell according to the transformation matrix $[-1 \ 0 \ 0, 0 \ 0 \ -1, 0.5 \ -0.5 \ 0]$ to avoid correlations during refinement. Thus, the orthorhombic c^* -axis became a triclinic b^* -axis. The length of the q -vectors along the plane that contains the Te net did not change. The component of the q -vectors along the shortest c^* -axis was reduced by 0.5 according to the transformation matrix. Similar transformation procedure was applied on $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ with a transformation matrix $[1 \ 1 \ 0, 0 \ 0 \ -1, -1 \ 0 \ 0]$.

Two crystals of Sm_2Te_5 and SmTe_2 from two different reaction batches were analyzed with single crystal X-ray diffraction studies. Both compounds were found to have the same stoichiometry (e.g. concentration of vacancies) and supercell parameters within the estimated statistical standard deviations.

Infrared (IR) Spectroscopy – Optical diffuse reflectance measurements were performed on single crystals of Sm_2Te_5 at room temperature. The spectra were recorded in the Mid-IR region ($6000 - 400 \text{ cm}^{-1}$) with a Nicolet 6700 FT-IR Spectrometer equipped with a diffuse reflectance collector from Spectra-Tech Inc.

Scanning Tunneling Microscopy (STM) of Sm_2Te_5 – The STM measurements were conducted in collaboration with Maria Iavarone at the Materials Science Division (MSD) at Argonne National Laboratory (ANL). STM measurements were performed with a low temperature home made STM at 4.2 K. The samples were cleaved under inert atmosphere and quickly cooled down at 4.2 K. Considering that the cleavage occurs between the van der Waals gap we expected the topmost layer, observable with the STM, to be the $\text{Te}^{1/2-}$ net. Topography images were acquired in constant current mode as well as in constant height mode and at different voltage tip-sample.

5.4. Results and Discussion

Subcell Description of RETe_2 and RE_2Te_5 – The average structure of RE_2Te_5 is an intergrowth of the two parent substructures RETe_2 and RETe_3 , Figure 5.5. The RETe_2 family adopts the Cu_2Sb structure type and has a rock salt type $[\text{RETe}]^+$ sublayer sandwiched between two square Te^{1-} nets, Figure 5.5A. The RETe_3 family adopts the NdTe_3 structure type and has a $[\text{RETe}]^+$ sublayer sandwiched between two square $\text{Te}^{1/2-}$

nets making RETe_3 slabs which stack along the b -axis creating van der Waals gaps, Figure 5.5B. The average RE_2Te_5 system adopts the space group Cmcm (Nd_2Te_5 structure type) and it consists of two puckered double layers of $[\text{RETe}]^+$ separated by a square net of Te^{1-} atoms forming RE_2Te_3 units. Each RE_2Te_3 unit is sandwiched by the planar nets of $\text{Te}^{1/2-}$ making a RE_2Te_5 slab. The slabs then stack along the b -axis creating van der Waals gaps, Figure 5.5C. The formula can be expressly written as $([\text{RETe}]^+)_2([\text{Te}]^{1/2-})_2[\text{Te}]^{1-}$. The RE atom is surrounded by nine Te atoms in a monocapped tetragonal antiprism geometry. The Te-Te distance in the square nets of Sm_2Te_5 is 3.0715(4) Å for both $\text{Te}^{1/2-}$ and Te^{1-} nets at 100 K.

Hypostoichiometry is very common in the REQ_{2-x} ($\text{Q} = \text{S}, \text{Se}, \text{Te}$) family. It originates from vacancies in the planar nets of Q that are mostly ordered for the sulfide¹³ and selenide¹⁴ and disordered for the telluride family.¹⁹ A lot of different phases have been characterized thermodynamically with small changes in the x value, e. g. SmS_{2-x} ¹⁵ and PrSe_{2-x} .¹⁶ We found that the Te^{1-} net (SmTe_{2-x} substructure) in the Sm_2Te_5 system has vacancies that actually are ordered making $\text{Sm}_2\text{Te}_{4.90(1)}$ the first rare-earth polytelluride compound with ordered vacancies.

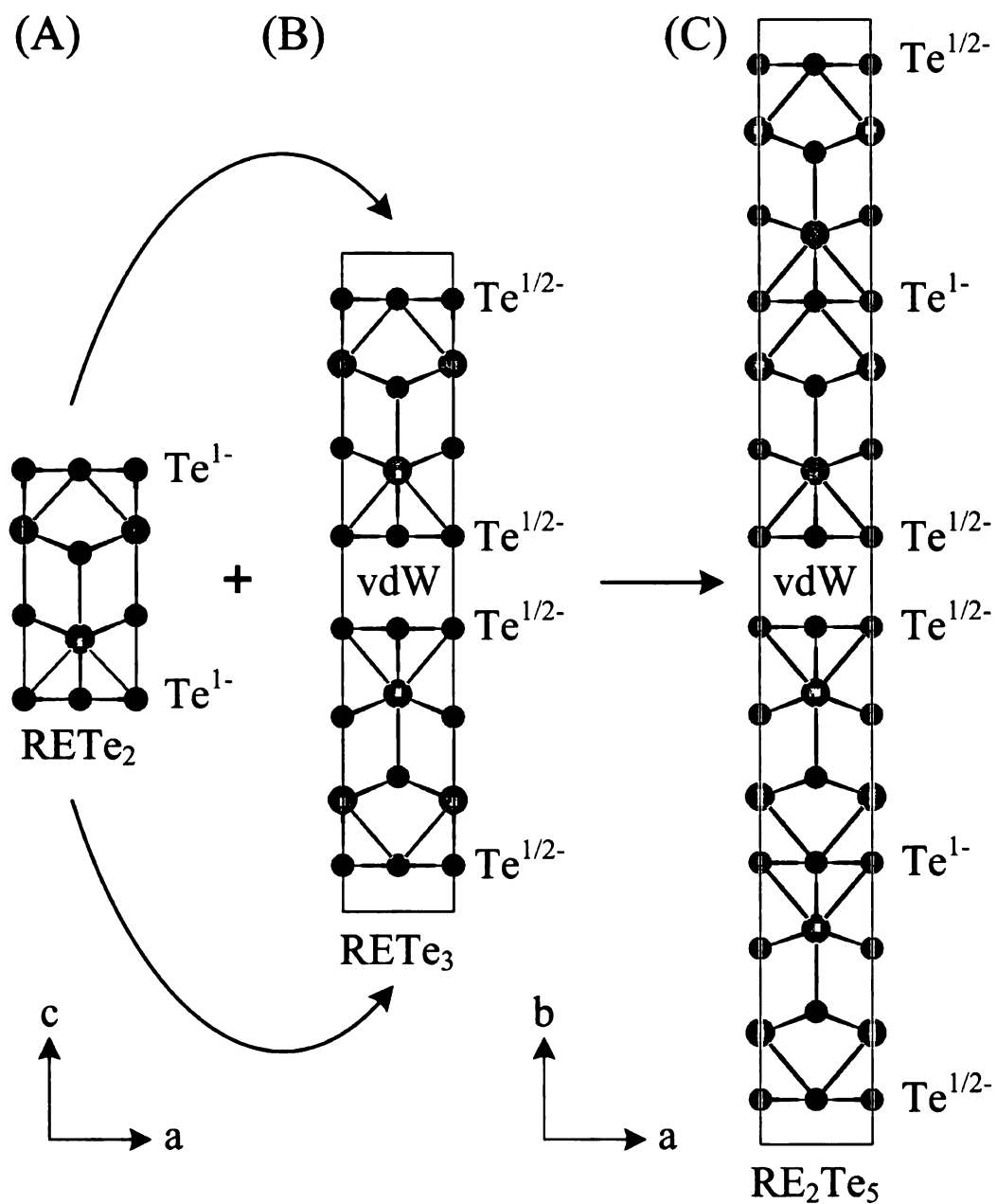


Figure 5.5. (A) The average structure of RETe_2 (Cu_2Sb - type) with square nets of Te^{1-} . (B) The average layered structure of RETe_3 (NdTe_3 - type) with square nets of $\text{Te}^{1/2-}$. (C) The hybrid average layered structure of RE_2Te_5 (Nd_2Te_5 - type) with square nets of both Te^{1-} and $\text{Te}^{1/2-}$. The van der Waals (vdW) gaps are indicated.

Subcell Description of $K_2Ag_4La_2Te_{10-x}$ – Another interesting example of intergrowth compound with two square Te nets of different electron count is $K_2Ag_4La_2Te_{10-x}$. The average layered structure of the quaternary adopts the orthorhombic space group Immm with cell parameter $a = 4.4599(2)$ Å, $b = 4.4849(2)$ Å, and $c = 50.353(2)$ Å at 100 K. It is composed by two distinct layers of two different substructures of $[LaTe_3]$ and $[K_2Ag_4Te_4]$, Figure 5.5. The two different layers alternate in a 1:1 ratio along the c -axis separated by a van der Waals gap.

The average oxidation state of the Te net atoms in the first substructure of $[LaTe_3]$ remains -0.5 with an average Te-Te distance of $3.1770(5)$ Å at 100 K. The second substructure, $[K_2Ag_4Te_4]$, is similar to the structure found in KCu_4S_3 .¹⁷ It is composed by two puckered $[AgTe]$ layers that are fused together sharing a common plane of Te atoms. Each $[AgTe]$ - layer is made up of ribbon tetrahedral $[AgTe_4]$ units that share edges in two dimensions. The difference, however, is that in $K_2Ag_4Te_4$, an extra Te atom exists in between these double layers. Interestingly, the additional Te atom creates a second planar net of Te atoms in the $[K_2Ag_4Te_4]$ layer with an apparent distance of $3.1770(4)$ Å at 100 K. The average oxidation state of the Te atoms in the shared Te net is 1-. Furthermore, this Te net was found to have vacancies that are actually long range ordered. The layers between the $[LaTe_3]$ slabs in $K_2Ag_4La_2Te_{10}$ are thicker in respect to the structurally similar $AMLaTe_4$ ($A = Na, K$; $M = Ag, Cu$) family.¹⁸

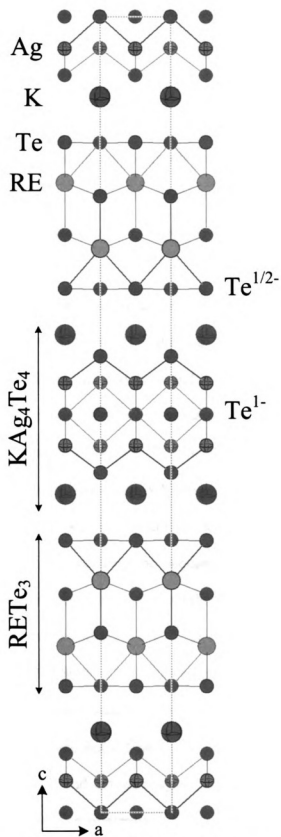


Figure 5.6. The average structure of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ with square nets of $\text{Te}^{1/2-}$ and Te^{1-} .

Supercell Description of Sm₂Te₅ Based on a Modulation q-vector – The hybrid CDWs in Sm₂Te₅ create a (3+2)-dimensional modulated incommensurate superstructure with two q-vectors at 100 K. A superspace crystallographic approach was necessary in order to solve the structure. A triclinic crystal system was the only possible option consistent with the number and orientation of the observed q-vectors. A stable refinement was achieved with P1($\alpha_1\beta_1\gamma_1, \alpha_2\beta_2\gamma_2$)0 superspace group. The two vectors are $q_1 = 0.3124(3)b^* + 1/2c^*$ and the weaker $q_2 = 0.3303(3)a^* + 0.3315(3)b^* + 0.349(1)c^*$. The labeling scheme is shown in Figure 5.7A.

The CDW distorted patterns of Te atoms in Sm₂Te₅ feature Te_x oligomers of different length, geometry and sequence from the ones observed so far in the rare-earth polytelluride family. Some similarities may be found in the parent substructures SmTe₃^{6c} and SmTe₂¹⁹ but the combination of the two q-vectors and the presence of occupational waves of vacancies create unique Te patterns. The majority of oligomers in the Te^{1/2-} net at 100 K are V-shaped trimers and occasionally N-shaped tetramers, Figure 5.8.

The main difference from RETe₃ though is the discontinuation of the same type of oligomers along the *a*-axis. Specifically, the sequence of trimers along *a*-axis now contains tetramers, dimers and sometimes even single Te atoms (shown with arrows in Figure 5.8). The Te-Te length distribution in Te^{1/2-} at 100 K varies from a minimum of 2.933(10) Å and maximum 3.208(10) Å with an average of 3.089(10) Å. The Te¹⁻ net at 100 K contains square-like octamers with a vacancy in the center. Furthermore, different sequence of dimers, V-shaped and linear trimers, L- and T-shaped tetramers, V-shaped pentamers, F-shaped hexamers, and defected square-like heptamers is observed due to vacancy ordering, Figure 5.9. The minimum Te-Te bond in the Te¹⁻ net at 100 K is

2.805(19) Å and it is the shortest Te-Te bond observed in the rare-earth polytelluride family. The maximum distance is 3.351(19) Å with an average of 3.083(19) Å.

Both Te nets remain distorted even above the first CDW transition temperature. The existence of the diagonal modulation vector creates distorted patterns with different sequence of oligomers. At 500 K the $\text{Te}^{1/2-}$ pattern consists mainly of alternating N-shaped tetramers and dimers, Figure 5.10. The majority of dimers are aligned diagonally in single chains and occasionally in double chains. The bond length distribution becomes very narrow with a minimum of 3.063(5) Å, maximum 3.098(5) Å and an average of 3.095(5) Å. The Te^{1-} net at 500 K does not show any of the square-like octamers but it contains sequence of monomers, dimers, V-shaped trimers, Z- and C-shaped pentamers with a linear Te atom, Figure 5.11. The minimum Te-Te bond is 2.953(10) Å, the maximum 3.211(11) Å with an average distance of 3.085(11) Å.

The temperature dependence of the q-vectors of $\text{Sm}_2\text{Te}_{5-x}$ surprisingly shows an opposite trend from the one observed for SmTe_3 .^{6c} The length of the q_1 -vector increases to 0.3233(8) at 450 K and the diagonal q_2 -vector decreases to $0.3100(8)a^* + 0.3268(8)b^* + 0.281(4)c^*$. At 500 K the q_1 -vector disappears and q_2 becomes shorter $0.315(1)a^* + 0.315(1)b^* + 0.351(6)c^*$. The q-vector temperature dependence for the SmTe_{2-x} substructure is negligible (see the supercell description of SmTe_2 based on a modulation q-vector section for more details).

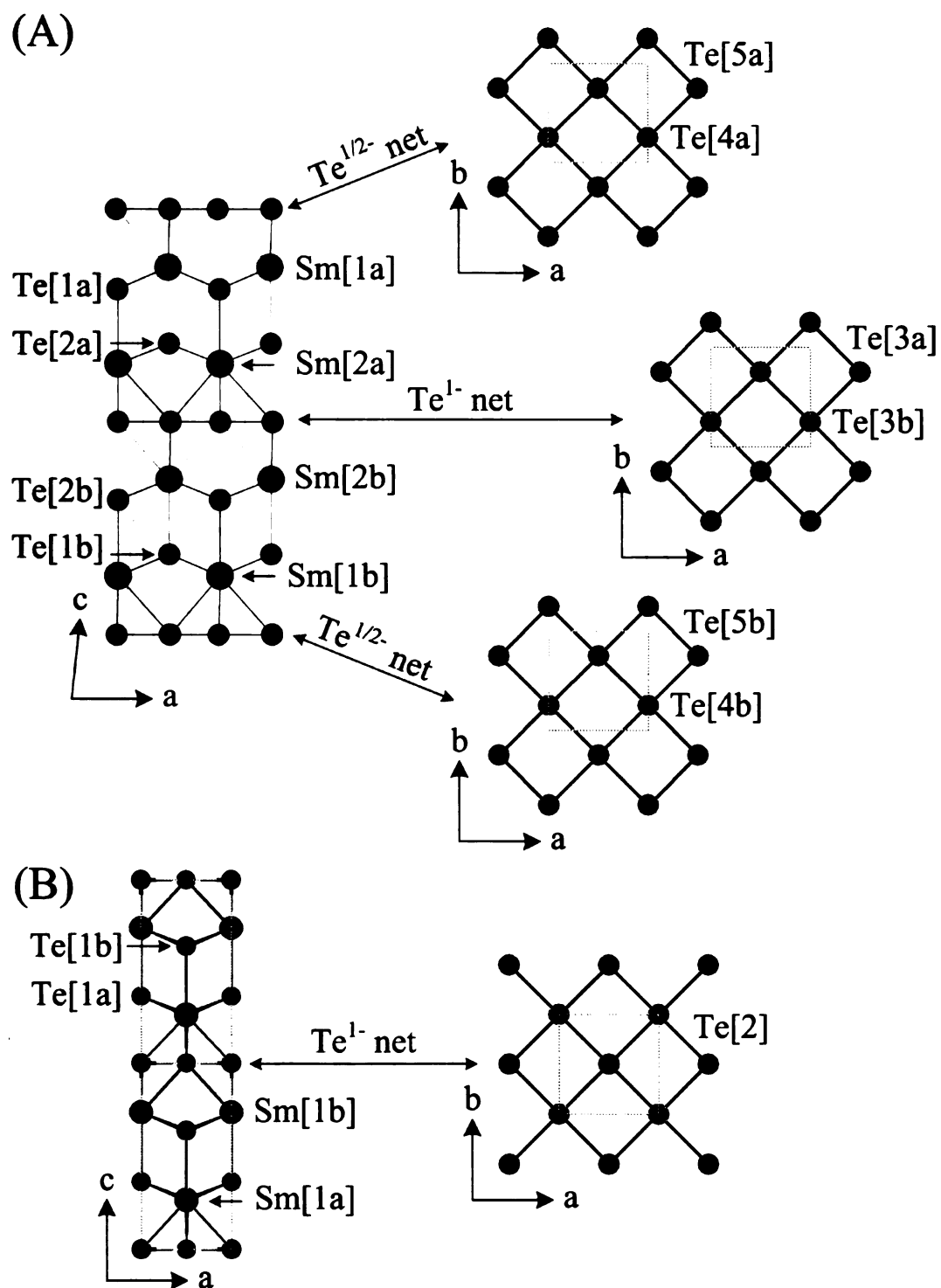


Figure 5.7. (A) Transformed cell of Sm_2Te_3 and labeling scheme used in the superspace refinement. (B) Cell labeling scheme in SmTe_2 supercell.

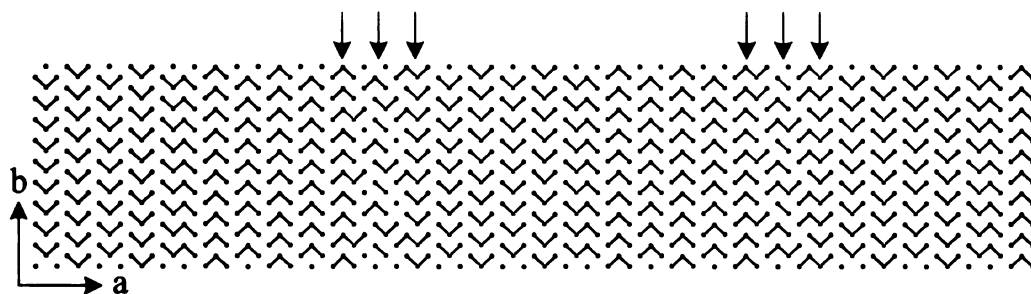


Figure 5.8. $\text{Te}^{1/2-}$ net of Sm_2Te_5 at 100 K with 3.017 Å bonding threshold.

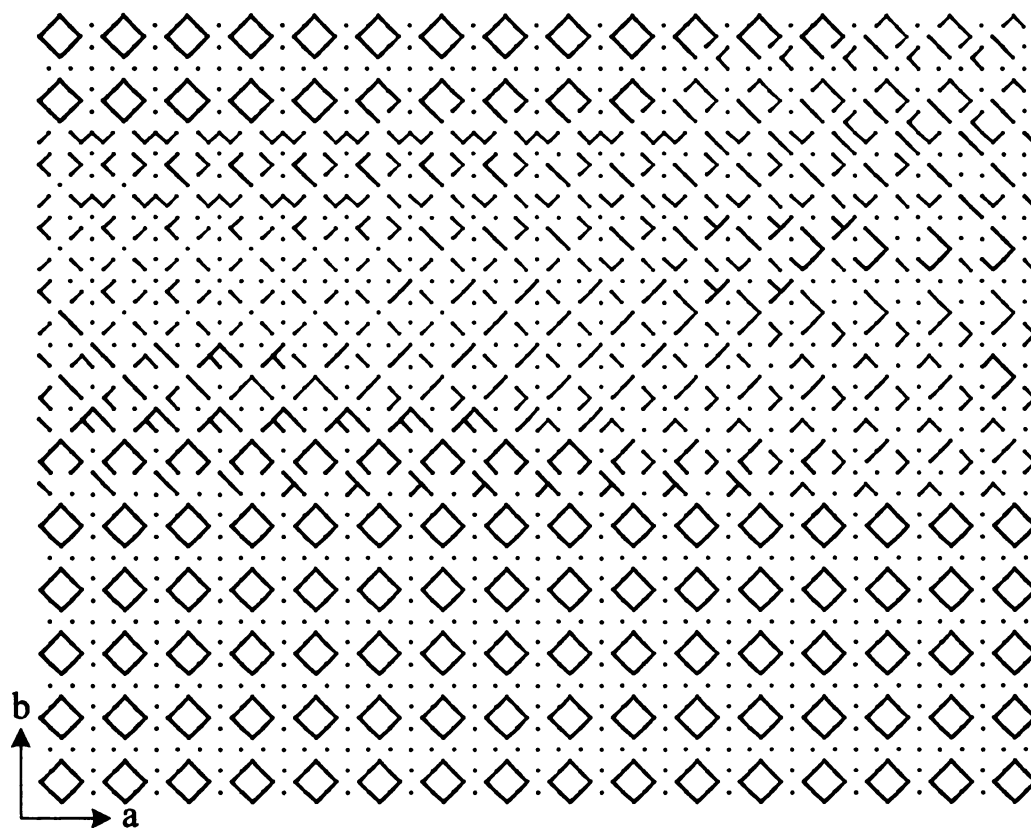


Figure 5.9. Te^{1-} net of Sm_2Te_5 at 100 K with 3.110 Å bonding threshold and 80% occupational cutoff.

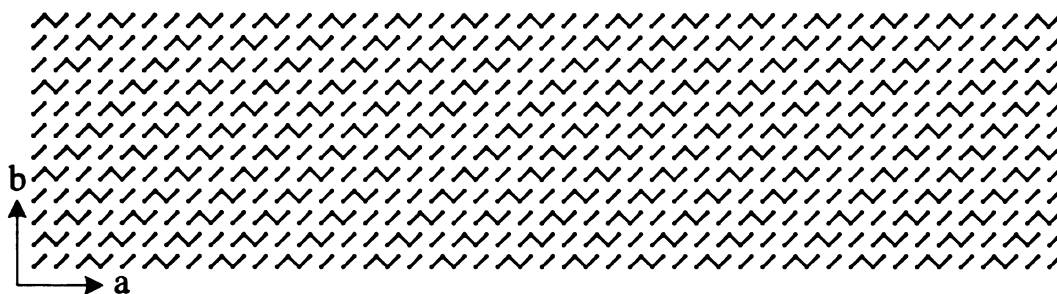


Figure 5.10. $\text{Te}^{1/2-}$ net of Sm_2Te_5 at 500 K with 3.074 Å bonding threshold.

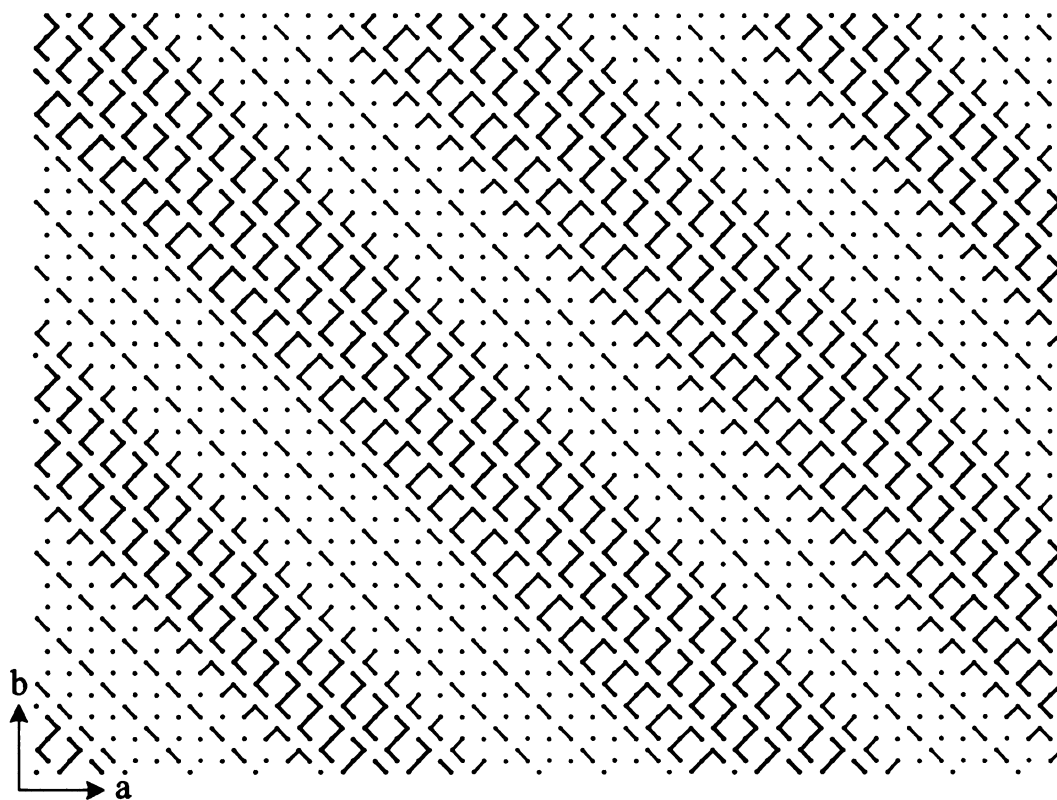


Figure 5.11. Te^{1-} net of Sm_2Te_5 at 500 K with 3.080 Å bonding threshold and 80% occupational cutoff.

Occupational modulation waves of vacancies in the Te^{1-} net of $\text{Sm}_2\text{Te}_{4.90(1)}$ – In the structure of $\text{Sm}_2\text{Te}_{5-x}$ there are two different crystallographic sites, $\text{Te}[3a]$ and $\text{Te}[3b]$, for the Te atoms in the Te^{1-} net. Interestingly, only one site, $\text{Te}[3a]$, is occupationally

distorted. The other site is fully occupied. The occupancy of Te[3a] atom modulates along the 4th and 5th dimension at 100 K creating a rather complicated pattern of vacancies. Figure 5.12 shows an example of the profile of the occupancy of Te[3a] along the t -direction at a fixed $u = 0.5$ section in which the occupancy becomes minimum. The coordinates t and u characterize the real three dimensional structure constructed as a perpendicular intersection with the superspace axis A_n ($n = 4$ for t and $n = 5$ for u) therefore $t = x_4 - q \cdot r$ where r is a positional vector in the three dimensional space. (see section 1.7.2 for more details). A contour plot of the occupancy along t and u directions can be found in Figure 5.13. The occupational modulation wave of Te[3a] is more simple at 500 K since there is only one q -vector. The profile of the occupancy along t is shown in Figure 5.14. The experimental Fourier map of Sm₂Te₅ at 100 K plotted along the modulation direction (t) in comparison with the calculated (fitted) position of Te[3a] is shown in Figure 5.15.

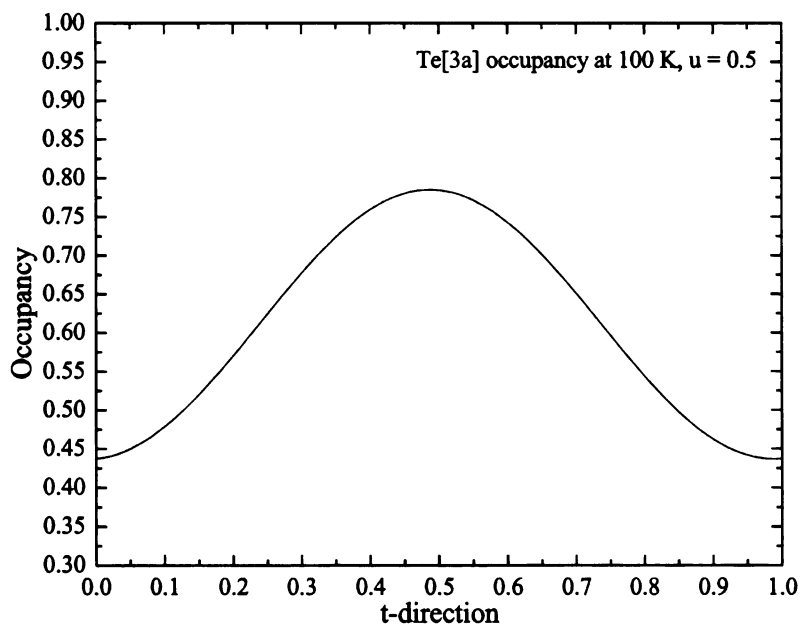


Figure 5.12. Profile of the occupancy of Te[3a] in Sm₂Te_{4.90(1)} at 100 K along the t -direction at a fixed $u = 0.5$ section.

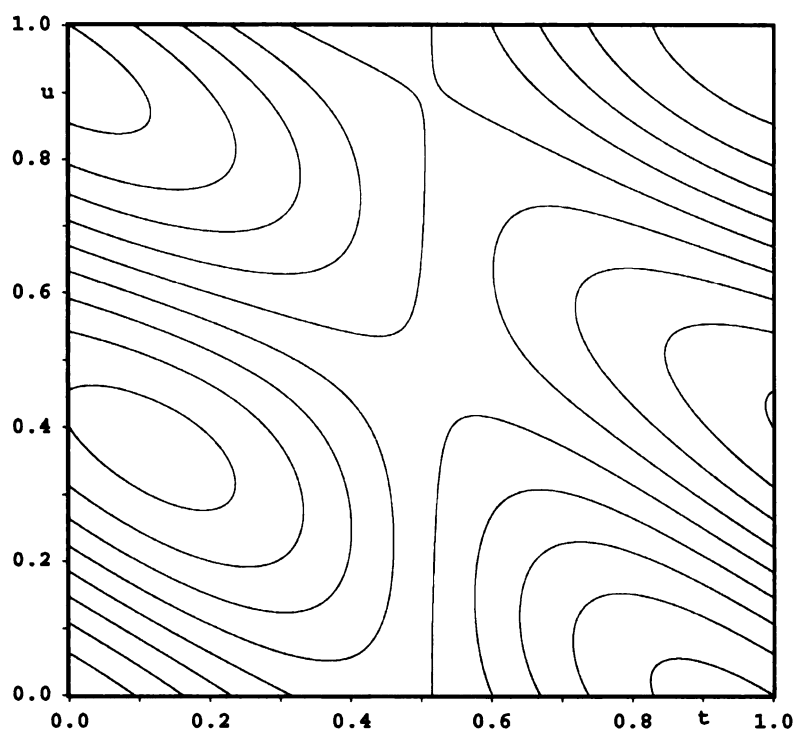


Figure 5.13. Contour plot of the occupancy of Te[3a] in $\text{Sm}_2\text{Te}_{4.90(1)}$ along the t - u space. One contour line per 0.1 (occupational fraction).

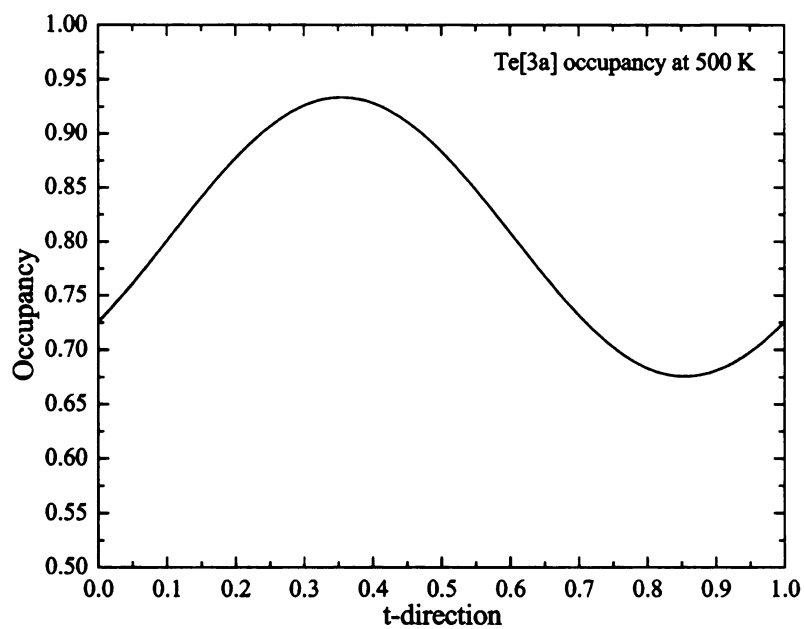


Figure 5.14. Profile of the occupancy of Te[3a] in $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K along the t -direction.

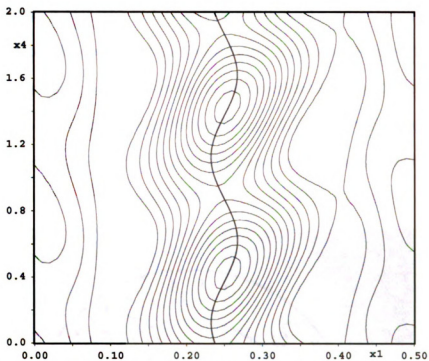


Figure 5.15. Experimental Fourier map of $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K plotted along the modulation direction (t). The central blue line represents the calculated (fitted) position of $\text{Te}[3a]$. One contour line per $0.75 \text{ e} \text{ \AA}^{-3}$. Summation of x_2 along 0.5-1.0 and $x_5 = 0.5$.

Scanning Tunneling Microscopy (STM) Study of Sm_2Te_5 – STM has been used widely to observe CDW modulations from atomic resolution images in direct space.²⁰ In order to verify the hybrid character of the CDW distortion in the $\text{Te}^{1/2-}$ net of Sm_2Te_5 we performed a low temperature STM (LT-STM) study. The STM experiment undertaken at 4.2 K clearly show an incommensurate CDW with wave vector in the $\text{Te}^{1/2-}$ plane along the diagonal of the Te-Te square net. The wave vector measured by Fourier transform of the STM topography images is in agreement with diffraction data. The CDW pattern revealed in Sm_2Te_5 is similar to the one observed in RETe_3 .^{6b, 21} However, an additional wave vector has been observed in this material that was not present in the tritelluride. This wave vector is in the direction of the Te-Te bond. The STM image of the Sm_2Te_5 surface is shown in Figure 5.16A, evidencing the distorted Te net with in-plane lattice parameter $a = 3.1(2) \text{ \AA}$. The fast Fourier transform analysis (FFT) of the STM image is

reported in Figure 5.16B. The peaks L correspond to the Te square lattice. The line cut from O to A, along the diagonal of the Te square net, is shown in Figure 5.16C. This line cut shows five peaks, one corresponding to the superlattice $2\pi/a$ and four intermediate peaks at 0.31, 0.38, 0.62, and 0.69. We identify $q_1 = 0.31$ as the CDW wave vector and the other peaks as the $1-2q_1$, $2q_1$, $1-q_1$ harmonics respectively. The line cut OL shows two additional peaks corresponding to $q_2 = 0.33$ and $2q_2 = 0.66$, Figure 5.16D.

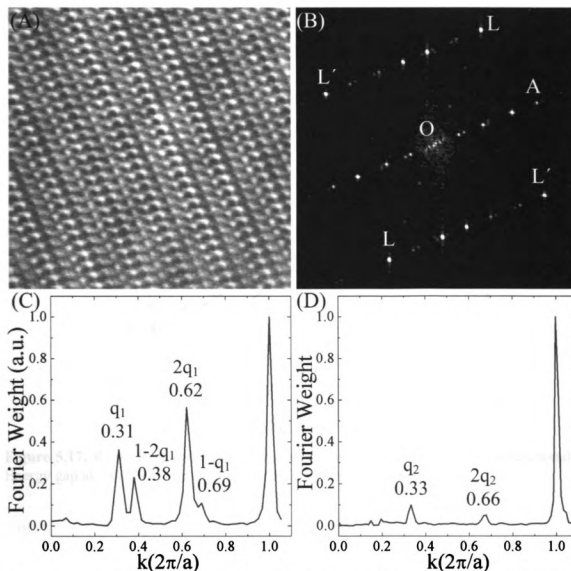


Figure 5.16. (A) STM image of the Sm_2Te_3 surface of $\text{Te}^{-1/2}$. (B) FFT of the STM image. The peaks L correspond to the Te square lattice. (C) Line cut plot from O to A, along the diagonal of the Te square net. (D) Line cut plot from O to L.

Infrared (IR) Spectroscopy of Sm_2Te_5 – The hybrid Sm_2Te_5 , like SmTe_3 , shows a metallic behavior since the CDW does not remove all the states from the Fermi level.^{9b} Despite this poor metallic character there are spectroscopically observed electronic transition. The energy gap was measured by infrared diffuse reflectance spectroscopy on single crystals of Sm_2Te_5 . The data showed a gap around 0.25 eV with a small discontinuity, Figure 5.17. This energy transitions can be attributed to the two CDW distorted Te nets with average charge of 0.5- and 1-.

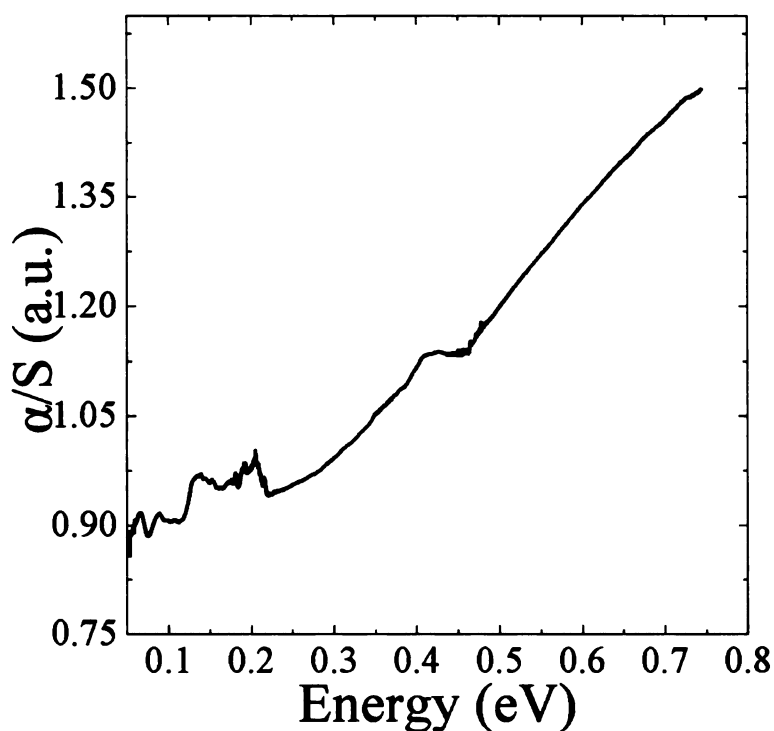


Figure 5.17. Room temperature infrared absorption spectrum of Sm_2Te_5 single crystals. Energy gap at ~ 0.25 eV corresponds to the CDW distorted Te nets.

Supercell Description of SmTe_{1.86(1)} Based on a Modulation q-vector – The distortions found in the Sm₂Te₅ compound revealed a modulation in the Te¹⁻ net that belongs to the SmTe₂ substructure.¹⁷ This led us to the reexamination of the modulated structure of SmTe₂ using a superspace crystallographic approach. The incommensurate superstructure of SmTe_{1.86(1)} was solved in the tetragonal P4($\alpha\beta^{1/2}$)($\beta-\alpha^{1/2}$)0 superspace group with two q-vector normal to each other with $q_1 = 0.2965(3)a^* + 0.2965(3)b^* + 1/2c^*$ and $q_2 = 0.2965(3)a^* - 0.2965(3)b^* + 1/2c^*$ at 100 K. A doubling of the subcell along the c-axis was necessary to avoid non-linear correlations between the rational and irrational components of the two q-vectors. Therefore, a centering vector of (0 0 $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$) was used with the corresponding superspace group notation of X4($\alpha\beta 0$)($\beta-\alpha 0$)0. The labeling scheme is shown in Figure 5.7B.

The CDW distorted Te nets in SmTe₂ possess two types of modulations. Positional and occupational distortions create a rather complicated pattern of Te_x²⁻ oligomers as can be seen in Figure 5.18. The bonding threshold was set to 3.110 Å in order to make a fair comparison with the corresponding pattern observed for Te¹⁻ in the Sm₂Te₅ phase. The majority of oligomers found in SmTe₂ have a linear shape of dimers and trimers. Occasionally single Te atoms, L-shaped tetramers and defected square-like oligomers (similar shape with the ones observed in Sm₂Te₅) with more than six Te atoms is found. The minimum Te-Te distance in the distorted net is 2.730(11) Å, the maximum 3.547(11) Å and the average values is 3.128(10) Å. The value of the occupational cutoff was taken equal to the average occupancy in order to obtain reasonable bond distances between atoms. The distribution of atoms/vacancies along the *t-u* plane is shown in the contour plot in Figure 5.19.

The q -vector dependence at high temperature (500 K) is negligible with cell parameters $a = 4.3787(4) \text{ \AA}$, $c = 8.9976(7) \text{ \AA}$ and $q_1 = 0.2974(3)a^* + 0.2974(3)b^* + 1/2c^*$ and $q_2 = 0.2974(3)a^* - 0.2974(3)b^* + 1/2c^*$.

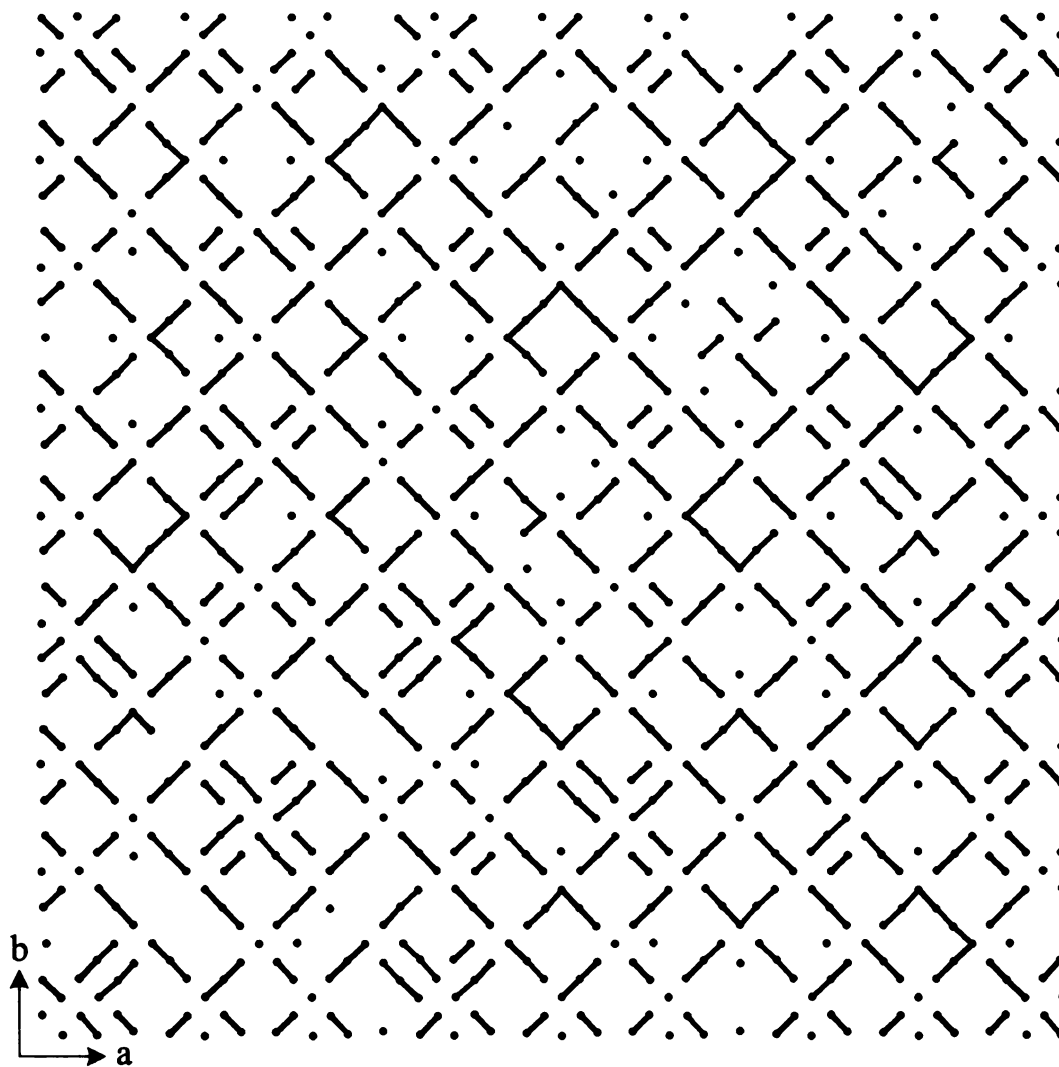


Figure 5.18. Te^{1-} net of SmTe_2 at 100 K with 3.110 $\text{\AA}$ bonding threshold and 86% occupational cutoff.

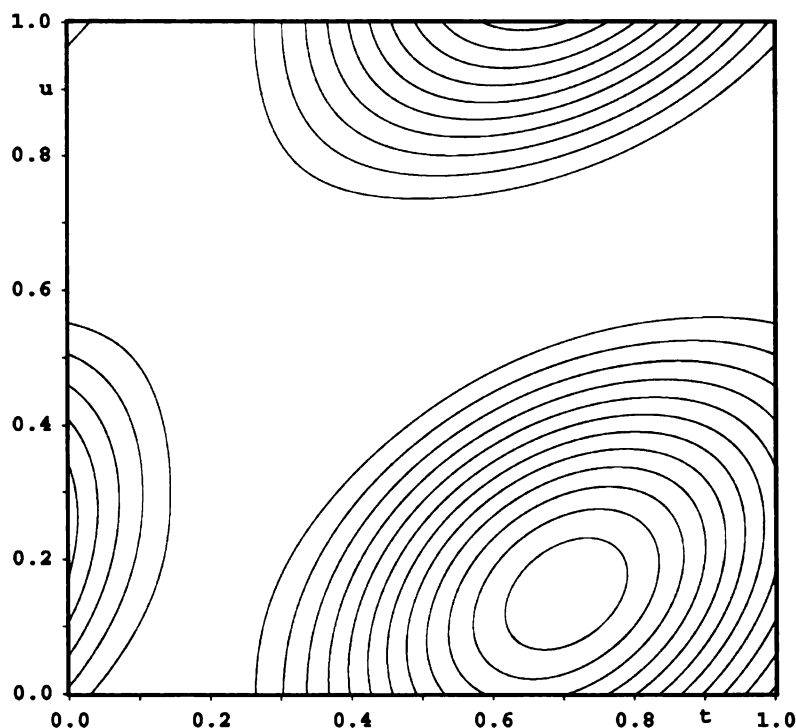


Figure 5.19. Contour plot of the occupancy of Te[2] in $\text{SmTe}_{1.86(1)}$ along the t - u space. One contour line per 0.05 (occupational fraction).

Supercell Description of $K_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ Based on a Modulation q -vector – The existence of two Te nets with different oxidation states created an incommensurate superstructure with two q -vectors at 100 K. There is one commensurate vector $q_1 = 1/3b^*$ and another incommensurate one $q_2 = 0.248(2)a^* + 0.166(2)b^* + 0.083(3)c^*$ for the orthorhombic (Immm) subcell. The intensity of the satellite reflections of q_2 -vector is ~ 20 times weaker than the intensity of the reflections of q_1 -vector. Two different approaches were used to solve the superstructure. In the first attempt, a three-fold subcell was used to clear the commensurate q -vector. A (3+1)-dimensional modulation with one positional and one occupational wave were then applied on the new monoclinic subcell (P2/m). All of the acceptable monoclinic superspace groups (P2, Pm, P2/m groups) gave an R-value for the observed satellite reflections to more than 30%. A triclinic P1

superspace group was the only acceptable solution with an agreement factor for all the observed reflections (main and satellites) of $\sim 6\%$. The total number of refined parameters was 2859.

In the second approach, a (3+2)-dimensional supercell was used in $C1(\alpha_1\beta_1\gamma_1)(\alpha_2\beta_2\gamma_2)0$ superspace group. The subcell in that case was transformed to avoid a large number of correlations according to the transformation matrix $[1\ 1\ 0\ 0\ 0\ -1\ -1\ 0\ 0]$ yielding cell parameters of $a = 6.3521(4)\text{ \AA}$, $b = 6.3531(4)\text{ \AA}$, $c = 25.4036(19)\text{ \AA}$, $\beta = 97.177(6)^\circ$, $q_1 = 0.3327(4)a^* + 0.3327(4)b^* + 0.334(2)c^*$, and $q_2 = 0.400(2)a^* - 0.072(2)b^* + 0.345(6)c^*$. The corresponding R-value was again $\sim 6\%$ with 1466 refined parameters. The second approach was chosen to be a more appropriate one since the same crystallographic solution was obtained with much less parameters, Figure 5.20.

From the observed distortions in the planar nets it seems that the first q_1 -vector affects mainly the position of the atoms in the $\text{Te}^{1/2-}$ net and the second q_2 -vector is responsible for the long range ordering of vacancies in the Te^{1-} net. The CDW distorted pattern of $\text{Te}^{1/2-}$ can be seen as a well ordered sequence of V-shaped trimers, Figure 5.21. The ideal pattern of identical oligomers comes from the fact that the modulation is commensurate. The minimum length in the Te-Te distance distribution is $2.87(4)\text{ \AA}$ and the maximum $3.49(6)\text{ \AA}$. The main difference of the Te^{1-} pattern from the $\text{Te}^{1/2-}$ one is the presence of ordered vacancies, Figure 5.22. The Te-Te length distribution in the Te^{1-} net is much narrower than the one found in the $\text{Te}^{1/2-}$ net with a minimum distance of $3.07(4)\text{ \AA}$, maximum $3.24(4)\text{ \AA}$ and average value of $3.16(4)\text{ \AA}$. The distribution of atoms/vacancies along the t-u plane is shown in the contour plot in Figure 5.23.

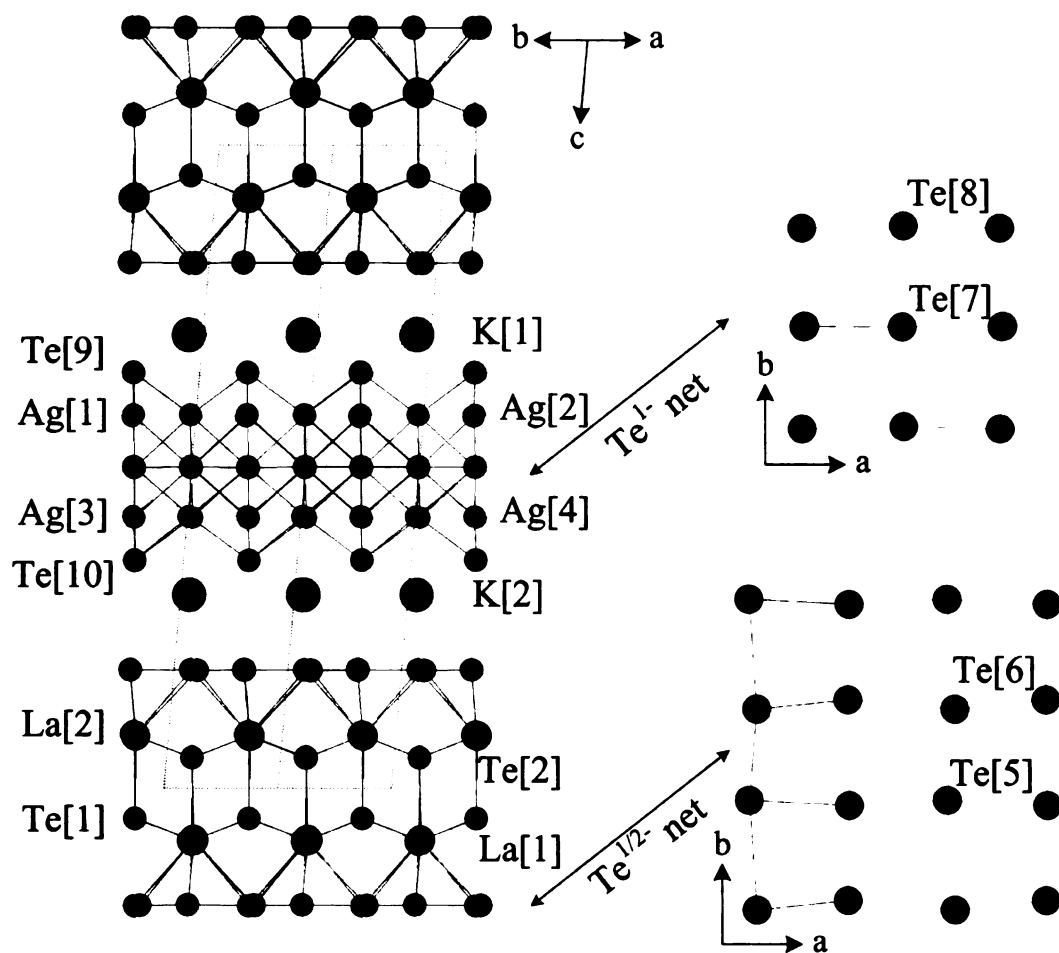


Figure 5.20. Transformed cell of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ and labels used in the superspace refinement at 100 K.

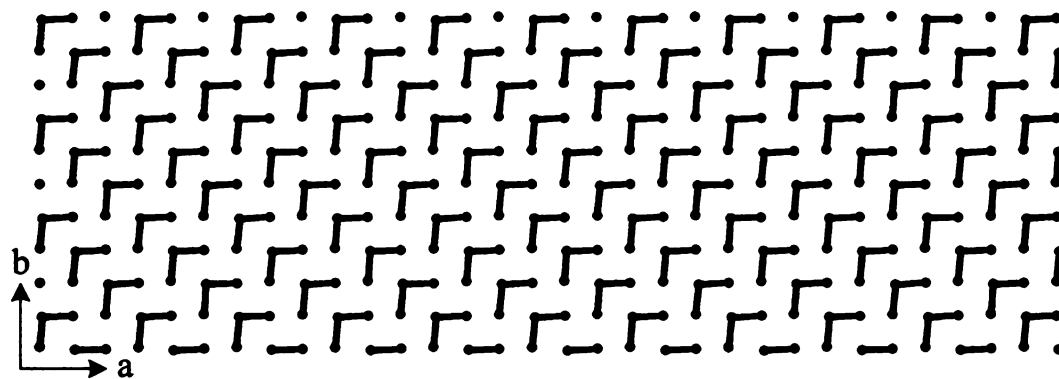


Figure 5.21. $\text{Te}^{1/2-}$ net of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with 3.017 Å bonding threshold showing trimers.

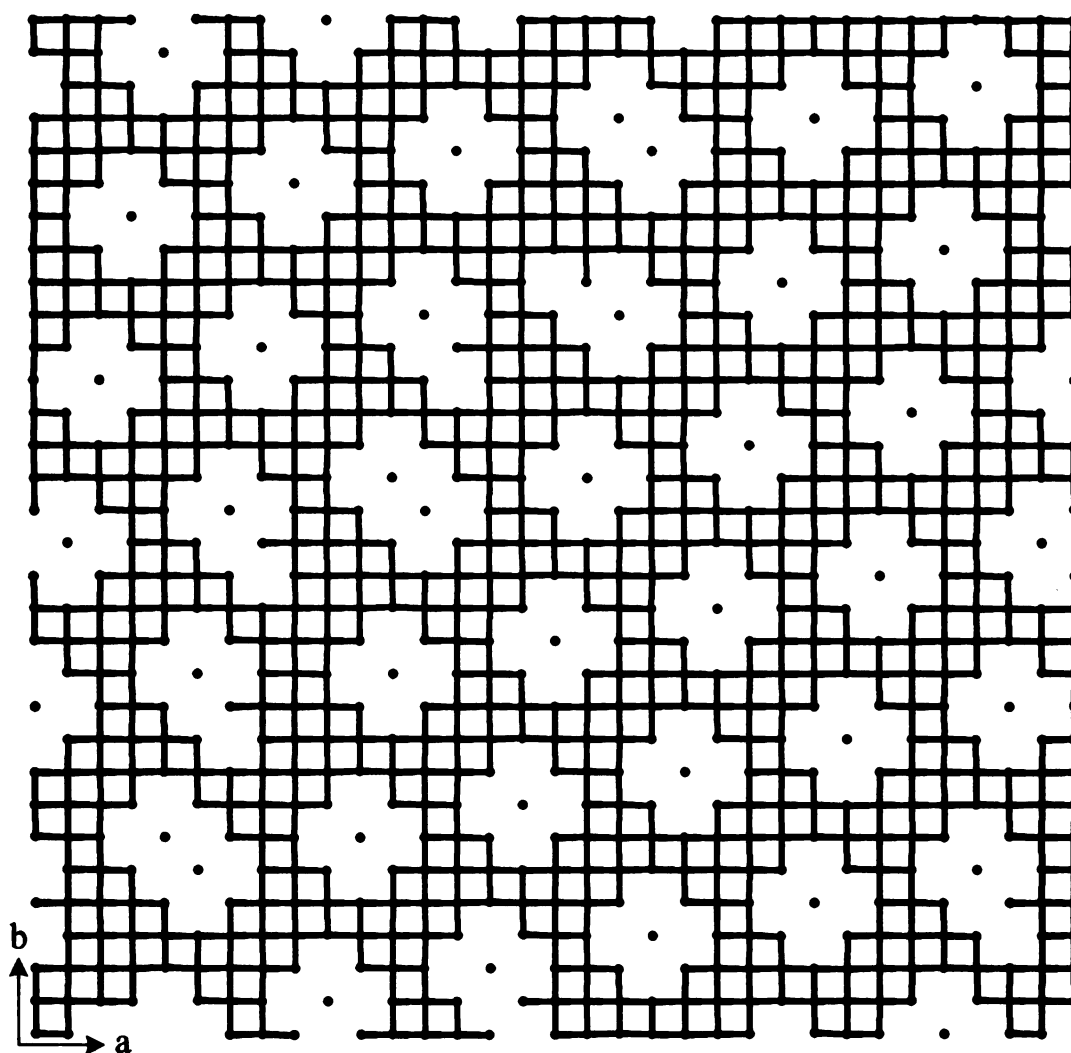


Figure 5.22. Te^{1-} net of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with 3.110 Å bonding threshold and 60% occupational cutoff.

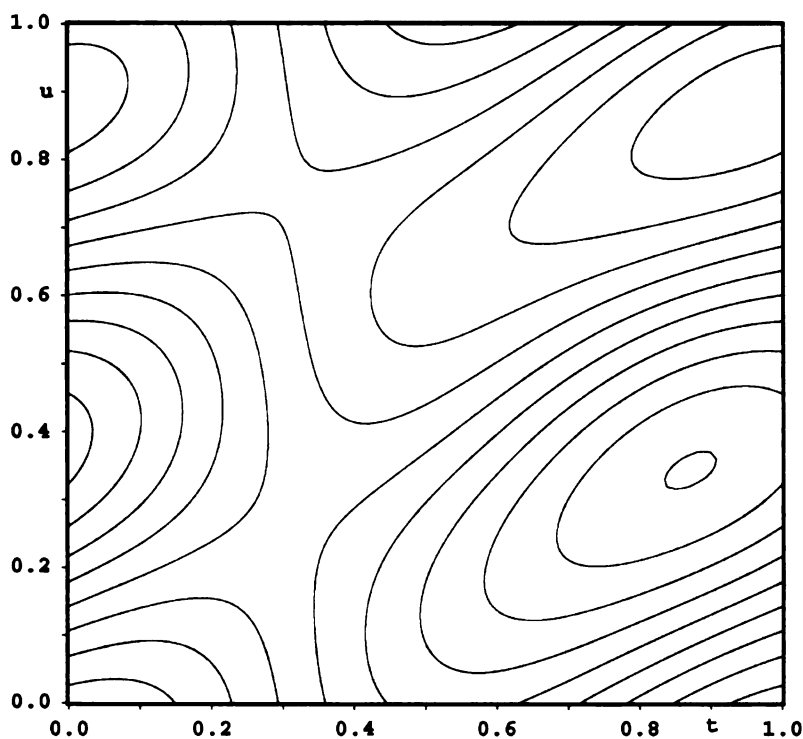


Figure 5.23. Contour plot of the occupancy of Te[2] in $\text{SmTe}_{1.86(1)}$ along the t - u space. One contour line per 0.05 (occupational fraction).

Band structure calculation of La_2Te_5 – The calculations were performed using the self-consistent full-potential linearized augmented plane wave method (LAPW)²² and the generalized gradient approximation (GGA)²³ for the exchange and correlation potential. The experimental cell constants and atomic coordinates from the crystal structure refinement of the average Sm_2Te_5 at 100 K were used as starting values. Volume optimization was used in order to find the minimum energy of the larger La_2Te_5 cell through a Murnaghan type fitting of the Equation of States.²⁴ Scalar relativistic corrections were included and a spin-orbit interaction was incorporated using a second variational procedure.²⁵ Directions in the Brillouin zone (BZ) of Cmc $\bar{m}$ space group are shown in Figure 5.29.²⁶ Interatomic forces were minimized within 0.1 mRy/bohr using a reverse-communication trust-region quasi-Newton method from the Port library.²⁷ The

values of the atomic radii were taken to be 2.7 a.u. for La atom and 2.5 a.u. for Te atoms, where a.u. is the atomic unit (0.529 Å). Convergence of the self-consistent iterations was performed for 150 k points inside the irreducible Brillouin zone to within 0.0001 Ry with a cutoff of -6.0 Ry between the valence and the core states. The calculations were performed using WIEN2K program.²⁸

Electronic band structure calculations performed on the undistorted (no CDW and vacancy ordering) structure of La_2Te_5 . The most important feature of the Fermi Surface (FS) of La_2Te_5 is the separation between the two bands located in the center of the FS (Γ point), Figure 5.28. These are Te p bands in character coming from the two Te nets with different oxidation states. The separation of the bands is such that the topology of the FS favors the formation of two nesting vectors. One vector along the b^* director with a length of 0.32(2) and a second vector along the diagonal of a^*-b^* plane at 0.35(2).²⁹ A weaker splitting of bands was found for the RETe_3 in respect to the RETe_2 due to the interactions between the Te layers separated by the van der Waals gap.³⁰ Although the distance of the Te bilayers separated by the van der Waals gap is essentially the same in both SmTe_3 and Sm_2Te_5 the presence of the additional Te^{1-} layer seems strongly to affect the nesting properties of the FS. The nesting vector from 0.28(2) for LaTe_3 increases significantly to 0.32(2) for La_2Te_5 in a similar fashion observed for KCuLaTe_4 .¹⁶

Band structure calculation of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ – The same calculation method and procedure that was used for La_2Te_5 were performed on the average Immm structure of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ (no CDW and vacancies). Directions in the Brillouin zone (BZ) of Immm space group are shown in Figure 5.33.²⁶ The bands that cross the Fermi surface are pronominally Te p in character. Additionally, some bands associated with the $[\text{K}_2\text{Ag}_4\text{Te}_4]$

layer cross the Fermi level but remain outside the nesting region of the bands of the distorted Te atoms, Figure 5.31. Similar behavior was observed for the layers of KCuLaTe_4 phase. There are seven bands that cross the Fermi level (Figure 5.32A-G) and create the Fermi surface topology shown in Figure 5.32H. The calculated nesting vector (shown in arrows in Figure 5.32H) is $0.35(2)$. The apparent difference of the FS of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ in respect with the surface calculated for LaTe_3 , KCuLaTe_4 , and La_2Te_5 is the existence of the band around the Γ point (Figure 5.32A). This band is located outside the nesting region and it is mainly Te p in character (Te atoms in the $[\text{K}_2\text{Ag}_4\text{Te}_4]$ layer).

5.5. Conclusions

The CDW distortions in the intergrowth $\text{Sm}_2\text{Te}_{5-x}$ compound have shown a unique hybrid character coming from the coupling of two individual q -vectors. The RE_2Te_5 family represents a rare example of composite structure that possesses two Te nets with different oxidation states, $\text{Te}^{1/2-}$ and Te^{1-} . In combination with occupational modulation waves of vacancies the new distorted Te patterns surprisingly are very different from the ones found in the two parent substructures. A similar behavior of simultaneous presence and coupling of two distinct CDW was found in the intergrowth $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10-x}$ compound as well. The new results reported here provide more information to the developing theory of two-dimensional CDW systems with a partially gapped Fermi surface.

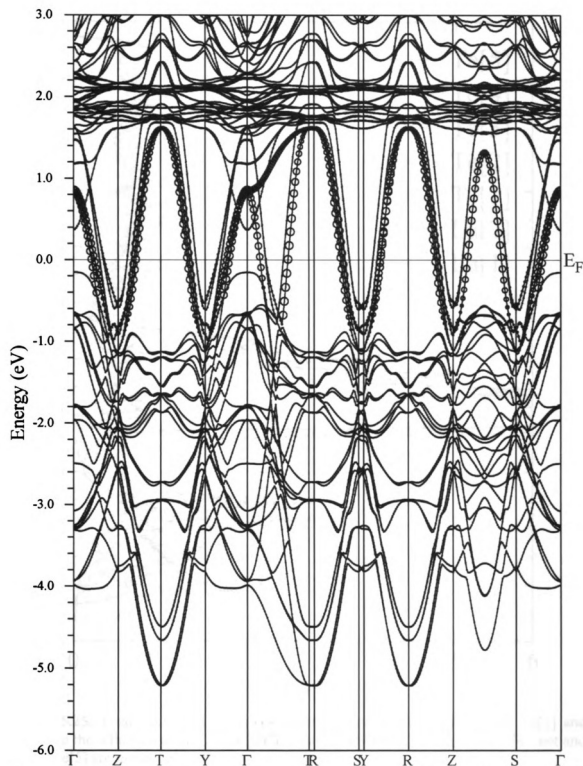


Figure 5.24. Band structure of La_2Te_5 near the Fermi level. $\text{Te}[3] p$ bands from the Te^{1-} net are drawn in open circles. The contribution of each orbital is proportional to the breadth of the circles tracing out the band. Only the bands that cross the Fermi surface are drawn in circles for clarity.

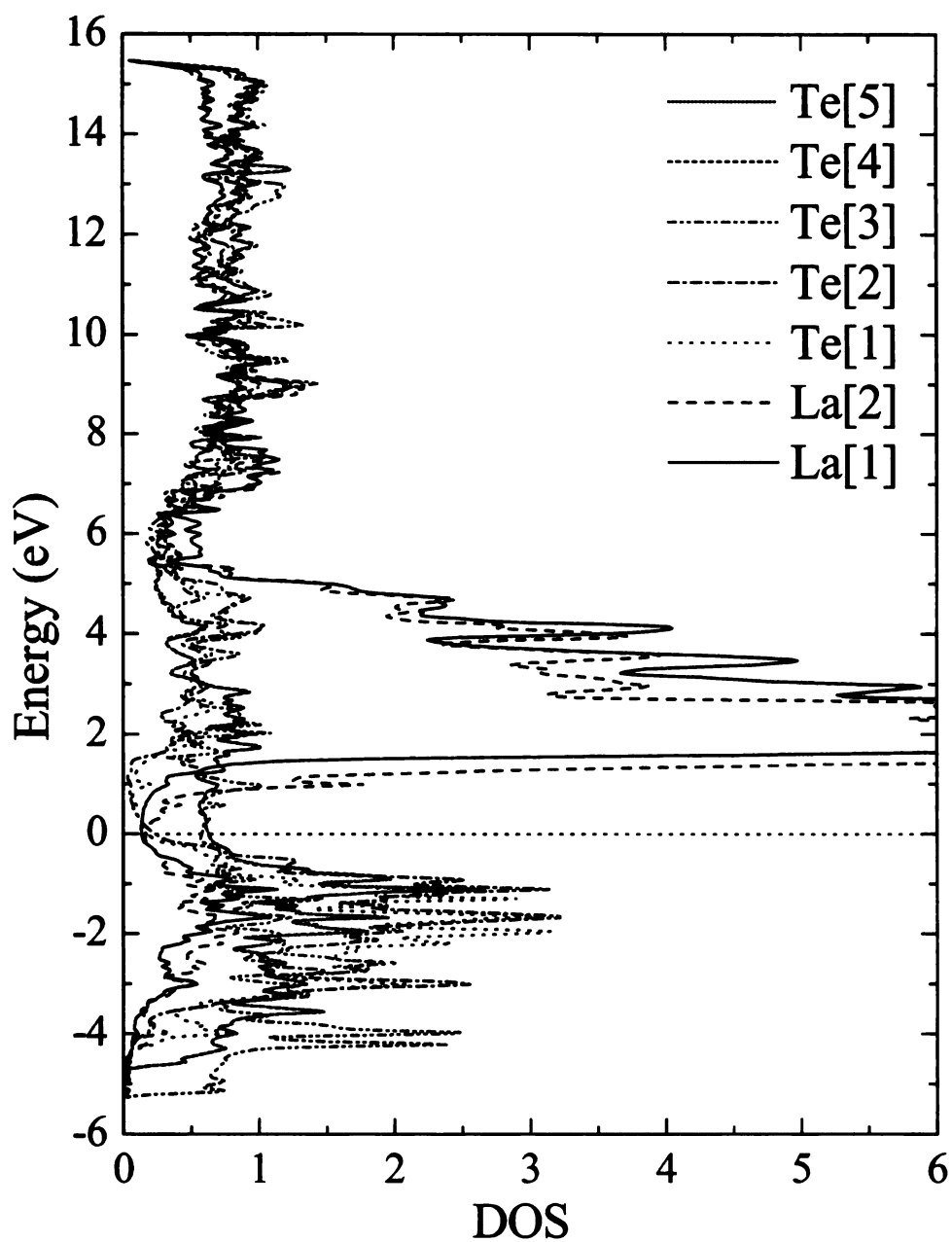


Figure 5.25. Total density of states (DOS) of La_2Te_5 near the Fermi level. Te[1] and Te[2] are the tellurium atoms in the [RETe] puckered layers, Te[3] is in the Te^{1-} net and Te[4], Te[5] are in the $\text{Te}^{1/2-}$ net.

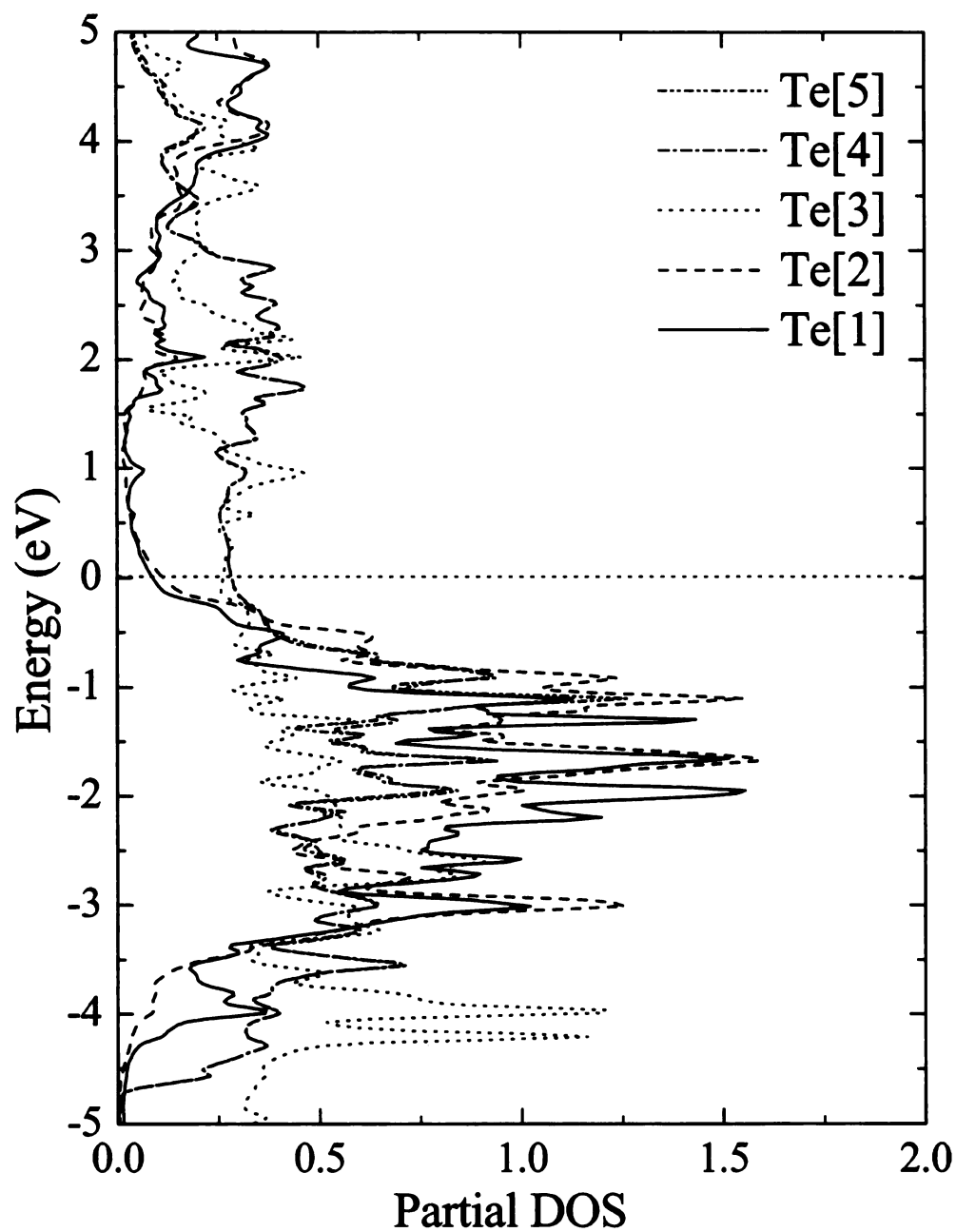


Figure 5.26. Partial density of states (DOS) of all Te p bands in La_2Te_5 near the Fermi level. Te[1] and Te[2] are the tellurium atoms in the [RETe] puckered layers, Te[3] is in the Te^{1-} net and Te[4], Te[5] are in the $\text{Te}^{1/2-}$ net.

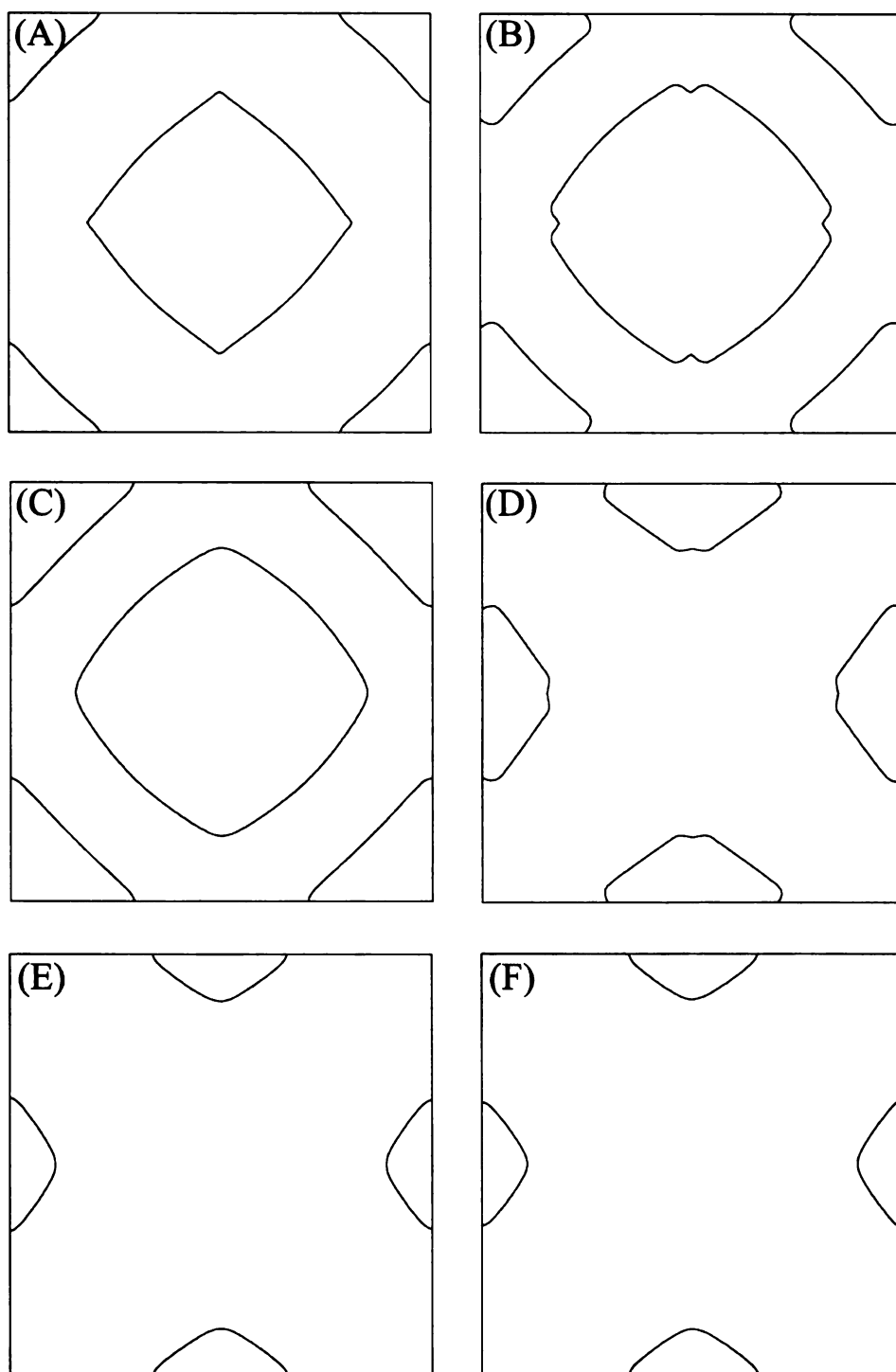


Figure 5.27. (A-F) Fermi surface topology of the six individual bands that cross the Fermi level of La_2Te_5 . Superposition of all six bands will give the total Fermi surface shown in Figure 5.28.

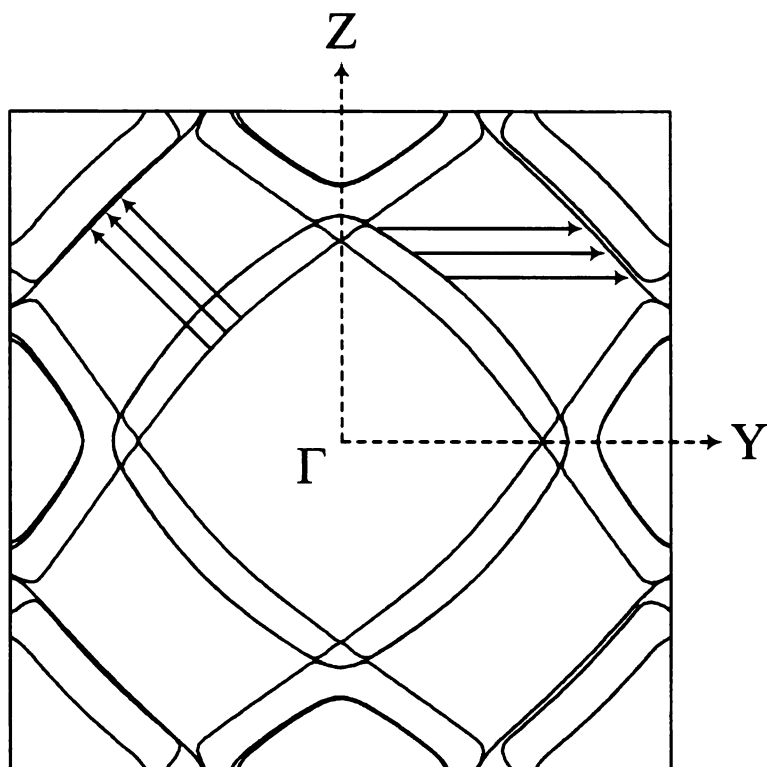


Figure 5.28. Calculated Fermi surface topology of La_2Te_5 . Possible nesting vectors with an average length of $q_1 = 0.32(2)$ along the b^* axis (Y point) and $q_2 = 0.35(2)$ along the diagonal are drawn in arrows.

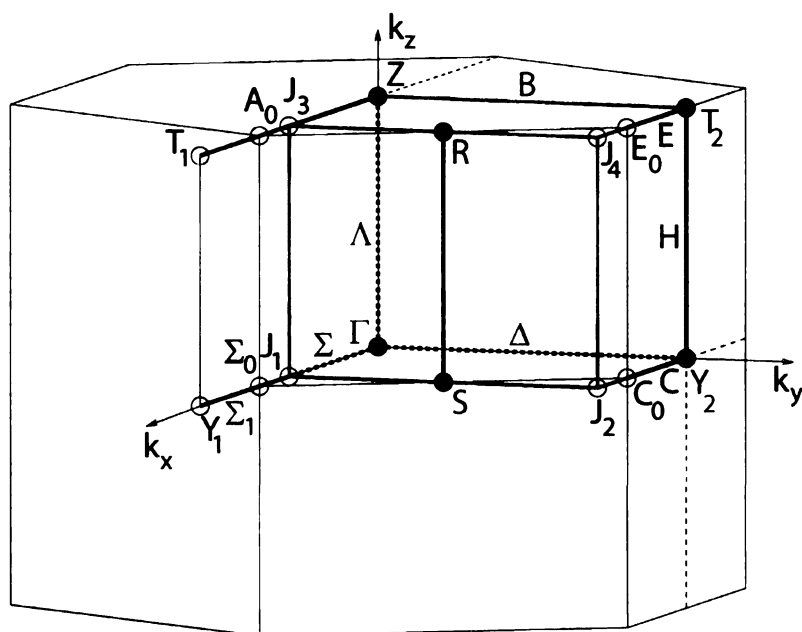


Figure 5.29. Brillouin zone of Cmc space group.²⁶

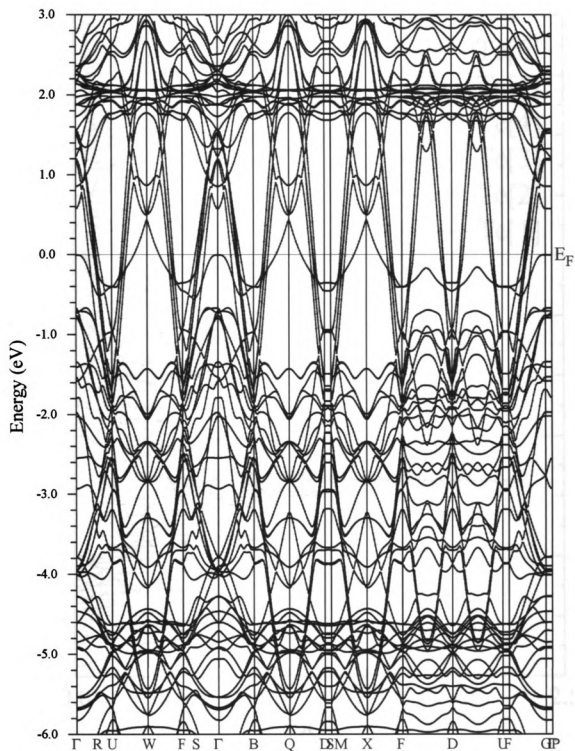


Figure 5.30. Band structure of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ near the Fermi level.

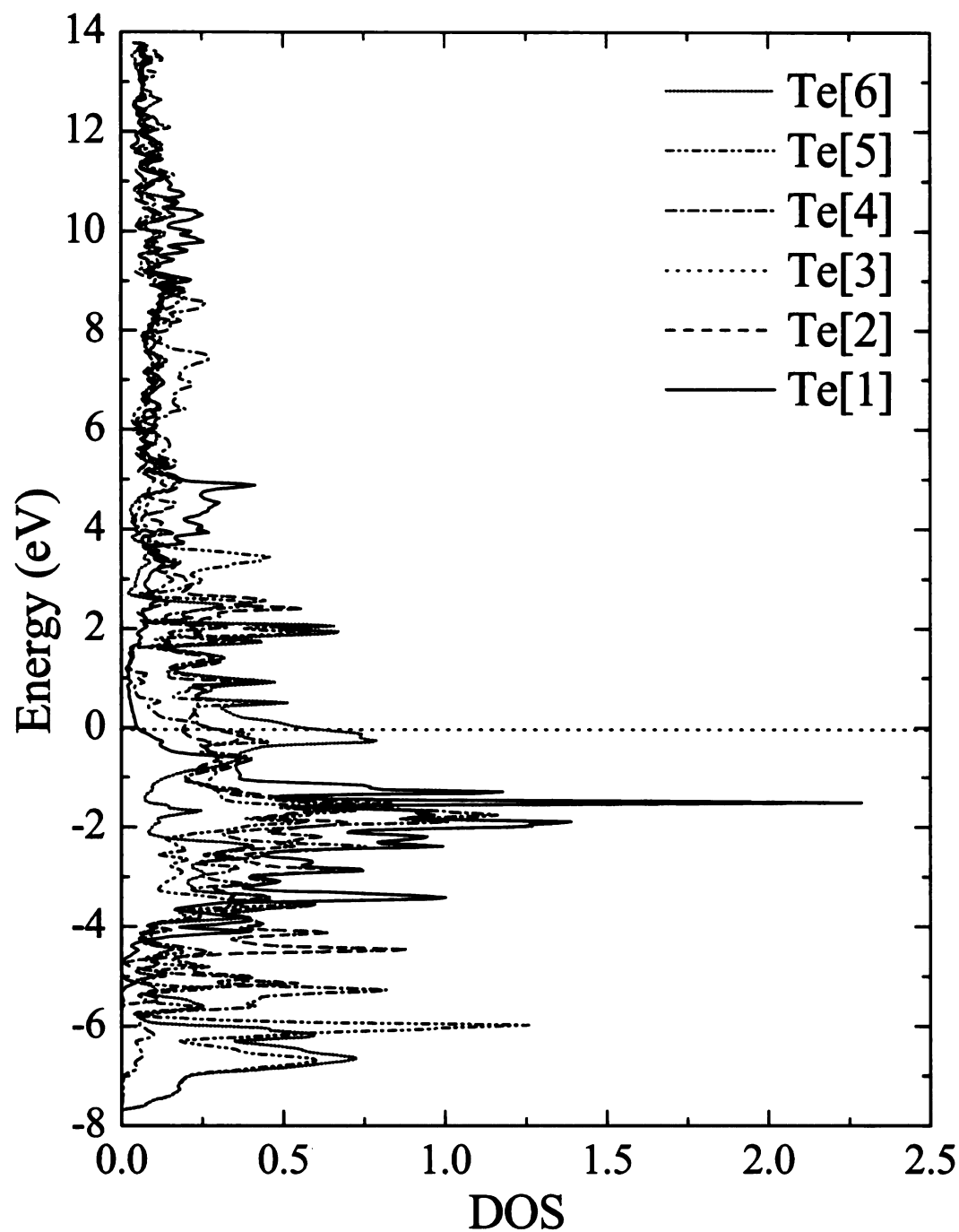


Figure 5.31. Partial density of states (DOS) of all Te p bands $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$ near the Fermi level. Te[1] and Te[2] are the tellurium atoms in the [RETe] puckered layers, Te[3] and Te[4] are in the $\text{Te}^{1/2-}$ net and Te[5], Te[6] are in the Te^{1-} net.

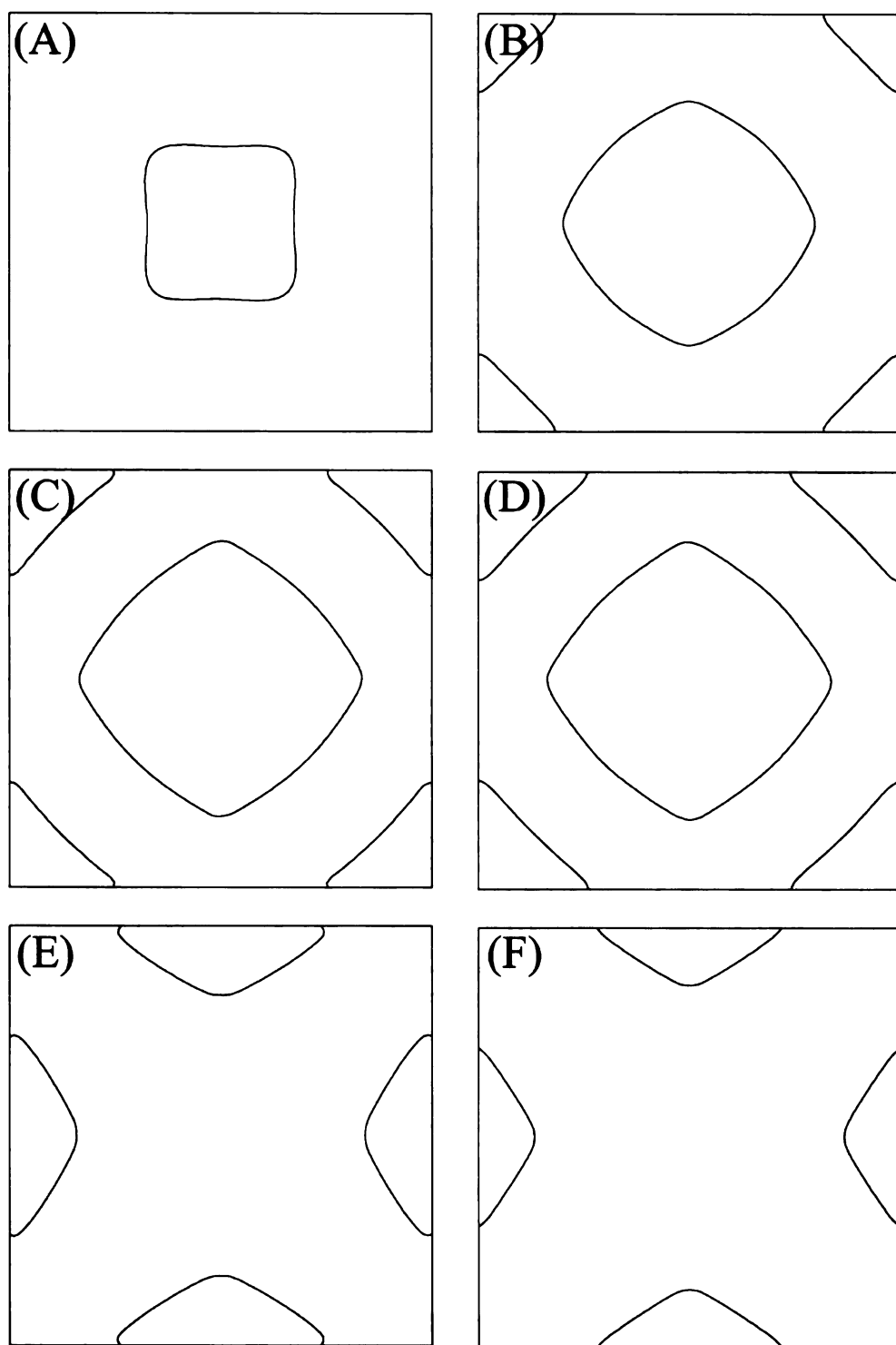


Figure 5.32. (A-G) Fermi surface topology of the seven individual bands that cross the Fermi level of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$. Superposition of all seven bands will give the Fermi surface (H).

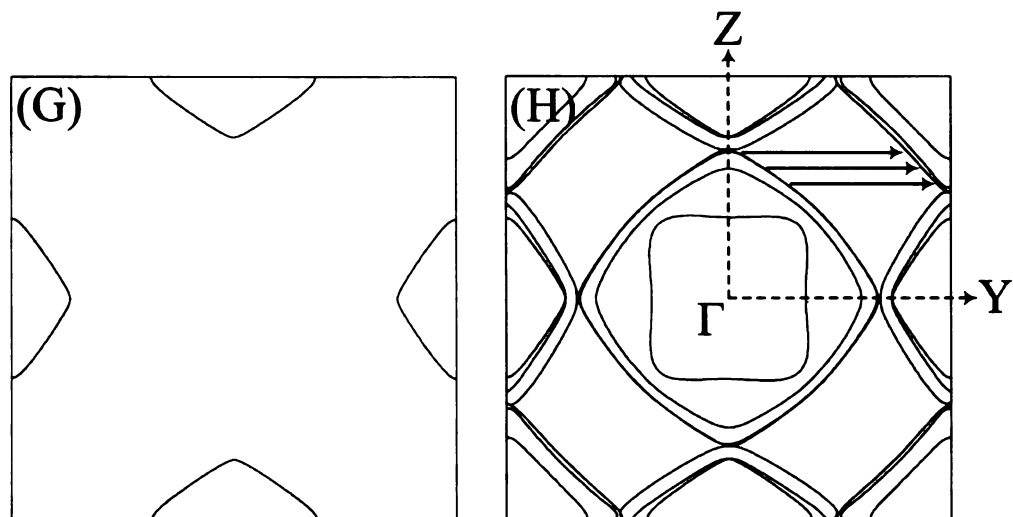


Figure 5.32. (Cont'd) (A-G) Fermi surface topology of the seven individual bands that cross the Fermi level of $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{10}$. Superposition of all seven bands will give the Fermi surface (H).

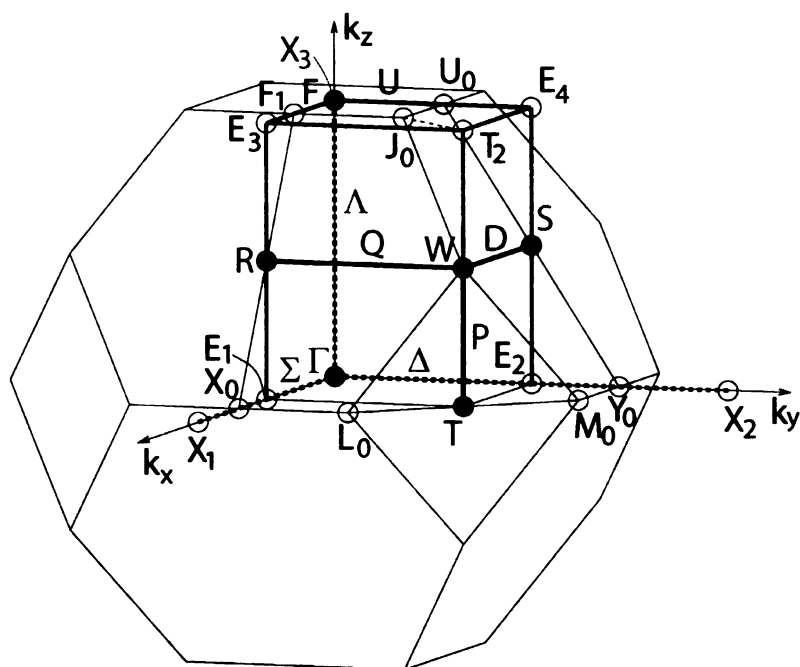


Figure 5.33. Brillouin zone of Immm space group.²⁶

Table 5.1. Crystal data and structure refinement for Sm₂Te_{4.90(1)} at 100 K.

Empirical formula	Sm ₂ Te _{4.90(1)}
Formula weight	938.7
Temperature	100.0(3) K
Crystal system	Triclinic
Space group	P1($\alpha_1\beta_1\gamma_1$)($\alpha_2\beta_2\gamma_2$)
Unit cell dimensions	$a = 4.3392(2) \text{ \AA}$, $\alpha = 90^\circ$ $b = 4.3483(2) \text{ \AA}$, $\beta = 95.679(4)^\circ$ $c = 21.8438(13) \text{ \AA}$, $\gamma = 90^\circ$
q-vector(1)	$0.3124(3)b^* + 1/2c^*$
q-vector(2)	$0.3303(3)a^* + 0.3315(3)b^* + 0.349(1)c^*$
Volume	$410.13(4) \text{ \AA}^3$
Z	2
Density (calculated)	7.5989 g/cm^3
Absorption coefficient	31.474 mm^{-1}
Crystal size	$0.33 \times 0.21 \times 0.02 \text{ mm}^3$
Theta range for data collection	1.80 to 30.19°
Index ranges	$-6 \leq h \leq 6$, $-6 \leq k \leq 6$, $-31 \leq l \leq 30$, $-1 \leq m, n \leq 1$
Reflections collected	73639 (7427 main + 66212 satellites)
Independent reflections	34375 (3969 main + 30406 satellites) [$R_{\text{int}} = 0.0703$]
Completeness to $\theta = 30.19^\circ$	95%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	34375 / 42 / 1100
Goodness-of-fit on F^2	1.43
Final R indices [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0587$, $wR_{\text{obs}} = 0.1981$
R indices (all data)	$R_{\text{all}} = 0.1658$, $wR_{\text{all}} = 0.2421$
Final R main indices [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0490$, $wR_{\text{obs}} = 0.1798$
R main indices (all data)	$R_{\text{all}} = 0.0521$, $wR_{\text{all}} = 0.1909$
Final R 1 st order satellites [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0872$, $wR_{\text{obs}} = 0.1987$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.2864$, $wR_{\text{all}} = 0.2633$
Final R 2 nd order satellites [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.1410$, $wR_{\text{obs}} = 0.3085$
R 2 nd order satellites (all data)	$R_{\text{all}} = 0.4981$, $wR_{\text{all}} = 0.4308$
Extinction coefficient	$0.00051(3)$
T_{min} and T_{max} coefficients	0.0095 and 0.5147
Largest diff. peak and hole	6.04 and $-6.75 \text{ e.\AA}^{-3}$
$R = \Sigma F_o - F_c / \Sigma F_o $, $wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0036I^2)$	

Table 5.2. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Sm[1a]	0	989	2499	1976	1	4(1)
	sin, 1	-15(4)	1(2)	0(1)		
	cos, 1	-51(2)	-2(2)	0(1)		
	sin, 2	3(2)	-5(2)	0(1)		
	cos, 2	0(2)	2(2)	0(1)		
	sin, 3	2(2)	-1(2)	0(1)		
	cos, 3	5(2)	-3(2)	1(1)		
	sin, 4	2(4)	1(3)	1(1)		
	cos, 4	5(4)	0(3)	0(1)		
Sm[1b]	0	-987(1)	-2497(1)	-1976(1)	1	4(1)
	sin, 1	49(3)	0(2)	0(1)		
	cos, 1	-34(3)	2(2)	0(1)		
	sin, 2	2(2)	0(2)	1(1)		
	cos, 2	-2(2)	3(2)	1(1)		
	sin, 3	-3(2)	-1(2)	-1(1)		
	cos, 3	4(2)	-6(2)	-1(1)		
	sin, 4	-4(4)	-1(3)	-1(1)		
	cos, 4	4(4)	-1(3)	-1(1)		
Sm[2b]	0	3079(2)	2499(2)	6135(1)	1	6(1)
	sin, 1	-2(2)	2(2)	1(1)		
	cos, 1	2(2)	1(2)	0(1)		
	sin, 2	-13(2)	-13(2)	0(1)		
	cos, 2	-3(2)	-9(2)	11(1)		
	sin, 3	-15(2)	20(2)	-3(1)		
	cos, 3	9(3)	9(2)	9(1)		
	sin, 4	-1(4)	-4(3)	-2(1)		
	cos, 4	2(4)	4(3)	1(1)		

Table 5.2. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Sm[2a]	0	-3054(2)	-2508(2)	-6127(1)	1	6(1)
	sin, 1	0(2)	2(2)	0(1)		
	cos, 1	-1(2)	-2(2)	1(1)		
	sin, 2	-7(3)	2(2)	7(1)		
	cos, 2	-21(2)	-17(2)	-8(1)		
	sin, 3	3(3)	0(2)	-8(1)		
	cos, 3	16(2)	-6(2)	-2(1)		
	sin, 4	0(4)	-2(3)	1(1)		
	cos, 4	3(4)	6(3)	1(1)		
Te[1b]	0	3823(3)	2493(3)	7606(1)	1	4(1)
	sin, 1	-4(3)	-1(2)	-1(1)		
	cos, 1	-6(3)	5(2)	0(1)		
	sin, 2	0(3)	6(3)	3(1)		
	cos, 2	0(3)	-4(3)	5(1)		
	sin, 3	1(3)	0(3)	2(1)		
	cos, 3	-3(3)	4(3)	3(1)		
	sin, 4	1(5)	1(4)	0(1)		
	cos, 4	-1(5)	2(4)	-3(1)		
Te[1a]	0	-3777(3)	-2512(3)	-7590(1)	1	4(1)
	sin, 1	-8(3)	6(2)	0(1)		
	cos, 1	-1(3)	-4(2)	-1(1)		
	sin, 2	7(3)	0(3)	4(1)		
	cos, 2	-2(3)	-5(3)	-1(1)		
	sin, 3	0(3)	0(3)	-2(1)		
	cos, 3	-5(3)	0(3)	-3(1)		
	sin, 4	6(5)	7(4)	-1(1)		
	cos, 4	3(5)	-3(4)	1(1)		

Table 5.2. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[2a]	0	1760(3)	2488(3)	3474(1)	1	4(1)
	sin, 1	6(3)	-5(2)	1(1)		
	cos, 1	3(3)	-2(2)	1(1)		
	sin, 2	-1(3)	-3(3)	2(1)		
	cos, 2	-15(3)	-8(3)	-1(1)		
	sin, 3	-3(3)	-3(3)	2(1)		
	cos, 3	-9(3)	-12(3)	2(1)		
	sin, 4	14(5)	0(4)	-1(1)		
	cos, 4	-2(5)	9(4)	0(1)		
Te[2b]	0	-1707(3)	-2515(3)	-3469(1)	1	4(1)
	sin, 1	6(3)	-7(2)	0(1)		
	cos, 1	1(3)	-1(2)	-1(1)		
	sin, 2	-10(3)	-5(3)	-1(1)		
	cos, 2	-14(3)	8(3)	3(1)		
	sin, 3	7(3)	-14(3)	0(1)		
	cos, 3	-3(3)	-7(3)	-3(1)		
	sin, 4	6(5)	-13(4)	-1(1)		
	cos, 4	1(5)	0(5)	3(1)		
Te[3a]	0	2534(5)	7602(4)	5003(1)	0.804(3)	17(1)
	sin, 1	-10(5)	-36(6)	3(1)		
	cos, 1	11(7)	68(7)	5(1)		
	sin, 2	-216(5)	-176(10)	1(1)		
	cos, 2	11(13)	-164(11)	0(1)		
	sin, 3	33(13)	-216(8)	-1(1)		
	cos, 3	211(5)	-91(13)	2(1)		
	sin, 4	-5(10)	43(7)	-2(2)		
	cos, 4	-34(9)	-15(10)	0(1)		

Table 5.2. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[3b]	0	-2470(4)	-7412(4)	-4999(1)	1	18(1)
	sin, 1	-5(4)	52(4)	4(1)		
	cos, 1	-10(5)	-47(5)	1(1)		
	sin, 2	-170(3)	-138(7)	-2(1)		
	cos, 2	5(10)	-124(8)	0(1)		
	sin, 3	-48(9)	147(6)	2(1)		
	cos, 3	-149(4)	78(9)	0(1)		
	sin, 4	7(7)	-10(6)	4(1)		
	cos, 4	14(7)	-16(6)	1(1)		
Te[4a]	0	471(4)	7492(3)	838(1)	1	5(1)
	sin, 1	2(11)	-8(3)	0(1)		
	cos, 1	248(3)	19(3)	-2(1)		
	sin, 2	6(4)	-1(3)	0(1)		
	cos, 2	6(4)	5(3)	0(1)		
	sin, 3	6(4)	-5(3)	1(1)		
	cos, 3	4(4)	-4(3)	-1(1)		
	sin, 4	-10(5)	-4(5)	2(1)		
	cos, 4	1(5)	-6(4)	-3(1)		
Te[4b]	0	-357(4)	-7514(3)	-820(1)	1	5(1)
	sin, 1	-101(8)	2(3)	-1(1)		
	cos, 1	180(5)	-9(3)	2(1)		
	sin, 2	-4(3)	-1(3)	0(1)		
	cos, 2	-3(4)	-2(3)	2(1)		
	sin, 3	1(4)	-2(3)	1(1)		
	cos, 3	-5(4)	2(3)	0(1)		
	sin, 4	-5(5)	-8(5)	-5(1)		
	cos, 4	-7(5)	-9(5)	-2(1)		

Table 5.2. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[5a]	0	5452(3)	2509(3)	840(1)	1	6(1)
	sin, 1	1(8)	-11(3)	0(1)		
	cos, 1	-180(3)	12(3)	0(1)		
	sin, 2	-3(3)	6(3)	1(1)		
	cos, 2	-2(3)	3(3)	1(1)		
	sin, 3	6(4)	-4(3)	-1(1)		
	cos, 3	2(4)	0(3)	0(1)		
	sin, 4	5(5)	-1(4)	2(1)		
	cos, 4	-3(5)	7(4)	3(1)		
Te[5b]	0	-5373(3)	-2488(3)	-823(1)	1	6(1)
	sin, 1	105(8)	0(3)	1(1)		
	cos, 1	-181(6)	2(3)	0(1)		
	sin, 2	4(3)	0(3)	1(1)		
	cos, 2	-2(3)	2(3)	0(1)		
	sin, 3	-5(4)	0(3)	-1(1)		
	cos, 3	-3(4)	1(3)	0(1)		
	sin, 4	-12(5)	2(4)	-5(1)		
	cos, 4	-7(6)	2(4)	0(1)		

Table 5.3. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Sm[1a]	0	4(1)	3(1)	5(1)	1(1)	1(1)	0(1)
	sin, 1	0(1)	0(1)	0(1)	0(1)	1(1)	0(1)
	cos, 1	-3(1)	1(1)	0(1)	-1(1)	0(1)	0(1)
	sin, 2	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)
	cos, 2	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	sin, 3	0(1)	-1(1)	0(1)	0(1)	0(1)	0(1)
	cos, 3	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	sin, 4	1(1)	0(1)	1(1)	0(1)	1(1)	1(1)
	cos, 4	-1(1)	1(1)	-1(1)	0(1)	1(1)	0(1)

Table 5.3. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Sm[1b]	0	4(1)	3(1)	5(1)	1(1)	1(1)	0(1)
	sin, 1	2(1)	-1(1)	0(1)	1(1)	0(1)	0(1)
	cos, 1	-2(1)	1(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 2	0(1)	0(1)	0(1)	0(1)	0(1)	1(1)
	sin, 3	0(1)	0(1)	0(1)	1(1)	0(1)	0(1)
	cos, 3	0(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	sin, 4	1(1)	1(1)	0(1)	-1(1)	0(1)	0(1)
	cos, 4	1(1)	0(1)	0(1)	-1(1)	0(1)	0(1)
Sm[2b]	0	5(1)	5(1)	8(1)	0(1)	1(1)	0(1)
	sin, 1	0(1)	-1(1)	0(1)	1(1)	0(1)	1(1)
	cos, 1	-1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	0(1)	-1(1)	0(1)	1(1)	0(1)	0(1)
	cos, 2	0(1)	-2(1)	2(1)	1(1)	1(1)	4(1)
	sin, 3	0(1)	2(1)	-1(1)	0(1)	1(1)	-2(1)
	cos, 3	-1(1)	0(1)	1(1)	2(1)	1(1)	3(1)
	sin, 4	0(1)	1(1)	0(1)	0(1)	-1(1)	1(1)
	cos, 4	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
Sm[2a]	0	5(1)	5(1)	8(1)	0(1)	1(1)	0(1)
	sin, 1	1(1)	0(1)	0(1)	0(1)	0(1)	-1(1)
	cos, 1	-1(1)	1(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	-1(1)	0(1)	1(1)	1(1)	0(1)	2(1)
	cos, 2	0(1)	-1(1)	-1(1)	-1(1)	-1(1)	-3(1)
	sin, 3	2(1)	1(1)	-1(1)	0(1)	0(1)	-3(1)
	cos, 3	1(1)	0(1)	0(1)	1(1)	1(1)	-2(1)
	sin, 4	1(1)	1(1)	0(1)	0(1)	-1(1)	0(1)
	cos, 4	0(1)	0(1)	0(1)	1(1)	0(1)	-1(1)

Table 5.3. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[1b]	0	4(1)	4(1)	5(1)	0(1)	1(1)	0(1)
	sin, 1	1(1)	0(1)	1(1)	0(1)	1(1)	0(1)
	cos, 1	-1(1)	1(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	1(1)	1(1)	0(1)	0(1)	0(1)	1(1)
	cos, 2	1(1)	0(1)	0(1)	0(1)	0(1)	2(1)
	sin, 3	0(1)	1(1)	0(1)	0(1)	0(1)	1(1)
	cos, 3	0(1)	1(1)	0(1)	1(1)	0(1)	1(1)
	sin, 4	0(1)	-1(1)	0(1)	-1(1)	-1(1)	0(1)
	cos, 4	1(1)	0(1)	1(1)	-1(1)	-1(1)	0(1)
Te[1a]	0	4(1)	4(1)	5(1)	0(1)	1(1)	0(1)
	sin, 1	-1(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	1(1)	-1(1)	1(1)	1(1)	0(1)	1(1)
	cos, 2	-1(1)	-1(1)	0(1)	0(1)	-1(1)	-1(1)
	sin, 3	1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 3	1(1)	1(1)	-1(1)	0(1)	0(1)	-2(1)
	sin, 4	0(1)	-1(1)	1(1)	1(1)	1(1)	1(1)
	cos, 4	0(1)	-2(1)	-1(1)	1(1)	-1(1)	-1(1)
Te[2a]	0	4(1)	4(1)	5(1)	0(1)	0(1)	0(1)
	sin, 1	-1(1)	0(1)	1(1)	0(1)	0(1)	-1(1)
	cos, 1	-1(1)	1(1)	0(1)	-1(1)	1(1)	0(1)
	sin, 2	-1(1)	-1(1)	1(1)	1(1)	0(1)	1(1)
	cos, 2	-1(1)	0(1)	1(1)	-1(1)	-1(1)	0(1)
	sin, 3	-2(1)	0(1)	1(1)	1(1)	1(1)	-1(1)
	cos, 3	0(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	sin, 4	2(1)	-1(1)	-2(1)	0(1)	-1(1)	1(1)
	cos, 4	0(1)	-2(1)	2(1)	0(1)	1(1)	0(1)

Table 5.3. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[2b]	0	4(1)	4(1)	5(1)	0(1)	0(1)	0(1)
	sin, 1	2(1)	-1(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	1(1)	0(1)	-1(1)	0(1)	1(1)
	sin, 2	-1(1)	0(1)	1(1)	0(1)	0(1)	0(1)
	cos, 2	0(1)	-1(1)	-2(1)	-1(1)	0(1)	2(1)
	sin, 3	-3(1)	-3(1)	2(1)	0(1)	0(1)	1(1)
	cos, 3	2(1)	0(1)	1(1)	-2(1)	0(1)	-1(1)
	sin, 4	-1(1)	3(1)	1(1)	0(1)	-1(1)	0(1)
	cos, 4	0(1)	1(1)	0(1)	-2(1)	1(1)	-1(1)
Te[3a]	0	21(1)	25(1)	7(1)	-2(1)	0(1)	0(1)
	sin, 1	-15(1)	1(2)	13(1)	0(1)	1(1)	0(1)
	cos, 1	6(1)	-7(1)	11(1)	-6(1)	1(1)	-3(1)
	sin, 2	9(1)	-13(1)	6(1)	-1(1)	1(1)	2(1)
	cos, 2	-4(1)	-8(1)	0(1)	-16(1)	1(1)	0(1)
	sin, 3	-1(1)	-11(1)	-2(1)	18(1)	-1(1)	1(1)
	cos, 3	8(1)	-9(1)	9(1)	-4(1)	3(1)	0(1)
	sin, 4	-1(2)	-2(2)	6(1)	4(1)	1(1)	-4(1)
	cos, 4	-2(2)	1(2)	3(2)	-7(1)	1(1)	0(1)
Te[3b]	0	21(1)	25(1)	7(1)	-2(1)	0(1)	0(1)
	sin, 1	6(1)	4(1)	-3(1)	0(1)	0(1)	5(1)
	cos, 1	3(1)	9(1)	2(1)	-4(1)	0(1)	-1(1)
	sin, 2	-2(1)	-19(1)	3(1)	-3(1)	-1(1)	-2(1)
	cos, 2	10(1)	6(1)	1(1)	-15(1)	-2(1)	0(1)
	sin, 3	-10(1)	4(2)	0(1)	-12(1)	-2(1)	2(1)
	cos, 3	6(1)	22(1)	-3(1)	-3(1)	0(1)	1(1)
	sin, 4	2(1)	4(1)	-5(1)	-1(1)	-3(1)	2(1)
	cos, 4	4(1)	2(1)	0(1)	1(1)	0(1)	-2(1)

Table 5.3. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[4a]	0	5(1)	4(1)	6(1)	0(1)	1(1)	0(1)
	sin, 1	-1(1)	-1(1)	0(1)	-1(1)	0(1)	0(1)
	cos, 1	4(1)	1(1)	-1(1)	4(1)	0(1)	1(1)
	sin, 2	1(1)	1(1)	0(1)	0(1)	0(1)	0(1)
	cos, 2	0(1)	0(1)	0(1)	1(1)	0(1)	0(1)
	sin, 3	-2(1)	0(1)	2(1)	1(1)	0(1)	0(1)
	cos, 3	-1(1)	1(1)	0(1)	0(1)	0(1)	1(1)
	sin, 4	-1(1)	-1(1)	-1(1)	0(1)	1(1)	1(1)
	cos, 4	-1(1)	0(1)	0(1)	1(1)	-2(1)	1(1)
Te[4b]	0	5(1)	4(1)	6(1)	0(1)	1(1)	0(1)
	sin, 1	0(1)	-2(1)	1(1)	-2(1)	0(1)	-1(1)
	cos, 1	2(1)	3(1)	0(1)	2(1)	1(1)	0(1)
	sin, 2	0(1)	-1(1)	1(1)	-1(1)	-1(1)	-1(1)
	cos, 2	0(1)	1(1)	0(1)	1(1)	-1(1)	1(1)
	sin, 3	3(1)	-1(1)	1(1)	-1(1)	0(1)	0(1)
	cos, 3	1(1)	-1(1)	-1(1)	0(1)	0(1)	-1(1)
	sin, 4	2(1)	3(1)	1(1)	0(1)	-1(1)	3(1)
	cos, 4	-1(1)	2(1)	-1(1)	0(1)	-1(1)	0(1)
Te[5a]	0	6(1)	5(1)	6(1)	0(1)	1(1)	0(1)
	sin, 1	0(1)	-1(1)	-1(1)	1(1)	1(1)	-2(1)
	cos, 1	-6(1)	1(1)	0(1)	-3(1)	0(1)	1(1)
	sin, 2	-3(1)	-1(1)	0(1)	0(1)	1(1)	0(1)
	cos, 2	-1(1)	0(1)	0(1)	0(1)	1(1)	0(1)
	sin, 3	-2(1)	0(1)	1(1)	1(1)	0(1)	0(1)
	cos, 3	0(1)	1(1)	0(1)	0(1)	1(1)	1(1)
	sin, 4	-2(1)	0(1)	-1(1)	1(1)	-1(1)	1(1)
	cos, 4	0(1)	3(1)	0(1)	-1(1)	-4(1)	-1(1)

Table 5.3. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[5b]	0	6(1)	5(1)	6(1)	0(1)	1(1)	0(1)
	sin, 1	4(1)	-2(1)	1(1)	3(1)	0(1)	1(1)
	cos, 1	-7(1)	2(1)	2(1)	-2(1)	0(1)	1(1)
	sin, 2	1(1)	0(1)	-1(1)	0(1)	1(1)	1(1)
	cos, 2	0(1)	-1(1)	0(1)	-1(1)	1(1)	0(1)
	sin, 3	2(1)	-1(1)	1(1)	-1(1)	0(1)	-1(1)
	cos, 3	1(1)	-2(1)	-1(1)	0(1)	0(1)	-1(1)
	sin, 4	1(1)	-2(1)	-1(1)	1(1)	-1(1)	2(1)
	cos, 4	-2(1)	2(1)	2(1)	-1(1)	-1(1)	0(1)

Table 5.4. Fourier components of the occupational modulation for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Te[3a]	sin, 1	0.047(9)
	cos, 1	0.009(5)
Te[3a]	sin, 2	0.082(13)
	cos, 2	-0.197(6)
Te[3a]	sin, 3	-0.153(10)
	cos, 3	0.147(12)
Te[3a]	sin, 4	0.011(13)
	cos, 4	-0.004(13)

Table 5.5. Bond lengths distributions [$\text{\AA}$] for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm[1a] - Te[1a] x 4	3.211(7)	3.192(7)	3.230(7)
Sm[1a] - Te[2a]	3.257(8)	3.247(8)	3.267(8)
Sm[1a] - Te[4a] x 2	3.296(8)	3.286(8)	3.310(8)
Sm[1a] - Te[5a] x 2	3.280(8)	3.236(8)	3.319(8)
Sm[1b] - Te[1b] x 4	3.200(7)	3.174(7)	3.221(7)
Sm[1b] - Te[2b]	3.246(8)	3.231(8)	3.264(8)
Sm[1b] - Te[4b] x 2	3.328(8)	3.316(8)	3.342(8)

Table 5.5. (Cont'd) Bond lengths distributions [Å] for Sm₂Te_{4.90(1)} at 100 K with e.s.d.'s in parentheses.

Sm[1b] - Te[5b]	3.306(9)	3.254(9)	3.351(9)
Sm[1b] - Te[5b]	3.325(9)	3.276(8)	3.374(8)
Sm[2b] - Te[1b]	3.199(8)	3.166(8)	3.234(8)
Sm[2b] - Te[2b] x 4	3.190(8)	3.170(8)	3.212(8)
Sm[2b] - Te[3a]	3.258(14)	3.114(13)	3.362(14)
Sm[2b] - Te[3a]	3.316(14)	3.208(13)	3.445(14)
Sm[2b] - Te[3b] x 2	3.282(10)	3.215(9)	3.354(9)
Sm[2a] - Te[1a]	3.180(8)	3.154(8)	3.200(8)
Sm[2a] - Te[2a] x 4	3.190(7)	3.163(7)	3.215(7)
Sm[2a] - Te[3a] x 2	3.273(14)	3.180(12)	3.387(12)
Sm[2a] - Te[3b]	3.248(11)	3.164(11)	3.323(11)
Sm[2a] - Te[3b]	3.305(11)	3.226(10)	3.395(11)
Te[3a] - Te[3b] x 4	3.083(19)	2.833(18)	3.351(19)
Te[4a] - Te[5a] x 4	3.075(10)	2.952(10)	3.196(10)
Te[4b] - Te[5b] x 3	3.068(10)	2.957(10)	3.184(10)
Te[4b] - Te[5b]	3.089(10)	2.970(10)	3.207(10)

Table 5.6. Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1a] - Sm[1a] - Te[1a] x 8	85.35(19)	84.67(18)	85.99(19)
Te[1a] - Sm[1a] - Te[1a] x 4	145.9(2)	145.4(2)	146.3(2)
Te[1a] - Sm[1a] - Te[2a] x 4	73.00(18)	72.38(17)	73.53(18)
Te[1a] - Sm[1a] - Te[4a] x 4	77.2(2)	75.5(2)	78.8(2)
Te[1a] - Sm[1a] - Te[4a] x 4	132.3(2)	129.7(2)	134.5(2)
Te[1a] - Sm[1a] - Te[5a] x 4	77.23(19)	76.70(19)	77.67(19)
Te[1a] - Sm[1a] - Te[5a] x 4	131.8(2)	131.3(2)	132.4(2)
Te[2a] - Sm[1a] - Te[4a] x 2	138.5(2)	138.2(2)	138.9(2)
Te[2a] - Sm[1a] - Te[5a] x 2	139.0(2)	138.4(2)	139.5(2)
Te[4a] - Sm[1a] - Te[4a] x 2	82.63(19)	82.24(19)	82.97(19)
Te[4a] - Sm[1a] - Te[5a] x 4	56.04(19)	54.00(18)	58.12(18)
Te[5a] - Sm[1a] - Te[5a] x 2	82.6(2)	82.5(2)	82.7(2)
Te[1b] - Sm[1b] - Te[1b] x 8	85.69(18)	84.94(18)	86.46(18)

Table 5.6. (Cont'd) Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 100 K with e.s.d.'s in parentheses.

Te[1b] - Sm[1b] - Te[1b] x 4	147.0(2)	146.4(2)	147.6(2)
Te[1b] - Sm[1b] - Te[2b] x 4	73.54(18)	73.09(18)	74.15(18)
Te[1b] - Sm[1b] - Te[4b] x 4	76.91(19)	75.29(19)	78.30(19)
Te[1b] - Sm[1b] - Te[4b] x 4	131.7(2)	129.5(2)	133.7(2)
Te[1b] - Sm[1b] - Te[5b] x 4	77.1(2)	76.42(19)	77.8(2)
Te[1b] - Sm[1b] - Te[5b] x 4	131.2(2)	130.5(2)	132.0(2)
Te[2b] - Sm[1b] - Te[4b] x 2	138.9(2)	138.5(2)	139.3(2)
Te[2b] - Sm[1b] - Te[5b] x 2	139.5(2)	138.7(2)	140.3(2)
Te[4b] - Sm[1b] - Te[4b] x 2	81.74(19)	81.42(19)	82.15(19)
Te[4b] - Sm[1b] - Te[5b] x 4	55.50(19)	53.47(19)	57.5(2)
Te[5b] - Sm[1b] - Te[5b] x 2	81.7(2)	81.5(2)	81.9(2)
Te[1b] - Sm[2b] - Te[2b] x 4	74.34(19)	73.67(19)	75.04(19)
Te[1b] - Sm[2b] - Te[3a] x 2	139.0(3)	136.4(3)	142.6(3)
Te[1b] - Sm[2b] - Te[3b] x 2	138.8(3)	136.6(3)	141.1(3)
Te[2b] - Sm[2b] - Te[2b] x 8	86.1(2)	85.63(19)	86.5(2)
Te[2b] - Sm[2b] - Te[2b] x 4	148.6(2)	147.1(2)	150.2(2)
Te[2b] - Sm[2b] - Te[3a] x 4	76.0(3)	72.8(3)	79.2(3)
Te[2b] - Sm[2b] - Te[3a] x 4	131.3(3)	127.7(3)	134.6(3)
Te[2b] - Sm[2b] - Te[3b] x 3	76.3(2)	74.4(2)	78.9(2)
Te[2b] - Sm[2b] - Te[3b] x 4	131.3(3)	128.4(3)	133.9(3)
Te[2b] - Sm[2b] - Te[3b]	75.1(2)	73.3(2)	77.0(2)
Te[3a] - Sm[2b] - Te[3a] x 2	83.1(3)	76.6(3)	88.4(3)
Te[3a] - Sm[2b] - Te[3b] x 4	56.0(3)	52.1(3)	60.9(3)
Te[3b] - Sm[2b] - Te[3b] x 2	82.8(3)	78.0(3)	87.1(3)
Te[1a] - Sm[2a] - Te[2a] x 4	74.23(18)	73.57(18)	74.98(18)
Te[1a] - Sm[2a] - Te[3a] x 2	138.7(3)	135.9(3)	141.6(3)
Te[1a] - Sm[2a] - Te[3b] x 2	139.0(2)	136.9(2)	141.9(2)
Te[2a] - Sm[2a] - Te[2a] x 8	86.00(18)	85.55(18)	86.55(18)
Te[2a] - Sm[2a] - Te[2a] x 4	148.5(2)	147.2(2)	149.9(2)
Te[2a] - Sm[2a] - Te[3a] x 4	76.5(3)	73.5(3)	80.2(3)
Te[2a] - Sm[2a] - Te[3a] x 4	131.6(3)	127.9(3)	135.8(3)
Te[2a] - Sm[2a] - Te[3b] x 4	76.1(2)	73.9(2)	78.2(2)
Te[2a] - Sm[2a] - Te[3b] x 4	131.4(3)	129.0(3)	133.6(3)
Te[3a] - Sm[2a] - Te[3a] x 2	83.0(3)	77.4(3)	87.9(3)

Table 5.6. (Cont'd) Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 100 K with e.s.d.'s in parentheses.

Te[3a] - Sm[2a] - Te[3b] x 4	56.3(3)	52.3(3)	61.4(3)
Te[3b] - Sm[2a] - Te[3b] x 2	83.1(3)	78.2(3)	87.0(3)
Sm[1b] - Te[1b] - Sm[1b] x 8	85.32(19)	84.80(19)	85.79(19)
Sm[1b] - Te[1b] - Sm[1b] x 4	147.0(2)	146.4(2)	147.7(2)
Sm[1b] - Te[1b] - Sm[2b] x 4	106.5(2)	105.9(2)	106.9(2)
Sm[1a] - Te[1a] - Sm[1a] x 8	85.01(18)	84.64(18)	85.49(18)
Sm[1a] - Te[1a] - Sm[1a] x 4	145.8(2)	145.3(2)	146.7(2)
Sm[1a] - Te[1a] - Sm[2a] x 4	107.1(2)	106.5(2)	107.5(2)
Sm[1a] - Te[2a] - Sm[2a] x 4	105.6(2)	104.8(2)	106.7(2)
Sm[2a] - Te[2a] - Sm[2a] x 8	85.77(19)	85.37(19)	86.19(19)
Sm[2a] - Te[2a] - Sm[2a] x 4	148.5(2)	147.4(2)	149.6(2)
Sm[1b] - Te[2b] - Sm[2b] x 4	105.6(2)	104.5(2)	106.7(2)
Sm[2b] - Te[2b] - Sm[2b] x 8	85.77(18)	85.54(18)	86.15(18)
Sm[2b] - Te[2b] - Sm[2b] x 4	148.7(3)	147.3(3)	150.1(3)
Sm[2b] - Te[3a] - Sm[2b] x 2	82.9(3)	81.7(3)	83.7(3)
Sm[2b] - Te[3a] - Sm[2a] x 4	122.8(5)	116.0(4)	129.9(5)
Sm[2b] - Te[3a] - Te[3b] x 4	61.6(3)	58.6(3)	64.6(3)
Sm[2b] - Te[3a] - Te[3b] x 4	118.2(4)	115.7(4)	121.7(4)
Sm[2a] - Te[3a] - Sm[2a] x 2	82.8(3)	82.2(3)	84.0(3)
Sm[2a] - Te[3a] - Te[3b] x 4	61.3(3)	57.5(3)	65.3(3)
Sm[2a] - Te[3a] - Te[3b] x 4	117.1(4)	113.0(4)	120.5(4)
Te[3b] - Te[3a] - Te[3b] x 8	90.1(5)	87.1(6)	94.3(5)
Te[3b] - Te[3a] - Te[3b] x 4	177.9(6)	175.5(6)	180
Sm[2b] - Te[3b] - Sm[2b] x 2	82.7(2)	81.5(2)	83.6(2)
Sm[2b] - Te[3b] - Sm[2a] x 4	123.0(4)	118.8(3)	127.8(4)
Sm[2b] - Te[3b] - Te[3a] x 4	61.5(3)	58.7(3)	64.4(3)
Sm[2b] - Te[3b] - Te[3a] x 4	117.2(4)	115.2(4)	119.9(4)
Sm[2a] - Te[3b] - Sm[2a] x 2	83.1(2)	82.3(2)	83.9(2)
Sm[2a] - Te[3b] - Te[3a] x 4	61.6(3)	59.8(3)	64.4(3)
Sm[2a] - Te[3b] - Te[3a] x 4	118.3(4)	116.4(4)	120.4(3)
Te[3a] - Te[3b] - Te[3a] x 8	90.2(5)	86.0(5)	93.3(5)
Te[3a] - Te[3b] - Te[3a] x 4	178.2(5)	175.0(6)	180
Sm[1a] - Te[4a] - Sm[1a] x 2	82.60(19)	82.23(19)	82.90(19)
Sm[1a] - Te[4a] - Te[5a] x 4	61.9(2)	60.86(19)	62.8(2)

Table 5.6. (Cont'd) Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 100 K with e.s.d.'s in parentheses.

Sm[1a] - Te[4a] - Te[5a] x 4	117.5(3)	114.2(3)	120.6(3)
Te[5a] - Te[4a] - Te[5a] x 8	90.0(3)	85.7(3)	94.3(3)
Te[5a] - Te[4a] - Te[5a] x 4	177.6(3)	175.3(3)	180
Sm[1b] - Te[4b] - Sm[1b] x 2	81.72(19)	81.31(18)	82.03(19)
Sm[1b] - Te[4b] - Te[5b] x 4	62.1(2)	61.49(19)	62.8(2)
Sm[1b] - Te[4b] - Te[5b] x 4	117.1(3)	114.5(3)	119.8(3)
Te[5b] - Te[4b] - Te[5b] x 8	90.0(3)	86.3(3)	93.8(3)
Te[5b] - Te[4b] - Te[5b] x 4	177.6(3)	175.5(3)	179.6(3)
Sm[1a] - Te[5a] - Sm[1a] x 2	82.6(2)	82.3(2)	82.9(2)
Sm[1a] - Te[5a] - Te[4a] x 4	62.3(2)	60.6(2)	63.9(2)
Sm[1a] - Te[5a] - Te[4a] x 4	117.9(3)	116.7(3)	119.1(3)
Te[4a] - Te[5a] - Te[4a] x 8	90.6(3)	86.7(3)	94.1(3)
Te[4a] - Te[5a] - Te[4a] x 4	177.6(3)	175.8(3)	180
Sm[1b] - Te[5b] - Sm[1b] x 2	81.7(2)	81.37(19)	82.07(19)
Sm[1b] - Te[5b] - Te[4b] x 4	62.6(2)	60.77(19)	64.3(2)
Sm[1b] - Te[5b] - Te[4b] x 4	117.6(2)	116.8(3)	118.4(3)
Te[4b] - Te[5b] - Te[4b] x 8	90.5(3)	86.7(3)	94.2(3)
Te[4b] - Te[5b] - Te[4b] x 4	177.5(3)	175.5(3)	180

Table 5.7. Crystal data and structure refinement for Sm₂Te_{4.90(1)} at 500 K.

Empirical formula	Sm ₂ Te _{4.90(1)}
Formula weight	926
Temperature	500.0(3) K
Wavelength	0.70926 Å
Crystal system	Triclinic
Space group	P1($\alpha\beta\gamma$)0
Unit cell dimensions	a = 4.3506(9) Å, α = 90° b = 4.3617(9) Å, β = 95.560(17)° c = 22.008(5) Å, γ = 90°
q-vector(1)	0.315(1)a* + 0.315(1)b* + 0.351(6)c*
Volume	415.66(15) Å ³
Z	2
Density (calculated)	7.396 g/cm ³
Absorption coefficient	30.712 mm ⁻¹
F(000)	758
Crystal size	0.33 x 0.21 x 0.02 mm ³
Theta range for data collection	1.86 to 29.18°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 6, -30 ≤ l ≤ 30, -1 ≤ m ≤ 1
Reflections collected	11293 (3282 main + 8011 satellites)
Independent reflections	9566 (2788 main + 6804 satellites) [R _{int} = 0.0517]
Completeness to θ = 29.18°	94%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9566 / 42 / 335
Goodness-of-fit on F ²	2.39
Final R indices [I > 3 σ (I)]	R _{obs} = 0.0459, wR _{obs} = 0.1663
R indices (all data)	R _{all} = 0.0920, wR _{all} = 0.2017
Final R main indices [I > 3 σ (I)]	R _{obs} = 0.0428, wR _{obs} = 0.1621
R main indices (all data)	R _{all} = 0.0467, wR _{all} = 0.1912
Final R 1 st order satellites [I > 3 σ (I)]	R _{obs} = 0.1127, wR _{obs} = 0.2492
R 1 st order satellites (all data)	R _{all} = 0.4093, wR _{all} = 0.3616
T _{min} and T _{max} coefficients	0.0095 and 0.5147
Largest diff. peak and hole	2.82 and -3.43 e.Å ⁻³
R = $\Sigma F_o - F_c / \Sigma F_o $, wR = $\{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and w = $1/(\sigma^2(I) + 0.0016I^2)$	

Table 5.8. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Sm[1a]	0	989	2499	1976	1	14(1)
	sin, 1	15	-8(4)	-1(1)		
	cos, 1	-3(4)	0(4)	1(1)		
Sm[1b]	0	-993(2)	-2491(2)	-1979(1)	1	14(1)
	sin, 1	-1(4)	-4(4)	1(1)		
	cos, 1	2(4)	-6(4)	0(1)		
Sm[2b]	0	3096(3)	2505(3)	6136(1)	1	16(1)
	sin, 1	-6(5)	-4(5)	7(1)		
	cos, 1	10(4)	11(4)	2(2)		
Sm[2a]	0	-3041(3)	-2491(3)	-6134(1)	1	16(1)
	sin, 1	-8(4)	-9(4)	-6(1)		
	cos, 1	4(4)	8(4)	-4(2)		
Te[1b]	0	3815(4)	2495(4)	7607(1)	1	13(1)
	sin, 1	-4(5)	-6(5)	3(1)		
	cos, 1	5(5)	1(5)	1(1)		
Te[1a]	0	-3798(4)	-2503(4)	-7593(1)	1	13(1)
	sin, 1	-5(5)	-4(5)	-3(1)		
	cos, 1	-1(5)	1(5)	-3(1)		
Te[2a]	0	1774(4)	2532(4)	3471(1)	1	14(1)
	sin, 1	-3(5)	4(5)	-1(1)		
	cos, 1	-4(5)	0(5)	-1(1)		
Te[2b]	0	-1694(4)	-2462(4)	-3473(1)	1	14(1)
	sin, 1	1(5)	-2(5)	3(1)		
	cos, 1	3(5)	3(5)	2(1)		
Te[3a]	0	2561(7)	7540(6)	4984(2)	0.804(3)	35(1)
	sin, 1	-65(20)	-55(20)	-2(3)		
	cos, 1	110(16)	132(14)	-3(2)		
Te[3b]	0	-2452(5)	-7465(5)	-5014(1)	1	35(1)
	sin, 1	-55(17)	-33(19)	1(2)		
	cos, 1	85(12)	97(9)	2(2)		

Table 5.8. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Te[4a]	0	434(5)	7489(4)	827(1)	1	19(1)
	sin, 1	2(7)	2(6)	-2(2)		
	cos, 1	-2(7)	0(6)	0(2)		
Te[4b]	0	-383(5)	-7517(5)	-839(1)	1	19(1)
	sin, 1	-8(7)	-2(7)	0(2)		
	cos, 1	-7(7)	4(7)	-1(2)		
Te[5a]	0	5412(4)	2480(4)	828(1)	1	20(1)
	sin, 1	-10(7)	-1(7)	-2(2)		
	cos, 1	-4(7)	-3(7)	-1(2)		
Te[5b]	0	-5425(4)	-2520(4)	-837(1)	1	20(1)
	sin, 1	-1(6)	-2(7)	0(2)		
	cos, 1	-1(7)	-4(6)	-2(2)		

Table 5.9. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm[1a]	0	13(1)	12(1)	17(1)	0(1)	2(1)	2(1)
	sin, 1	0(1)	-1(1)	0(1)	0(1)	0(1)	-1(1)
	cos, 1	-1(1)	1(1)	-1(1)	-1(1)	-1(1)	0(1)
Sm[1b]	0	13(1)	12(1)	17(1)	0(1)	2(1)	2(1)
	sin, 1	1(1)	-1(1)	0(1)	0(1)	1(1)	1(1)
	cos, 1	1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
Sm[2b]	0	14(1)	14(1)	21(1)	0(1)	1(1)	1(1)
	sin, 1	0(1)	0(1)	1(1)	0(1)	1(1)	2(1)
	cos, 1	1(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
Sm[2a]	0	14(1)	14(1)	21(1)	0(1)	1(1)	1(1)
	sin, 1	-1(1)	0(1)	1(1)	0(1)	-2(1)	-1(1)
	cos, 1	0(1)	1(1)	-1(1)	0(1)	1(1)	0(1)
Te[1b]	0	13(1)	12(1)	16(1)	0(1)	2(1)	1(1)
	sin, 1	0(1)	-1(1)	1(1)	1(1)	1(1)	1(1)
	cos, 1	0(1)	-1(1)	0(1)	0(1)	0(1)	0(1)

Table 5.9. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Te[1a]	0	13(1)	12(1)	16(1)	0(1)	2(1)	1(1)
	sin, 1	0(1)	1(1)	-1(1)	0(1)	-1(1)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	-1(1)	0(1)	0(1)
Te[2a]	0	13(1)	12(1)	18(1)	0(1)	1(1)	2(1)
	sin, 1	-1(1)	0(1)	-2(1)	0(1)	-2(1)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	1(1)	0(1)	0(1)
Te[2b]	0	13(1)	12(1)	18(1)	0(1)	1(1)	2(1)
	sin, 1	0(1)	0(1)	-1(1)	0(1)	1(1)	0(1)
	cos, 1	1(1)	1(1)	-1(1)	0(1)	1(1)	0(1)
Te[3a]	0	43(1)	43(1)	19(1)	-3(1)	1(1)	2(1)
	sin, 1	-8(3)	-6(3)	1(2)	-9(2)	1(2)	-1(2)
	cos, 1	10(3)	8(3)	-6(2)	-1(2)	3(2)	-3(2)
Te[3b]	0	43(1)	43(1)	19(1)	-3(1)	1(1)	2(1)
	sin, 1	8(3)	12(3)	1(2)	-12(2)	-2(1)	1(1)
	cos, 1	15(2)	16(3)	-2(2)	-1(3)	-3(1)	3(1)
Te[4a]	0	20(1)	18(1)	20(1)	1(1)	3(1)	1(1)
	sin, 1	0(1)	0(1)	-2(1)	-1(1)	-1(1)	-2(1)
	cos, 1	-1(1)	-1(1)	-1(1)	0(1)	0(1)	1(1)
Te[4b]	0	20(1)	18(1)	20(1)	1(1)	3(1)	1(1)
	sin, 1	0(1)	0(1)	2(1)	0(1)	0(1)	0(1)
	cos, 1	1(1)	0(1)	0(1)	0(1)	0(1)	1(1)
Te[5a]	0	20(1)	19(1)	21(1)	1(1)	2(1)	2(1)
	sin, 1	-1(1)	0(1)	1(1)	1(1)	0(1)	1(1)
	cos, 1	1(1)	1(1)	1(1)	0(1)	0(1)	-1(1)
Te[5b]	0	20(1)	19(1)	21(1)	1(1)	2(1)	2(1)
	sin, 1	-1(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	1(1)	-1(1)	0(1)	-1(1)

Table 5.10. Fourier components of the occupational modulation for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Atom	Wave	Occupational component
Te[3a]	sin, 1	-0.114(14)
	cos, 1	-0.06(3)

Table 5.11. Bond lengths distributions [Å] for Sm₂Te_{4.90(1)} at 500 K with estimated standard deviations in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm[1a] - Te[1a] x 4	3.222(3)	3.221(3)	3.223(3)
Sm[1a] - Te[2a]	3.274(4)	3.270(4)	3.279(4)
Sm[1a] - Te[4a] x 2	3.333(4)	3.330(4)	3.336(4)
Sm[1a] - Te[5a]	3.329(4)	3.322(4)	3.336(4)
Sm[1a] - Te[5a]	3.321(4)	3.316(4)	3.326(4)
Sm[1b] - Te[1b] x 2	3.211(3)	3.207(3)	3.216(3)
Sm[1b] - Te[1b]	3.204(3)	3.203(3)	3.205(3)
Sm[1b] - Te[1b]	3.218(3)	3.215(3)	3.221(3)
Sm[1b] - Te[2b]	3.273(4)	3.267(4)	3.279(4)
Sm[1b] - Te[4b]	3.322(4)	3.317(4)	3.328(4)
Sm[1b] - Te[4b]	3.308(4)	3.307(4)	3.309(4)
Sm[1b] - Te[5b] x 2	3.313(4)	3.309(4)	3.317(4)
Sm[2b] - Te[1b]	3.223(5)	3.213(4)	3.233(4)
Sm[2b] - Te[2b]	3.182(4)	3.172(4)	3.193(4)
Sm[2b] - Te[2b]	3.202(4)	3.197(4)	3.206(4)
Sm[2b] - Te[2b]	3.193(4)	3.192(4)	3.194(4)
Sm[2b] - Te[2b]	3.212(4)	3.204(4)	3.220(4)
Sm[2b] - Te[3a]	3.325(8)	3.299(8)	3.353(8)
Sm[2b] - Te[3a]	3.345(8)	3.313(7)	3.378(7)
Sm[2b] - Te[3b] x 2	3.324(6)	3.303(6)	3.345(6)
Sm[2a] - Te[1a]	3.196(5)	3.188(5)	3.203(5)
Sm[2a] - Te[2a] x 2	3.190(4)	3.184(4)	3.197(4)
Sm[2a] - Te[2a] x 2	3.204(4)	3.203(4)	3.205(4)
Sm[2a] - Te[3a]	3.260(8)	3.230(8)	3.290(8)
Sm[2a] - Te[3a]	3.291(8)	3.267(7)	3.316(8)
Sm[2a] - Te[3b]	3.274(6)	3.257(6)	3.291(6)
Sm[2a] - Te[3b]	3.289(6)	3.268(5)	3.310(5)
Te[3a] - Te[3b] x 4	3.085(11)	2.961(11)	3.211(11)
Te[4a] - Te[5a] x 2	3.090(5)	3.085(5)	3.095(5)
Te[4a] - Te[5a] x 2	3.076(5)	3.073(5)	3.079(5)
Te[4b] - Te[5b] x 2	3.095(5)	3.092(5)	3.098(5)
Te[4b] - Te[5b] x 2	3.068(5)	3.063(5)	3.073(5)

Table 5.12. Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 500 K with estimated standard deviations in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1a] - Sm[1a] - Te[1a] x 8	85.22(8)	85.09(7)	85.34(7)
Te[1a] - Sm[1a] - Te[1a] x 4	145.90(11)	145.73(11)	146.07(11)
Te[1a] - Sm[1a] - Te[2a] x 2	73.41(9)	73.27(9)	73.55(9)
Te[1a] - Sm[1a] - Te[4a] x 4	77.18(9)	77.11(9)	77.26(9)
Te[1a] - Sm[1a] - Te[4a] x 4	131.71(9)	131.56(9)	131.87(9)
Te[1a] - Sm[1a] - Te[5a] x 4	77.14(9)	76.97(9)	77.31(9)
Te[1a] - Sm[1a] - Te[5a] x 4	131.39(10)	131.29(10)	131.49(10)
Te[1a] - Sm[1a] - Te[2a] x 2	72.86(9)	72.63(9)	73.08(9)
Te[2a] - Sm[1a] - Te[4a] x 2	139.29(10)	139.12(10)	139.45(10)
Te[2a] - Sm[1a] - Te[5a]	139.45(10)	139.27(9)	139.63(9)
Te[2a] - Sm[1a] - Te[5a]	138.83(9)	138.62(8)	139.03(8)
Te[4a] - Sm[1a] - Te[4a] x 2	81.82(10)	81.80(10)	81.84(10)
Te[4a] - Sm[1a] - Te[5a] x 4	55.16(9)	55.13(9)	55.18(9)
Te[5a] - Sm[1a] - Te[5a] x 2	81.73(10)	81.60(10)	81.86(10)
Te[1b] - Sm[1b] - Te[1b] x 6	85.67(8)	85.64(8)	85.71(8)
Te[1b] - Sm[1b] - Te[1b] x 2	85.17(8)	85.09(8)	85.25(8)
Te[1b] - Sm[1b] - Te[1b] x 4	147.21(11)	147.02(11)	147.40(11)
Te[1b] - Sm[1b] - Te[2b] x 3	73.93(9)	73.83(9)	74.04(9)
Te[1b] - Sm[1b] - Te[4b] x 4	76.56(9)	76.38(9)	76.73(9)
Te[1b] - Sm[1b] - Te[4b] x 2	131.62(11)	131.52(11)	131.72(11)
Te[1b] - Sm[1b] - Te[5b] x 4	76.55(9)	76.45(9)	76.65(9)
Te[1b] - Sm[1b] - Te[5b] x 4	130.85(10)	130.67(10)	131.03(10)
Te[1b] - Sm[1b] - Te[4b] x 2	130.82(10)	130.74(10)	130.90(10)
Te[1b] - Sm[1b] - Te[2b]	73.28(9)	73.15(9)	73.40(9)
Te[2b] - Sm[1b] - Te[4b] x 2	138.95(10)	138.83(10)	139.06(10)
Te[2b] - Sm[1b] - Te[5b] x 2	139.27(10)	139.22(10)	139.32(10)
Te[4b] - Sm[1b] - Te[4b] x 2	82.27(11)	82.25(11)	82.29(11)
Te[4b] - Sm[1b] - Te[5b] x 3	55.56(10)	55.53(10)	55.58(10)
Te[4b] - Sm[1b] - Te[5b]	54.99(9)	54.90(9)	55.09(9)
Te[5b] - Sm[1b] - Te[5b] x 2	82.02(10)	81.96(10)	82.07(10)
Te[1b] - Sm[2b] - Te[2b] x 4	74.31(10)	74.03(10)	74.59(10)
Te[1b] - Sm[2b] - Te[3a] x 2	139.28(19)	138.33(19)	140.22(19)
Te[1b] - Sm[2b] - Te[3b] x 2	139.26(16)	138.60(15)	139.92(16)

Table 5.12. (Cont'd) Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 500 K with estimated standard deviations in parentheses.

Te[2b] - Sm[2b] - Te[2b] x 6	86.19(10)	86.01(10)	86.37(10)
Te[2b] - Sm[2b] - Te[2b] x 4	148.91(14)	148.24(13)	149.56(13)
Te[2b] - Sm[2b] - Te[3a] x 4	76.33(19)	75.24(19)	77.41(19)
Te[2b] - Sm[2b] - Te[3a] x 4	130.73(19)	129.33(19)	132.14(19)
Te[2b] - Sm[2b] - Te[3b] x 4	76.26(15)	75.54(15)	76.98(15)
Te[2b] - Sm[2b] - Te[3b] x 4	130.69(17)	129.57(17)	131.83(17)
Te[2b] - Sm[2b] - Te[2b] x 2	85.42(9)	85.29(9)	85.56(9)
Te[3a] - Sm[2b] - Te[3a] x 2	81.7(2)	79.9(2)	83.5(2)
Te[3a] - Sm[2b] - Te[3b] x 4	55.3(2)	54.9(2)	55.6(2)
Te[3b] - Sm[2b] - Te[3b] x 2	81.61(17)	80.35(16)	82.90(16)
Te[1a] - Sm[2a] - Te[2a] x 3	73.95(10)	73.68(10)	74.23(10)
Te[1a] - Sm[2a] - Te[2a]	74.64(10)	74.31(10)	74.97(10)
Te[1a] - Sm[2a] - Te[3a] x 2	138.36(17)	137.55(17)	139.17(18)
Te[1a] - Sm[2a] - Te[3b] x 2	138.40(16)	137.60(15)	139.20(16)
Te[2a] - Sm[2a] - Te[2a] x 6	86.02(9)	85.85(9)	86.19(9)
Te[2a] - Sm[2a] - Te[2a] x 4	148.59(14)	147.99(14)	149.20(14)
Te[2a] - Sm[2a] - Te[3a] x 4	75.96(19)	74.83(19)	77.11(19)
Te[2a] - Sm[2a] - Te[3a] x 4	131.3(2)	129.8(2)	132.7(2)
Te[2a] - Sm[2a] - Te[3b] x 4	75.88(15)	75.08(15)	76.69(15)
Te[2a] - Sm[2a] - Te[3b] x 4	131.27(17)	130.12(17)	132.40(17)
Te[2a] - Sm[2a] - Te[2a] x 2	85.43(10)	85.28(10)	85.58(10)
Te[3a] - Sm[2a] - Te[3a] x 2	83.3(2)	81.7(2)	84.8(2)
Te[3a] - Sm[2a] - Te[3b] x 4	56.2(2)	55.7(2)	56.7(2)
Te[3b] - Sm[2a] - Te[3b] x 2	83.32(18)	81.93(17)	84.69(16)
Sm[1b] - Te[1b] - Sm[1b] x 8	85.46(9)	85.33(9)	85.59(9)
Sm[1b] - Te[1b] - Sm[1b] x 4	147.21(12)	146.94(12)	147.48(12)
Sm[1b] - Te[1b] - Sm[2b] x 4	106.46(10)	106.36(10)	106.57(10)
Sm[1a] - Te[1a] - Sm[1a] x 8	85.19(7)	85.14(7)	85.24(8)
Sm[1a] - Te[1a] - Sm[1a] x 4	145.90(12)	145.58(12)	146.22(12)
Sm[1a] - Te[1a] - Sm[2a] x 4	107.35(10)	107.14(10)	107.55(10)
Sm[1a] - Te[2a] - Sm[2a] x 3	105.20(10)	104.85(10)	105.54(10)
Sm[1a] - Te[2a] - Sm[2a]	106.21(11)	105.93(11)	106.49(11)
Sm[2a] - Te[2a] - Sm[2a] x 8	85.85(10)	85.81(10)	85.88(10)
Sm[2a] - Te[2a] - Sm[2a] x 4	148.59(14)	148.22(14)	148.96(14)

Table 5.12. (Cont'd) Bond angles distributions [°] for Sm₂Te_{4.90(1)} at 500 K with estimated standard deviations in parentheses.

Sm[1b] - Te[2b] - Sm[2b] x 3	105.15(11)	104.80(11)	105.50(11)
Sm[1b] - Te[2b] - Sm[2b]	105.95(10)	105.62(10)	106.28(10)
Sm[2b] - Te[2b] - Sm[2b] x 8	85.84(9)	85.76(9)	85.92(9)
Sm[2b] - Te[2b] - Sm[2b] x 4	148.90(14)	148.33(14)	149.47(14)
Sm[2b] - Te[3a] - Sm[2b] x 2	81.67(15)	81.21(15)	82.16(16)
Sm[2b] - Te[3a] - Sm[2a] x 4	123.8(3)	121.2(2)	126.4(3)
Sm[2b] - Te[3a] - Te[3b] x 4	62.11(19)	60.75(17)	63.48(18)
Sm[2b] - Te[3a] - Te[3b] x 4	117.4(3)	116.9(2)	117.9(2)
Sm[2a] - Te[3a] - Sm[2a] x 2	83.23(16)	83.09(16)	83.39(17)
Sm[2a] - Te[3a] - Te[3b] x 4	61.70(19)	60.40(18)	63.0(2)
Sm[2a] - Te[3a] - Te[3b] x 4	118.0(3)	117.6(2)	118.4(3)
Te[3b] - Te[3a] - Te[3b] x 8	90.0(3)	89.7(3)	90.3(3)
Te[3b] - Te[3a] - Te[3b] x 4	179.6(3)	179.5(4)	179.9(3)
Sm[2b] - Te[3b] - Sm[2b] x 2	81.62(12)	81.37(13)	81.87(13)
Sm[2b] - Te[3b] - Sm[2a] x 4	123.9(2)	121.91(19)	125.9(2)
Sm[2b] - Te[3b] - Te[3a] x 4	62.4(2)	61.36(19)	63.4(2)
Sm[2b] - Te[3b] - Te[3a] x 4	117.5(2)	117.3(2)	117.7(2)
Sm[2a] - Te[3b] - Sm[2a] x 2	83.31(13)	82.92(13)	83.70(13)
Sm[2a] - Te[3b] - Te[3a] x 4	61.51(19)	60.54(18)	62.48(19)
Sm[2a] - Te[3b] - Te[3a] x 4	117.9(2)	117.8(2)	118.1(2)
Te[3a] - Te[3b] - Te[3a] x 8	90.3(3)	89.7(3)	90.9(3)
Te[3a] - Te[3b] - Te[3a] x 4	179.7(3)	179.4(4)	179.9(2)
Sm[1a] - Te[4a] - Sm[1a] x 2	81.82(10)	81.69(10)	81.95(10)
Sm[1a] - Te[4a] - Te[5a] x 4	62.37(10)	62.23(10)	62.50(10)
Sm[1a] - Te[4a] - Te[5a] x 4	117.41(14)	117.31(15)	117.51(15)
Te[5a] - Te[4a] - Te[5a] x 8	89.89(13)	89.81(13)	89.97(13)
Te[5a] - Te[4a] - Te[5a] x 4	179.75(17)	179.62(18)	179.87(16)
Sm[1b] - Te[4b] - Sm[1b] x 2	82.26(10)	82.17(10)	82.36(10)
Sm[1b] - Te[4b] - Te[5b] x 4	62.21(10)	62.14(10)	62.29(10)
Sm[1b] - Te[4b] - Te[5b] x 2	117.29(14)	117.17(14)	117.42(14)
Sm[1b] - Te[4b] - Te[5b] x 2	118.17(15)	118.14(15)	118.21(15)
Te[5b] - Te[4b] - Te[5b] x 6	89.65(13)	89.55(13)	89.75(13)
Te[5b] - Te[4b] - Te[5b] x 4	179.50(17)	179.41(16)	179.59(18)
Te[5b] - Te[4b] - Te[5b] x 2	90.65(13)	90.57(13)	90.72(13)

Table 5.12. (Cont'd) Bond angles distributions [°] for $\text{Sm}_2\text{Te}_{4.90(1)}$ at 500 K with estimated standard deviations in parentheses.

Sm[1a] - Te[5a] - Sm[1a] x 2	81.73(10)	81.65(10)	81.81(10)
Sm[1a] - Te[5a] - Te[4a] x 4	62.72(10)	62.66(11)	62.78(11)
Sm[1a] - Te[5a] - Te[4a] x 4	117.71(14)	117.65(14)	117.78(14)
Te[4a] - Te[5a] - Te[4a] x 8	90.41(13)	90.29(13)	90.52(13)
Te[4a] - Te[5a] - Te[4a] x 4	179.75(17)	179.65(18)	179.84(17)
Sm[1b] - Te[5b] - Sm[1b] x 2	82.02(10)	81.95(10)	82.08(10)
Sm[1b] - Te[5b] - Te[4b] x 4	62.59(10)	62.44(10)	62.73(10)
Sm[1b] - Te[5b] - Te[4b] x 4	117.87(14)	117.78(14)	117.97(14)
Te[4b] - Te[5b] - Te[4b] x 4	90.65(13)	90.55(13)	90.74(13)
Te[4b] - Te[5b] - Te[4b] x 4	179.50(16)	179.45(17)	179.55(16)
Te[4b] - Te[5b] - Te[4b] x 4	89.81(13)	89.70(13)	89.92(13)

Table 5.13. Crystal data and structure refinement for SmTe_{1.86(1)} at 100 K.

Empirical formula	SmTe _{1.86(1)}
Formula weight	380
Temperature	100.0(3) K
Crystal system	Tetragonal
Space group	X4($\alpha\beta 0$)($\beta-\alpha 0$)0
Centering vector	(0 0 $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$)
Unit cell dimensions	a = 4.3520(3) Å, $\alpha = 90^\circ$ b = 4.3520(3) Å, $\beta = 90^\circ$ c = 17.8902(7) Å, $\gamma = 90^\circ$
q-vector(1)	0.2965(3)a* + 0.2965(3)b*
q-vector(2)	0.2965(3)a* + -0.2965(3)b*
Volume	338.84(4) Å ³
Z	4
Density (calculated)	7.4474 g/cm ³
Absorption coefficient	32.191 mm ⁻¹
Crystal size	0.12 x 0.08 x 0.01 mm ³
Theta range for data collection	1.86 to 29.14°
Index ranges	-6<=h<=6, -6<=k<=6, -24<=l<=24, -1<=m, n<=1
Reflections collected	38830 (1259 main + 37571 satellites)
Independent reflections	4099 (454 main + 3645 satellites) [R _{int} = 0.0736]
Completeness to $\theta = 29.14^\circ$	100%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4099 / 0 / 133
Goodness-of-fit on F ²	1.29
Final R indices [I>2 σ (I)]	R _{obs} = 0.0419, wR _{obs} = 0.1006
R indices (all data)	R _{all} = 0.0949, wR _{all} = 0.1233
Final R main indices [I>2 σ (I)]	R _{obs} = 0.0212, wR _{obs} = 0.0633
R main indices (all data)	R _{all} = 0.0228, wR _{all} = 0.0664
Final R 1 st order satellites [I>2 σ (I)]	R _{obs} = 0.0628, wR _{obs} = 0.1214
R 1 st order satellites (all data)	R _{all} = 0.1060, wR _{all} = 0.1362
Final R 2 nd order satellites [I>2 σ (I)]	R _{obs} = 0.1535, wR _{obs} = 0.2719
R 2 nd order satellites (all data)	R _{all} = 0.4056, wR _{all} = 0.4644
T _{min} and T _{max} coefficients	0.0482 and 0.7227
Largest diff. peak and hole	3.19 and -1.97 e.Å ⁻³
R = $\Sigma F_o - F_c / \Sigma F_o $, wR = $\{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and w = $1/(\sigma^2(I)+0.0016I^2)$	

Table 5.14. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Sm[1a]	0	2549	2549	1356	1	7(1)
	sin, 1	-38(4)	-42(5)	0		
	cos, 1	0	0	31(1)		
	sin, 2	-42(5)	38(4)	0		
	cos, 2	0	0	31(1)		
	sin, 3	17(3)	16(5)	0		
	cos, 3	0	0	9(1)		
	sin, 4	-16(5)	17(3)	0		
	cos, 4	0	0	9(1)		
Sm[1b]	0	-2451	-2451	-1356(1)	1	7(1)
	sin, 1	-24(4)	-28(5)	0		
	cos, 1	0	0	-31(1)		
	sin, 2	-28(5)	24(4)	0		
	cos, 2	0	0	-31(1)		
	sin, 3	8(3)	0(5)	0		
	cos, 3	0	0	-7(1)		
	sin, 4	0(5)	8(3)	0		
	cos, 4	0	0	-7(1)		
Te[1a]	0	2549	2549	3149(2)	1	7(1)
	sin, 1	-2(6)	7(6)	0		
	cos, 1	0	0	26(1)		
	sin, 2	7(6)	2(6)	0		
	cos, 2	0	0	26(1)		
	sin, 3	-11(3)	4(6)	0		
	cos, 3	0	0	0(1)		
	sin, 4	-4(6)	-11(3)	0		
	cos, 4	0	0	0(1)		

Table 5.14. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[1b]	0	-2451	-2451	-3157(1)	1	2(1)
	sin, 1	15(5)	23(5)	0		
	cos, 1	0	0	-22(1)		
	sin, 2	23(5)	-15(5)	0		
	cos, 2	0	0	-22(1)		
	sin, 3	-2(3)	7(6)	0		
	cos, 3	0	0	-2(1)		
	sin, 4	-7(6)	-2(3)	0		
	cos, 4	0	0	-2(1)		
Te[2]	0	2549	7549	-16(1)	1	24(1)
	sin, 1	-209(6)	-472(8)	0		
	cos, 1	0	0	-2(2)		
	sin, 2	-260(6)	237(8)	0		
	cos, 2	0	0	-12(2)		
	sin, 3	-124(4)	-25(14)	0		
	cos, 3	0	0	1(2)		
	sin, 4	-16(11)	-235(6)	0		
	cos, 4	0	0	-2(2)		

Table 5.15. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm[1a]	0	5(1)	5(1)	11(1)	0	0	0
	sin, 1	0	0	0	0	-2(1)	2(1)
	cos, 1	0(1)	0(1)	3(1)	0(1)	0	0
	sin, 2	0	0	0	0	2(1)	2(1)
	cos, 2	0(1)	0(1)	3(1)	0(1)	0	0
	sin, 3	0	0	0	0	1(1)	-1(1)
	cos, 3	0(1)	-1(1)	4(1)	-4(1)	0	0
	sin, 4	0	0	0	0	1(1)	1(1)
	cos, 4	-1(1)	0(1)	4(1)	4(1)	0	0

Table 5.15. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses.

Sm[1b]	0	7(1)	7(1)	8(1)	0	0	0
	sin, 1	0	0	0	0	1(1)	-3(1)
	cos, 1	-1(1)	2(1)	-2(1)	0(1)	0	0
	sin, 2	0	0	0	0	-3(1)	0(1)
	cos, 2	2(1)	-1(1)	-2(1)	0(1)	0	0
	sin, 3	0	0	0	0	1(1)	-1(1)
	cos, 3	1(1)	0(1)	0(1)	0(1)	0	0
	sin, 4	0	0	0	0	1(1)	1(1)
	cos, 4	0(1)	1(1)	0(1)	0(1)	0	0
Te[1a]	0	6(1)	6(1)	11(1)	0	0	0
	sin, 1	0	0	0	0	-2(1)	1(1)
	cos, 1	1(1)	-1(1)	-1(1)	0(1)	0	0
	sin, 2	0	0	0	0	1(1)	2(1)
	cos, 2	-1(1)	1(1)	-1(1)	0(1)	0	0
	sin, 3	0	0	0	0	0(1)	0(1)
	cos, 3	1(1)	1(1)	3(1)	-1(1)	0	0
	sin, 4	0	0	0	0	0(1)	0(1)
	cos, 4	1(1)	1(1)	3(1)	1(1)	0	0
Te[1b]	0	1(1)	1(1)	4(1)	0	0	0
	sin, 1	0	0	0	0	1(1)	-2(1)
	cos, 1	1(1)	1(1)	-3(1)	0(1)	0	0
	sin, 2	0	0	0	0	-2(1)	-1(1)
	cos, 2	1(1)	1(1)	-3(1)	0(1)	0	0
	sin, 3	0	0	0	0	0(1)	-1(1)
	cos, 3	0(1)	0(1)	1(1)	-1(1)	0	0
	sin, 4	0	0	0	0	1(1)	0(1)
	cos, 4	0(1)	0(1)	1(1)	1(1)	0	0

Table 5.15. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses

Te[2]	0	14(1)	49(1)	8(1)	2(1)	0	0
	sin, 1	0	0	0	0	5(1)	16(1)
	cos, 1	-6(2)	32(2)	-2(1)	-9(1)	0	0
	sin, 2	0	0	0	0	0(1)	-1(2)
	cos, 2	-11(2)	17(2)	5(1)	14(1)	0	0
	sin, 3	0	0	0	0	3(1)	9(2)
	cos, 3	-11(1)	31(1)	-1(1)	19(2)	0	0
	sin, 4	0	0	0	0	2(1)	10(1)
	cos, 4	-16(1)	8(1)	2(1)	-12(1)	0	0

Table 5.16. Fourier components of the occupational modulation for $\text{Sm1 Te}_{1.8}$ at 100.0 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Te[2]	sin, 1	0
	cos, 1	-0.155(12)
Te[2]	sin, 2	0
	cos, 2	-0.182(12)
Te[2]	sin, 3	0
	cos, 3	-0.023(7)
Te[2]	sin, 4	0
	cos, 4	-0.140(7)

Table 5.17. Bond lengths distributions [$\text{\AA}$] for $\text{SmTe}_{1.86(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Sm[1a] - Te[1a]	3.208(5)	3.162(8)	3.238(8)
Sm[1a] - Te[1b] x 4	3.197(6)	3.152(6)	3.239(6)
Sm[1a] - Te[2] x 4	3.268(8)	3.166(8)	3.464(9)
Sm[1b] - Te[1a] x 4	3.202(6)	3.167(6)	3.234(6)
Sm[1b] - Te[1b]	3.221(4)	3.174(7)	3.239(7)
Sm[1b] - Te[2] x 4	3.235(7)	3.187(8)	3.303(8)
Te[2] - Te[2] x 3	3.128(10)	2.730(11)	3.547(11)

Table 5.18. Bond angles distributions [°] for SmTe_{1.86(1)} at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1a] - Sm[1a] - Te[1b] x 4	74.23(12)	72.80(10)	76.11(10)
Te[1a] - Sm[1a] - Te[2] x 4	138.0(3)	134.6(2)	144.3(2)
Te[1b] - Sm[1a] - Te[1b] x 8	85.77(18)	85.07(19)	86.71(17)
Te[1b] - Sm[1a] - Te[1b] x 4	148.49(12)	145.81(18)	152.10(19)
Te[1b] - Sm[1a] - Te[2] x 8	75.5(2)	72.8(2)	79.2(3)
Te[1b] - Sm[1a] - Te[2] x 8	131.2(2)	127.2(2)	135.7(2)
Te[2] - Sm[1a] - Te[2] x 4	87.1(2)	80.4(3)	89.4(2)
Te[2] - Sm[1a] - Te[2] x 8	56.9(2)	50.9(3)	63.2(2)
Te[1a] - Sm[1b] - Te[1a] x 8	85.6(2)	85.04(19)	86.51(19)
Te[1a] - Sm[1b] - Te[1a] x 4	148.01(13)	145.09(18)	151.44(18)
Te[1a] - Sm[1b] - Te[1b] x 4	74.02(17)	72.49(17)	75.79(18)
Te[1a] - Sm[1b] - Te[2] x 8	75.3(3)	71.9(2)	79.2(3)
Te[1a] - Sm[1b] - Te[2] x 8	131.8(3)	126.0(3)	138.1(3)
Te[1b] - Sm[1b] - Te[2] x 4	137.3(2)	135.11(17)	140.5(3)
Te[2] - Sm[1b] - Te[2] x 4	85.9(2)	80.7(2)	89.1(2)
Te[2] - Sm[1b] - Te[2] x 8	58.0(3)	49.4(3)	65.4(3)
Sm[1a] - Te[1a] - Sm[1b] x 4	106.03(15)	104.53(12)	107.46(17)
Sm[1b] - Te[1a] - Sm[1b] x 8	85.65(18)	84.96(15)	86.30(17)
Sm[1b] - Te[1a] - Sm[1b] x 4	147.98(16)	145.5(2)	150.7(2)
Sm[1a] - Te[1b] - Sm[1a] x 8	85.77(17)	85.23(17)	86.38(16)
Sm[1a] - Te[1b] - Sm[1a] x 4	148.44(13)	145.62(19)	150.97(19)
Sm[1a] - Te[1b] - Sm[1b] x 4	105.77(18)	104.24(17)	107.19(16)
Sm[1a] - Te[2] - Sm[1a] x 2	83.8(2)	81.48(17)	85.9(3)
Sm[1a] - Te[2] - Sm[1b] x 4	123.4(3)	114.4(3)	131.9(3)
Sm[1a] - Te[2] - Te[2] x 4	61.7(2)	56.9(2)	66.5(2)
Sm[1a] - Te[2] - Te[2] x 4	117.4(3)	114.2(2)	121.2(3)
Sm[1b] - Te[2] - Sm[1b] x 2	84.8(2)	83.70(19)	85.8(3)
Sm[1b] - Te[2] - Te[2] x 4	61.0(2)	57.56(18)	65.3(2)
Sm[1b] - Te[2] - Te[2] x 4	118.2(3)	111.9(3)	122.6(3)
Te[2] - Te[2] - Te[2] x 8	89.1(3)	84.1(3)	92.5(4)
Te[2] - Te[2] - Te[2] x 4	177.7(4)	173.7(4)	179.7(3)

Table 5.19. Crystal data and structure refinement for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K.

Empirical formula	$K_2Ag_4La_2Te_{9.61(1)}$
Formula weight	2012.4
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Triclinic
Space group	$C1(\alpha_1\beta_1\gamma_1)(\alpha_2\beta_2\gamma_2)0$
Unit cell dimensions	$a = 6.3521(4)$ Å, $\alpha = 90^\circ$ $b = 6.3531(4)$ Å, $\beta = 97.177(6)^\circ$ $c = 25.4036(19)$ Å, $\gamma = 90^\circ$
q-vector(1)	$0.3327(4)a^* + 0.3327(4)b^* + 0.334(2)c^*$
q-vector(2)	$0.400(2)a^* - 0.072(2)b^* + 0.345(6)c^*$
Volume	$1017.14(12)$ Å ³
Z	2
Density (calculated)	6.5687 g/cm ³
Absorption coefficient	21.69 mm ⁻¹
Crystal size	$0.19 \times 0.16 \times 0.08$ mm ³
Theta range for data collection	1.56 to 29.23°
Index ranges	$-9 \leq h \leq 9$, $-9 \leq k \leq 8$, $-35 \leq l \leq 35$, $-1 \leq m$, $n \leq 1$
Reflections collected	37838 (4271 main + 33567 satellites)
Independent reflections	32687 (3745 main + 28993 satellites) [$R_{int} = 0.0982$]
Completeness to $\theta = 18.01^\circ$	95%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	32687 / 0 / 1466
Goodness-of-fit on F^2	1.29
Final R indices [$I > 3\sigma(I)$]	$R_{obs} = 0.0633$, $wR_{obs} = 0.1476$
R indices (all data)	$R_{all} = 0.2151$, $wR_{all} = 0.1787$
Final R main indices [$I > 3\sigma(I)$]	$R_{obs} = 0.0569$, $wR_{obs} = 0.1402$
R main indices (all data)	$R_{all} = 0.0651$, $wR_{all} = 0.1427$
Final R 1 st order satellites [$I > 3\sigma(I)$]	$R_{obs} = 0.0811$, $wR_{obs} = 0.1692$
R 1 st order satellites (all data)	$R_{all} = 0.2758$, $wR_{all} = 0.2225$
Final R 2 nd order satellites [$I > 3\sigma(I)$]	$R_{obs} = 0.1428$, $wR_{obs} = 0.2926$
R 2 nd order satellites (all data)	$R_{all} = 0.6862$, $wR_{all} = 0.7711$
T_{min} and T_{max} coefficients	0.1100 and 0.8843
Largest diff. peak and hole	5.05 and -3.56 e.Å ⁻³

$$R = \sum ||F_o| - |F_c|| / \sum |F_o|, wR = \{ \sum [w(|F_o|^2 - |F_c|^2)^2] / \sum [w(|F_o|^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$$

Table 5.20. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
La[1]	0	2913	15	826	1	9(1)
	sin, 1	43(13)	-32(17)	-8(3)		
	cos, 1	-46(13)	60(10)	11(2)		
	sin, 2	1(4)	5(5)	-1(1)		
	cos, 2	-3(3)	1(4)	0(1)		
	sin, 3	-3(5)	0(6)	-2(1)		
	cos, 3	3(4)	9(5)	0(2)		
	sin, 4	-5(4)	1(4)	1(1)		
	cos, 4	4(4)	4(5)	0(1)		
La[2]	0	-2913(1)	16(1)	-823(1)	1	8(1)
	sin, 1	-68(5)	52(10)	-12(1)		
	cos, 1	25(20)	-34(15)	4(3)		
	sin, 2	0(3)	1(5)	-1(1)		
	cos, 2	-2(3)	4(4)	0(1)		
	sin, 3	-5(5)	6(7)	0(1)		
	cos, 3	4(5)	-10(6)	1(1)		
	sin, 4	-3(4)	4(5)	0(1)		
	cos, 4	2(4)	-7(5)	1(1)		
Te[1]	0	7739(3)	12(3)	482(1)	1	11(1)
	sin, 1	-2(2)	-6(2)	-7(3)		
	cos, 1	4(2)	-2(3)	9(2)		
	sin, 2	4(4)	0(5)	2(1)		
	cos, 2	4(4)	-6(5)	-1(1)		
	sin, 3	-4(5)	9(6)	1(2)		
	cos, 3	4(5)	-5(7)	1(2)		
	sin, 4	-9(5)	-1(5)	-1(1)		
	cos, 4	6(6)	2(5)	0(2)		

Table 5.20. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[2]	0	-7739(3)	13(3)	-479(1)	1	7(1)
	sin, 1	-12(3)	9(3)	-7(1)		
	cos, 1	10(4)	3(4)	3(2)		
	sin, 2	0(4)	-1(5)	1(1)		
	cos, 2	-2(3)	1(5)	-1(1)		
	sin, 3	2(5)	5(6)	0(1)		
	cos, 3	-2(5)	-4(6)	-1(1)		
	sin, 4	0(4)	6(5)	0(1)		
	cos, 4	1(4)	0(5)	0(1)		
Te[3]	0	934(3)	2515(3)	1833(1)	1	10(1)
	sin, 1	25(60)	-95(50)	-1(1)		
	cos, 1	-214(6)	195(30)	3(1)		
	sin, 2	5(4)	8(5)	1(1)		
	cos, 2	-1(5)	0(6)	-1(1)		
	sin, 3	9(6)	-2(6)	0(1)		
	cos, 3	4(6)	-4(7)	1(1)		
	sin, 4	-1(5)	4(7)	0(1)		
	cos, 4	5(5)	-12(6)	0(1)		
Te[4]	0	937(4)	-2503(4)	1831(1)	1	13(1)
	sin, 1	-5(80)	165(70)	-3(3)		
	cos, 1	291(5)	-235(50)	11(1)		
	sin, 2	2(5)	-14(6)	0(1)		
	cos, 2	10(5)	-11(7)	-1(1)		
	sin, 3	2(7)	6(8)	0(2)		
	cos, 3	8(6)	-9(7)	-1(2)		
	sin, 4	-5(5)	5(6)	0(1)		
	cos, 4	3(5)	-3(6)	-1(1)		

Table 5.20. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[5]	0	-901(4)	2496(4)	-1844(1)	1	12(1)
	sin, 1	255(30)	-275(16)	-13(1)		
	cos, 1	-105(70)	-45(80)	2(4)		
	sin, 2	-6(5)	-1(6)	0(1)		
	cos, 2	-7(5)	-7(5)	-2(1)		
	sin, 3	5(6)	2(7)	0(2)		
	cos, 3	-7(6)	4(7)	1(2)		
	sin, 4	-1(5)	2(6)	-1(1)		
	cos, 4	-1(5)	3(6)	0(1)		
Te[6]	0	-897(4)	-2486(4)	-1832(1)	1	14(1)
	sin, 1	-225(20)	238(5)	-4(1)		
	cos, 1	85(70)	15(70)	2(2)		
	sin, 2	7(5)	-4(7)	1(1)		
	cos, 2	-1(5)	18(6)	1(1)		
	sin, 3	-3(6)	7(8)	0(2)		
	cos, 3	-4(6)	10(7)	-1(2)		
	sin, 4	3(5)	9(6)	0(1)		
	cos, 4	-1(5)	7(7)	1(1)		
Te[7]	0	13(5)	33(5)	5007(1)	1	23(1)
	sin, 1	67(3)	15(18)	2(1)		
	cos, 1	5(20)	-61(6)	3(1)		
	sin, 2	-54(16)	-16(10)	0(2)		
	cos, 2	54(16)	23(8)	0(2)		
	sin, 3	-12(8)	13(9)	-1(2)		
	cos, 3	9(8)	8(9)	-1(2)		
	sin, 4	-18(6)	-75(6)	0(2)		
	cos, 4	1(9)	5(30)	-3(2)		

Table 5.20. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[8]	0	5032(5)	26(5)	5008(1)	0.607(4)	23(1)
	sin, 1	19(11)	0(12)	3(2)		
	cos, 1	34(8)	-36(5)	7(2)		
	sin, 2	1(10)	12(11)	1(3)		
	cos, 2	17(9)	13(10)	-4(2)		
	sin, 3	1(12)	7(13)	3(3)		
	cos, 3	8(9)	11(11)	-3(3)		
	sin, 4	-17(9)	-19(11)	3(2)		
	cos, 4	-10(11)	-15(14)	-3(3)		
Te[9]	0	4272(3)	45(3)	3530(1)	1	11(1)
	sin, 1	13(10)	2(9)	1(2)		
	cos, 1	33(4)	-29(3)	8(1)		
	sin, 2	-1(5)	-2(5)	2(2)		
	cos, 2	-7(4)	0(5)	-4(1)		
	sin, 3	5(5)	-7(6)	2(2)		
	cos, 3	-1(5)	-1(6)	-1(2)		
	sin, 4	-8(5)	-2(6)	-2(2)		
	cos, 4	-3(5)	-6(5)	-2(2)		
Te[10]	0	-4277(3)	47(3)	-3566(1)	1	33(1)
	sin, 1	17(3)	-26(7)	-27(4)		
	cos, 1	0(6)	-20(8)	-13(8)		
	sin, 2	6(10)	-13(6)	24(4)		
	cos, 2	33(5)	2(7)	11(7)		
	sin, 3	-3(6)	3(8)	2(2)		
	cos, 3	1(6)	-11(7)	0(2)		
	sin, 4	-7(12)	-35(12)	-3(13)		
	cos, 4	28(6)	-25(15)	34(2)		

Table 5.20. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Ag[1]	0	2099(4)	2556(4)	4203(1)	1	19(1)
	sin, 1	35(4)	15(6)	7(5)		
	cos, 1	1(11)	-16(6)	16(2)		
	sin, 2	-17(12)	-32(10)	-5(2)		
	cos, 2	38(7)	-26(11)	-2(2)		
	sin, 3	10(10)	-13(9)	-2(2)		
	cos, 3	19(8)	-10(10)	1(2)		
	sin, 4	-23(8)	-38(12)	2(3)		
	cos, 4	14(11)	-24(16)	-7(2)		
Ag[2]	0	2130(4)	-2448(4)	4203(1)	1	23(1)
	sin, 1	86(14)	15(20)	9(1)		
	cos, 1	45(20)	-77(5)	3(3)		
	sin, 2	-58(10)	-15(10)	-10(2)		
	cos, 2	30(16)	-23(8)	-6(3)		
	sin, 3	-15(18)	4(16)	-6(5)		
	cos, 3	42(10)	33(8)	13(3)		
	sin, 4	1(8)	-37(8)	-1(4)		
	cos, 4	-13(6)	-6(16)	-10(2)		
Ag[3]	0	-2076(4)	2568(5)	-4229(1)	1	36(1)
	sin, 1	65(11)	15(18)	-14(4)		
	cos, 1	-35(19)	-59(7)	-12(4)		
	sin, 2	-15(20)	-33(13)	31(3)		
	cos, 2	83(9)	34(12)	6(9)		
	sin, 3	15(20)	15(30)	9(8)		
	cos, 3	52(10)	69(10)	-19(5)		
	sin, 4	-30(8)	-82(11)	-1(7)		
	cos, 4	-7(14)	-15(30)	19(2)		

Table 5.20. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Ag[4]	0	-2121(5)	-2437(5)	-4244(1)	1	42(1)
	sin, 1	74(8)	-15(20)	-28(7)		
	cos, 1	-15(20)	-66(8)	-23(8)		
	sin, 2	-25(40)	8(11)	24(3)		
	cos, 2	135(11)	-20(10)	6(7)		
	sin, 3	-49(11)	53(13)	-5(3)		
	cos, 3	15(20)	-15(20)	0(4)		
	sin, 4	44(11)	-121(11)	-7(8)		
	cos, 4	19(19)	-15(50)	20(4)		
K[1]	0	8979(9)	53(9)	2953(2)	1	12(1)
	sin, 1	-37(18)	-31(15)	-2(3)		
	cos, 1	56(14)	-40(13)	9(2)		
	sin, 2	0(13)	5(16)	0(3)		
	cos, 2	8(13)	1(16)	-3(3)		
	sin, 3	15(20)	-25(20)	2(4)		
	cos, 3	36(16)	5(20)	0(4)		
	sin, 4	7(18)	15(18)	2(4)		
	cos, 4	-28(15)	-22(17)	-6(4)		
K[2]	0	1008(9)	34(11)	6978(2)	1	19(1)
	sin, 1	72(16)	-91(11)	-15(4)		
	cos, 1	55(20)	-5(30)	-10(5)		
	sin, 2	18(15)	-6(18)	4(4)		
	cos, 2	-28(14)	-6(18)	1(4)		
	sin, 3	5(20)	-5(30)	-1(5)		
	cos, 3	-33(17)	-35(20)	1(5)		
	sin, 4	-27(17)	38(19)	1(4)		
	cos, 4	-18(18)	15(20)	2(4)		

Table 5.21. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La[1]	0	6(1)	5(1)	17(1)	-2(1)	2(1)	0(1)
	sin, 1	-1(1)	-1(1)	2(1)	1(1)	-1(1)	0(1)
	cos, 1	2(1)	4(1)	-1(1)	-2(1)	0(1)	-1(1)
	sin, 2	-1(1)	1(1)	-1(1)	-1(1)	2(1)	0(1)
	cos, 2	1(1)	-1(1)	1(1)	0(1)	-1(1)	0(1)
	sin, 3	0(1)	-1(1)	0(2)	1(1)	0(1)	0(1)
	cos, 3	-2(1)	0(1)	1(2)	-1(1)	-1(1)	1(1)
	sin, 4	1(1)	-1(1)	0(1)	1(1)	0(1)	2(1)
	cos, 4	0(1)	-1(1)	-1(1)	0(1)	-1(1)	-1(1)
La[2]	0	8(1)	9(1)	8(1)	0(1)	1(1)	0(1)
	sin, 1	4(1)	4(1)	-1(1)	-3(1)	1(1)	0(1)
	cos, 1	-1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	sin, 2	-1(1)	0(1)	0(1)	1(1)	0(1)	1(1)
	cos, 2	1(1)	1(1)	3(1)	0(1)	0(1)	-1(1)
	sin, 3	-1(1)	3(2)	1(1)	-3(1)	0(1)	-1(1)
	cos, 3	-1(1)	2(2)	-1(1)	-2(2)	0(1)	2(1)
	sin, 4	1(1)	-3(1)	2(1)	1(1)	1(1)	1(1)
	cos, 4	0(1)	1(2)	1(1)	2(1)	1(1)	1(1)
Te[1]	0	8(1)	4(1)	21(1)	3(1)	3(1)	1(1)
	sin, 1	0(1)	0(1)	2(1)	0(1)	1(1)	-1(1)
	cos, 1	0(1)	0(1)	-2(1)	1(1)	-1(1)	1(1)
	sin, 2	-1(1)	0(2)	2(2)	0(1)	1(1)	0(1)
	cos, 2	0(1)	-2(1)	1(2)	2(1)	-3(1)	0(1)
	sin, 3	3(1)	3(2)	-1(2)	-1(1)	2(1)	-1(1)
	cos, 3	0(2)	-2(2)	1(2)	1(1)	-1(1)	0(2)
	sin, 4	2(1)	0(1)	-1(2)	2(1)	-1(1)	0(1)
	cos, 4	2(1)	1(1)	-1(2)	1(1)	1(1)	0(1)

Table 5.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[2]	0	6(1)	10(1)	4(1)	-4(1)	0(1)	1(1)
	sin, 1	-1(1)	-2(1)	1(1)	1(1)	0(1)	-1(1)
	cos, 1	0(1)	-1(1)	0(1)	0(1)	0(1)	-1(1)
	sin, 2	-1(1)	1(1)	0(1)	-1(1)	0(1)	0(1)
	cos, 2	1(1)	0(1)	-1(1)	1(1)	1(1)	0(1)
	sin, 3	0(1)	-2(2)	0(2)	1(1)	0(1)	-1(1)
	cos, 3	-1(1)	-2(2)	2(1)	2(1)	1(1)	-1(1)
	sin, 4	-1(1)	1(1)	1(1)	0(1)	0(1)	0(1)
	cos, 4	0(1)	0(1)	-1(1)	-2(1)	0(1)	0(1)
Te[3]	0	11(1)	12(1)	7(1)	-4(1)	1(1)	-1(1)
	sin, 1	7(1)	-3(2)	-1(1)	-4(2)	1(1)	2(1)
	cos, 1	-2(2)	-5(1)	-1(1)	5(1)	1(1)	-3(1)
	sin, 2	1(1)	0(2)	0(1)	-2(1)	1(1)	0(1)
	cos, 2	0(1)	-1(2)	-1(1)	-2(1)	-1(1)	1(1)
	sin, 3	-1(1)	1(2)	-1(2)	2(1)	0(1)	1(2)
	cos, 3	-1(1)	0(2)	0(2)	1(2)	0(1)	-1(1)
	sin, 4	0(1)	1(2)	-1(1)	1(1)	-1(1)	1(1)
	cos, 4	0(1)	1(2)	0(1)	1(1)	0(1)	0(1)
Te[4]	0	13(1)	14(1)	13(1)	-2(1)	2(1)	-1(1)
	sin, 1	-14(1)	9(3)	-1(1)	1(3)	-1(1)	1(1)
	cos, 1	4(4)	12(3)	-1(1)	-10(1)	2(1)	-4(1)
	sin, 2	1(1)	-2(2)	1(2)	1(2)	0(1)	0(1)
	cos, 2	-1(1)	-1(2)	1(2)	5(1)	-1(1)	1(1)
	sin, 3	0(2)	1(2)	1(2)	-1(3)	2(1)	1(2)
	cos, 3	0(2)	-1(2)	3(2)	7(1)	-1(1)	-1(2)
	sin, 4	0(2)	1(2)	-1(1)	-1(1)	1(1)	0(2)
	cos, 4	-2(1)	0(2)	0(2)	-1(1)	-1(1)	1(1)

Table 5.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[5]	0	13(1)	12(1)	11(1)	-3(1)	2(1)	0(1)
	sin, 1	8(4)	5(3)	1(1)	-9(1)	-3(1)	4(1)
	cos, 1	13(2)	-9(2)	0(1)	1(3)	0(1)	-1(1)
	sin, 2	0(1)	-1(2)	-1(1)	0(1)	-1(1)	0(1)
	cos, 2	2(1)	-1(2)	-1(1)	3(1)	0(1)	0(1)
	sin, 3	-2(2)	-1(2)	0(2)	2(2)	-1(1)	1(2)
	cos, 3	1(2)	1(2)	0(2)	3(2)	-1(1)	-1(2)
	sin, 4	0(1)	-1(2)	0(1)	0(1)	1(1)	0(1)
	cos, 4	1(1)	0(2)	-1(1)	2(1)	1(1)	0(1)
Te[6]	0	10(1)	10(1)	21(1)	-1(1)	2(1)	1(1)
	sin, 1	-5(2)	-5(2)	2(1)	6(1)	2(1)	-1(1)
	cos, 1	-5(2)	6(2)	2(1)	1(2)	0(1)	0(1)
	sin, 2	1(1)	0(2)	-1(2)	0(2)	1(1)	0(1)
	cos, 2	-3(1)	1(2)	2(2)	4(1)	1(1)	0(1)
	sin, 3	-1(1)	-1(2)	3(2)	3(2)	0(1)	-1(2)
	cos, 3	0(2)	1(2)	0(2)	2(2)	1(1)	-1(2)
	sin, 4	0(1)	1(2)	0(2)	1(2)	-1(1)	1(1)
	cos, 4	0(1)	1(2)	-1(2)	-3(1)	0(1)	0(1)
Te[7]	0	26(1)	28(1)	15(1)	1(1)	1(1)	0(1)
	sin, 1	0(1)	2(1)	-1(1)	0(1)	-1(1)	-2(1)
	cos, 1	2(1)	0(2)	0(1)	3(1)	1(1)	-1(1)
	sin, 2	2(3)	-3(3)	-4(2)	-1(2)	0(1)	-2(2)
	cos, 2	-8(2)	-6(2)	5(2)	-2(2)	0(1)	-1(2)
	sin, 3	1(3)	3(3)	-4(2)	-2(2)	1(1)	-1(2)
	cos, 3	5(2)	-4(3)	-2(3)	-1(2)	0(2)	0(2)
	sin, 4	0(4)	-7(2)	2(2)	0(2)	0(1)	1(2)
	cos, 4	-11(2)	-1(3)	3(2)	-1(1)	0(1)	-1(2)

Table 5.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[8]	0	15(1)	16(1)	21(1)	0(1)	2(1)	1(1)
	sin, 1	-3(2)	-3(2)	0(2)	1(2)	-4(1)	0(1)
	cos, 1	-4(2)	-4(2)	5(2)	4(1)	-2(2)	2(2)
	sin, 2	4(4)	5(3)	6(3)	-3(2)	1(2)	2(3)
	cos, 2	10(3)	2(4)	0(3)	0(2)	0(2)	-5(3)
	sin, 3	-5(3)	-1(4)	1(6)	3(2)	-1(3)	1(3)
	cos, 3	3(4)	-1(4)	-9(4)	1(3)	-3(3)	1(3)
	sin, 4	-8(3)	6(4)	0(4)	0(2)	0(3)	1(3)
	cos, 4	5(4)	5(4)	6(3)	-2(2)	4(2)	-6(2)
Te[9]	0	10(1)	8(1)	16(1)	-2(1)	3(1)	-2(1)
	sin, 1	1(1)	-1(1)	2(2)	0(1)	1(1)	0(1)
	cos, 1	1(1)	1(1)	7(1)	0(1)	0(1)	0(1)
	sin, 2	-3(1)	-4(2)	9(2)	2(1)	1(1)	-1(1)
	cos, 2	-2(1)	-1(2)	-4(3)	-1(1)	-1(1)	0(1)
	sin, 3	-1(2)	-2(2)	4(3)	0(1)	0(2)	0(2)
	cos, 3	2(1)	0(2)	-7(2)	-1(1)	-2(1)	1(1)
	sin, 4	0(1)	1(2)	-5(2)	-1(1)	-3(1)	-1(1)
	cos, 4	1(1)	-4(2)	0(2)	1(1)	1(2)	0(1)
Te[10]	0	10(1)	12(1)	78(2)	1(1)	8(1)	6(1)
	sin, 1	2(1)	1(1)	32(7)	1(1)	6(1)	1(1)
	cos, 1	0(1)	-2(1)	21(9)	0(1)	2(2)	0(1)
	sin, 2	2(1)	6(2)	-55(8)	1(1)	-7(2)	-1(2)
	cos, 2	1(1)	-1(2)	-26(15)	0(1)	-2(2)	1(2)
	sin, 3	2(2)	-2(3)	-8(3)	0(2)	0(2)	-1(2)
	cos, 3	-1(2)	4(2)	-1(4)	-2(1)	0(2)	2(2)
	sin, 4	0(2)	-1(3)	5(30)	0(2)	-2(5)	-1(2)
	cos, 4	3(1)	5(2)	-73(3)	2(1)	-12(2)	2(2)

Table 5.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Ag[1]	0	19(1)	20(1)	17(1)	3(1)	-1(1)	4(1)
	sin, 1	0(2)	4(2)	6(2)	-1(2)	1(1)	0(1)
	cos, 1	5(1)	6(2)	4(2)	-5(1)	-1(1)	2(1)
	sin, 2	2(2)	-2(2)	-4(2)	-2(1)	3(2)	-2(3)
	cos, 2	-4(2)	-4(2)	2(2)	0(2)	4(2)	-8(2)
	sin, 3	2(2)	0(3)	1(3)	-4(2)	6(3)	-4(3)
	cos, 3	-1(2)	-4(2)	6(2)	-4(2)	6(3)	-7(2)
	sin, 4	2(2)	-2(2)	1(2)	3(2)	1(2)	0(3)
	cos, 4	-4(2)	-3(2)	-3(2)	2(2)	2(1)	-5(2)
Ag[2]	0	24(1)	22(1)	25(1)	-8(1)	7(1)	6(1)
	sin, 1	-2(2)	2(2)	8(1)	5(1)	6(1)	8(1)
	cos, 1	5(1)	4(2)	-1(2)	-3(2)	0(2)	-1(2)
	sin, 2	-1(2)	-6(2)	-10(2)	-7(2)	-7(2)	-7(2)
	cos, 2	-1(2)	-3(3)	-4(3)	-4(3)	1(2)	-1(3)
	sin, 3	-3(3)	0(3)	-8(7)	-1(4)	-4(5)	-3(4)
	cos, 3	3(2)	-3(2)	16(4)	8(2)	12(2)	7(2)
	sin, 4	6(2)	-1(3)	-2(3)	-3(4)	-3(2)	-1(3)
	cos, 4	-1(3)	-5(2)	-5(2)	-8(2)	0(2)	-5(2)
Ag[3]	0	25(1)	31(1)	52(2)	4(1)	0(1)	-8(1)
	sin, 1	2(2)	5(2)	14(3)	2(2)	-5(3)	-7(3)
	cos, 1	5(1)	2(2)	3(5)	6(1)	9(2)	8(3)
	sin, 2	-9(2)	-4(3)	-27(3)	-6(2)	0(4)	7(5)
	cos, 2	-4(3)	2(3)	-5(8)	-5(2)	-12(2)	-17(3)
	sin, 3	-2(3)	0(3)	-13(11)	-6(2)	-5(9)	-2(6)
	cos, 3	-3(2)	-2(3)	26(6)	3(3)	-20(3)	-13(2)
	sin, 4	5(3)	4(5)	-3(6)	2(4)	6(2)	9(2)
	cos, 4	-6(3)	-12(3)	-15(3)	-11(2)	-1(3)	2(4)

Table 5.21. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_2\text{Ag}_4\text{La}_2\text{Te}_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Ag[4]	0	33(1)	36(2)	59(2)	0(1)	11(1)	-3(2)
	sin, 1	5(2)	7(3)	18(3)	-9(3)	0(2)	7(2)
	cos, 1	5(2)	10(3)	6(6)	-8(3)	2(2)	-3(3)
	sin, 2	-10(4)	-2(3)	-12(3)	12(4)	5(4)	-7(7)
	cos, 2	-12(3)	-2(3)	3(5)	13(4)	-15(2)	24(3)
	sin, 3	1(4)	5(3)	9(4)	-5(2)	13(3)	-15(4)
	cos, 3	-7(3)	3(4)	-1(5)	3(3)	-3(6)	6(7)
	sin, 4	-3(3)	4(5)	5(5)	4(6)	-19(2)	14(3)
	cos, 4	-5(2)	-10(3)	-9(4)	15(3)	2(7)	4(6)
K[1]	0	16(2)	13(2)	7(2)	0(1)	2(1)	-2(2)
	sin, 1	7(3)	-6(3)	1(2)	1(2)	0(2)	-6(2)
	cos, 1	7(3)	7(3)	1(2)	-4(2)	1(2)	1(3)
	sin, 2	1(4)	6(6)	-2(4)	4(3)	-2(3)	4(4)
	cos, 2	-8(3)	13(5)	-2(4)	-3(3)	1(3)	4(4)
	sin, 3	-1(6)	-2(10)	0(5)	0(4)	2(4)	2(8)
	cos, 3	-9(4)	22(5)	2(4)	0(4)	0(4)	15(4)
	sin, 4	-5(4)	-2(5)	2(4)	0(4)	3(3)	-5(4)
	cos, 4	1(4)	-6(5)	-2(4)	0(3)	0(3)	-5(4)
K[2]	0	11(2)	26(3)	19(2)	-7(2)	1(1)	4(2)
	sin, 1	4(2)	8(3)	-5(3)	-6(2)	1(2)	-1(2)
	cos, 1	3(2)	0(4)	-2(3)	-3(3)	5(2)	-2(3)
	sin, 2	-1(4)	-8(6)	4(5)	2(4)	1(4)	1(5)
	cos, 2	2(3)	-5(6)	-3(5)	0(4)	-6(3)	6(4)
	sin, 3	-4(5)	11(12)	9(6)	-1(5)	-1(5)	6(7)
	cos, 3	-7(4)	24(7)	3(7)	0(4)	-6(4)	9(5)
	sin, 4	4(4)	-5(6)	-5(5)	0(4)	-1(4)	-7(4)
	cos, 4	-1(4)	4(6)	0(5)	0(4)	-2(4)	-1(5)

Table 5.22. Fourier components of the occupational modulation for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Te[8]	sin, 1	-0.017(10)
	cos, 1	-0.022(10)
Te[8]	sin, 2	0.12(2)
	cos, 2	0.04(4)
Te[8]	sin, 3	-0.01(2)
	cos, 3	-0.02(3)
Te[8]	sin, 4	-0.01(5)
	cos, 4	0.107(16)

Table 5.23. Bond lengths distributions [$\text{\AA}$] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
La[1] - Te[1] x 4	3.293(19)	3.247(19)	3.335(19)
La[1] - Te[2]	3.29(2)	3.273(20)	3.312(20)
La[1] - Te[3] x 2	3.38(3)	3.32(2)	3.46(2)
La[1] - Te[4] x 2	3.39(4)	3.35(5)	3.43(4)
La[2] - Te[1]	3.29(2)	3.27(2)	3.30(2)
La[2] - Te[2] x 4	3.292(20)	3.253(16)	3.328(16)
La[2] - Te[5] x 2	3.42(4)	3.38(4)	3.46(4)
La[2] - Te[6] x 2	3.41(3)	3.28(2)	3.53(2)
Te[3] - Te[4] x 4	3.20(6)	2.90(6)	3.49(6)
Te[4] - K[1] x 2	3.64(5)	3.49(4)	3.78(5)
Te[5] - Te[6] x 4	3.18(6)	2.87(4)	3.45(4)
Te[7] - Te[8] x 4	3.16(4)	3.07(4)	3.24(4)
Te[7] - Ag[1] x 2	3.03(4)	2.99(3)	3.07(4)
Te[7] - Ag[2] x 2	3.03(4)	2.97(4)	3.07(4)
Te[7] - Ag[3] x 2	2.96(5)	2.86(5)	3.03(5)
Te[7] - Ag[4] x 2	2.93(6)	2.84(6)	2.99(6)
Te[8] - Te[10]	3.59(6)	3.34(4)	3.74(7)
Te[8] - Ag[1] x 2	3.05(3)	3.00(4)	3.10(3)
Te[8] - Ag[2] x 2	3.02(4)	2.87(4)	3.09(4)
Te[8] - Ag[3] x 2	2.98(5)	2.82(5)	3.05(5)

Table 5.23. (Cont'd) Bond lengths distributions [Å] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[8] - Ag[4] x 2	2.91(5)	2.73(6)	3.06(5)
Te[9] - Ag[1] x 2	2.82(3)	2.78(3)	2.92(3)
Te[9] - Ag[2] x 2	2.81(4)	2.77(4)	2.85(4)
Te[9] - K[1] x 4	3.50(4)	3.44(4)	3.55(4)
Te[10] - Ag[3] x 2	2.82(6)	2.72(5)	2.94(6)
Te[10] - Ag[4] x 2	2.81(7)	2.74(7)	2.93(6)
Te[10] - K[2] x 4	3.46(6)	3.35(5)	3.52(6)
Ag[1] - Ag[2] x 4	3.18(4)	3.06(3)	3.30(3)
Ag[3] - Ag[4] x 4	3.18(6)	2.98(6)	3.42(6)

Table 5.24. Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - La[1] - Te[1] x 4	149.4(7)	148.5(7)	150.2(7)
Te[1] - La[1] - Te[1] x 8	86.0(5)	85.6(5)	86.2(5)
Te[1] - La[1] - Te[2] x 4	74.7(5)	74.0(5)	75.5(5)
Te[1] - La[1] - Te[3] x 4	75.4(9)	74.1(8)	76.7(9)
Te[1] - La[1] - Te[3] x 4	130.6(10)	129.0(10)	132.1(10)
Te[1] - La[1] - Te[4] x 4	75.6(11)	72.3(10)	78.6(11)
Te[1] - La[1] - Te[4] x 4	130.7(12)	125.3(12)	136.3(12)
Te[2] - La[1] - Te[3] x 2	138.6(8)	137.6(8)	139.6(8)
Te[2] - La[1] - Te[4] x 2	138.3(10)	136.7(9)	139.9(10)
Te[3] - La[1] - Te[3] x 2	83.0(9)	82.1(8)	83.9(8)
Te[3] - La[1] - Te[4] x 4	56.4(11)	51.3(11)	61.1(10)
Te[4] - La[1] - Te[4] x 2	83.2(11)	80.9(12)	85.1(11)
Te[1] - La[2] - Te[2] x 4	74.7(4)	74.3(5)	75.1(5)
Te[1] - La[2] - Te[5] x 2	138.8(7)	137.4(7)	140.1(7)
Te[1] - La[2] - Te[6] x 2	138.4(6)	137.5(7)	139.8(6)
Te[2] - La[2] - Te[2] x 4	149.5(6)	148.6(5)	150.3(5)
Te[2] - La[2] - Te[2] x 8	86.0(5)	85.7(5)	86.4(6)
Te[2] - La[2] - Te[5] x 4	130.5(7)	125.4(7)	135.7(6)
Te[2] - La[2] - Te[5] x 4	75.6(6)	72.5(6)	78.8(7)
Te[2] - La[2] - Te[6] x 4	130.6(6)	129.1(7)	132.1(7)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[2] - La[2] - Te[6] x 4	75.6(5)	74.2(6)	76.9(6)
Te[5] - La[2] - Te[5] x 2	82.2(8)	79.9(9)	84.1(7)
Te[5] - La[2] - Te[6] x 4	55.4(8)	50.2(5)	60.2(5)
Te[6] - La[2] - Te[6] x 2	82.8(7)	82.2(5)	83.8(6)
La[1] - Te[1] - La[1] x 4	149.4(7)	148.7(7)	150.4(7)
La[1] - Te[1] - La[1] x 8	86.1(5)	85.9(5)	86.3(5)
La[1] - Te[1] - La[2] x 4	105.3(5)	104.7(5)	105.9(5)
La[1] - Te[2] - La[2] x 4	105.2(5)	104.3(5)	106.3(5)
La[2] - Te[2] - La[2] x 4	149.5(5)	149.0(5)	149.9(5)
La[2] - Te[2] - La[2] x 8	86.0(4)	85.6(4)	86.4(4)
La[1] - Te[3] - La[1] x 2	83.0(5)	82.3(5)	83.7(5)
La[1] - Te[3] - Te[4] x 4	61.9(10)	59.0(8)	65.3(10)
La[1] - Te[3] - Te[4] x 4	117.7(11)	115.7(11)	119.1(9)
La[1] - Te[3] - K[1] x 4	126.1(14)	122.1(12)	130.2(13)
Te[4] - Te[3] - Te[4] x 4	174.8(18)	171.4(15)	179.8(15)
Te[4] - Te[3] - Te[4] x 8	89.5(16)	86.8(17)	92.5(18)
Te[4] - Te[3] - K[1] x 4	64.3(10)	62.5(11)	66.3(11)
Te[4] - Te[3] - K[1] x 4	116.4(11)	111.6(10)	121.4(10)
La[1] - Te[4] - La[1] x 2	82.9(5)	82.3(5)	83.3(6)
La[1] - Te[4] - Te[3] x 4	118.4(11)	112.4(9)	124.3(9)
La[1] - Te[4] - Te[3] x 4	61.7(10)	59.5(9)	63.6(10)
La[1] - Te[4] - K[1] x 4	124.9(16)	118.6(16)	131.6(16)
Te[3] - Te[4] - Te[3] x 4	174.0(18)	170.2(12)	180(2)
Te[3] - Te[4] - Te[3] x 8	89.8(16)	87.6(17)	93.1(19)
Te[3] - Te[4] - K[1] x 4	116.2(12)	113.2(13)	119.6(13)
Te[3] - Te[4] - K[1] x 4	64.6(11)	60.1(10)	68.7(11)
K[1] - Te[4] - K[1] x 2	76.8(10)	76.1(10)	77.7(10)
La[2] - Te[5] - La[2] x 2	82.1(5)	81.7(4)	82.4(5)
La[2] - Te[5] - Te[6] x 4	62.0(8)	59.7(9)	64.4(9)
La[2] - Te[5] - Te[6] x 4	117.0(10)	110.3(8)	123.8(7)
La[2] - Te[5] - K[2] x 4	127.4(15)	122.3(10)	132.5(11)
Te[6] - Te[5] - Te[6] x 4	174.0(17)	170.1(16)	179.0(16)
Te[6] - Te[5] - Te[6] x 8	89.9(14)	87.1(16)	93.1(16)
Te[6] - Te[5] - K[2] x 4	65.6(11)	61.5(9)	69.9(10)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[6] - Te[5] - K[2] x 4	115.9(12)	112.2(14)	119.4(14)
La[2] - Te[6] - La[2] x 2	82.8(5)	82.1(4)	83.7(4)
La[2] - Te[6] - Te[5] x 4	118.0(9)	114.6(13)	121.4(12)
La[2] - Te[6] - Te[5] x 4	62.6(8)	58.4(6)	67.7(7)
La[2] - Te[6] - K[2] x 4	126.5(13)	121.3(9)	132.2(9)
Te[5] - Te[6] - Te[5] x 4	174.1(16)	170.8(14)	179.2(9)
Te[5] - Te[6] - Te[5] x 8	89.4(13)	86.7(12)	92.8(15)
Te[5] - Te[6] - K[2] x 4	115.0(11)	109.6(10)	120.0(10)
Te[5] - Te[6] - K[2] x 4	64.5(10)	62.6(10)	66.6(11)
Te[8] - Te[7] - Te[8] x 4	178.9(12)	176.7(11)	180
Te[8] - Te[7] - Te[8] x 8	90.2(10)	87.7(10)	93.0(10)
Te[8] - Te[7] - Ag[1] x 4	121.5(10)	120.3(10)	122.5(9)
Te[8] - Te[7] - Ag[1] x 4	58.1(8)	55.3(8)	60.2(8)
Te[8] - Te[7] - Ag[2] x 4	121.9(11)	119.5(10)	124.0(11)
Te[8] - Te[7] - Ag[2] x 4	58.7(9)	57.6(9)	59.7(9)
Te[8] - Te[7] - Ag[3] x 4	58.1(11)	54.7(11)	60.1(11)
Te[8] - Te[7] - Ag[3] x 4	122.8(13)	120.1(12)	126.2(14)
Te[8] - Te[7] - Ag[4] x 4	57.0(11)	53.5(10)	60.6(10)
Te[8] - Te[7] - Ag[4] x 4	122.5(13)	120.0(13)	126.1(13)
Ag[1] - Te[7] - Ag[1] x 2	95.9(8)	94.8(8)	97.8(8)
Ag[1] - Te[7] - Ag[2] x 4	63.4(9)	61.4(10)	65.5(10)
Ag[1] - Te[7] - Ag[3] x 4	115.0(14)	110.3(15)	118.3(14)
Ag[1] - Te[7] - Ag[4] x 2	177.1(13)	173.1(14)	179.9(14)
Ag[1] - Te[7] - Ag[4] x 2	82.0(13)	75.5(13)	85.6(13)
Ag[2] - Te[7] - Ag[2] x 2	95.9(10)	94.0(9)	98.9(9)
Ag[2] - Te[7] - Ag[3] x 2	177.8(15)	174.6(15)	180
Ag[2] - Te[7] - Ag[3] x 2	82.7(14)	77.2(14)	85.6(13)
Ag[2] - Te[7] - Ag[4] x 4	116.1(14)	111.0(17)	119.8(15)
Ag[3] - Te[7] - Ag[3] x 2	98.8(14)	95.2(14)	105.2(15)
Ag[3] - Te[7] - Ag[4] x 4	65.5(13)	60.1(12)	73.2(13)
Ag[4] - Te[7] - Ag[4] x 2	99.9(14)	96.1(14)	106.9(15)
Te[7] - Te[8] - Te[7] x 4	178.9(12)	177.8(12)	180
Te[7] - Te[8] - Te[7] x 8	89.8(10)	88.1(10)	92.4(9)
Te[7] - Te[8] - Te[10] x 4	89.8(8)	89.0(8)	90.6(8)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[7] - Te[8] - Ag[1] x 4	58.1(8)	57.1(8)	59.1(8)
Te[7] - Te[8] - Ag[1] x 4	121.4(10)	119.9(10)	122.9(10)
Te[7] - Te[8] - Ag[2] x 4	58.3(9)	56.6(9)	60.1(10)
Te[7] - Te[8] - Ag[2] x 4	121.4(11)	119.9(10)	124.1(10)
Te[7] - Te[8] - Ag[3] x 4	122.3(14)	120.3(13)	125.8(13)
Te[7] - Te[8] - Ag[3] x 4	57.5(10)	55.0(10)	59.4(11)
Te[7] - Te[8] - Ag[4] x 4	122.7(14)	119.9(14)	125.4(14)
Te[7] - Te[8] - Ag[4] x 4	57.1(10)	54.9(10)	59.4(10)
Te[10] - Te[8] - Ag[1] x 2	131.5(11)	129.5(11)	132.8(11)
Te[10] - Te[8] - Ag[2] x 2	132.2(12)	131.1(12)	133.7(12)
Te[10] - Te[8] - Ag[3] x 2	49.7(11)	47.1(11)	55.0(12)
Te[10] - Te[8] - Ag[4] x 2	49.9(11)	47.1(11)	55.3(12)
Ag[1] - Te[8] - Ag[1] x 2	95.8(10)	94.6(10)	98.5(10)
Ag[1] - Te[8] - Ag[2] x 4	63.3(9)	61.2(9)	66.3(10)
Ag[1] - Te[8] - Ag[3] x 4	115.3(13)	111.1(13)	117.8(13)
Ag[1] - Te[8] - Ag[4] x 2	177.8(15)	174.6(15)	179.9(15)
Ag[1] - Te[8] - Ag[4] x 2	81.5(12)	76.5(12)	85.3(12)
Ag[2] - Te[8] - Ag[2] x 2	95.8(11)	94.0(11)	99.1(11)
Ag[2] - Te[8] - Ag[3] x 2	177.6(15)	172.1(16)	180
Ag[2] - Te[8] - Ag[3] x 2	83.1(13)	78.7(14)	85.4(14)
Ag[2] - Te[8] - Ag[4] x 4	116.0(13)	113.1(14)	119.7(14)
Ag[3] - Te[8] - Ag[3] x 2	98.8(16)	94.9(14)	107.4(14)
Ag[3] - Te[8] - Ag[4] x 4	65.4(12)	61.5(12)	71.6(13)
Ag[4] - Te[8] - Ag[4] x 2	99.9(16)	94.6(16)	108.6(16)
Ag[1] - Te[9] - Ag[1] x 2	105.9(9)	105.1(9)	106.9(9)
Ag[1] - Te[9] - Ag[2] x 4	68.9(10)	66.6(10)	70.2(10)
Ag[1] - Te[9] - K[1] x 4	74.7(9)	73.4(9)	75.5(9)
Ag[1] - Te[9] - K[1] x 4	139.8(10)	138.0(10)	140.7(10)
Ag[2] - Te[9] - Ag[2] x 2	105.9(11)	103.0(10)	108.0(11)
Ag[2] - Te[9] - K[1] x 4	75.1(10)	73.7(9)	77.8(10)
Ag[2] - Te[9] - K[1] x 4	139.7(11)	137.7(11)	141.5(11)
K[1] - Te[9] - K[1] x 4	130.7(10)	128.9(10)	132.2(10)
K[1] - Te[9] - K[1] x 8	80.0(10)	78.8(10)	81.0(11)
Te[8] - Te[10] - Ag[3] x 2	53.6(14)	50.6(14)	57.3(13)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[8] - Te[10] - Ag[4] x 2	52.3(13)	48.9(14)	55.2(14)
Te[8] - Te[10] - K[2] x 4	113.6(11)	111.6(10)	117.2(10)
Ag[3] - Te[10] - Ag[3] x 2	107(2)	101.0(18)	114.1(18)
Ag[3] - Te[10] - Ag[4] x 4	68.7(16)	65.5(14)	71.6(13)
Ag[3] - Te[10] - K[2] x 4	139.5(14)	137.5(13)	142.1(13)
Ag[3] - Te[10] - K[2] x 4	73.3(12)	71.3(12)	74.8(12)
Ag[4] - Te[10] - Ag[4] x 2	106(2)	99.3(19)	110(2)
Ag[4] - Te[10] - K[2] x 4	139.1(14)	137.3(15)	141.7(14)
Ag[4] - Te[10] - K[2] x 4	73.8(13)	71.2(11)	75.3(13)
K[2] - Te[10] - K[2] x 4	133.3(19)	126.8(14)	138(2)
K[2] - Te[10] - K[2] x 8	80.9(14)	78.3(12)	83.6(13)
Te[7] - Ag[1] - Te[7] x 2	95.8(9)	93.5(9)	100.0(8)
Te[7] - Ag[1] - Te[8] x 4	63.3(9)	61.6(8)	64.5(9)
Te[7] - Ag[1] - Te[9] x 4	113.5(11)	110.9(11)	114.7(11)
Te[7] - Ag[1] - Ag[2] x 4	58.3(9)	56.8(10)	59.2(10)
Te[7] - Ag[1] - Ag[2] x 4	122.1(12)	119.8(11)	125.6(11)
Te[8] - Ag[1] - Te[8] x 2	95.8(10)	94.8(10)	97.6(10)
Te[8] - Ag[1] - Te[9] x 2	78.7(9)	76.6(9)	80.1(8)
Te[8] - Ag[1] - Te[9] x 2	175.3(12)	173.7(11)	179.0(11)
Te[8] - Ag[1] - Ag[2] x 4	58.0(9)	54.9(8)	59.5(9)
Te[8] - Ag[1] - Ag[2] x 4	121.6(11)	119.7(10)	123.3(10)
Te[9] - Ag[1] - Te[9] x 2	105.9(9)	103.8(8)	107.1(8)
Te[9] - Ag[1] - Ag[2] x 4	55.4(8)	54.1(8)	56.6(8)
Te[9] - Ag[1] - Ag[2] x 4	124.2(11)	122.4(11)	126.3(11)
Ag[2] - Ag[1] - Ag[2] x 4	178.6(12)	176.4(13)	180
Ag[2] - Ag[1] - Ag[2] x 8	90.3(11)	88.8(11)	91.8(11)
Te[7] - Ag[2] - Te[7] x 2	95.9(10)	93.6(8)	99.4(9)
Te[7] - Ag[2] - Te[8] x 4	63.6(9)	61.1(9)	65.6(9)
Te[7] - Ag[2] - Te[9] x 4	114.0(12)	112.1(12)	117.2(10)
Te[7] - Ag[2] - Ag[1] x 4	121.1(13)	120.0(13)	122.7(13)
Te[7] - Ag[2] - Ag[1] x 4	58.4(9)	57.4(10)	60.5(9)
Te[8] - Ag[2] - Te[8] x 2	95.8(11)	93.6(10)	99.3(10)
Te[8] - Ag[2] - Te[9] x 2	79.4(10)	77.4(10)	82.2(10)
Te[8] - Ag[2] - Te[9] x 2	174.4(14)	172.8(15)	175.9(15)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[8] - Ag[2] - Ag[1] x 4	121.7(12)	118.6(12)	125.9(12)
Te[8] - Ag[2] - Ag[1] x 4	58.8(9)	57.5(8)	61.5(9)
Te[9] - Ag[2] - Te[9] x 2	105.9(11)	102.6(9)	108.2(11)
Te[9] - Ag[2] - Ag[1] x 4	124.7(13)	121.9(12)	127.0(13)
Te[9] - Ag[2] - Ag[1] x 4	55.8(8)	54.9(8)	57.3(9)
Ag[1] - Ag[2] - Ag[1] x 4	178.2(13)	174.9(11)	180
Ag[1] - Ag[2] - Ag[1] x 8	89.6(10)	87.4(10)	91.3(10)
Te[7] - Ag[3] - Te[7] x 2	98.9(16)	94.1(12)	106.7(14)
Te[7] - Ag[3] - Te[8] x 4	64.5(12)	62.0(12)	68.6(14)
Te[7] - Ag[3] - Te[10] x 4	112.3(17)	107.4(17)	116.6(16)
Te[7] - Ag[3] - Ag[4] x 4	56.8(13)	53.3(14)	59.3(14)
Te[7] - Ag[3] - Ag[4] x 4	122.6(19)	117.0(18)	130.5(18)
Te[7] - Ag[3] - K[2] x 2	94.0(13)	90.6(14)	96.3(13)
Te[7] - Ag[3] - K[2] x 2	166.6(17)	159.7(16)	171.0(16)
Te[8] - Ag[3] - Te[8] x 2	98.9(17)	94.4(13)	106.8(15)
Te[8] - Ag[3] - Te[10] x 2	76.7(14)	68.7(14)	81.9(13)
Te[8] - Ag[3] - Te[10] x 2	175(2)	169(3)	179.8(16)
Te[8] - Ag[3] - Ag[4] x 4	56.4(12)	52.3(10)	59.4(12)
Te[8] - Ag[3] - Ag[4] x 4	122.0(17)	118.4(19)	126.1(16)
Te[8] - Ag[3] - K[2] x 4	120.8(16)	114.3(14)	126.1(15)
Te[10] - Ag[3] - Te[10] x 2	107(2)	103(2)	110(2)
Te[10] - Ag[3] - Ag[4] x 4	55.6(14)	54.0(12)	57.3(13)
Te[10] - Ag[3] - Ag[4] x 4	125(2)	121.7(18)	127.3(19)
Te[10] - Ag[3] - K[2] x 4	61.3(13)	59.2(12)	64.2(13)
Ag[4] - Ag[3] - Ag[4] x 4	177(2)	174.7(19)	179.8(15)
Ag[4] - Ag[3] - Ag[4] x 8	89.5(15)	86.4(15)	92.2(14)
Ag[4] - Ag[3] - K[2] x 4	65.6(14)	62.7(14)	68.2(14)
Ag[4] - Ag[3] - K[2] x 4	114.9(19)	110.7(16)	119.0(17)
Te[7] - Ag[4] - Te[7] x 2	99.8(17)	95.0(17)	108.5(16)
Te[7] - Ag[4] - Te[8] x 4	65.6(13)	61.8(12)	68.9(14)
Te[7] - Ag[4] - Te[10] x 4	113.4(18)	107.5(16)	118.0(15)
Te[7] - Ag[4] - Ag[3] x 4	123(2)	116(2)	130(2)
Te[7] - Ag[4] - Ag[3] x 4	57.8(14)	53.2(12)	60.9(14)
Te[7] - Ag[4] - K[2] x 2	94.1(14)	90.5(14)	97.0(14)

Table 5.24. (Cont'd) Bond angles distributions [°] for $K_2Ag_4La_2Te_{9.61(1)}$ at 100 K with e.s.d.'s in parentheses.

Te[7] - Ag[4] - K[2] x 2	166.1(18)	159.3(18)	170.0(17)
Te[8] - Ag[4] - Te[8] x 2	99.9(18)	95.7(19)	106.9(17)
Te[8] - Ag[4] - Te[10] x 2	77.8(16)	69.9(15)	83.0(16)
Te[8] - Ag[4] - Te[10]	175(2)	171(2)	180(2)
Te[8] - Ag[4] - Ag[3] x 4	123.2(19)	120.2(18)	127.7(19)
Te[8] - Ag[4] - Ag[3] x 4	58.2(13)	54.4(11)	61.6(12)
Te[8] - Ag[4] - K[2] x 4	121.9(17)	116.5(15)	125.8(14)
Te[8] - Ag[4] - Te[10]	176(2)	172(2)	180(2)
Te[10] - Ag[4] - Te[10] x 2	105(2)	103(2)	107(2)
Te[10] - Ag[4] - Ag[3] x 4	124(2)	122(2)	127(2)
Te[10] - Ag[4] - Ag[3] x 4	55.7(14)	53.2(13)	58.1(14)
Te[10] - Ag[4] - K[2] x 4	61.0(13)	59.8(13)	62.8(14)
Ag[3] - Ag[4] - Ag[3] x 4	177(2)	174(2)	180(2)
Ag[3] - Ag[4] - Ag[3] x 8	90.5(16)	88.0(16)	92.7(17)
Ag[3] - Ag[4] - K[2] x 4	113.5(18)	109.3(17)	117.3(18)
Ag[3] - Ag[4] - K[2] x 4	64.8(15)	62.0(15)	67.1(16)
Te[4] - K[1] - Te[4] x 2	76.8(12)	75.9(12)	77.6(13)
Te[4] - K[1] - Te[9] x 4	136.4(14)	132.9(14)	139.6(14)
Te[4] - K[1] - Te[9] x 4	85.6(11)	83.1(9)	88.2(11)
Te[9] - K[1] - Te[9] x 4	130.7(12)	129.6(12)	132.0(12)
Te[9] - K[1] - Te[9] x 8	80.0(10)	79.0(9)	80.7(10)
Te[10] - K[2] - Te[10] x 4	133.3(18)	130.4(17)	136.4(17)
Te[10] - K[2] - Te[10] x 8	80.9(12)	79.7(11)	82.9(12)
Te[10] - K[2] - Ag[3] x 4	45.5(11)	43.1(10)	47.4(11)
Te[10] - K[2] - Ag[3] x 4	94.1(14)	91.8(13)	96.9(14)
Te[10] - K[2] - Ag[4] x 4	45.2(11)	43.0(11)	46.9(11)
Te[10] - K[2] - Ag[4] x 4	93.4(14)	90.7(14)	96.6(13)

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Chapter 6

Reactions of Europium Metal (Eu) with Coinage Metals (Cu and Ag) in Polychalcogenide Flux: Distorted Tellurium Nets of Eu²⁺ compounds

6.1. Introduction

Rare-earth metals (RE) usually form isostructural compounds due to similar chemical nature. In the polychalcogenide chemistry most of the RE atoms stabilize in the 3+ state. In general, only a few RE atoms are known to exist in the 2+ oxidation state including Sm, Eu, Tm and Yb with Eu^{2+} being the most stable cation. Although europium is stable in the 3+ oxidation state mainly in oxides (Eu_2O_3)¹ when combined with a chalcogen atom it usually adopts a 2+ valence. The reason is that the energy level of the f-orbitals of europium is lower with respect to the energy of the p-orbitals of the chalcogen (especially Se or Te) so that Eu^{3+} always gets reduced by the chalcogen atom to Eu^{2+} . In the case of the sulfide analogues, the energy level of S p-orbitals is comparable to the energy of Eu^{3+} and therefore sometimes the 2+ oxidation state can be stabilized. A few examples of compounds with mixed valent $\text{Eu}^{2+}/\text{Eu}^{3+}$ and S include the misfit layered phase $[(\text{EuS})_{1.5}]_{1.15}\text{NbS}_2$ ² and cubic Eu_3S_4 .³

Recently, we have shown that a change in the radius of RE^{3+} (from La to Tm) has an effect on the length of the periodicity (q-vector) of the CDW modulation in the square nets of tellurium in the RETe_3 series.⁴ The chemical pressure applied on the nets due to this lanthanide contraction is increased as the RE^{3+} radius gets smaller. In this situation, the average Te-Te distances become shorter and the overlap of the Te p-orbitals increases. Therefore, the shape and width of the p-bands that are responsible for the CDW distortion are affected and an overall change in the nesting properties of the Fermi surface occurs. Eu^{2+} is generally bigger than La^{3+} , the first and larger member of the RE^{3+} series.⁵ Thus, compounds with square nets of Te coordinated with Eu^{2+} will represent the extreme case of minimum chemical pressure among the rare-earth polytellurides. The

short list of Eu-containing polytelluride compounds with square nets of Te includes $\text{Cu}_{0.66}\text{EuTe}_2$,⁶ $\text{KCu}_2\text{EuTe}_4$,⁶ $\text{Na}_{0.2}\text{Ag}_{2.8}\text{EuTe}_4$ ⁶ and $\text{K}_{0.65}\text{Ag}_2\text{Eu}_{1.35}\text{Te}_4$.⁷ Although the supercell of the later phase only was characterized with conventional crystallographic techniques, reexamination of the AM_2EuTe_4 ($\text{A} = \text{Na, K, Rb, Cs}$; $\text{M} = \text{Cu, Ag}$) series and $\text{Cu}_{0.66}\text{EuTe}_2$ with the application of multidimensional crystallographic approach is important to reveal and understand the details behind their CDW distortion.⁴

The structure of AM_2EuTe_4 consists of square nets of Te attached on the one side of tetragonal antiprismatic coordinated europium atoms. The other tetragonal side of the antiprism is composed by puckered $[\text{MTe}]^-$ layers making a polar $[\text{M}_2\text{EuTe}_4]^-$ slab. The slabs stack along the c-axis and they are separated by A^+ atoms and van der Waals gaps. We found that the q-vector changes tremendously by changing the size of the alkali metal cation A^+ . The component of the q-vector for the smaller Na-containing analogs is ~ 0.31 and for the bigger Cs phases is ~ 0.26 . The planar Te net layer-layer separation increases with the size of the A^+ . A similar behavior of the effect of the CDW distortion with the change of the cross-plane dimensionality of the compound was recently reported for the AMRETe_4 ($\text{A} = \text{Na, K}$; $\text{M} = \text{Cu, Ag}$; $\text{RE} = \text{La, Ce}$) family.⁸ The AM_2EuTe_4 compounds not only represent another interesting example of this behavior but they also give the possibility of examination of how small steps in change in dimensionality affect the CDW distortions. Surprisingly, the behavior found in the quaternary and Cu_xEuTe_2 phases suggests that there is a competition between dimensionality (cross-plane interactions) and chemical pressure (in plane interactions) with opposite trends in the length of the CDW modulations.

6.2. Experimental Section

6.2.1. Reagents

The following reagents were used as obtained. Potassium metal, analytical reagent, Aldrich Chemical Co., Milwaukee, WI; Sodium metal, analytical reagent, Aldrich Chemical Co., Milwaukee, WI; Rubidium metal, analytical reagent, Johnson Matthey/AESAR Group, Seabrook, NH; Cesium metal, analytical reagent, Johnson Matthey/AESAR Group, Seabrook, NH; Europium metal, 99.9% pure, ~ 2mm turnings, Chinese Rare Earth Information Center, Inner Mongolia, China; Tellurium chunks, Tellurex Corp, Traverse City, MI; N, N – Dimethylformamide (DMF), ACS reagent grade, Spectrum Chemicals, New Brunswick, NJ; Diethyl ether anhydrous, ACS reagent grade, Columbus Chemical Industries, Columbus, WI.

Activated Copper – Copper metal (40 mesh, Cerac, Milwaukee, WI) was first activated by washing it with copious amounts of dilute hydrochloric acid. This step was necessary to remove the oxide layer from the fine particles (powder) and to ensure stoichiometric reaction of Cu.

Potassium Telluride, K_2Te – 5.836 g (0.15 mol) K was sliced in small pieces (~ 3 mm) in a N_2 filled glovebox and combined with 9.523 g (0.075 mol) Te in a 1000 mL single neck round bottom flask. A Teflon coated magnetic stir bar was added in the flask as well. The flask were connected to a glass adapter with a stopcock joint and removed from the glovebox. The flask and adapter was then connected to a dry condenser apparatus and chilled to -78 C using a dry ice/acetone bath. Approximately 800 mL of pure NH_3 were condensed, under N_2 atmosphere, onto the reagents, yielding a purple solution. The solution was kept under stirring and maintained at -78 C for up to 16 hours.

The dry ice/acetone mixture was removed and the NH_3 was allowed to evaporate off as the flask warmed up to room temperature under a constant flow of N_2 for ~ 6 hours. The resulting brown powder (K_2Te) was evacuated on a Schlenck line for ~ 4 hours and taken into a N_2 filled glovebox. The product was ground to a fine powder with a mortar and pestle and placed into a screw-capped vial in the glovebox.

Sodium Telluride, Na_2Te – The procedure was the same as described above for K_2Te . 3.448 g (0.15 mol) Na was sliced in small pieces (~ 3 mm) and combined with 9.523 g (0.075 mol) Te. The product had a white-light gray color and was stored in the same manner as for K_2Te .

Rubidium Telluride, Rb_2Te – 8.589 g (0.10 mol) of liquid Rb was transferred in a 1000 mL triple neck round bottom flask in a N_2 filled glovebox. The Rb metal was kept in liquid state by placing the ingot / ampoule of Rb on a hot plate. A hot glass pipette was used for transferring the liquid Rb into the flask. The middle neck of the flask was connected to a glass adapter with a stopcock joint. The other two necks were closed using a glass stop joint and the flask was removed from the glovebox. The flask and adapter was then connected to a dry condenser apparatus and chilled to -78°C using a dry ice/acetone bath. Approximately 400 mL of pure NH_3 were condensed, under N_2 atmosphere, onto the alkali metal, yielding a purple solution. 6.411 g (0.05 mol) of Te and a Teflon coated magnetic stir bar were added. Another ~ 400 mL of pure NH_3 were added in the mixture. The solution was kept under stirring and maintained at -78°C for up to 16 hours. The dry ice/acetone mixture was removed and the NH_3 was allowed to evaporate off as the flask warmed up to room temperature under a constant flow of N_2 for ~ 6 hours. The resulting dark green powder (Rb_2Te) was evacuated on a Schlenck line for

~ 4 hours and taken into a N₂ filled glovebox. The product was ground to a fine powder with a mortar and pestle and placed into a screw-capped vial in the glovebox.

Cesium Telluride, Cs₂Te – The procedure was the same as described above for Rb₂Te. 10.135 g (0.076 mol) Cs was used with 4.865 g (0.048 mol) Te. The product had a light green / yellow color and was stored in the same manner as for Rb₂Te.

6.2.2. Synthesis

AM₂EuTe₄ (*A* = K, Na, Rb, Cs; *M* = Cu, Ag) – A_{1-x}M₂Eu_{1+x}Te₄ was synthesized from a mixture of A₂Te (*A* = K, Na, Rb, Cs; 0.500 mmol), *M* (*M* = Cu, Ag; 0.125 mmol), Eu (0.125 mmol), and Te (2.0 mmol) that was sealed under vacuum in a quartz tube and heated to 700 °C for 5 days. The tube was then cooled to 300 °C at a rate of 4 °C/h, followed by quenching to room temperature at a rate of 10 °C/h. The excess A₂Te_y flux was washed off with N,N-dimethylformamide under nitrogen to reveal very thin red-purple plate-shaped crystals.

Cu_{0.63}EuTe₂ – Cu_{0.63}EuTe₂ was synthesized from a mixture of 0.298 g Rb₂Te (1.0 mmol) 0.032 g Cu (0.5 mmol), 0.038 g Eu (0.25 mmol) and 0.510 g Te (4.0 mmol) that was sealed under high vacuum in a 13 mm quartz ampoule. The ampoule was heated to 400 °C for 12 h, kept at that temperature for 12 h, heated to 850 °C in 24 h, and kept at that temperature for 6 days. The tube was then cooled to 400 °C at a rate of 4 °C h⁻¹, and then quenched to room temperature in 4 h. The excess Rb₂Te_x flux was removed under nitrogen to reveal red-brown square plate-like crystals. The crystals were air and water stable. EDS analysis on several crystals confirmed the absence of Rb from the flux and the hypostoichiometry of Cu. The average composition obtained from the

semiquantitative analysis was $\text{Cu}_{0.6(1)}\text{Eu}_{1.0(1)}\text{Te}_{2.0(1)}$. Several tries using direct combination or halide flux gave a mixture of the ternary phase and binary EuTe.

6.2.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – All the temperature dependent measurements were performed on the same single crystal for some of the AM_2EuTe_4 compounds ($A = \text{K, Na, Rb, Cs}$; $M = \text{Cu, Ag}$). Single crystals were quenched from room temperature to 100 K. The heating rate for warming ramps was ~ 200 K/h. Typical acquisition time was ~ 24 h. Summary table of crystal data and detailed crystallographic table reports for each individual AM_2EuTe_4 analogue and temperature can be found in tables 6.2-6.46. Detailed tables for $\text{Cu}_{0.63}\text{EuTe}_2$ are reported in tables 6.47-6.52. Intensity data were collected on a STOE IPDS II diffractometer equipped with a graphite monochromatized Mo radiation ($\lambda = 0.71073$ Å) and an Image Plate (IP) detector. The data were collected with an ω -scan technique from 0 - 180° and an arbitrary ϕ -angle. Data reduction was performed with the X-Area package.⁹ The length determination and refinement of the q-vectors was performed with the Peaklist 1.06 software part of the X-Area suite using a least square refinement algorithm. An analytical absorption correction was performed (X-Shape within X-Area) and all structures were refined with JANA2000 software.¹⁰ Direct

methods of SHELXTL software¹¹ were used to find the atomic positions in the subcell. Temperature was controlled by an Oxford Cryostream 700 Plus cryostat.

Satellite reflections of first order were observed and used for the refinement of the quaternary AM_2EuTe_4 compounds ($A = K, Na, Rb, Cs$; $M = Cu, Ag$). A single modulation wave for positional and thermal parameters was used. Only the symmetry allowed Fourier terms were refined.

Satellite reflections of first order for both q-vectors and mixed order reflections ($q_1 + q_2, q_1 - q_2$) were observed at 100 K and used for the refinement of the ternary $Cu_{0.63}EuTe_2$. Four modulation waves ($q_1, q_2, q_1 + q_2, q_1 - q_2$) for positional and temperature parameters were used. Fourier terms were freely refined based on the symmetry elements of the superspace group. All the examined superspace groups (centrosymmetric and noncentrosymmetric orthorhombic and centrosymmetric monoclinic ones) gave R-values for the satellites to more than 40%.

Infrared (IR) Spectroscopy – Optical diffuse reflectance measurements were performed on single crystals of all AM_2EuTe_4 members at room temperature. The spectra were recorded in the Mid-IR region ($6000 - 400\text{ cm}^{-1}$) with a Nicolet 6700 FT-IR Spectrometer equipped with a diffuse reflectance collector from Spectra-Tech Inc.

Magnetic Susceptibility Measurements – A MPMS Quantum Design SQUID magnetometer was used to measure the magnetic response of some of the AM_2EuTe_4 compounds over the range of 2-300 K. Single crystals of each sample were measured parallel and perpendicular to the applied magnetic field in respect to the plate geometry of the crystals. A perpendicular field corresponds to a magnetization direction along the c-axis. A parallel magnetic field corresponds to a random direction along the ab-plane. A

field dependent magnetic susceptibility at 300 K was first investigated in the range of 0 – 1 T to ensure a linear response of the magnetization. Subsequent temperature dependent studies were then performed at a constant field of 3,000 G. The effective magnetic moment, μ_{eff} , was calculated from the following formula:

$$\mu_{\text{eff}} = 2.818 \times \sqrt{\chi_M \cdot T}$$

where χ_M is the inverse of the slope taken from the linear region of the $1/\chi_M$ vs T plot (χ_M is the molar magnetic susceptibility).

6.3. Results and Discussion

Subcell Description of AM_2EuTe_4 – The average structure of AM_2EuTe_4 adopts the polar space group P4mm in agreement with previous work.⁶ It consists of square antiprismatic europium atoms sandwiched between a puckered anti-PbO type layer of $[MTe]^-$ and a square net of tellurium atoms making a polar $[M_2EuTe_4]^-$ slab, Figure 6.1. The slabs then stack along the c-axis, charge balanced with A^+ cations, creating van der Waals gaps. The formula can be more expressly written as $A^+([MTe]^-)_2(Eu)^{2+}[Te_2]^-$ that gives an average electron count on the Te atoms of the square net of -0.5. The Eu-Te distances in the antiprism are 3.322(3) Å and 3.440(8) Å for $NaAg_2EuTe_4$, Figure 6.2A. The A^+ site has a square antiprismatic geometry with A-Te distances 3.347(3) Å and 3.466(8) Å, Figure 6.2B. The Te-Te distances in the square net are 3.1538(4) Å, Figure 6.2C. In the quaternary AM_2EuTe_4 series for $A = Na$ and K , the alkali metal site was found to be mixed-occupied with the Eu metal by single crystal diffraction analysis. The similar atomic radii and same square antiprismatic site environment of these atoms can facilitate such disorder.

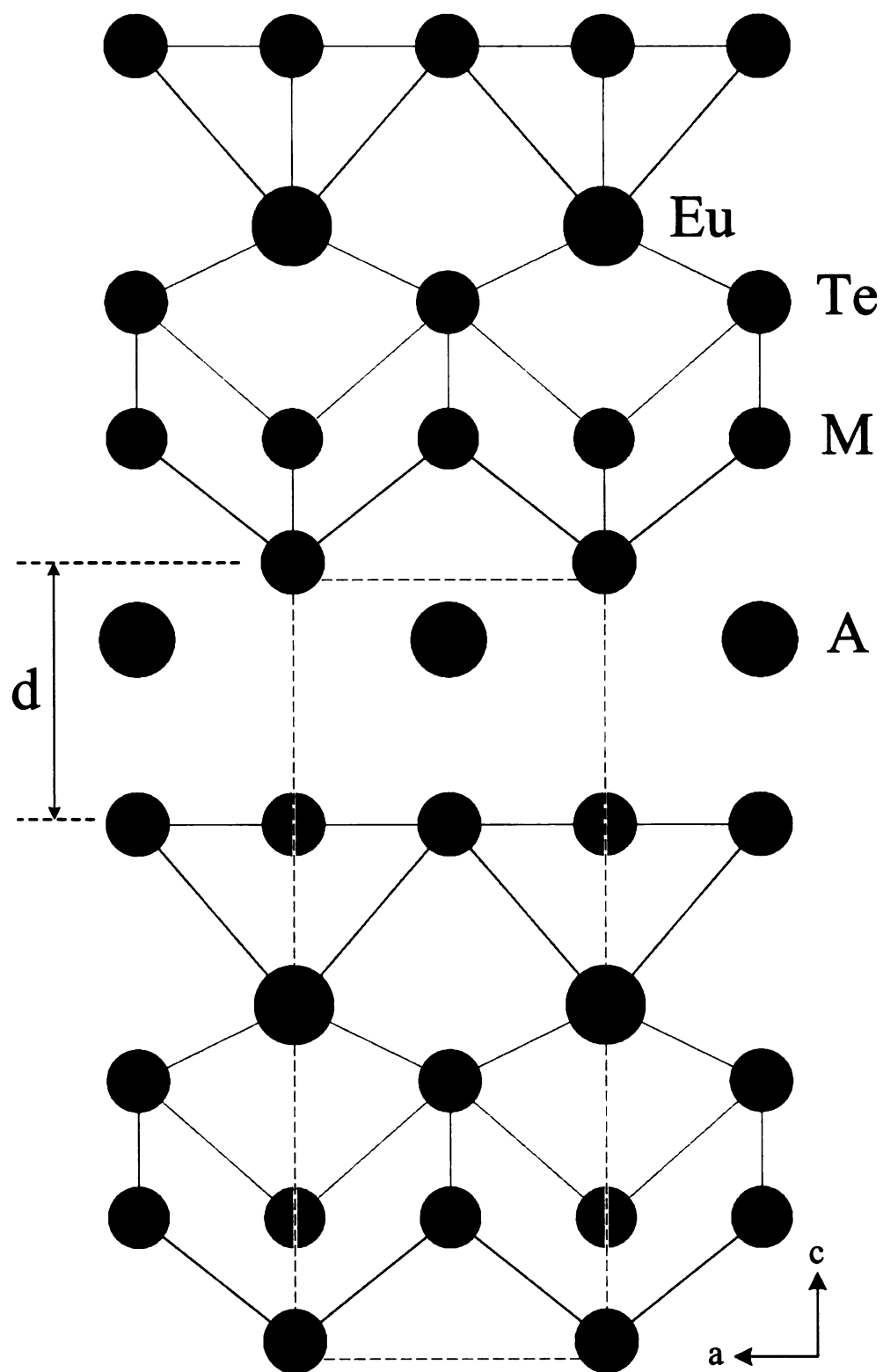


Figure 6.1. Undistorted structure of AM_2EuTe_4 . The interplanar separation d changes from ~ 3.7 Å in the Na^+ , to ~ 4.2 Å in the K^+ , to ~ 4.7 Å in the Rb^+ , and to ~ 5.1 Å in the Cs^+ analogues.

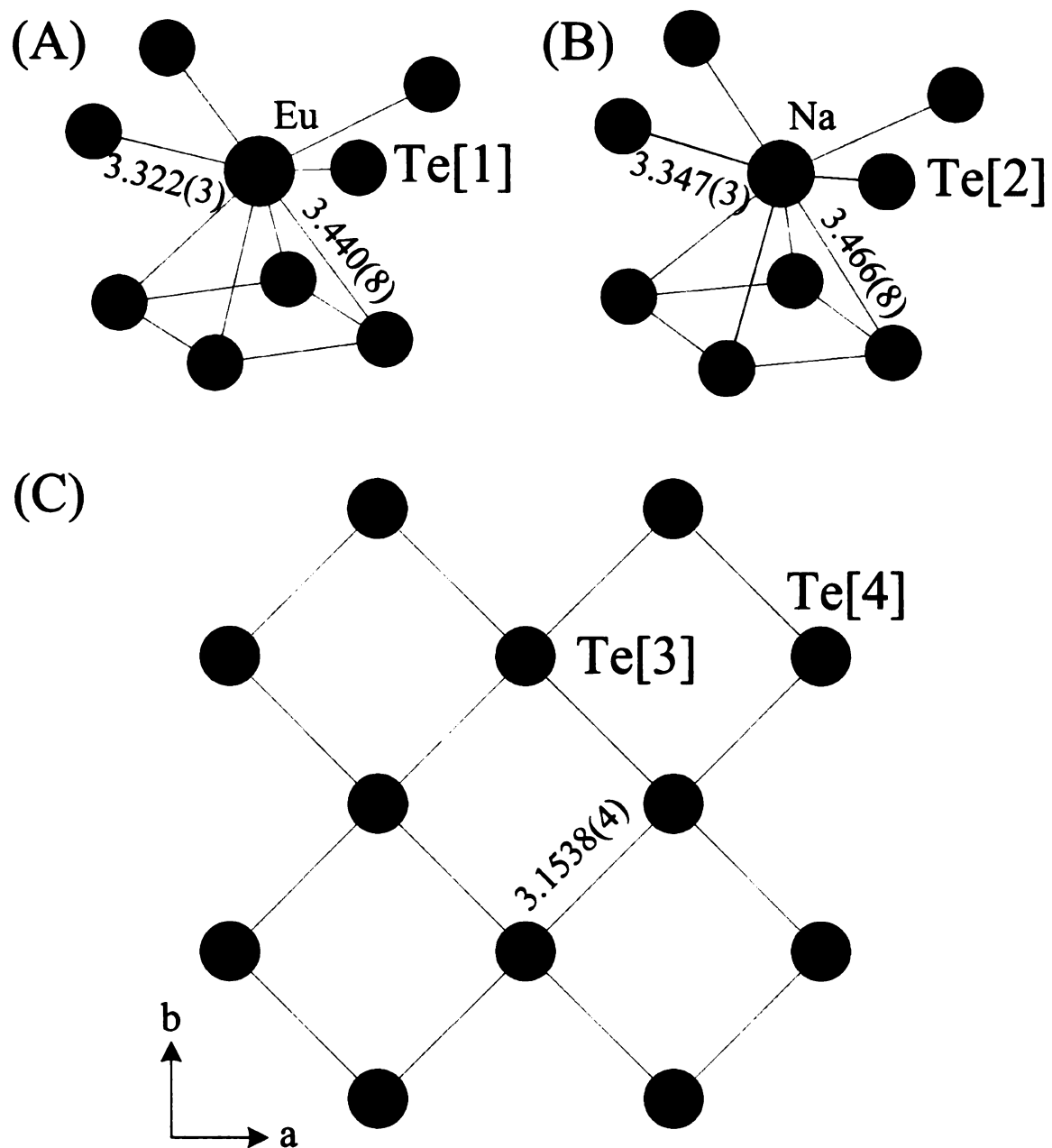


Figure 6.2. (A) Coordination geometry and environment of Eu in $\text{NaAg}_2\text{EuTe}_4$. (B) Coordination geometry and environment of Na in $\text{NaAg}_2\text{EuTe}_4$. (C) Square net of Te atoms in the subcell of $\text{NaAg}_2\text{EuTe}_4$.

Subcell Description of $\text{Cu}_{0.63}\text{EuTe}_2$ – The undistorted structure of $\text{Cu}_{0.63}\text{EuTe}_2$ crystallizes in the space group $P4/nmm$ and adopts the CaMnBi_2 structure type. It consists of europium atoms surrounded by eight tellurium atoms in a square antiprismatic geometry. The europium atoms are sandwiched between an anti-PbO type layer of $[\text{CuTe}]^-$ and a square net of tellurium atoms, Figure 6.3. The structure is very similar to the quaternary AM_2EuTe_4 phases if the alkali metal is replaced by a europium atom. Interestingly, the copper site found to be partially occupied with a refined fraction of 0.63(2). Although partial occupancy on this copper site is unusual in the polytelluride family it has been observed in the isostructural family of antimonides M_xLaSb_2 ($\text{M} = \text{Zn}, \text{Co}, \text{Mn}$ and Cu with $x = 0.52 - 0.87$).¹² The formula can be more expressly written as $[\text{M}_x\text{Te}]^{(2-x)-}\text{Eu}^{2+}[\text{Te}]^{x-}$ with an average electron count on the Te atoms of the square net of -0.63(2). The Eu-Te distances in the antiprism are 3.3193(6) Å and 3.4705(8) Å and the Te-Te distances in the square net are 3.1648(4) Å at 100 K.

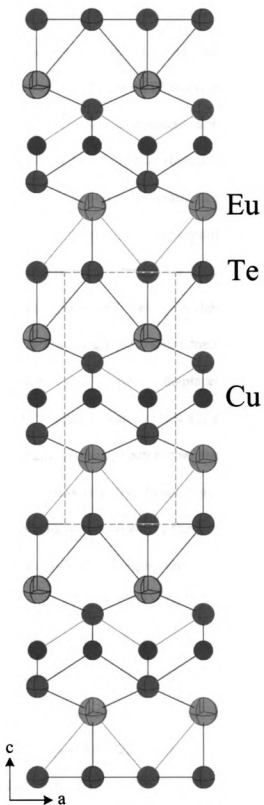


Figure 6.3. Undistorted structure of Cu_xEuTe_2

Supercell Description of AM_2EuTe_4 Based on a Modulation q -vector – The AM_2EuTe_4 series ($A = Na, K, Rb, Cs$; $M = Cu, Ag$) adopt the $Pm(0\beta 1/2)0$ superspace group. The tetragonal symmetry of the subcell ($P4mm$) is lost now due to the distortion. The q -vector possesses an incommensurate component along b^* and a commensurate one along c^* in the form $q = \beta b^* + 1/2c^*$. The irrational component is always along the longer b -axis of the ab -plane that contains the planar Te net for all the analogues. The distortion is mainly located in the planar $Te^{1/2-}$ net creating a wide distribution of Te-Te distances as can be seen in Figure 6.4 (distances for $CsAg_2EuTe_4$ at 100 K). The atomic displacement of the Te atoms (Te[3] and Te[4]) in the planar net along the a -axis (x direction) is at least two orders of magnitude larger than the displacements found along the other two directions, Figure 6.5. The atomic displacements along the b and c -axis (y and z directions), are shown in Figure 6.6 and Figure 6.7 respectively.

Interestingly, the length of the q -vector changes significantly as a function of alkali metal, and appears to be less sensitive to the nature of the coinage metal. The q -vector is ~ 0.31 for all the Na-analogues, 0.28 for the K-phases and 0.26 for Rb- and Cs-members. Specifically, for $NaCu_2EuTe_4$ the q -vector is 0.3122(7) and for $NaAg_2EuTe_4$ is 0.3134(6) at 100 K. For KCu_2EuTe_4 and KAg_2EuTe_4 the q -vectors are 0.2822(6) and 0.2853(5) respectively. Finally, $RbCu_2EuTe_4$ has a q -vector of 0.2656(8), for $RbAg_2EuTe_4$ is 0.2625(7) and for $CsAg_2EuTe_4$ is 0.2631(6). The difference in the cell parameters containing the planar Te net (ab -plane) between the members with different alkali metal is smaller than 3% ($a = 4.3692(7)$ Å, $b = 4.3790(6)$ Å for $NaCu_2EuTe_4$ and $a = 4.4911(6)$ Å, $b = 4.5068(7)$ Å for $CsAg_2EuTe_4$). Similarly, the difference in a and b cell parameters between the analogues with different coinage metal (from the smaller Cu to

the larger Ag) is negligible. The Eu-Te^{1/2-} distances (3.41 - 3.44 Å) remain practically unchanged within the AM₂EuTe₄ family. The distances that are affected the most from the occupation of the A site (A = Na, K, Rb and Cs) are related to the separation between the polar [M₂EuTe₄]⁻ slabs. In more details, the separation of the Te^{1/2-} and Te²⁻ (from the [MTe]⁻ layer) planar nets in the Na-analogues is ~ 3.7 Å. This distance increases to ~ 4.2 Å in the K-substituted members, and becomes ~ 4.7 Å and ~ 5.1 Å in Rb- and Cs-containing phases respectively, Figure 6.1. The dependence of the CDW modulations to the third cross plane dimension was first observed (presented in Chapter 4) in the AMRETe₄ (A = Na, K; M = Cu, Ag; RE = La, Ce) family. The AM₂EuTe₄ family shows similar behavior and furthermore illustrates how CDW distortions are affected by gradually changing the cross plane interactions.

The distorted Te patterns in the AM₂EuTe₄ family have the same type of oligomers (mostly trimers and tetramers) with the ones observed in the RETe₃ series.¹³ In Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 100 K the minimum Te-Te distance in the net is 2.961(3) Å and the maximum 3.234(4) Å with an average of 3.094(4) Å. By taking 3.024 Å to be the Te-Te bonding threshold, the net can be conveniently viewed as a sequence of trimers and tetramers, Figure 6.. In Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄, the minimum and maximum Te-Te distance is 2.984(5) Å and 3.284(5) Å at 100 K and the Te pattern looks similar with the one in the Cu-analogue showing the same oligomers in a slightly different sequence, Figure 6.. The distorted Te net in the K-members shows a larger number of tetramers over trimers in respect with the Na-members and occasionally single Te atoms, Figures 6.15-6.16. The Te-Te bond distribution for KCu₂EuTe₄ has a minimum distance of 2.934(4) Å and maximum 3.284(4) Å. In K_{0.97(2)}Ag₂Eu_{1.03(2)}Te₄ these distances are

2.940(5) Å and 3.398(6) Å respectively. The Te patterns of the Rb- and Cs-members contain a more frequent number of columns of single Te atoms from the patterns of the K-analogues, Figures 6.17-6.19. The minimum Te-Te distance for RbCu₂EuTe₄ at 100 K is 2.932(5) Å and the maximum is 3.320(5) Å. In RbAg₂EuTe₄ the minimum is 3.167(3) Å and maximum 3.181(3) Å. Finally, for CsAg₂EuTe₄, the shorter Te-Te distances are 2.937(2) Å and the longer ones 3.442(3) Å at 100 K.

The temperature dependence of the q-vector seems negligible from 100 K to 300 K as measured for the two end members, Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ and CsAg₂EuTe₄. Specifically, the q-vector of Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ from 0.3134(6)b* + 1/2c* at 100 K becomes 0.3118(5)b* + 1/2c* at 300 K. The q-vector of CsAg₂EuTe₄ is 0.2631(6)b* + 1/2c* at 100 K and 0.2650(6) + 1/2c* at 300 K. The changes in the distorted Te patterns with temperature are small with minor differences in the sequence of the oligomers. The modulated Te pattern of Na_{0.80(2)}Ag₂Eu_{1.20(2)}Te₄ at 300 K is shown in Figure 6. and for CsAg₂EuTe₄ in Figure 6.20. The Te-Te bond distribution becomes broader with a minimum of 2.973(3) Å and maximum of 3.329(4) Å for Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 300 K and 2.951(2) Å and 3.453(2) Å for CsAg₂EuTe₄ respectively.

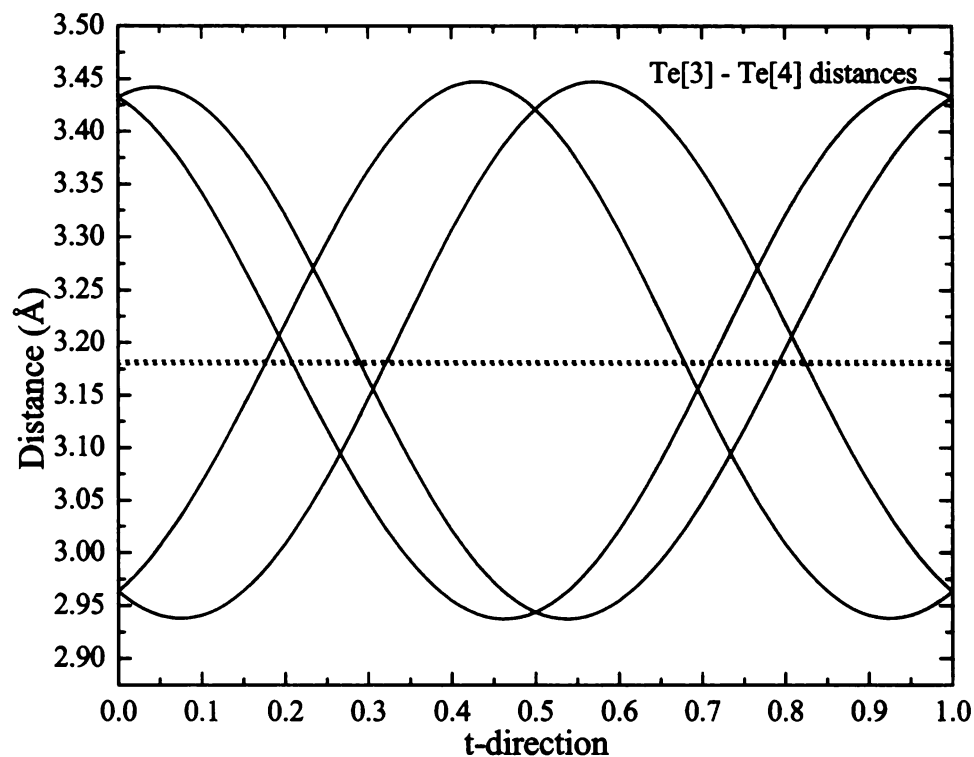


Figure 6.4. Representative plot of the Te[3]-Te[4] distances found in the distorted net of $\text{CsAg}_2\text{EuTe}_4$ from the superspace analysis based on a q -vector as a function of t -direction. Dashed lines represent the average (undistorted) Te-Te distances.

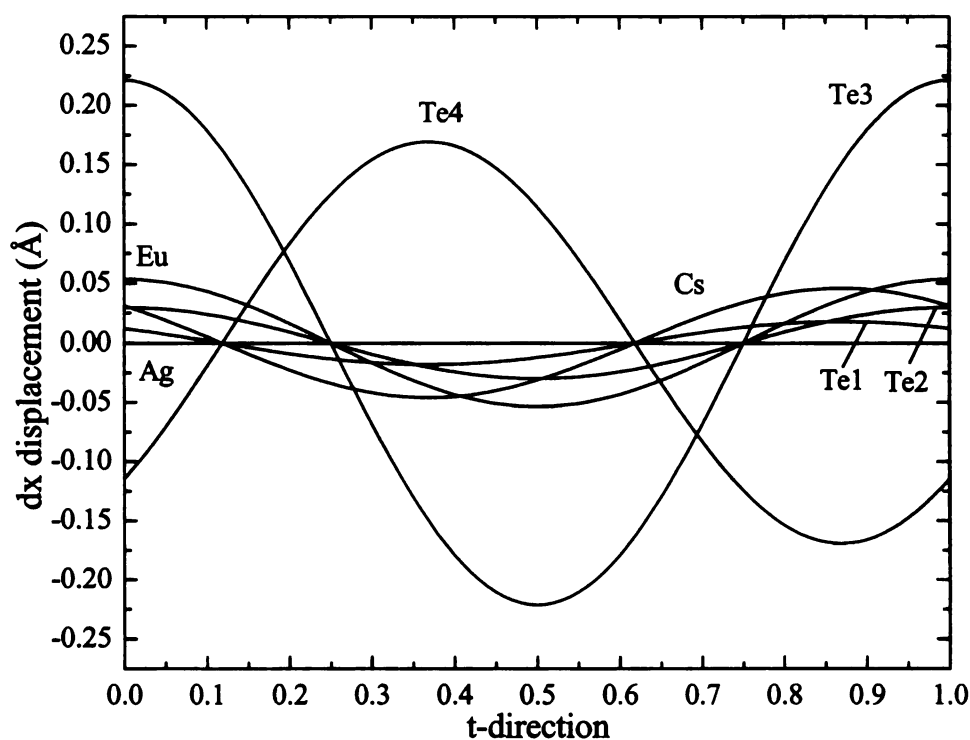


Figure 6.5. Plot of the positional displacement (Å) along x -axis of all the atoms in the $\text{CsAg}_2\text{EuTe}_4$ supercell as a function of t -direction.

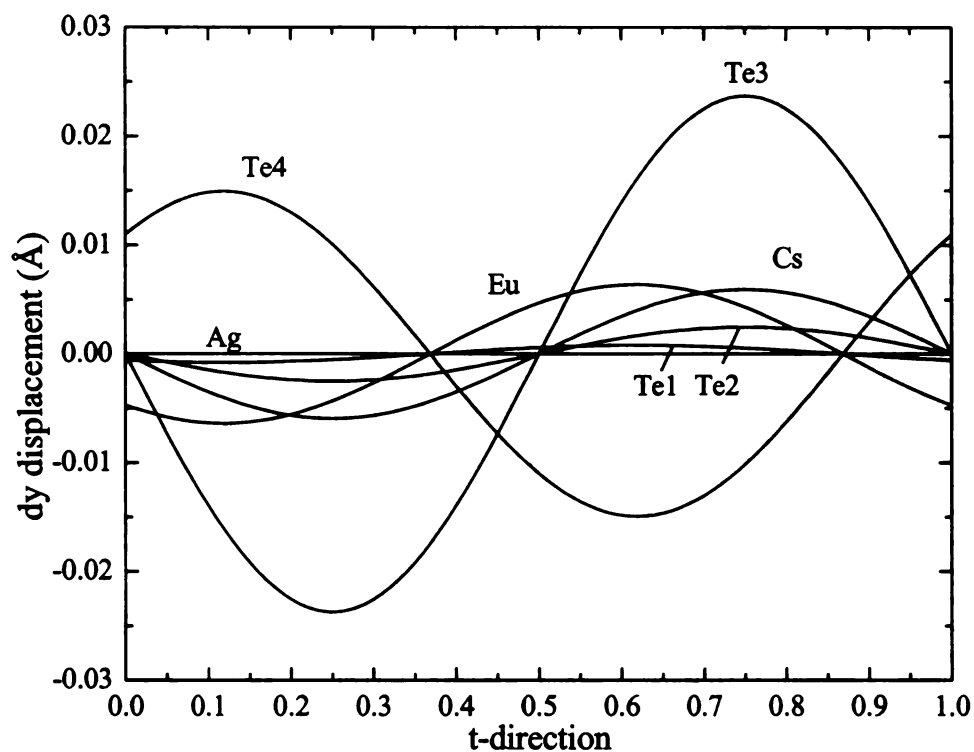


Figure 6.6. Plot of the positional displacement (Å) along y-axis of all the atoms in the CsAg₂EuTe₄ supercell as a function of t-direction.

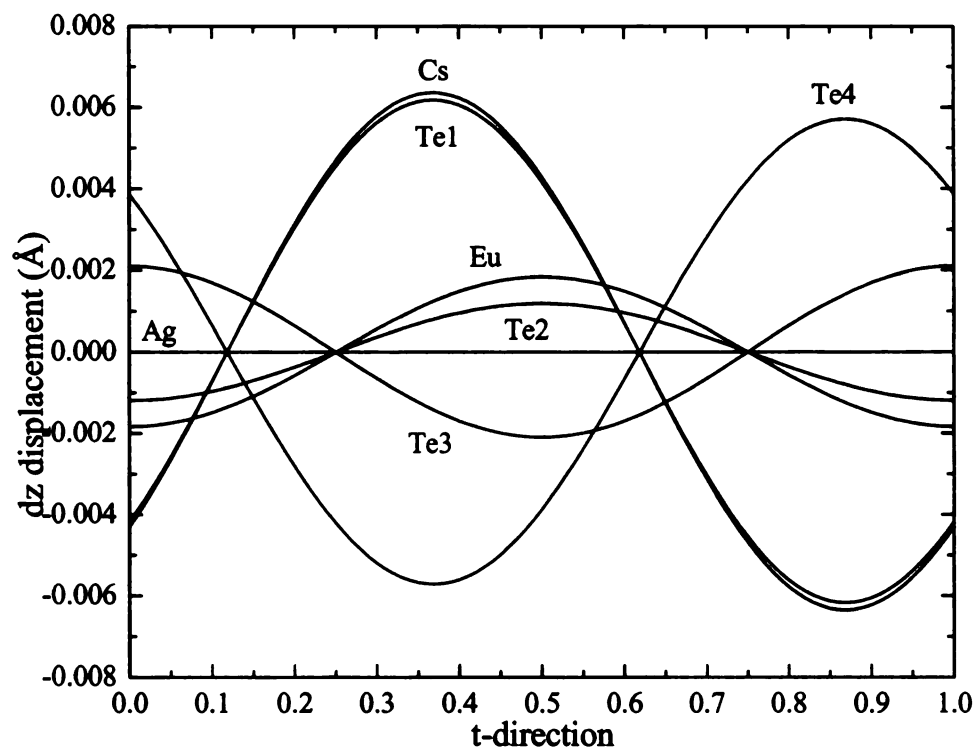


Figure 6.7. Plot of the positional displacement (Å) along z-axis of all the atoms in the CsAg₂EuTe₄ supercell as a function of t-direction.

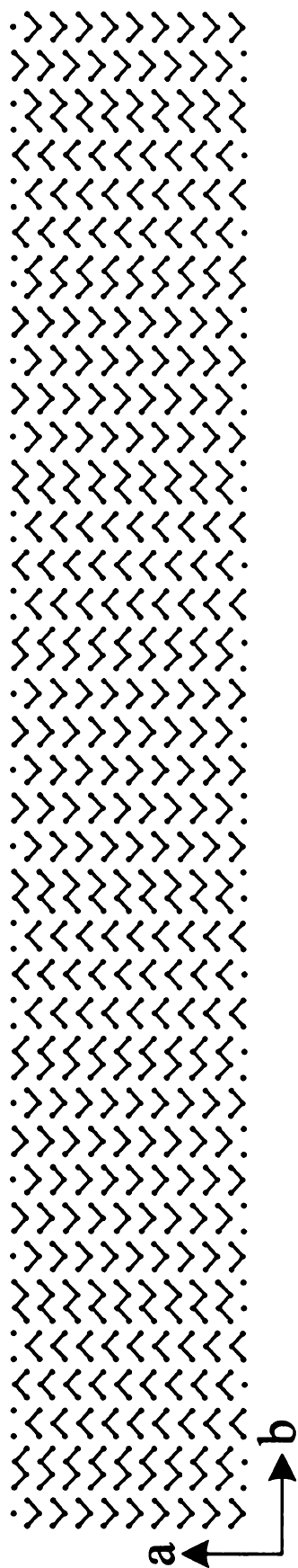


Figure 6.8. $\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$ at 100 K with $q = 0.3122(7)b^* + 1/2c^*$ and 3.024 Å bonding threshold.

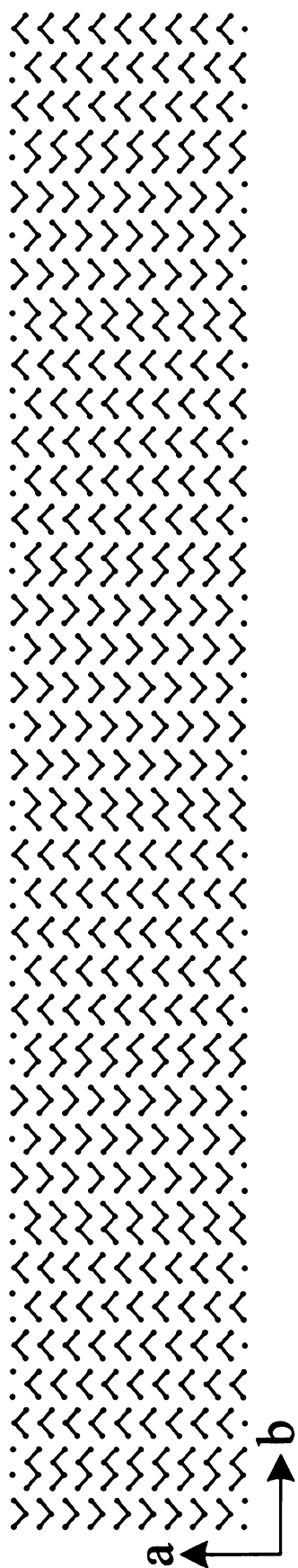


Figure 6.9. $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 100 K with $q = 0.3134(6)b^* + 1/2c^*$ and 3.048 Å bonding threshold.

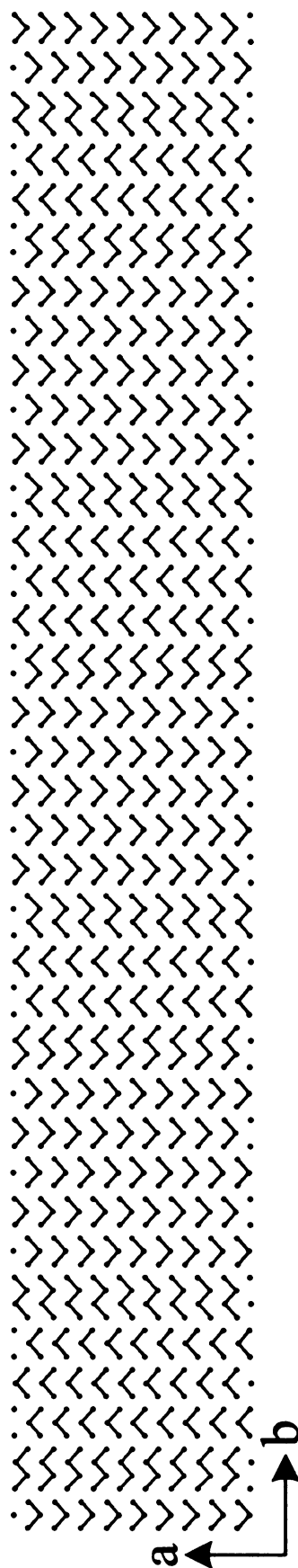


Figure 6.10. $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 300 K with $q = 0.3118(5)b^* + 1/2c^*$ and 3.058 Å bonding threshold.

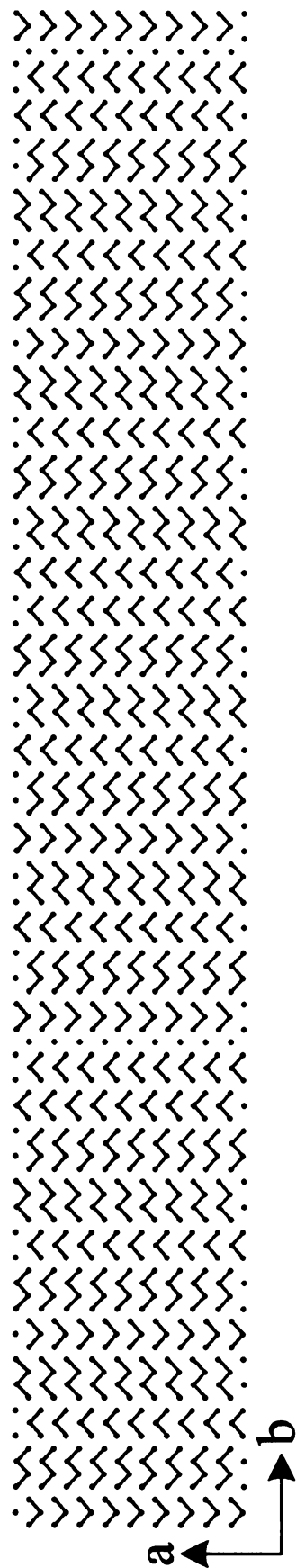


Figure 6.11. $\text{KCu}_2\text{EuTe}_4$ at 100 K with $q = 0.2822(6)b^* + 1/2c^*$ and 3.030 Å bonding threshold.

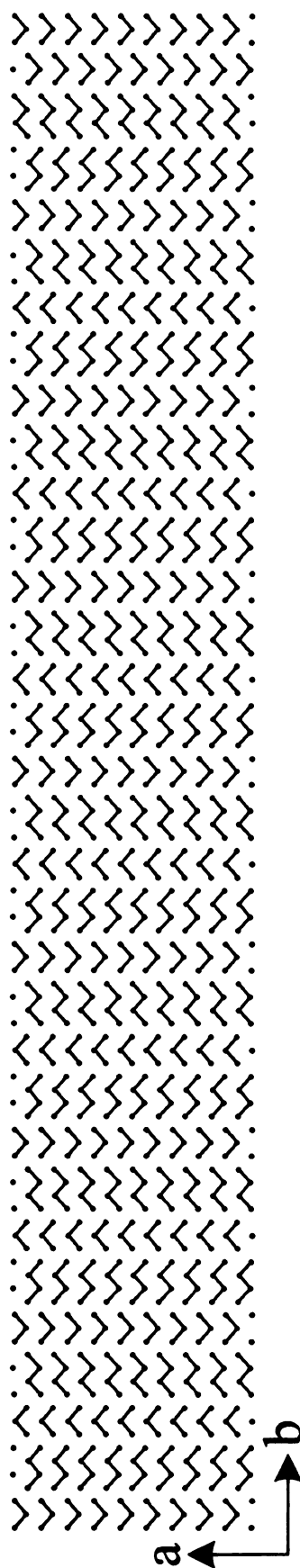


Figure 6.12. $\text{K}_{0.97(2)}\text{Ag}_2\text{Eu}_{1.03(2)}\text{Te}_4$ at 100 K with $q = 0.2853(5)b^* + 1/2c^*$ and 3.069 Å bonding threshold.

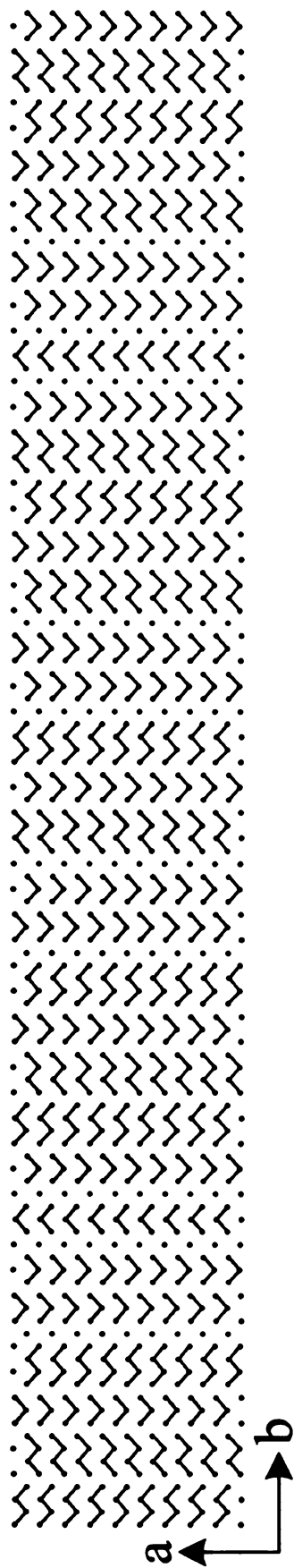


Figure 6.13. RbCu₂EuTe₄ at 100 K with $q = 0.2656(8)b^* + 1/2c^*$ and 3.023 Å bonding threshold.

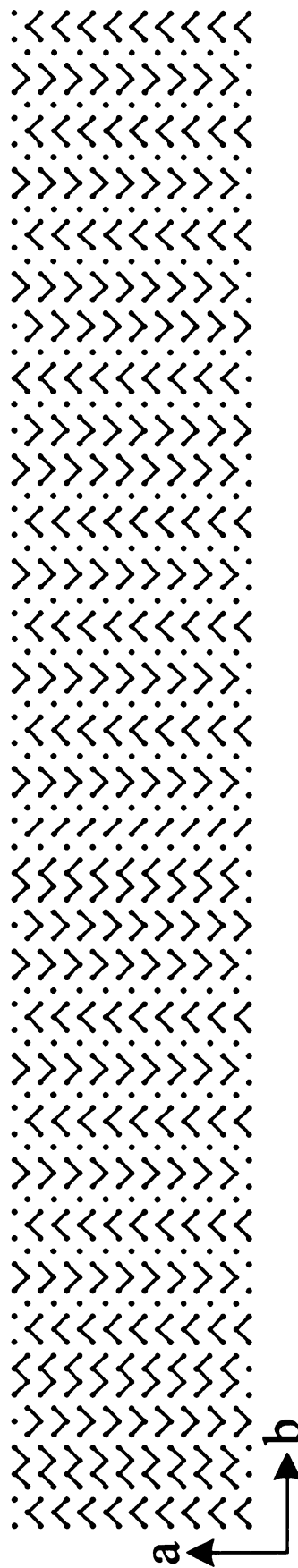


Figure 6.14. RbAg₂EuTe₄ at 100 K with $q = 0.2625(7)b^* + 1/2c^*$ and 3.167 Å bonding threshold.

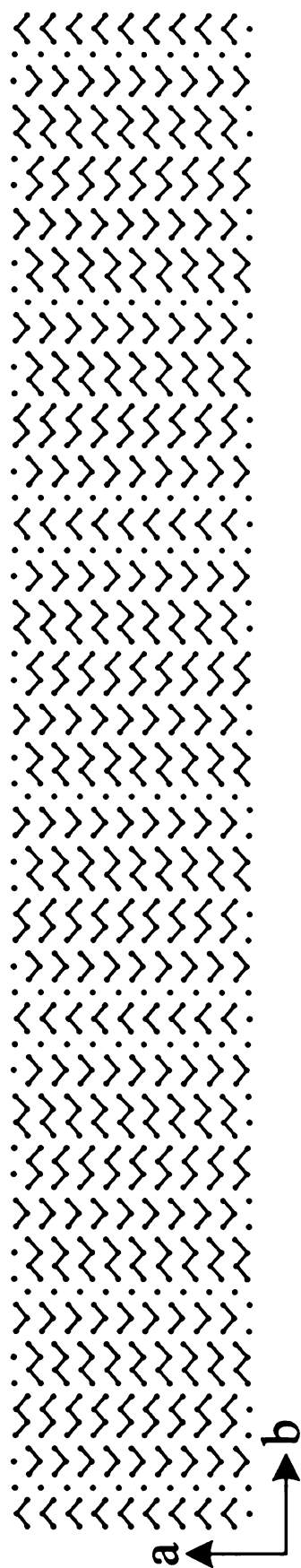


Figure 6.15. CsAg₂EuTe₄ at 100 K with $q = 0.2631(6)b^* + 1/2c^*$ and 3.060 Å bonding threshold.

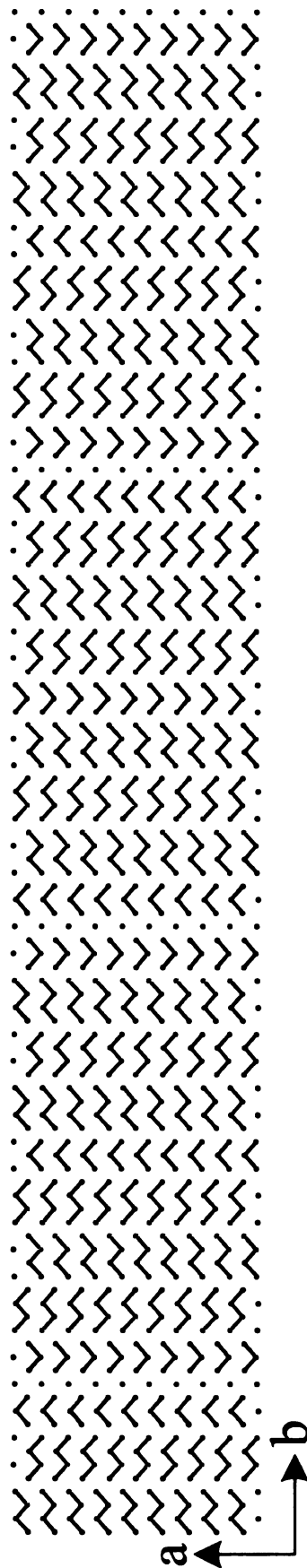


Figure 6.16. CsAg₂EuTe₄ at 300 K with $q = 0.2650(6)b^* + 1/2c^*$ and 3.080 Å bonding threshold.

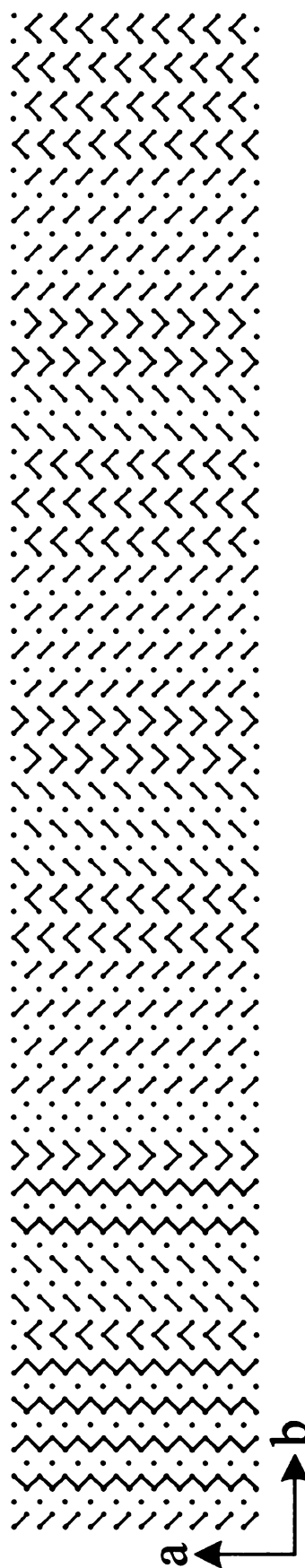


Figure 6.17. Cu_{0.63(2)}EuTe₂ at 100 K with $q_1 = 0.2910(2)b^* + 1/2c^*$ and $q_2 = 0.3557(3)b^*$ and 3.118 Å bonding threshold.

Supercell Description of Cu_{0.63}EuTe₂ Based on a Modulation q-vector – Although the average structure of Cu_{0.63}EuTe₂ and AM₂EuTe₄ are similar, the distortions and supercell of the former compound are very different from the ones observed in the latter phases. Cu_{0.63}EuTe₂ possesses two incommensurate modulation q-vectors with $q_1 = 0.2910(2)b^* + 1/2c^*$ and $q_2 = 0.3557(3)b^*$ and it crystallizes in Pm(0 β_1 1/2)(0 β_2 0)0 superspace group. In order to obtain a stable refinement and avoid non-linear correlations between the rational and irrational components of the modulation vectors a doubling of the cell along the c-axis was performed to clear the rational part. Therefore a centering vector of (0 0 $\frac{1}{2}$ $\frac{1}{2}$ 0) and a corresponding superspace group notation of Xm(0 β_1 0)(0 β_2 0)0 were used.

The distortion is mainly located in the planar nets of Te. The distribution of Te-Te distances has a minimum of 2.934(5) Å, maximum 3.280(6) Å and an average value of 3.158(6) Å, Figure 6.8. The atomic displacements of the Te atoms (Te[2a] and Te[2b]) in the net along the a-axis (x direction) are comparable to the displacements found along the other two directions, Figure 6.9. The atomic displacements along the b and c-axis (y and z directions), are shown in Figure 6.10 and Figure 6.11 respectively for u = 0.5. The sequence of oligomers of the distorted Te nets of Cu_{0.63}EuTe₂ is very different from the ones observed in the quaternary AM₂EuTe₄ series. The pattern can be seen conventionally as a sequence of mainly trimers, dimers, and single Te atoms. The noticeable differences of this pattern are the absence of tetramers and most importantly the presence of infinite zigzag Te chains running along the a-axis. The minimum Te-Te distance in the zigzag chains is 3.070(5) Å and the maximum 3.116(5) Å. The chains that are oriented perpendicular to the direction of the modulation vectors result from the

similar magnitude of distortions occurred along the two directions in the ab-plane. This is a rare feature taking into account that this interconnection between oligomers (monomers to form chains) in a normal direction to the modulation wave occurs at a temperature (100 K) far away from the CDW transition temperature (> 300 K). Similar type of interconnected atoms was observed for the RETe_3 family close to the CDW transition temperature.⁴

It is surprising that the $\text{Cu}_{0.63(2)}\text{EuTe}_2$ phase has two q-vectors in respect to the quaternary compounds given the fact that both subcells are structurally almost the same. Furthermore, there is only one type of distorted Te net with an average oxidation state of $-0.63(2)$ e/Te in the structure with no apparent difference in the electron count between the distorted Te nets. Different average oxidation states on distorted Te nets in a compound are known to create multiple hybrid q-vectors like in Sm_2Te_5 (Chapter 5). Actually, the ternary phase is packed even more symmetrically along the long c-axis since there is only one type of atoms (Eu) in between the layers. Therefore, a uniform distribution of charge on the Te nets is expected. On the other hand, the possible weak ordering of Cu vacancies cannot be responsible for the appearance of the second q-vector. The supercell structure refines with no problems without the application of occupational waves on the Cu-site and the change in the residual intensities is negligible. The agreement factor of all the observed reflections (main and satellites) decreases only by $\sim 0.02\%$ when ordering of Cu-vacancies is assumed.

The existence and length of the two vectors can be rationalized from the comparison of the cell parameters and distances found in $\text{Cu}_{0.63(2)}\text{EuTe}_2$ and quaternary $\text{ACu}_2\text{EuTe}_4$ phases. The value of the atomic radius of Eu (1.25 Å) is between the ones for

Na (1.18 Å) and K (1.51 Å). Following the trend of the length of the q-vector with chemical pressure we expect the value of the q-vector component for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ to be between the corresponding values for $\text{NaCu}_2\text{EuTe}_4$ and $\text{KCu}_2\text{EuTe}_4$. Indeed, the ternary phase has a vector of $q_1 = 0.2910(2)b^*$ whose length lies between $0.3122(7)b^*$ ($\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$) and $0.2822(6)b^*$ ($\text{KCu}_2\text{EuTe}_4$). The second vector of $\text{Cu}_{0.63(2)}\text{EuTe}_2$ can be seen as a result of the change in separation distance of the planar distorted $\text{Te}^{1/2-}$ nets. From the Rb quaternary analogue to Na the separation between the Te nets decreases while the length of the q-vector increases. Specifically, the separation length in $\text{RbCu}_2\text{EuTe}_4$ is ~ 11.5 Å, for $\text{KCu}_2\text{EuTe}_4$ is ~ 11.2 Å, and in $\text{NaCu}_2\text{EuTe}_4$ becomes ~ 10.6 Å. Their q-vectors are ~ 0.26 , 0.28 , and 0.31 respectively. Interestingly, $\text{Cu}_{0.63(2)}\text{EuTe}_2$ has the shortest c-axis among the quaternaries with a value of ~ 10.1 Å although Eu^{2+} is bigger than Na^+ . This is because of the stronger Eu-Te interactions compared with the Na-Te ones that make the length of the bonds in the former case shorter. Thus we expect the length of the q-vector component to be at least longer than 0.31 . Factually, the second vector of the ternary phase is $q_2 = 0.3557(3)b^*$.

The interactions along the third-dimension (c-axis) increase as the separation distance of the planar Te nets decreases moving from the bigger Cs^+ to the smaller Na^+ . When the alkali metal is replaced by Eu^{2+} atoms the cross-plane interactions are even stronger since the Eu-Te overlap of orbitals is greater than the overlap in the A-Te (A = alkali metal) case. In that sense the $\text{Cu}_{0.63}\text{EuTe}_2$ member has an enhanced three-dimensional character in respect to the quaternary phases with no apparent van der Waals gap. Therefore, the gradual change in the dimensionality will have an effect on the shape of the bands and the topology of the Fermi surface.

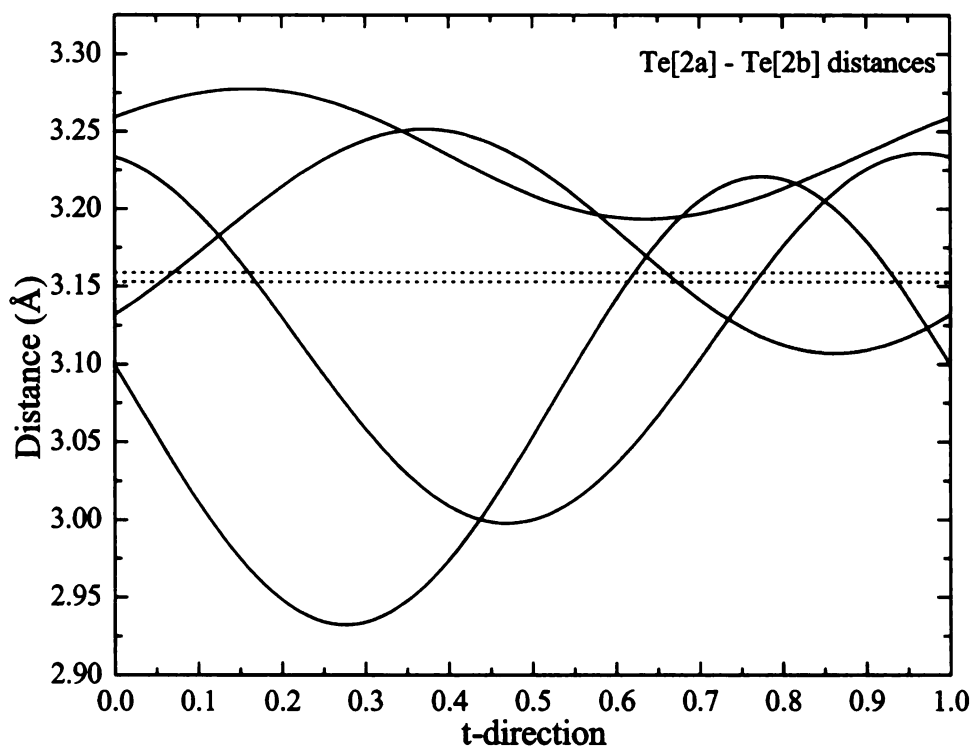


Figure 6.8. The Te[3]-Te[4] distances found in the distorted net of $\text{Cu}_{0.63(2)}\text{EuTe}_2$ from the superspace analysis based on a q-vector as a function of t-direction. Dashed lines represent the average (undistorted) Te-Te distances.

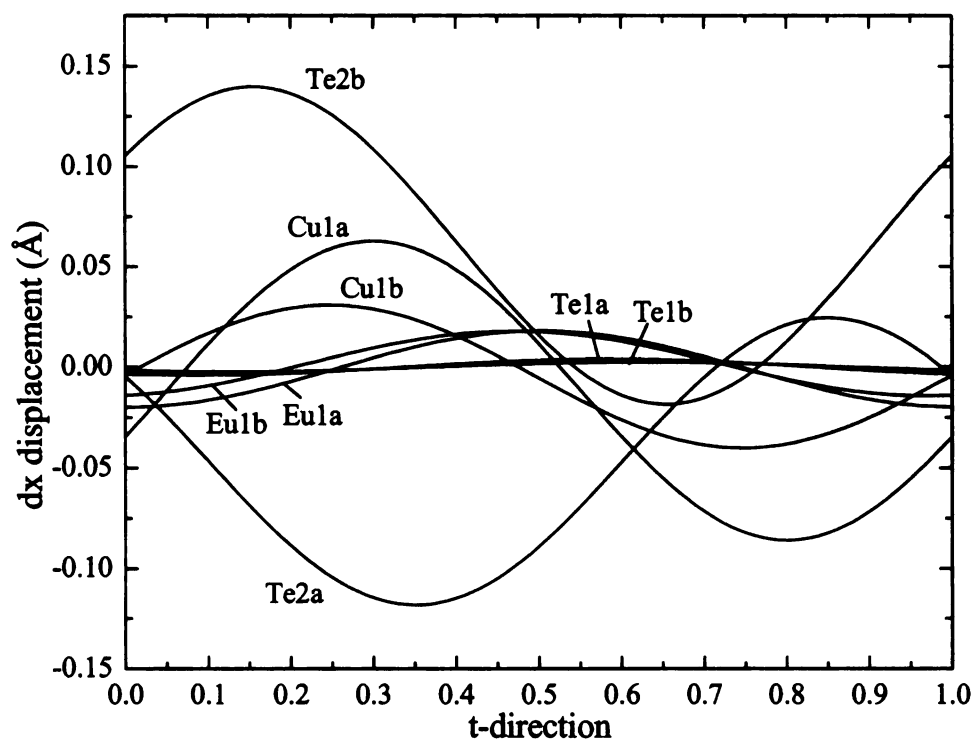


Figure 6.9. Plot of the positional displacement (Å) along x-axis of all the atoms in the $\text{Cu}_{0.63(2)}\text{EuTe}_2$ supercell as a function of t-direction for $u = 0.5$.

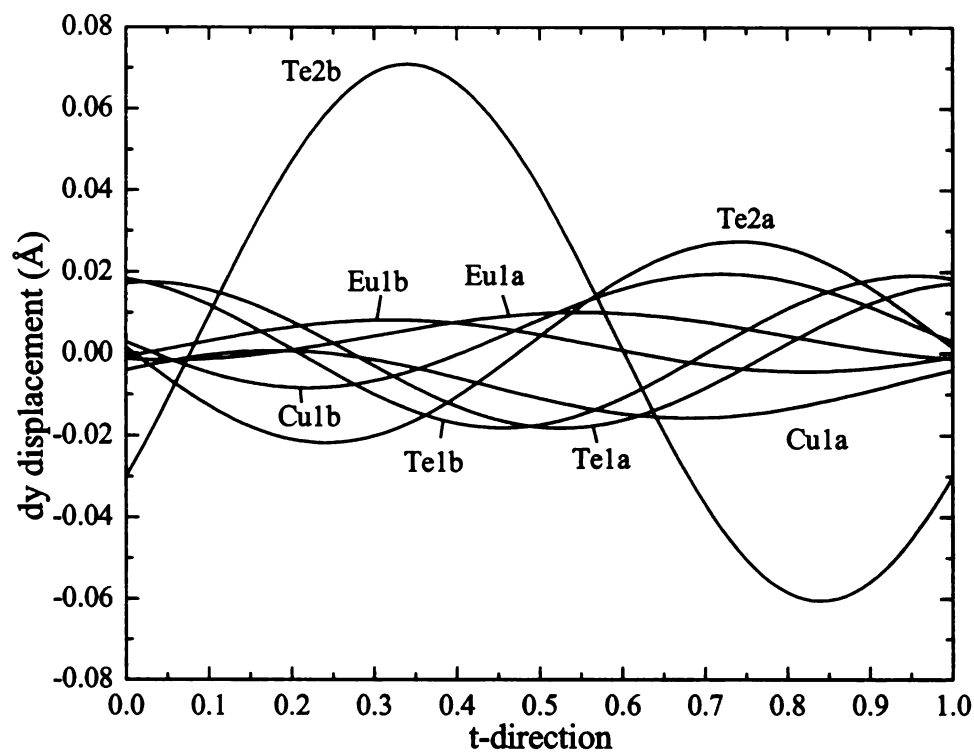


Figure 6.10. Plot of the positional displacement (Å) along y-axis of all the atoms in the $\text{Cu}_{0.63(2)}\text{EuTe}_2$ supercell as a function of t-direction for $u = 0.5$.

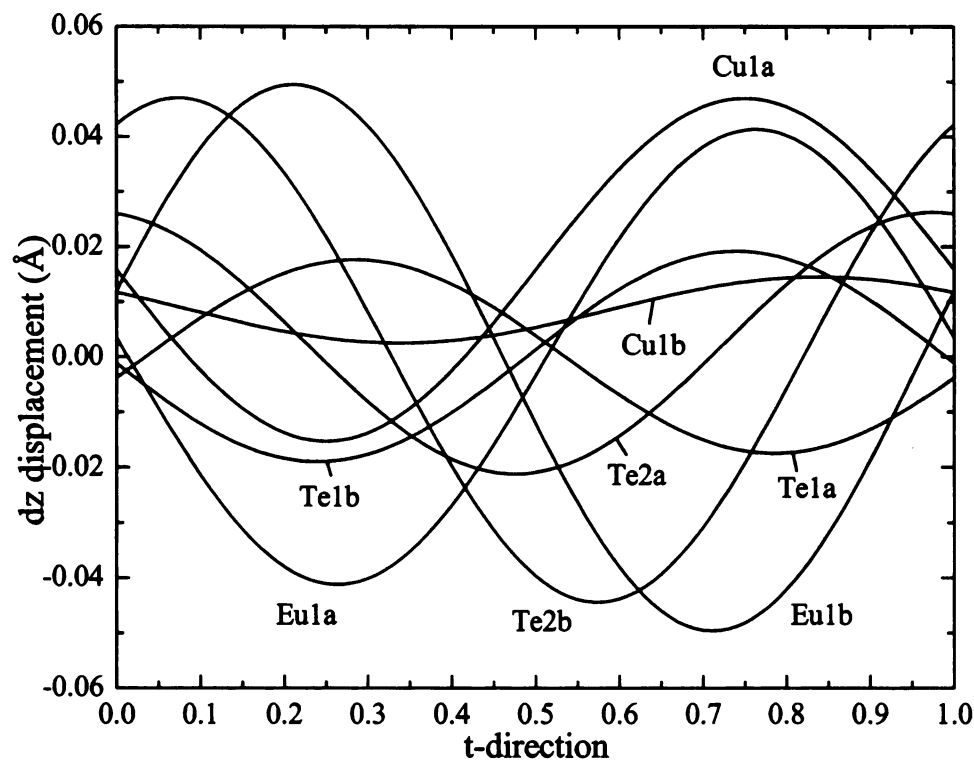


Figure 6.11. Plot of the positional displacement (Å) along z-axis of all the atoms in the $\text{Cu}_{0.63(2)}\text{EuTe}_2$ supercell as a function of t-direction for $u = 0.5$.

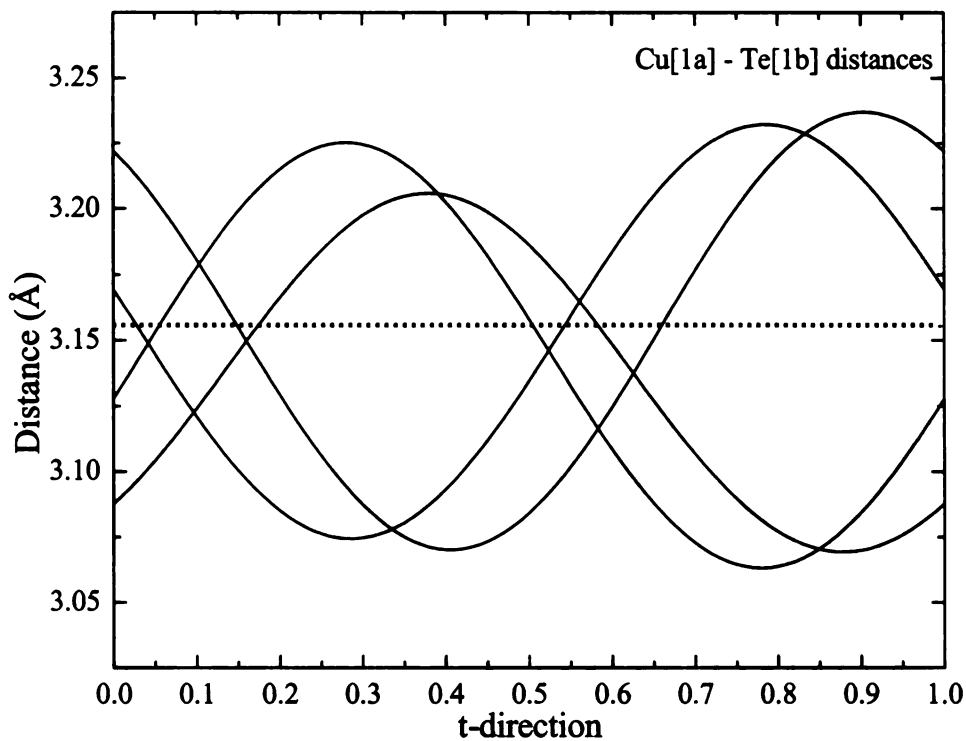


Figure 6.12. The Cu[1a]-Cu[1b] distances found in the distorted net of $\text{Cu}_{0.63(2)}\text{EuTe}_2$ from the superspace analysis based on a q-vector as a function of t-direction. Dashed lines represent the average (undistorted) Cu-Cu distances.

Magnetic Susceptibility Measurements of AM_2EuTe_4 – Variable temperature magnetic susceptibility data for most of the AM_2EuTe_4 analogues was measured in the range of 2-300 K at 3000 G. The material exhibit Curie-Weiss behavior. A representative susceptibility plot for $\text{NaAg}_2\text{EuTe}_4$ is shown in Figure 6.13. A μ_{eff} value of $7.64 \mu_{\text{B}}$ and a Weiss constant of -1 K were estimated by linear fitting of the $1/\chi_{\text{M}}$ vs T data. This value is consistent with an f^7 configuration or Eu^{2+} ($7.9 - 8.0 \mu_{\text{B}}$) and is very different from that expected for Eu^{3+} ($3.3 - 3.5 \mu_{\text{B}}$).

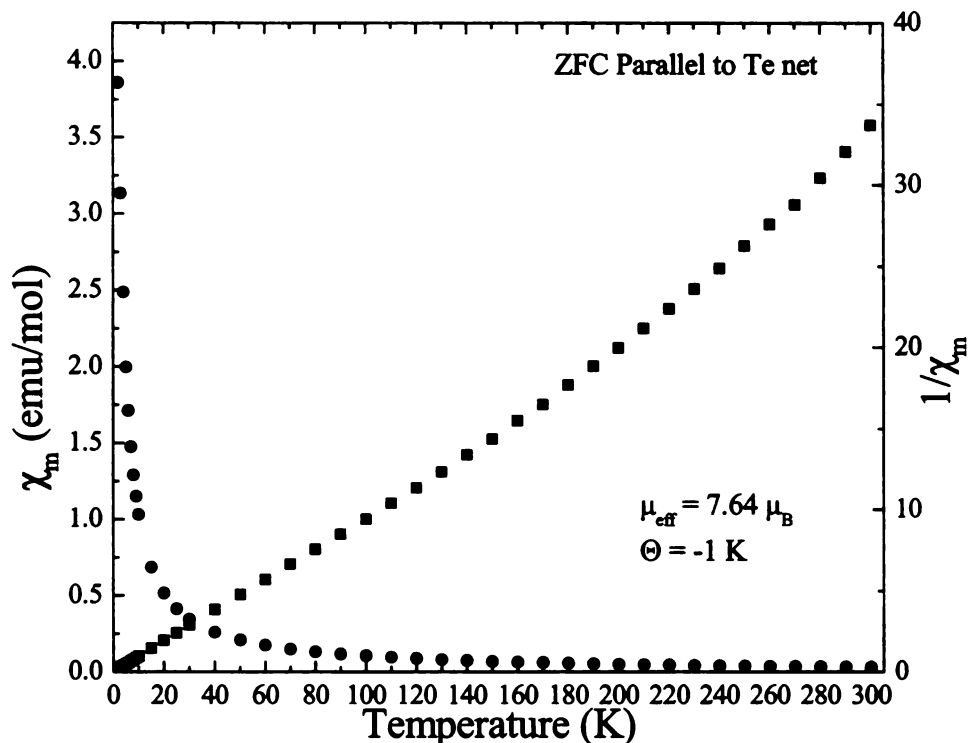


Figure 6.13. Temperature dependent magnetic susceptibility for NaAg₂EuTe₄.

Infrared (IR) Spectroscopy – Electronic transitions which can be assigned to the CDW energy gap of the Te-net were observed by IR diffuse reflectance measurements. The energy values are between 0.28(2) eV for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ and 0.08(2) eV for CsAg₂EuTe₄ at room temperature, Table 6.1. The corresponding energy gap for Cu_{0.63(2)}EuTe₂ is 0.16(2) eV. A representative plot of the apparent gap for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ is shown in Figure 6.14.

Table 6.1. Minimum and maximum distances of Te-Te within the net (X-ray diffraction at 100K) and room temperature energy gap values of all $A_{1-x}M_2Eu_{1+x}Te_4$ ($A = K, Na, Rb, Cs$; $M = Cu, Ag$) quaternary compounds and $Cu_{0.63(2)}EuTe_2$.

Compound	Minimum distance (Å)	Maximum distance (Å)	Energy gap (eV)
$Na_{0.80(2)}Cu_2Eu_{1.20(2)}Te_4$	2.961(3)	3.234(4)	0.26(2)
$Na_{0.81(2)}Ag_2Eu_{1.19(2)}Te_4$	2.984(5)	3.284(5)	0.28(2)
KCu_2EuTe_4	2.934(4)	3.284(4)	0.21(2)
$K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$	2.940(5)	3.398(6)	0.23(2)
$RbCu_2EuTe_4$	2.932(5)	3.320(5)	0.11(2)
$RbAg_2EuTe_4$	3.167(3)	3.181(3)	0.09(2)
$CsAg_2EuTe_4$	2.937(2)	3.442(3)	0.08(2)
$Cu_{0.63(2)}EuTe_2$	2.934(5)	3.280(6)	0.16(2)

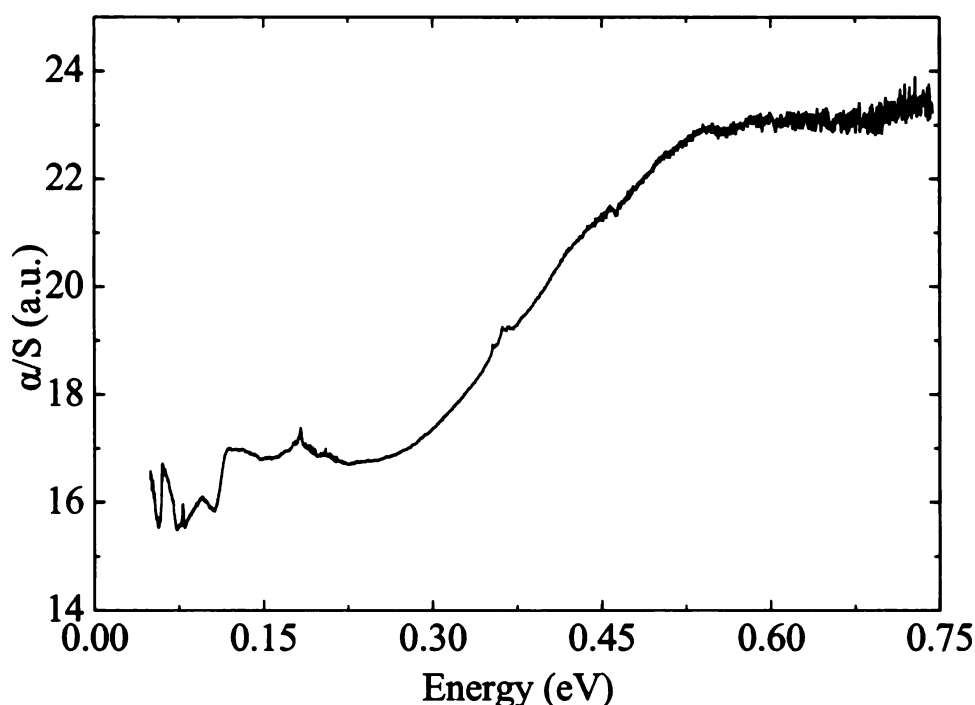


Figure 6.14. Typical room temperature infrared absorption spectrum of $Na_{0.81(2)}Ag_2Eu_{1.19(2)}Te_4$ showing energy gap at around 0.28 eV.

Band structure calculation of ACu_2LuTe_4 – The calculations were performed using the self-consistent full-potential linearized augmented plane wave method

(LAPW)¹⁴ and the generalized gradient approximation (GGA)¹⁵ for the exchange and correlation potential. The experimental cell constants and atomic coordinates from the crystal structure refinement of the average undistorted ACu₂EuTe₄ (A = Na, K, and Rb) compounds in Pmm2 were used. The volume optimization for KCu₂LuTe₄ gave a minimum energy at a volume difference of ~ 3%. This difference was assumed to be negligible since the nesting vector of the Fermi surface ranges ± 0.02 in length and a more energetically accurate calculation would not give extra details. Furthermore, the Fermi energy level was shifted by one electron in order to compensate the difference between the charges of Eu²⁺ and Eu³⁺. Directions in the Brillouin zone (BZ) of Pmm2 space group are shown in Figure 6.19.¹⁶ Interatomic forces were minimized within 0.1 mRy/bohr using a reverse-communication trust-region quasi-Newton method from the Port library.¹⁷ Scalar relativistic corrections were included and a spin-orbit interaction was incorporated using a second variational procedure.¹⁸ The values of the atomic radii were taken to be: 2.5 a.u. for alkali metal atom, 2.3 a.u. for Cu atom, 2.5 a.u. for Lu atom and 2.4 a.u. for Te atoms, where a.u. is the atomic unit (0.529 Å). Convergence of the self-consistent iterations was performed for 50 k points inside the irreducible BZ to within 0.0001 Ry with a cutoff of -6.0 Ry between the valence and the core states. The calculations were performed using WIEN2K program.¹⁹

The band structure of NaCu₂LuTe₄ showed that two Te p bands nearly parallel to each other cross the Fermi level, Figure 6.15. This indicated that a small perturbation of the Fermi level is not going to change significantly the Fermi surface topology for NaM₂LuTe₄. Indeed, the modulations found in the Na/Eu disordered Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ phase that contains a distorted Te net with an average oxidation

state of 0.60(4) (different from the average electron count of 0.5 found in the other quaternary analogues) possesses a q-vector that follows the expected trend.

The theoretical calculation on ACu_2LuTe_4 ($A = Na, K, \text{ and } Rb$) verified that the Fermi surface topology in these compounds favors the formation of a nesting vector (q-vector) along the b-axis. The length of the vector decreases from 0.30(1) to 0.26(1) for $NaCu_2LuTe_4$ to $RbCu_2LuTe_4$ respectively and this is consistent with the experimental results. The representative shape of the Fermi surface topology of the two bands of $NaCu_2LuTe_4$ that cross the Fermi level is shown in Figure 6.16A-B and the overall Fermi surface is shown in Figure 6.16C.

Band structure calculation of Cu_xLuTe_2 – The same calculation method and procedure that was used for ACu_2LuTe_4 were performed on the average structure of $CuLuTe_2$ (no CDW and vacancies). Directions in the Brillouin zone (BZ) of Pmmn space group are shown in Figure 6.20.¹⁶ The bands around the Fermi level that are still Te p in character are more dispersed from the ones found in the quaternary phases, Figure 6.17. This makes the Fermi surface more complex and sensitive to small changes in the Fermi level. This is apparent from the calculated Fermi topologies at three different Fermi levels that correspond to three different concentrations of x for Cu atoms, namely $x = 0, 1/3$, and $2/3$. The Fermi level for $x = 0$ was calculated from the $CuLuTe_2$ substructure (no vacancies, $x = 1$) after removing one electron from the system (charged cell). The intermediate Fermi level energies were calculated by linear interpolation between the two values of $x = 0$ and $x = 1$. Interestingly, the Fermi surface of $CuLuTe_2$ ($x = 1$) does not favor spanning of the bands since the topology does not have parallel regions in which nesting can occur, Figure 6.18A. An electron deficient situation like in $Cu_{2/3}LuTe_2$ the

Fermi level is lowered since there are less electrons ($x < 1$) in the system. This small shift in energy gives a different Fermi surface topology that starts to have bands that are almost parallel to each, Figure 6.18B. This creates a more favorable geometry in which nesting may develop. This is more apparent when the Fermi level is shifted even more in the case of $\text{Cu}_{1/2}\text{LuTe}_2$ that clearly posses two bands with a nesting vector of 0.38(2), Figure 6.18C. Finally, in the hypothetical situation of one electron energy shift of the Fermi level there are two bands that cross the Fermi surface. One band is located in the center (around the Γ point) of the Fermi surface (Figure 6.18D) and the other band that crosses the surface more than once is located at the edges (Figure 6.18E). The overall topology gives two possible parallel nesting vectors with lengths of 0.39(2) and 0.44(2), Figure 6.18F that is qualitatively in good agreement with the experimental observation.

These results qualitatively describe the experimental observations and give some insight for the stability of the Cu deficient compounds vs the fully occupied one. It seems that is necessary to remove electrons from the CuLuTe_2 system in order to have the Fermi level in such position that nesting is favorable. The only flexible way for the system to adopt this required configuration is to create vacancies in the Cu plane. This gives a reasonable answer to the hypostoichiometry that is always found in the Cu_xLuTe_2 family and may be even in the M_xLaSb_2 ($\text{M} = \text{Zn}, \text{Co}, \text{Mn}$ and Cu with $x = 0.52 - 0.87$) series.¹²

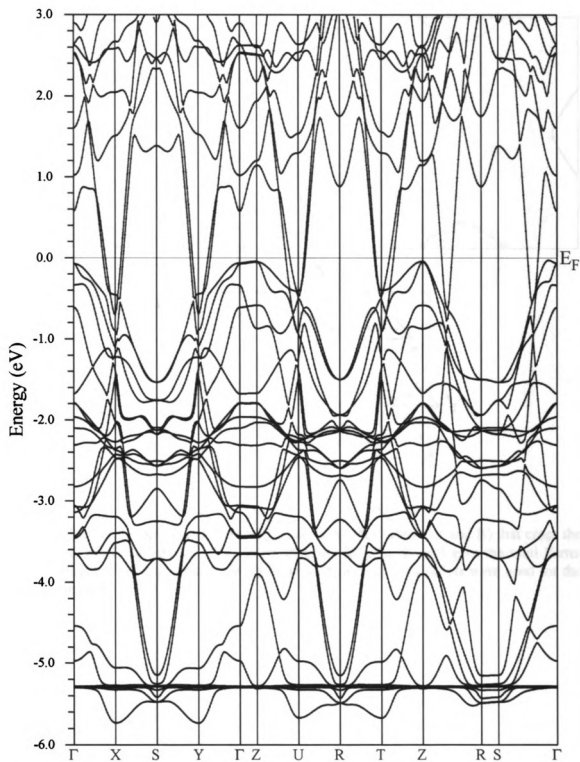


Figure 6.15. Band structure of NaCu₂LuTe₄ near the Fermi level.

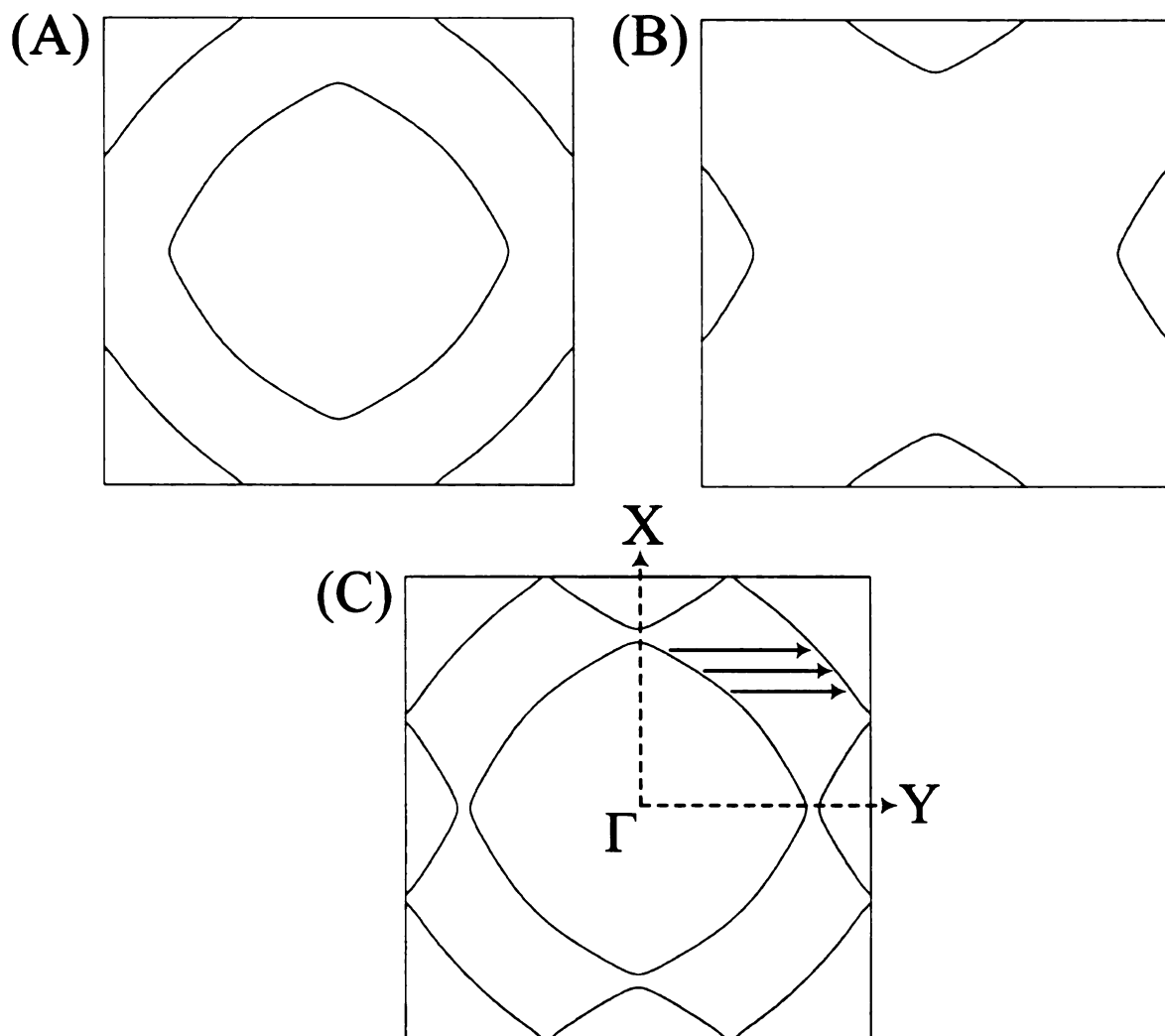


Figure 6.16. Fermi surface topology of the two individual bands (A and B) that cross the Fermi level of $\text{NaCu}_2\text{LuTe}_4$. (C) Superposition of these bands will give the total Fermi surface. Possible nesting vectors are drawn in arrows. 51×51 k points were used for the calculation of the Fermi surface.

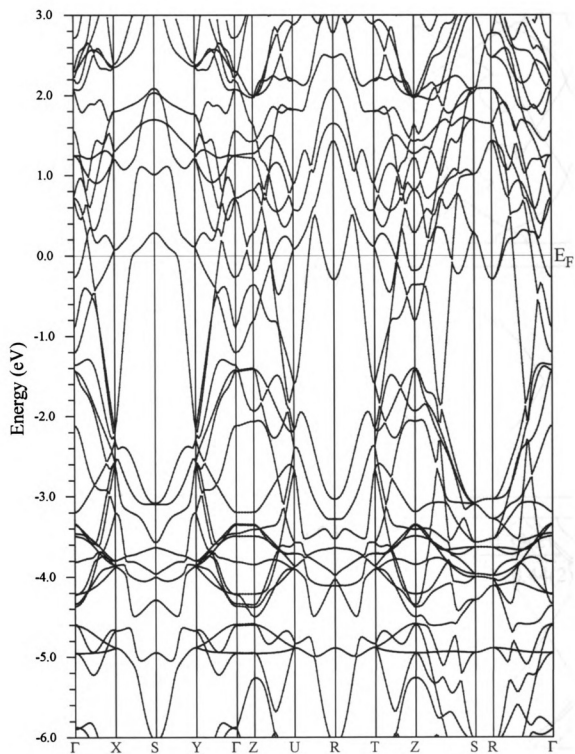


Figure 6.17. Band structure of CuLuTe₂ near the Fermi level.

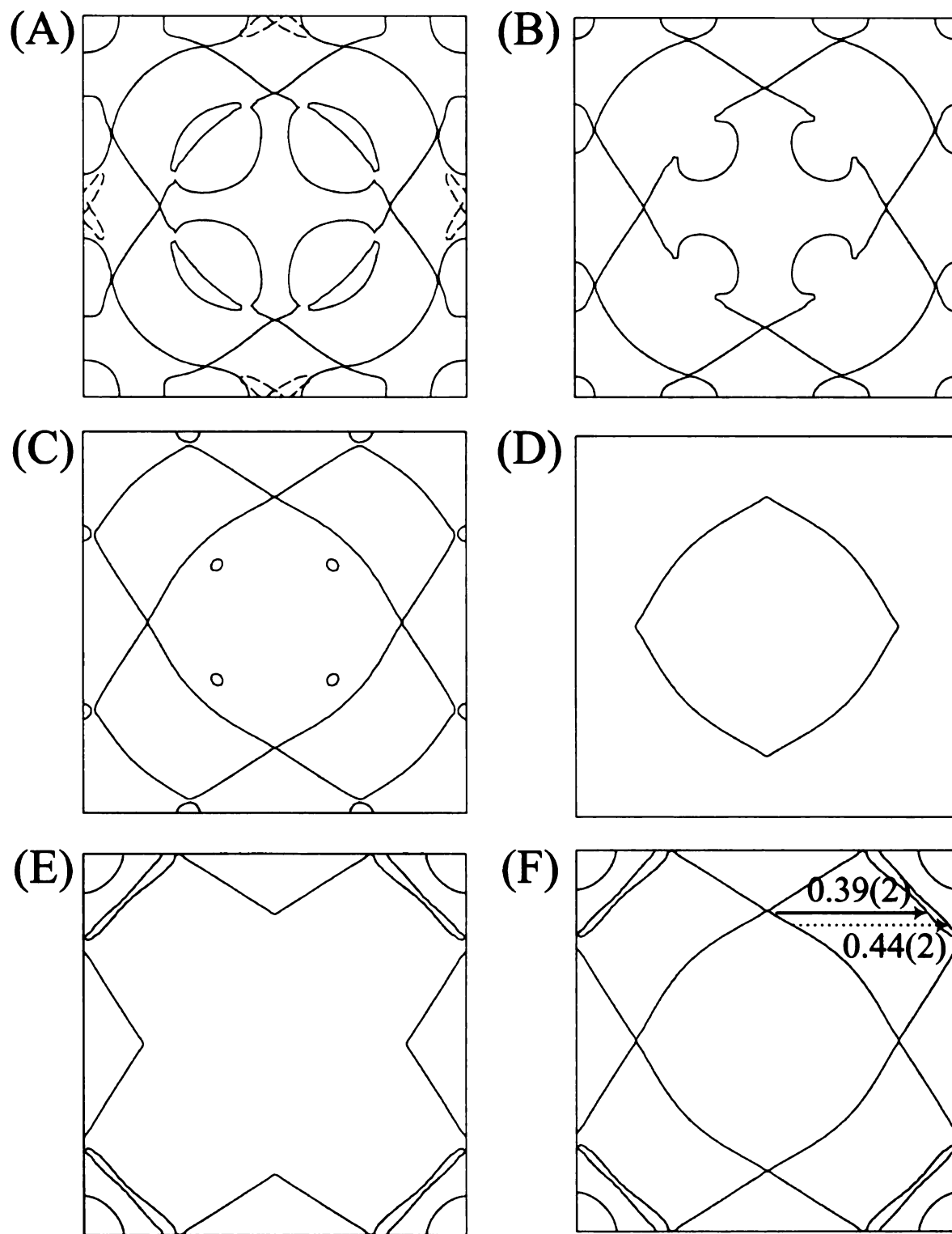


Figure 6.18. Fermi surface topology for Cu_xLuTe_2 . (A) $x = 1$. (B) $x = 2/3$. (C) $x = 1/3$. (D) The first band that crosses the Fermi surface for $x = 0$. (E) The second band that crosses the Fermi surface for $x = 0$. (F) Superposition of bands (D and E) that gives the total Fermi surface topology for $x = 0$ with possible nesting vectors drawn in arrows. 51 x 51 k points were used for the calculation of the Fermi surface.

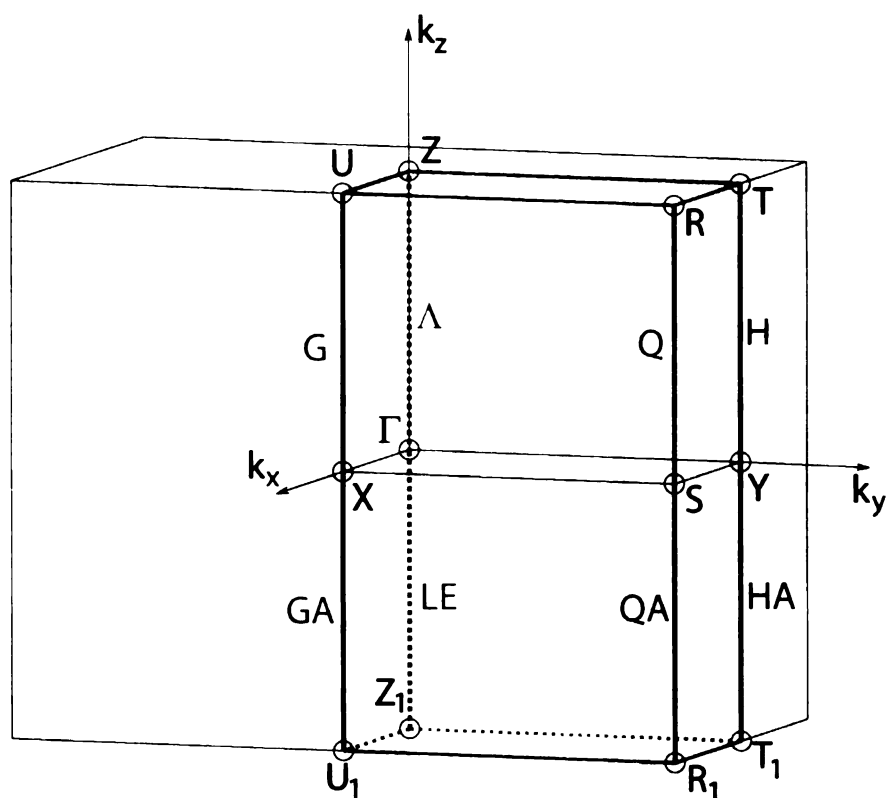


Figure 6.19. Brillouin zone of Pmm2 space group.¹⁶

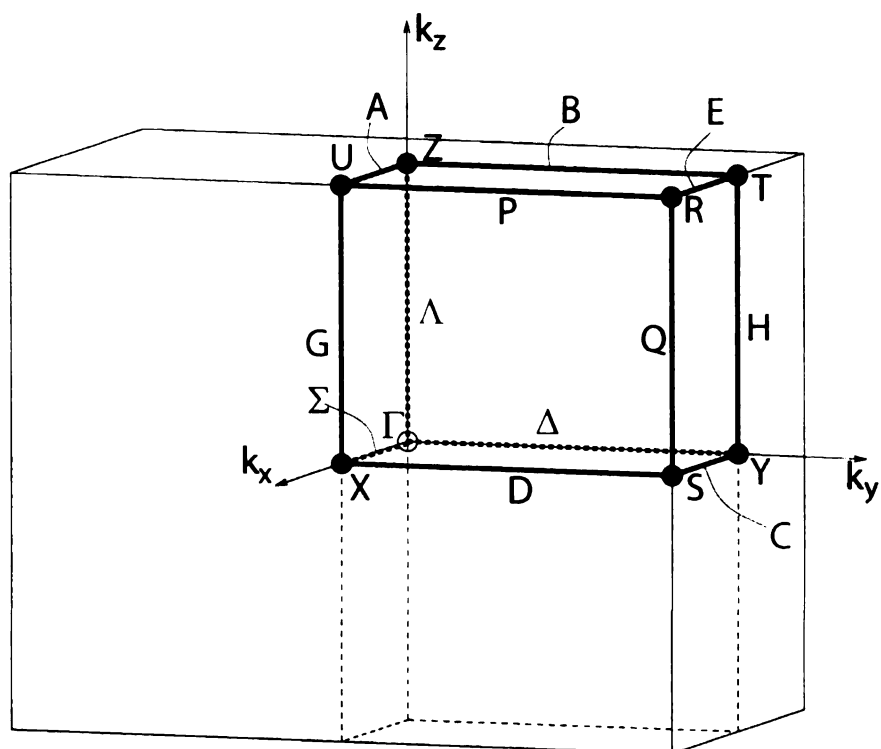


Figure 6.20. Brillouin zone of Pmmn space group.¹⁶

6.4. Conclusions

The AM_2EuTe_4 series ($A = Na, K, Rb, Cs$; $M = Cu, Ag$) seems to be the missing link between the $RETe_3$ and $AMRETe_4$ ($RE = \text{Rare earth}$; $A = Na, K$; $M = Cu, Ag$) compounds. A continuous variation of increasing dimensionality from RbM_2EuTe_4 to NaM_2EuTe_4 seems to have an opposite trend from the chemical pressure effect. The q -vector increases (from ~ 0.26 to ~ 0.31) with the cross-plane interactions between the distorted Te nets. At the same time the length of the q -vector decreases with increasing the size of the atoms. This suggests that the two types of dimensionality changes, cross plane (third-dimension) and in plane (chemical pressure) have competing effects on the CDW distortions. In the case of $RETe_3$, $AMRETe_4$, and AM_2EuTe_4 where a well defined van der Waals is present, the system seems to distort with an intermediate q -vector that results from the two competing phenomena. The energetic cost from the two possible different q -vector lengths can be relieved through the van der Waals gap that decreases the strain that is created from the two different periodicities in the system. The extended three-dimensional interactions in Cu_xEuTe_2 force the system to preserve the two different modulation vectors coming from the two competing effects since there is no van der Waals gap. Therefore, one vector is created due to chemical pressure (size of Eu) and another vector from the cross-plane interactions.

The new results reported here add more information to the understanding of CDW distortions and the effect of the structure on the CDW modulations. This gives some clues on the anomalous behavior of temperature and RE size that was observed in the $RETe_3$ family. A temperature difference would most likely affect the van der Waals gap (cross-plane interaction between the Te nets) more than the size of the RE atom.

Similarly, a change in the size of the RE (chemical pressure) from LaTe_3 to TmTe_3 would not affect significantly the spacing of the distorted Te nets. Therefore the average q -vector resulting from the two different effects (chemical pressure and dimensionality) should have a diverging trend depended on the most favorable interaction. In this extent, a more conclusive experiment would be the application of physical pressure that most probably will affect the van der Waals gap even more and contrast the two competing trends.

Table 6.2. Crystal data and structure refinement for Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 100 K.

Empirical formula	Na _{0.80(2)} Cu ₂ Eu _{1.20(2)} Te ₄
Formula weight	838.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.3692(7) Å, α = 90° b = 4.3790(6) Å, β = 90° c = 10.5877(18) Å, γ = 90°
q-vector	0.3122(7)b* + 1/2c*
Volume	202.57(5) Å ³
Z	1
Density (calculated)	6.8690 g/cm ³
Absorption coefficient	28.385 mm ⁻¹
F(000)	350
Crystal size	0.21 x 0.10 x 0.01 mm ³
Theta range for data collection	1.74 to 29.01°
Index ranges	-5 ≤ h ≤ 5, -5 ≤ k ≤ 5, -14 ≤ l ≤ 14, -1 ≤ m ≤ 1
Reflections collected	5406 (1756 main + 3650 satellites)
Independent reflections	2744 (979 main + 1765 satellites) [R _{int} = 0.0348]
Completeness to θ = 29.01°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2744 / 28 / 123
Goodness-of-fit on F ²	1.21
Final R indices [I > 2σ(I)]	R _{obs} = 0.0271, wR _{obs} = 0.0764
R indices (all data)	R _{all} = 0.0513, wR _{all} = 0.0847
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0215, wR _{obs} = 0.0685
R main indices (all data)	R _{all} = 0.0249, wR _{all} = 0.0713
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0675, wR _{obs} = 0.1010
R 1 st order satellites (all data)	R _{all} = 0.1912, wR _{all} = 0.1230
T _{min} and T _{max} coefficients	0.0451 and 0.7883
Largest diff. peak and hole	1.88 and -1.18 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²) ²] / Σ[w(F _o ⁴)]} ^{1/2} and w = 1/(σ ² (I) + 0.0016I ²)	

Table 6.3. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu[1]	0	0	0	2749	0.566(9)	7(1)
	sin, 1	7(6)	4(3)	0(2)		
	cos, 1	6(5)	-5(4)	0(2)		
Eu[2]	0	5001(2)	5000	7737(1)	0.629(10)	11(1)
	sin, 1	-77(2)	-21(7)	0(1)		
	cos, 1	90(3)	-18(6)	0(1)		
Te[1]	0	5000(5)	5000	3747(2)	1	8(1)
	sin, 1	-34(2)	2(1)	1(1)		
	cos, 1	-14(1)	-6(3)	0(1)		
Te[2]	0	10004(5)	0	6681(2)	1	11(1)
	sin, 1	-32(2)	-1(2)	0(1)		
	cos, 1	19(1)	-2(3)	0(1)		
Te[3]	0	4995(6)	0	235(2)	1	9(1)
	sin, 1	-18(1)	19(8)	-1(1)		
	cos, 1	-249(6)	-1(1)	-12(2)		
Te[4]	0	9992(6)	5000	221(2)	1	8(1)
	sin, 1	18(1)	-14(8)	-1(1)		
	cos, 1	253(5)	1(1)	-11(2)		
Cu[1]	0	10010(9)	5000	5222(4)	1	11(1)
	sin, 1	-286(15)	-2(1)	-27(4)		
	cos, 1	20(1)	-31(11)	2(1)		
Cu[2]	0	4994(10)	0	5211(4)	1	23(1)
	sin, 1	224(16)	0(1)	-26(5)		
	cos, 1	-15(1)	2(13)	2(1)		
Na[1]	0	0	0	2749	0.434(9)	7(1)
	sin, 1	7(6)	4(3)	0(2)		
	cos, 1	6(5)	-5(4)	0(2)		
Na[2]	0	5001	5000	7737	0.371(10)	11(1)
	sin, 1	-77(2)	-21(7)	0(1)		
	cos, 1	90(3)	-18(6)	0(1)		

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 6.4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu[1]	0	2(1)	8(1)	12(1)	0	1(1)	0
	sin, 1	1(1)	-1(1)	0(1)	1(1)	1(1)	-1(1)
	cos, 1	0(1)	-1(1)	0(1)	-1(1)	1(1)	1(1)
Eu[2]	0	9(1)	11(1)	13(1)	0	0(1)	0
	sin, 1	-3(1)	-2(1)	1(1)	0(1)	-1(1)	-1(1)
	cos, 1	4(1)	3(1)	-1(1)	0(1)	1(1)	-1(1)
Te[1]	0	3(1)	8(1)	14(1)	0	0(1)	0
	sin, 1	-1(1)	0(1)	-1(1)	0(1)	1(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	0(1)	-1(1)
Te[2]	0	7(1)	8(1)	17(1)	0	1(1)	0
	sin, 1	-1(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	1(1)	0(1)	0(1)	0(1)	0(1)	1(1)
Te[3]	0	9(1)	5(1)	12(1)	0	1(1)	0
	sin, 1	-1(1)	0(1)	0(1)	1(1)	0(1)	2(1)
	cos, 1	-11(1)	-1(1)	6(1)	0(1)	-2(1)	0(1)
Te[4]	0	10(1)	5(1)	8(1)	0	-1(1)	0
	sin, 1	1(1)	0(1)	0(1)	-3(1)	0(1)	1(1)
	cos, 1	12(1)	0(1)	-6(1)	0(1)	0(1)	0(1)
Cu[1]	0	12(2)	11(2)	11(1)	0	6(1)	0
	sin, 1	-12(2)	0(2)	2(2)	0(1)	-5(1)	0(1)
	cos, 1	1(1)	0(1)	0(1)	-2(2)	0(1)	1(2)
Cu[2]	0	19(2)	33(2)	15(1)	0	-8(1)	0
	sin, 1	9(2)	1(3)	-9(2)	0(1)	1(1)	0(1)
	cos, 1	-1(1)	0(1)	1(1)	6(2)	0(1)	-2(2)
Na[1]	0	2(1)	8(1)	12(1)	0	1(1)	0
	sin, 1	1(1)	-1(1)	0(1)	1(1)	1(1)	-1(1)
	cos, 1	0(1)	-1(1)	0(1)	-1(1)	1(1)	1(1)
Na[2]	0	9(1)	11(1)	13(1)	0	0(1)	0
	sin, 1	-3(1)	-2(1)	1(1)	0(1)	-1(1)	-1(1)
	cos, 1	4(1)	3(1)	-1(1)	0(1)	1(1)	-1(1)

Table 6.5. Bond lengths distributions [Å] for $\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu[1] - Te[1] x 4	3.286(3)	3.272(3)	3.300(3)
Eu[1] - Te[3] x 2	3.406(4)	3.323(4)	3.489(4)
Eu[1] - Te[4] x 2	3.419(3)	3.408(3)	3.431(3)
Eu[1] - Cu[1] x 2	3.454(5)	3.433(5)	3.477(5)
Eu[1] - Cu[2] x 2	3.442(6)	3.361(8)	3.525(8)
Te[1] - Cu[1] x 2	2.683(6)	2.612(7)	2.755(7)
Te[1] - Cu[2] x 2	2.684(5)	2.670(4)	2.700(4)
Te[2] - Cu[1] x 2	2.681(4)	2.661(4)	2.701(4)
Te[2] - Cu[2] x 2	2.685(6)	2.609(8)	2.764(8)
Te[2] - Eu[2] x 4	3.290(3)	3.261(3)	3.319(3)
Te[3] - Te[4] x 4	3.094(4)	2.961(3)	3.234(4)
Te[3] - Eu[2] x 2	3.435(3)	3.415(3)	3.454(3)
Te[4] - Eu[2] x 2	3.417(3)	3.388(4)	3.446(4)
Cu[1] - Cu[2] x 4	3.098(7)	2.965(7)	3.237(7)
Cu[1] - Eu[2] x 2	3.447(5)	3.423(7)	3.472(7)
Cu[2] - Eu[2] x 2	3.458(5)	3.430(6)	3.487(6)

Table 6.6. Bond angles distributions [°] for $\text{Na}_{0.80(2)}\text{Cu}_2\text{Eu}_{1.20(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu[1] - Te[1] x 8	83.58(7)	83.37(7)	83.78(7)
Te[1] - Eu[1] - Te[1] x 4	140.56(9)	140.44(9)	140.67(9)
Te[1] - Eu[1] - Te[3] x 4	80.31(8)	79.25(8)	81.42(8)
Te[1] - Eu[1] - Te[3] x 4	133.24(9)	132.60(9)	133.86(8)
Te[1] - Eu[1] - Te[4] x 4	80.31(7)	78.98(7)	81.62(7)
Te[1] - Eu[1] - Te[4] x 4	133.26(9)	131.56(9)	134.93(9)
Te[1] - Eu[1] - Cu[1] x 4	46.93(12)	45.05(12)	48.82(12)
Te[1] - Eu[1] - Cu[1] x 4	99.34(12)	98.18(11)	100.50(11)
Te[1] - Eu[1] - Cu[2] x 4	46.94(7)	46.58(7)	47.30(7)
Te[1] - Eu[1] - Cu[2] x 4	99.27(11)	98.01(11)	100.49(11)
Te[3] - Eu[1] - Te[3] x 2	79.82(8)	79.50(8)	80.09(9)
Te[3] - Eu[1] - Te[4] x 4	53.91(7)	51.95(7)	55.87(7)

Table 6.6. (Cont'd) Bond angles distributions [°] for Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Eu[1] - Cu[1] x 4	126.38(13)	123.96(13)	128.81(12)
Te[3] - Eu[1] - Cu[2] x 2	100.63(15)	100.26(16)	101.05(15)
Te[3] - Eu[1] - Cu[2] x 2	179.43(16)	179.23(16)	179.64(16)
Te[4] - Eu[1] - Te[4] x 2	79.69(8)	79.39(8)	79.94(8)
Te[4] - Eu[1] - Cu[1] x 2	100.83(8)	100.61(8)	101.11(8)
Te[4] - Eu[1] - Cu[1] x 2	177.81(15)	176.65(15)	180
Te[4] - Eu[1] - Cu[2] x 4	126.33(11)	124.47(11)	128.14(11)
Cu[1] - Eu[1] - Cu[1] x 2	78.73(10)	78.05(10)	79.32(10)
Cu[1] - Eu[1] - Cu[2] x 4	53.38(12)	51.55(13)	55.26(14)
Cu[2] - Eu[1] - Cu[2] x 2	78.80(17)	78.18(18)	79.38(19)
Eu[1] - Te[1] - Eu[1] x 8	83.58(7)	83.14(7)	84.01(7)
Eu[1] - Te[1] - Eu[1] x 4	140.56(9)	140.53(9)	140.58(9)
Eu[1] - Te[1] - Cu[1] x 4	69.89(11)	68.79(11)	71.04(12)
Eu[1] - Te[1] - Cu[1] x 4	137.49(6)	137.12(6)	137.85(6)
Eu[1] - Te[1] - Cu[2] x 4	69.56(16)	68.37(16)	70.74(16)
Eu[1] - Te[1] - Cu[2] x 4	137.6(2)	135.10(19)	140.1(2)
Cu[1] - Te[1] - Cu[1] x 2	108.86(19)	107.8(2)	109.8(2)
Cu[1] - Te[1] - Cu[2] x 4	70.33(19)	67.26(18)	73.37(19)
Cu[2] - Te[1] - Cu[2] x 2	109.41(18)	108.80(17)	109.91(17)
Cu[1] - Te[2] - Cu[1] x 2	109.62(16)	109.32(16)	109.83(16)
Cu[1] - Te[2] - Cu[2] x 4	70.52(14)	67.58(17)	73.54(18)
Cu[1] - Te[2] - Eu[2] x 4	69.67(12)	68.44(14)	70.93(14)
Cu[1] - Te[2] - Eu[2] x 4	137.76(14)	135.70(18)	139.86(18)
Cu[2] - Te[2] - Cu[2] x 2	109.0(2)	108.1(2)	109.9(2)
Cu[2] - Te[2] - Eu[2] x 4	69.88(11)	68.52(11)	71.23(12)
Cu[2] - Te[2] - Eu[2] x 4	137.56(10)	136.94(8)	138.19(8)
Eu[2] - Te[2] - Eu[2] x 8	83.45(8)	83.44(8)	83.46(8)
Eu[2] - Te[2] - Eu[2] x 4	140.24(9)	139.87(9)	140.60(8)
Eu[1] - Te[3] - Eu[1] x 2	79.82(8)	79.50(9)	80.09(9)
Eu[1] - Te[3] - Te[4] x 4	63.32(8)	61.19(8)	65.45(8)
Eu[1] - Te[3] - Te[4] x 4	117.08(9)	116.49(11)	117.75(11)
Eu[1] - Te[3] - Eu[2] x 4	126.26(9)	123.39(9)	129.05(9)
Te[4] - Te[3] - Te[4] x 8	90.25(11)	85.91(12)	94.62(13)
Te[4] - Te[3] - Te[4] x 4	177.04(13)	175.41(13)	179.50(11)

Table 6.6. (Cont'd) Bond angles distributions [°] for Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Te[4] - Te[3] - Eu[2] x 4	62.95(7)	62.05(7)	63.87(7)
Te[4] - Te[3] - Eu[2] x 4	116.66(11)	113.61(11)	119.63(12)
Eu[2] - Te[3] - Eu[2] x 2	79.21(8)	79.16(9)	79.25(8)
Eu[1] - Te[4] - Eu[1] x 2	79.65(7)	79.44(8)	79.81(8)
Eu[1] - Te[4] - Te[3] x 4	62.81(8)	61.83(8)	63.87(8)
Eu[1] - Te[4] - Te[3] x 4	116.79(11)	114.11(11)	119.48(12)
Eu[1] - Te[4] - Eu[2] x 4	126.26(10)	124.35(10)	128.18(9)
Te[3] - Te[4] - Te[3] x 8	90.25(12)	86.01(12)	94.67(13)
Te[3] - Te[4] - Te[3] x 4	177.05(13)	175.42(12)	179.49(11)
Te[3] - Te[4] - Eu[2] x 4	63.46(9)	61.67(8)	65.33(9)
Te[3] - Te[4] - Eu[2] x 4	117.03(10)	116.10(10)	117.85(9)
Eu[2] - Te[4] - Eu[2] x 2	79.41(7)	79.17(7)	79.64(7)
Eu[1] - Cu[1] - Eu[1] x 2	78.68(11)	77.97(13)	79.32(14)
Eu[1] - Cu[1] - Te[1] x 4	63.25(11)	61.77(12)	64.71(13)
Eu[1] - Cu[1] - Te[2] x 2	85.80(10)	85.46(9)	86.19(12)
Eu[1] - Cu[1] - Te[2] x 2	164.22(17)	163.03(18)	165.04(16)
Eu[1] - Cu[1] - Cu[2] x 4	63.09(15)	61.98(14)	64.31(15)
Eu[1] - Cu[1] - Cu[2] x 4	116.4(2)	113.2(2)	119.6(2)
Eu[1] - Cu[1] - Eu[2] x 4	126.62(14)	124.36(17)	128.82(16)
Te[1] - Cu[1] - Te[1] x 2	108.86(18)	107.8(2)	109.8(2)
Te[1] - Cu[1] - Te[2] x 4	109.52(16)	106.64(19)	112.36(19)
Te[1] - Cu[1] - Cu[2] x 4	54.76(15)	52.51(15)	57.05(17)
Te[1] - Cu[1] - Cu[2] x 4	124.83(18)	123.31(18)	126.19(18)
Te[1] - Cu[1] - Eu[2] x 2	86.12(15)	84.04(19)	88.2(2)
Te[1] - Cu[1] - Eu[2] x 2	164.8(2)	163.4(3)	166.3(3)
Te[2] - Cu[1] - Te[2] x 2	109.52(18)	108.5(2)	110.4(2)
Te[2] - Cu[1] - Cu[2] x 4	54.77(15)	53.74(14)	55.90(14)
Te[2] - Cu[1] - Cu[2] x 4	125.4(2)	121.7(3)	129.0(3)
Te[2] - Cu[1] - Eu[2] x 4	63.51(12)	62.57(14)	64.40(14)
Cu[2] - Cu[1] - Cu[2] x 8	90.1(2)	85.5(2)	94.8(3)
Cu[2] - Cu[1] - Cu[2] x 4	176.9(2)	175.0(2)	179.6(2)
Cu[2] - Cu[1] - Eu[2] x 4	63.53(14)	61.55(15)	65.54(16)
Cu[2] - Cu[1] - Eu[2] x 4	116.74(16)	115.67(17)	117.72(17)
Eu[2] - Cu[1] - Eu[2] x 2	78.72(11)	78.10(13)	79.32(13)

Table 6.6. (Cont'd) Bond angles distributions [°] for Na_{0.80(2)}Cu₂Eu_{1.20(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Eu[1] - Cu[2] - Eu[1] x 2	78.80(13)	78.18(15)	79.38(15)
Eu[1] - Cu[2] - Te[1] x 4	63.48(12)	62.82(14)	64.12(14)
Eu[1] - Cu[2] - Te[2] x 2	86.13(17)	83.7(2)	88.6(2)
Eu[1] - Cu[2] - Te[2] x 2	164.8(2)	161.4(3)	168.2(3)
Eu[1] - Cu[2] - Cu[1] x 4	63.61(16)	61.57(15)	65.73(17)
Eu[1] - Cu[2] - Cu[1] x 4	116.77(18)	115.85(19)	117.77(18)
Eu[1] - Cu[2] - Eu[2] x 4	126.73(16)	124.20(18)	129.26(17)
Te[1] - Cu[2] - Te[1] x 2	109.4(2)	108.2(2)	110.3(2)
Te[1] - Cu[2] - Te[2] x 4	109.63(19)	106.9(2)	112.4(2)
Te[1] - Cu[2] - Cu[1] x 4	54.79(14)	54.01(14)	55.62(14)
Te[1] - Cu[2] - Cu[1] x 4	125.5(2)	122.3(3)	128.7(3)
Te[1] - Cu[2] - Eu[2] x 2	85.94(11)	85.55(8)	86.31(8)
Te[1] - Cu[2] - Eu[2] x 2	164.28(19)	163.3(2)	164.82(18)
Te[2] - Cu[2] - Te[2] x 2	109.0(2)	108.1(2)	109.9(2)
Te[2] - Cu[2] - Cu[1] x 4	54.85(15)	52.72(15)	57.09(17)
Te[2] - Cu[2] - Cu[1] x 4	124.92(19)	123.43(18)	126.29(18)
Te[2] - Cu[2] - Eu[2] x 4	63.31(11)	61.85(11)	64.79(12)
Cu[1] - Cu[2] - Cu[1] x 8	90.4(2)	86.3(2)	94.6(3)
Cu[1] - Cu[2] - Cu[1] x 4	177.1(2)	175.4(2)	179.6(2)
Cu[1] - Cu[2] - Eu[2] x 4	63.12(13)	62.22(11)	64.12(11)
Cu[1] - Cu[2] - Eu[2] x 4	116.52(19)	113.6(2)	119.5(2)
Eu[2] - Cu[2] - Eu[2] x 2	78.59(13)	78.23(15)	78.88(15)
Te[2] - Eu[2] - Te[2] x 8	83.51(5)	82.60(5)	84.41(5)
Te[2] - Eu[2] - Te[2] x 4	140.23(7)	140.12(7)	140.35(7)
Te[2] - Eu[2] - Te[3] x 4	80.62(8)	79.03(8)	82.16(8)
Te[2] - Eu[2] - Te[3] x 4	133.32(8)	130.70(8)	135.92(8)
Te[2] - Eu[2] - Te[4] x 4	80.61(8)	80.43(8)	80.79(8)
Te[2] - Eu[2] - Te[4] x 4	133.28(10)	132.72(10)	133.85(10)
Te[2] - Eu[2] - Cu[1] x 4	46.86(6)	46.75(6)	46.98(6)
Te[2] - Eu[2] - Cu[1] x 4	99.13(11)	97.79(11)	100.47(11)
Te[2] - Eu[2] - Cu[2] x 4	46.73(14)	44.89(14)	48.51(14)
Te[2] - Eu[2] - Cu[2] x 4	99.08(12)	97.69(12)	100.44(12)
Te[3] - Eu[2] - Te[3] x 2	79.24(7)	78.87(7)	79.51(7)
Te[3] - Eu[2] - Te[4] x 4	53.69(8)	51.55(8)	55.82(8)

Table 6.7. Crystal data and structure refinement for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K.

Empirical formula	Na _{0.81(2)} Ag ₂ Eu _{1.19(2)} Te ₄
Formula weight	926.9
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.4185(6) Å, α = 90° b = 4.4435(7) Å, β = 90° c = 11.0767(17) Å, γ = 90°
q-vector	0.3134(6)b* + 1/2c*
Volume	217.48(6) Å ³
Z	1
Density (calculated)	7.0749 g/cm ³
Absorption coefficient	25.987 mm ⁻¹
F(000)	385
Crystal size	0.16 x 0.09 x 0.01 mm ³
Theta range for data collection	3.10 to 28.94°
Index ranges	-5 ≤ h ≤ 5, -6 ≤ k ≤ 6, -15 ≤ l ≤ 15, -1 ≤ m ≤ 1
Reflections collected	5470 (1725 main + 3745 satellites)
Independent reflections	3175 (1071 main + 2104 satellites) [R _{int} = 0.0293]
Completeness to θ = 28.94°	97%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3175 / 28 / 122
Goodness-of-fit on F ²	2.43
Final R indices [I > 2σ(I)]	R _{obs} = 0.0577, wR _{obs} = 0.1431
R indices (all data)	R _{all} = 0.0854, wR _{all} = 0.1747
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0512, wR _{obs} = 0.1436
R main indices (all data)	R _{all} = 0.0550, wR _{all} = 0.1732
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0880, wR _{obs} = 0.1411
R 1 st order satellites (all data)	R _{all} = 0.1986, wR _{all} = 0.1800
T _{min} and T _{max} coefficients	0.0897 and 0.8062
Largest diff. peak and hole	5.89 and -7.48 e.Å ⁻³

$$R = \sum |F_o| - |F_c| / \sum |F_o|, wR = \{ \sum [w(|F_o|^2 - |F_c|^2)^2] / \sum [w(|F_o|^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$$

Table 6.8. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu[1]	0	0	0	2749	0.577(14)	14(1)
	sin, 1	37(9)	0(3)	-6(3)		
	cos, 1	33(8)	1(3)	-5(2)		
Eu[2]	0	5021(4)	5000	8021(2)	0.605(14)	11(1)
	sin, 1	68(3)	3(5)	-1(2)		
	cos, 1	-95(4)	2(4)	1(3)		
Te[1]	0	5039(8)	5000	3688(3)	1	12(1)
	sin, 1	38(3)	1(1)	0(2)		
	cos, 1	17(1)	-2(3)	0(1)		
Te[2]	0	20(8)	0	7023(3)	1	11(1)
	sin, 1	30(3)	0(2)	0(2)		
	cos, 1	-22(2)	0(3)	0(1)		
Te[3]	0	4998(8)	0	393(4)	1	15(1)
	sin, 1	31(1)	32(6)	-1(1)		
	cos, 1	250(11)	-4(1)	-8(3)		
Te[4]	0	7(8)	5000	387(4)	1	13(1)
	sin, 1	-35(1)	-26(6)	-1(1)		
	cos, 1	-285(10)	3(1)	-9(3)		
Ag[1]	0	9911(7)	5000	5371(4)	1	9(1)
	sin, 1	228(13)	-3(1)	-16(3)		
	cos, 1	-27(2)	-25(7)	2(1)		
Ag[2]	0	4953(7)	0	5363(5)	1	15(1)
	sin, 1	-212(15)	2(1)	-26(4)		
	cos, 1	24(2)	21(7)	3(1)		
Na[1]	0	0	0	2749	0.423(14)	14(1)
	sin, 1	37(9)	0(3)	-6(3)		
	cos, 1	33(8)	1(3)	-5(2)		
Na[2]	0	5021	5000	8021	0.395(14)	11(1)
	sin, 1	68(3)	3(5)	-1(2)		
	cos, 1	-95(4)	2(4)	1(3)		

Table 6.9. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu[1]	0	13(1)	15(1)	14(1)	0	6(1)	0
	sin, 1	-2(1)	0(1)	-4(1)	-1(1)	-5(1)	-1(1)
	cos, 1	-2(1)	0(1)	-3(1)	2(1)	-4(1)	1(1)
Eu[2]	0	15(1)	1(1)	17(1)	0	2(1)	0
	sin, 1	-5(1)	0(1)	0(1)	0(1)	-1(1)	-1(1)
	cos, 1	7(1)	0(1)	0(1)	0(1)	2(1)	-1(1)
Te[1]	0	12(1)	9(1)	15(1)	0	6(1)	0
	sin, 1	-3(1)	0(1)	2(1)	0(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	1(1)	0(1)	0(1)	0(1)
Te[2]	0	15(1)	1(1)	16(1)	0	4(1)	0
	sin, 1	-2(1)	0(1)	1(1)	0(1)	-1(1)	0(1)
	cos, 1	2(1)	0(1)	-1(1)	0(1)	1(1)	0(1)
Te[3]	0	30(1)	7(1)	9(1)	0	2(1)	0
	sin, 1	-1(1)	0(1)	1(1)	-3(1)	0(1)	-1(1)
	cos, 1	-9(2)	-3(1)	4(1)	0(1)	3(1)	0(1)
Te[4]	0	13(1)	8(1)	18(1)	0	0(1)	0
	sin, 1	3(1)	0(1)	0(1)	2(1)	1(1)	0(1)
	cos, 1	22(2)	-1(1)	-3(1)	0(1)	9(1)	0(1)
Ag[1]	0	6(1)	11(1)	11(1)	0	-6(1)	0
	sin, 1	-1(2)	-5(1)	-1(1)	1(1)	5(1)	0(1)
	cos, 1	0(1)	1(1)	0(1)	5(1)	-1(1)	0(1)
Ag[2]	0	11(1)	9(1)	26(1)	0	7(1)	0
	sin, 1	9(2)	-5(1)	-5(2)	0(1)	6(1)	0(1)
	cos, 1	-1(1)	1(1)	1(1)	-3(1)	-1(1)	0(1)
Na[1]	0	13(1)	15(1)	14(1)	0	6(1)	0
	sin, 1	-2(1)	0(1)	-4(1)	-1(1)	-5(1)	-1(1)
	cos, 1	-2(1)	0(1)	-3(1)	2(1)	-4(1)	1(1)
Na[2]	0	15(1)	1(1)	17(1)	0	2(1)	0
	sin, 1	-5(1)	0(1)	0(1)	0(1)	-1(1)	-1(1)
	cos, 1	7(1)	0(1)	0(1)	0(1)	2(1)	-1(1)

Table 6.10. Bond lengths distributions [Å] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu[1] - Te[1] x 2	3.307(4)	3.292(4)	3.323(4)
Eu[1] - Te[1] x 2	3.330(4)	3.319(4)	3.341(4)
Eu[1] - Te[3] x 2	3.379(6)	3.322(7)	3.438(7)
Eu[1] - Te[4] x 2	3.392(5)	3.378(5)	3.404(5)
Eu[2] - Te[2] x 4	3.323(4)	3.293(4)	3.352(4)
Eu[2] - Te[3] x 2	3.442(5)	3.430(5)	3.452(5)
Eu[2] - Te[4] x 2	3.432(6)	3.392(6)	3.472(6)
Te[1] - Ag[1]	2.934(6)	2.859(7)	3.011(7)
Te[1] - Ag[1]	2.849(6)	2.798(7)	2.899(7)
Te[1] - Ag[2] x 2	2.896(5)	2.878(5)	2.915(5)
Te[1] - Na[1] x 2	3.330(4)	3.319(4)	3.341(4)
Te[1] - Na[1] x 2	3.307(4)	3.292(4)	3.323(4)
Te[2] - Ag[1] x 2	2.880(4)	2.866(4)	2.893(4)
Te[2] - Ag[2]	2.899(7)	2.794(8)	3.002(8)
Te[2] - Ag[2]	2.852(7)	2.788(8)	2.919(8)
Te[2] - Na[2] x 4	3.322(4)	3.292(3)	3.353(4)
Te[3] - Te[4] x 4	3.133(5)	2.984(5)	3.284(5)
Te[3] - Na[1] x 2	3.379(6)	3.319(7)	3.437(7)
Te[3] - Na[2] x 2	3.442(5)	3.430(5)	3.452(5)
Te[4] - Na[1] x 2	3.392(5)	3.378(5)	3.404(5)
Te[4] - Na[2] x 2	3.424(5)	3.367(6)	3.481(6)
Ag[1] - Ag[2] x 2	3.122(5)	3.000(6)	3.244(6)
Ag[1] - Ag[2] x 2	3.147(5)	3.026(6)	3.271(6)

Table 6.11. Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu[1] - Te[1] x 2	84.41(10)	84.10(10)	84.72(11)
Te[1] - Eu[1] - Te[1] x 6	83.47(9)	83.37(9)	83.57(9)
Te[1] - Eu[1] - Te[1] x 4	141.50(13)	141.21(13)	141.80(13)
Te[1] - Eu[1] - Te[3] x 4	79.45(11)	78.54(11)	80.36(11)
Te[1] - Eu[1] - Te[3] x 4	133.12(10)	132.49(10)	133.73(9)

Table 6.11. (Cont'd) Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Eu[1] - Te[4] x 4	79.06(9)	77.59(10)	80.56(9)
Te[1] - Eu[1] - Te[4] x 4	133.66(14)	131.34(13)	136.01(13)
Te[3] - Eu[1] - Te[3] x 2	81.66(12)	81.62(14)	81.68(11)
Te[3] - Eu[1] - Te[4] x 4	55.19(9)	52.88(9)	57.56(9)
Te[4] - Eu[1] - Te[4] x 2	81.88(11)	81.66(11)	82.01(11)
Te[2] - Eu[2] - Te[2] x 4	83.93(9)	83.08(9)	84.79(9)
Te[2] - Eu[2] - Te[2] x 4	83.35(9)	83.31(9)	83.40(9)
Te[2] - Eu[2] - Te[2] x 4	141.13(13)	141.00(12)	141.26(12)
Te[2] - Eu[2] - Te[3] x 4	79.62(9)	78.15(9)	81.12(9)
Te[2] - Eu[2] - Te[3] x 4	133.14(12)	130.37(11)	135.91(11)
Te[2] - Eu[2] - Te[4] x 4	79.92(10)	79.46(10)	80.38(10)
Te[2] - Eu[2] - Te[4] x 4	133.04(10)	132.51(10)	133.57(10)
Te[2] - Eu[2] - Ag[1] x 2	97.26(12)	96.49(12)	98.01(12)
Te[2] - Eu[2] - Ag[1] x 2	48.55(8)	48.42(8)	48.67(8)
Te[3] - Eu[2] - Te[3] x 2	80.45(10)	79.94(10)	80.86(10)
Te[3] - Eu[2] - Te[4] x 4	54.19(10)	51.72(10)	56.75(11)
Te[3] - Eu[2] - Ag[1] x 2	128.09(11)	126.21(12)	129.91(12)
Te[4] - Eu[2] - Te[4] x 2	80.24(12)	79.99(13)	80.48(13)
Te[4] - Eu[2] - Ag[1]	176.15(15)	174.60(16)	177.71(16)
Te[4] - Eu[2] - Ag[1]	103.59(14)	102.30(15)	104.92(15)
Eu[1] - Te[1] - Eu[1] x 6	83.70(11)	83.51(11)	83.88(11)
Eu[1] - Te[1] - Eu[1] x 4	141.50(14)	141.28(15)	141.72(15)
Eu[1] - Te[1] - Ag[1] x 2	72.11(13)	71.42(12)	72.79(13)
Eu[1] - Te[1] - Ag[1] x 4	136.08(8)	135.57(9)	136.56(8)
Eu[1] - Te[1] - Ag[2] x 2	71.91(14)	70.22(14)	73.63(14)
Eu[1] - Te[1] - Ag[2] x 2	135.5(2)	133.4(2)	137.7(2)
Eu[1] - Te[1] - Eu[1] x 2	84.41(11)	84.34(11)	84.48(11)
Eu[1] - Te[1] - Ag[1] x 2	73.48(13)	72.64(13)	74.35(13)
Eu[1] - Te[1] - Ag[2] x 2	72.88(14)	71.58(14)	74.16(14)
Eu[1] - Te[1] - Ag[2] x 2	137.4(2)	135.1(2)	139.7(2)
Ag[1] - Te[1] - Ag[1] x 2	99.63(19)	99.0(2)	100.2(2)
Ag[1] - Te[1] - Ag[2] x 4	65.31(16)	63.59(16)	67.08(16)
Ag[2] - Te[1] - Ag[2] x 2	100.25(18)	99.94(18)	100.47(18)
Eu[2] - Te[2] - Eu[2] x 4	83.95(10)	83.71(10)	84.17(11)

Table 6.11. (Cont'd) Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Eu[2] - Te[2] - Eu[2] x 4	83.35(7)	83.31(7)	83.40(7)
Eu[2] - Te[2] - Eu[2] x 4	141.14(14)	140.79(14)	141.49(14)
Eu[2] - Te[2] - Ag[1] x 2	71.59(13)	70.26(13)	72.91(13)
Eu[2] - Te[2] - Ag[1] x 2	135.77(19)	134.39(19)	137.12(19)
Eu[2] - Te[2] - Ag[2] x 4	72.39(13)	71.76(13)	73.04(13)
Eu[2] - Te[2] - Ag[2] x 4	136.25(8)	135.51(9)	137.02(8)
Eu[2] - Te[2] - Ag[1] x 2	72.93(13)	71.98(13)	73.88(13)
Eu[2] - Te[2] - Ag[1] x 2	137.61(19)	136.12(19)	139.13(19)
Ag[1] - Te[2] - Ag[1] x 2	101.03(17)	100.96(16)	101.07(17)
Ag[1] - Te[2] - Ag[2] x 2	65.40(14)	63.82(15)	66.97(16)
Ag[1] - Te[2] - Ag[2] x 2	66.58(14)	64.18(16)	69.05(16)
Ag[2] - Te[2] - Ag[2] x 2	100.4(2)	99.4(2)	101.3(2)
Eu[1] - Te[3] - Eu[1] x 2	81.66(14)	81.62(15)	81.68(13)
Eu[1] - Te[3] - Eu[2] x 4	125.39(12)	122.63(13)	128.17(13)
Eu[1] - Te[3] - Te[4] x 4	62.68(12)	60.59(12)	64.88(13)
Eu[1] - Te[3] - Te[4] x 4	117.49(14)	116.39(14)	118.55(14)
Eu[2] - Te[3] - Eu[2] x 2	80.42(12)	80.11(13)	80.64(13)
Eu[2] - Te[3] - Te[4] x 4	62.71(11)	62.04(10)	63.29(11)
Eu[2] - Te[3] - Te[4] x 4	117.28(17)	114.31(19)	120.2(2)
Te[4] - Te[3] - Te[4] x 4	90.51(15)	85.66(16)	95.59(19)
Te[4] - Te[3] - Te[4] x 4	89.55(9)	89.08(10)	90.27(9)
Te[4] - Te[3] - Te[4] x 4	176.95(16)	175.16(18)	179.80(19)
Eu[1] - Te[4] - Eu[1] x 2	81.83(13)	81.68(14)	81.91(12)
Eu[1] - Te[4] - Eu[2] x 4	125.29(12)	122.83(13)	127.69(13)
Eu[1] - Te[4] - Te[3] x 4	62.17(11)	61.65(11)	62.64(11)
Eu[1] - Te[4] - Te[3] x 4	117.52(17)	114.35(19)	120.6(2)
Eu[2] - Te[4] - Eu[2] x 2	80.25(13)	79.99(14)	80.48(14)
Eu[2] - Te[4] - Te[3] x 4	63.13(12)	61.16(12)	65.14(13)
Eu[2] - Te[4] - Te[3] x 4	116.99(15)	115.84(14)	118.03(14)
Te[3] - Te[4] - Te[3] x 4	90.37(14)	85.23(16)	95.61(18)
Te[3] - Te[4] - Te[3] x 4	89.55(10)	89.08(9)	90.27(10)
Te[3] - Te[4] - Te[3] x 4	176.86(16)	174.95(17)	179.8(2)
Te[1] - Ag[1] - Te[1] x 2	99.63(19)	99.0(2)	100.2(2)
Te[1] - Ag[1] - Te[2] x 2	115.37(15)	113.30(18)	117.45(17)

Table 6.11. (Cont'd) Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Ag[1] - Ag[2] x 2	57.83(15)	55.58(14)	60.18(16)
Te[1] - Ag[1] - Ag[2] x 4	122.15(17)	120.82(17)	123.53(17)
Te[1] - Ag[1] - Te[2] x 2	113.02(15)	110.85(18)	115.18(17)
Te[1] - Ag[1] - Ag[2] x 2	56.78(14)	55.11(15)	58.46(16)
Te[2] - Ag[1] - Te[2] x 2	100.98(18)	100.5(2)	101.4(2)
Te[2] - Ag[1] - Ag[2] x 2	57.57(14)	56.55(15)	58.61(14)
Te[2] - Ag[1] - Ag[2] x 2	124.3(2)	121.2(2)	127.4(3)
Te[2] - Ag[1] - Ag[2] x 2	56.26(14)	55.41(14)	57.17(14)
Te[2] - Ag[1] - Ag[2] x 2	122.3(2)	119.4(2)	125.3(2)
Ag[2] - Ag[1] - Ag[2] x 4	90.87(17)	86.73(19)	95.2(2)
Ag[2] - Ag[1] - Ag[2] x 4	89.58(13)	89.20(12)	90.14(12)
Ag[2] - Ag[1] - Ag[2] x 4	177.41(19)	175.5(2)	179.7(2)
Te[1] - Ag[2] - Te[1] x 2	100.21(19)	99.3(2)	101.0(2)
Te[1] - Ag[2] - Te[2] x 2	115.06(16)	112.50(18)	117.54(18)
Te[1] - Ag[2] - Te[2] x 2	113.35(16)	110.86(19)	115.87(19)
Te[1] - Ag[2] - Ag[1] x 2	57.91(14)	57.30(13)	58.57(13)
Te[1] - Ag[2] - Ag[1] x 4	123.6(2)	120.0(3)	127.2(3)
Te[1] - Ag[2] - Ag[1] x 2	56.33(14)	55.66(14)	57.04(14)
Te[2] - Ag[2] - Te[2] x 2	100.4(2)	99.4(2)	101.3(2)
Te[2] - Ag[2] - Ag[1] x 4	57.16(14)	54.89(14)	59.43(15)
Te[2] - Ag[2] - Ag[1] x 4	122.24(18)	121.09(18)	123.53(17)
Ag[1] - Ag[2] - Ag[1] x 8	89.97(17)	85.9(2)	94.1(2)
Ag[1] - Ag[2] - Ag[1] x 4	177.39(19)	175.6(2)	179.7(2)

Table 6.12. Crystal data and structure refinement for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 300 K.

Empirical formula	Na _{0.81(2)} Ag ₂ Eu _{1.19(2)} Te ₄
Formula weight	926.9
Temperature	300.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.4376(5) Å, α = 90° b = 4.4599(7) Å, β = 90° c = 11.1258(14) Å, γ = 90°
q-vector	0.3118(5)b* + 1/2c*
Volume	220.19(5) Å ³
Z	1
Density (calculated)	6.9876 g/cm ³
Absorption coefficient	25.666 mm ⁻¹
F(000)	386
Crystal size	0.16 x 0.09 x 0.01 mm ³
Theta range for data collection	1.69 to 29.02°
Index ranges	-5 ≤ h ≤ 5, -6 ≤ k ≤ 6, -15 ≤ l ≤ 15, -1 ≤ m ≤ 1
Reflections collected	5559 (1754 main + 3805 satellites)
Independent reflections	3187 (1073 main + 2114 satellites) [R _{int} = 0.0328]
Completeness to θ = 29.02°	95%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3187 / 26 / 121
Goodness-of-fit on F ²	1.32
Final R indices [I > 2σ(I)]	R _{obs} = 0.0342, wR _{obs} = 0.0801
R indices (all data)	R _{all} = 0.0609, wR _{all} = 0.1000
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0224, wR _{obs} = 0.0651
R main indices (all data)	R _{all} = 0.0251, wR _{all} = 0.0682
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.0829, wR _{obs} = 0.1240
R 1 st order satellites (all data)	R _{all} = 0.1807, wR _{all} = 0.1779
Extinction coefficient	0.00010(7)
T _{min} and T _{max} coefficients	0.0897 and 0.8062
Largest diff. peak and hole	1.65 and -1.67 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.13. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 300 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu[1]	0	0	0	2749	0.5854	21(1)
	sin, 1	61(7)	-7(2)	6(2)		
	cos, 1	54(7)	8(3)	6(2)		
Eu[2]	0	5000(2)	5000	8017(1)	0.605(14)	15(1)
	sin, 1	59(3)	8(3)	-1(1)		
	cos, 1	-82(4)	5(2)	1(2)		
Te[1]	0	4995(6)	5000	3690(2)	1	14(1)
	sin, 1	37(3)	-1(1)	1(1)		
	cos, 1	16(1)	1(2)	0(1)		
Te[2]	0	-4(6)	0	7018(2)	1	15(1)
	sin, 1	22(3)	1(2)	1(1)		
	cos, 1	-16(2)	1(2)	0(1)		
Te[3]	0	4982(6)	0	340(3)	1	18(1)
	sin, 1	31(1)	-41(4)	-2(1)		
	cos, 1	293(7)	4(1)	-15(2)		
Te[4]	0	9982(6)	5000	331(3)	1	16(1)
	sin, 1	-36(1)	38(4)	-2(1)		
	cos, 1	-349(7)	-4(1)	-15(2)		
Ag[1]	0	9959(6)	5000	5325(3)	1	22(1)
	sin, 1	180(14)	0(1)	-11(3)		
	cos, 1	-18(2)	3(5)	1(1)		
Ag[2]	0	4955(6)	0	5310(3)	1	27(1)
	sin, 1	-88(17)	-2(1)	-11(3)		
	cos, 1	9(2)	-25(5)	1(1)		
Na[1]	0	0	0	2749	0.4146	21(1)
	sin, 1	61(7)	-7(2)	6(2)		
	cos, 1	54(7)	8(3)	6(2)		
Na[2]	0	5000	5000	8017	0.395(14)	15(1)
	sin, 1	59(3)	8(3)	-1(1)		
	cos, 1	-82(4)	5(2)	1(2)		

Table 6.14. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Na}_{0.81(2)}\text{Ag}_2\text{Eu}_{1.19(2)}\text{Te}_4$ at 300 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu[1]	0	24(1)	26(1)	14(1)	0	-2(1)	0
	sin, 1	5(1)	-2(1)	1(1)	-4(1)	-3(1)	2(1)
	cos, 1	4(1)	-2(1)	1(1)	5(1)	-3(1)	-3(1)
Eu[2]	0	11(1)	8(1)	24(1)	0	1(1)	0
	sin, 1	5(1)	0(1)	-1(1)	-1(1)	-1(1)	2(1)
	cos, 1	-6(1)	1(1)	1(1)	-1(1)	1(1)	1(1)
Te[1]	0	15(1)	16(1)	11(1)	0	1(1)	0
	sin, 1	2(1)	-1(1)	0(1)	0(1)	1(1)	0(1)
	cos, 1	1(1)	-1(1)	0(1)	1(1)	0(1)	0(1)
Te[2]	0	11(1)	9(1)	25(1)	0	-1(1)	0
	sin, 1	-1(1)	0(1)	0(1)	0(1)	-1(1)	0(1)
	cos, 1	1(1)	0(1)	0(1)	0(1)	1(1)	0(1)
Te[3]	0	19(1)	17(1)	18(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	-4(1)	0(1)	1(1)
	cos, 1	2(2)	2(1)	-4(1)	0(1)	-1(1)	0(1)
Te[4]	0	21(1)	13(1)	14(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	5(1)	0(1)	-1(1)
	cos, 1	-3(1)	1(1)	1(1)	0(1)	1(1)	0(1)
Ag[1]	0	19(1)	28(1)	20(1)	0	-1(1)	0
	sin, 1	1(1)	-1(1)	-2(1)	1(1)	4(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	7(1)	0(1)	1(1)
Ag[2]	0	31(1)	24(1)	26(1)	0	2(1)	0
	sin, 1	-2(2)	1(1)	0(1)	-1(1)	3(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	-8(1)	0(1)	-4(1)
Na[1]	0	24(1)	26(1)	14(1)	0	-2(1)	0
	sin, 1	5(1)	-2(1)	1(1)	-4(1)	-3(1)	2(1)
	cos, 1	4(1)	-2(1)	1(1)	5(1)	-3(1)	-3(1)
Na[2]	0	11(1)	8(1)	24(1)	0	1(1)	0
	sin, 1	5(1)	0(1)	-1(1)	-1(1)	-1(1)	2(1)
	cos, 1	-6(1)	1(1)	1(1)	-1(1)	1(1)	1(1)

Table 6.15. Bond lengths distributions [Å] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu[1] - Te[1] x 4	3.335(3)	3.316(3)	3.354(3)
Eu[1] - Te[3]	3.443(4)	3.403(4)	3.485(4)
Eu[1] - Te[3]	3.433(4)	3.352(4)	3.514(4)
Eu[1] - Te[4] x 2	3.455(3)	3.431(3)	3.479(3)
Eu[2] - Te[2] x 4	3.338(3)	3.311(3)	3.364(3)
Eu[2] - Te[3] x 2	3.416(3)	3.397(3)	3.435(3)
Eu[2] - Te[4]	3.404(4)	3.347(4)	3.464(4)
Eu[2] - Te[4]	3.395(4)	3.308(4)	3.481(4)
Te[1] - Ag[1]	2.881(5)	2.825(7)	2.938(7)
Te[1] - Ag[1]	2.857(5)	2.817(7)	2.897(7)
Te[1] - Ag[2] x 2	2.867(3)	2.855(3)	2.879(3)
Te[1] - Na[1] x 4	3.332(3)	3.310(3)	3.354(3)
Te[2] - Ag[1] x 2	2.920(3)	2.913(4)	2.927(4)
Te[2] - Ag[2]	2.936(6)	2.888(7)	2.982(7)
Te[2] - Ag[2]	2.907(6)	2.878(7)	2.938(7)
Te[2] - Na[2] x 4	3.335(3)	3.309(3)	3.362(3)
Te[3] - Te[4] x 4	3.150(3)	2.973(3)	3.329(4)
Te[3] - Na[1]	3.433(4)	3.352(4)	3.514(4)
Te[3] - Na[1]	3.443(4)	3.403(4)	3.485(4)
Te[3] - Na[2] x 2	3.416(3)	3.397(3)	3.435(3)
Te[4] - Na[1] x 2	3.455(3)	3.431(3)	3.479(3)
Te[4] - Na[2]	3.394(4)	3.308(4)	3.481(4)
Te[4] - Na[2]	3.405(4)	3.347(4)	3.464(4)
Ag[1] - Ag[2] x 4	3.148(5)	3.067(6)	3.228(6)

Table 6.16. Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 300 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu[1] - Te[1] x 4	83.94(8)	83.47(8)	84.41(8)
Te[1] - Eu[1] - Te[1] x 4	83.47(6)	83.34(6)	83.60(6)
Te[1] - Eu[1] - Te[1] x 4	141.40(8)	141.09(8)	141.70(8)
Te[1] - Eu[1] - Te[3] x 4	79.71(8)	79.00(8)	80.43(8)

Table 6.16. (Cont'd) Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 300 K with e.s.d.'s in parentheses.

Te[1] - Eu[1] - Te[3] x 4	132.98(6)	132.53(6)	133.41(6)
Te[1] - Eu[1] - Te[4] x 4	79.55(7)	77.70(7)	81.43(7)
Te[1] - Eu[1] - Te[4] x 4	133.03(10)	129.86(10)	136.25(10)
Te[3] - Eu[1] - Te[3] x 2	80.37(8)	79.80(9)	80.93(9)
Te[3] - Eu[1] - Te[4] x 4	54.29(6)	51.06(6)	57.62(6)
Te[4] - Eu[1] - Te[4] x 2	80.48(7)	80.36(6)	80.57(6)
Te[2] - Eu[2] - Te[2] x 4	83.85(6)	83.08(6)	84.63(7)
Te[2] - Eu[2] - Te[2] x 4	83.37(6)	83.28(6)	83.46(6)
Te[2] - Eu[2] - Te[2] x 4	141.07(8)	140.97(8)	141.18(8)
Te[2] - Eu[2] - Te[3] x 4	79.28(6)	77.64(6)	80.94(6)
Te[2] - Eu[2] - Te[3] x 4	133.41(9)	130.48(8)	136.33(8)
Te[2] - Eu[2] - Te[4] x 4	79.46(7)	78.67(7)	80.27(7)
Te[2] - Eu[2] - Te[4] x 4	133.32(7)	132.64(7)	133.98(6)
Te[3] - Eu[2] - Te[3] x 2	81.58(7)	81.38(7)	81.67(7)
Te[3] - Eu[2] - Te[4] x 4	54.95(7)	51.90(7)	58.11(8)
Te[4] - Eu[2] - Te[4] x 2	81.48(8)	81.05(9)	81.85(9)
Eu[1] - Te[1] - Eu[1] x 4	84.03(8)	84.02(8)	84.04(8)
Eu[1] - Te[1] - Eu[1] x 4	83.47(7)	83.34(7)	83.60(7)
Eu[1] - Te[1] - Eu[1] x 4	141.40(9)	141.13(9)	141.66(9)
Eu[1] - Te[1] - Ag[1] x 4	72.11(10)	71.68(10)	72.53(11)
Eu[1] - Te[1] - Ag[1] x 4	136.34(6)	135.94(6)	136.75(6)
Eu[1] - Te[1] - Ag[2] x 4	71.52(13)	70.47(13)	72.58(13)
Eu[1] - Te[1] - Ag[2] x 4	136.41(18)	135.21(18)	137.60(18)
Eu[1] - Te[1] - Na[1] x 4	84.03(8)	84.02(8)	84.04(8)
Ag[1] - Te[1] - Ag[1] x 2	101.31(16)	100.89(18)	101.71(18)
Ag[1] - Te[1] - Ag[2] x 4	66.32(16)	65.33(16)	67.33(16)
Ag[2] - Te[1] - Ag[2] x 2	102.11(13)	101.64(13)	102.55(13)
Eu[2] - Te[2] - Eu[2] x 4	83.92(7)	83.72(7)	84.12(7)
Eu[2] - Te[2] - Eu[2] x 4	83.37(5)	83.28(5)	83.46(5)
Eu[2] - Te[2] - Eu[2] x 4	141.08(9)	140.78(9)	141.38(9)
Eu[2] - Te[2] - Ag[1] x 4	72.58(11)	71.59(12)	73.55(11)
Eu[2] - Te[2] - Ag[1] x 4	136.23(16)	135.17(16)	137.28(16)
Eu[2] - Te[2] - Ag[2] x 4	73.09(11)	72.52(11)	73.66(11)
Eu[2] - Te[2] - Ag[2] x 4	136.13(6)	135.83(6)	136.43(6)

Table 6.16. (Cont'd) Bond angles distributions [°] for Na_{0.81(2)}Ag₂Eu_{1.19(2)}Te₄ at 300 K with e.s.d.'s in parentheses.

Ag[1] - Te[2] - Ag[1] x 2	99.63(12)	99.37(12)	99.85(12)
Ag[1] - Te[2] - Ag[2] x 4	65.05(12)	63.63(14)	66.44(14)
Ag[2] - Te[2] - Ag[2] x 2	98.83(18)	98.43(19)	99.23(19)
Eu[1] - Te[3] - Eu[1] x 2	80.37(9)	79.80(10)	80.93(10)
Eu[1] - Te[3] - Eu[2] x 4	125.45(8)	122.70(9)	128.23(9)
Eu[1] - Te[3] - Te[4] x 4	63.17(8)	61.09(8)	65.38(9)
Eu[1] - Te[3] - Te[4] x 4	117.08(10)	115.86(10)	118.14(10)
Eu[2] - Te[3] - Eu[2] x 2	81.53(8)	80.97(8)	81.97(8)
Eu[2] - Te[3] - Te[4] x 4	62.29(7)	61.44(7)	63.22(7)
Eu[2] - Te[3] - Te[4] x 4	117.48(11)	114.27(12)	120.68(13)
Te[4] - Te[3] - Te[4] x 4	90.42(10)	85.29(11)	95.83(13)
Te[4] - Te[3] - Te[4] x 4	89.52(7)	88.91(7)	90.51(7)
Te[4] - Te[3] - Te[4] x 4	176.33(11)	174.24(12)	179.65(14)
Eu[1] - Te[4] - Eu[1] x 2	80.40(8)	79.77(8)	80.92(8)
Eu[1] - Te[4] - Eu[2] x 4	125.49(9)	122.21(10)	128.70(9)
Eu[1] - Te[4] - Te[3] x 4	62.63(8)	61.58(8)	63.66(8)
Eu[1] - Te[4] - Te[3] x 4	117.18(12)	113.65(12)	120.59(13)
Eu[2] - Te[4] - Eu[2] x 2	81.48(8)	81.05(9)	81.85(9)
Eu[2] - Te[4] - Te[3] x 4	62.87(8)	60.55(8)	65.24(9)
Eu[2] - Te[4] - Te[3] x 4	117.42(9)	116.29(9)	118.34(10)
Te[3] - Te[4] - Te[3] x 4	90.50(10)	85.06(10)	96.12(13)
Te[3] - Te[4] - Te[3] x 4	89.52(7)	88.91(6)	90.51(7)
Te[3] - Te[4] - Te[3] x 4	176.17(11)	173.97(12)	179.64(14)
Te[1] - Ag[1] - Te[1] x 2	101.31(15)	100.89(17)	101.71(17)
Te[1] - Ag[1] - Te[2] x 4	114.51(13)	112.85(17)	116.19(17)
Te[1] - Ag[1] - Ag[2] x 4	56.81(13)	55.51(13)	58.15(14)
Te[1] - Ag[1] - Ag[2] x 4	122.67(14)	122.19(14)	123.15(14)
Te[2] - Ag[1] - Te[2] x 2	99.60(14)	99.21(15)	99.94(16)
Te[2] - Ag[1] - Ag[2] x 4	57.72(12)	56.96(12)	58.49(12)
Te[2] - Ag[1] - Ag[2] x 4	123.26(18)	121.1(2)	125.5(2)
Ag[2] - Ag[1] - Ag[2] x 8	90.26(17)	87.9(2)	92.7(2)
Ag[2] - Ag[1] - Ag[2] x 4	178.17(18)	177.3(2)	179.40(18)
Te[1] - Ag[2] - Te[1] x 2	102.10(15)	101.72(17)	102.46(17)
Te[1] - Ag[2] - Te[2] x 2	114.56(14)	113.40(19)	115.69(19)

Table 6.17. Crystal data and structure refinement for $\text{KCu}_2\text{EuTe}_4$ at 100 K.

Empirical formula	$\text{KCu}_2\text{EuTe}_4$
Formula weight	828.5
Temperature	100 K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	$\text{Pm}(0\beta 1/2)0$
Unit cell dimensions	$a = 4.3862(5)$ Å, $\alpha = 90^\circ$ $b = 4.4074(7)$ Å, $\beta = 90^\circ$ $c = 11.2228(16)$ Å, $\gamma = 90^\circ$
q-vector	$0.2822(6)\mathbf{b}^* + 1/2\mathbf{c}^*$
Volume	$216.96(5)$ Å ³
Z	1
Density (calculated)	6.3395 g/cm ³
Absorption coefficient	25.527 mm ⁻¹
F(000)	348
Crystal size	$0.27 \times 0.04 \times 0.01$ mm ³
Theta range for data collection	3.01 to 29.43°
Index ranges	$-6 \leq h \leq 5$, $-6 \leq k \leq 6$, $-15 \leq l \leq 15$, $-1 \leq m \leq 1$
Reflections collected	4925 (1533 main + 3392 satellites)
Independent reflections	2923 (983 main + 1940 satellites) [$R_{\text{int}} = 0.0472$]
Completeness to $\theta = 29.43^\circ$	93%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2923 / 0 / 121
Goodness-of-fit on F^2	1.92
Final R indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0527$, $wR_{\text{obs}} = 0.1308$
R indices (all data)	$R_{\text{all}} = 0.0814$, $wR_{\text{all}} = 0.1401$
Final R main indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0418$, $wR_{\text{obs}} = 0.1199$
R main indices (all data)	$R_{\text{all}} = 0.0431$, $wR_{\text{all}} = 0.1201$
Final R 1 st order satellites [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.1162$, $wR_{\text{obs}} = 0.1867$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.2513$, $wR_{\text{all}} = 0.2298$
Extinction coefficient	$0.00042(7)$
T_{min} and T_{max} coefficients	0.0359 and 0.7776
Largest diff. peak and hole	4.03 and -2.89 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o $, $wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.18. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu	0	0	0	2749	1	11(1)
	sin, 1	-73(4)	-3(3)	-3(2)		
	cos, 1	-65(4)	3(3)	-2(1)		
Te[1]	0	5004(4)	5000	3639(1)	1	11(1)
	sin, 1	-25(3)	0(2)	1(2)		
	cos, 1	-11(2)	0(3)	0(1)		
Te[2]	0	9994(4)	0	6373(2)	1	12(1)
	sin, 1	-48(3)	2(1)	2(2)		
	cos, 1	22(2)	4(3)	-1(1)		
Te[3]	0	5002(6)	0	362(2)	1	12(1)
	sin, 1	-33(1)	-22(8)	0(1)		
	cos, 1	-293(6)	3(1)	-2(3)		
Te[4]	0	17(6)	5000	359(2)	1	13(1)
	sin, 1	37(1)	8(9)	0(1)		
	cos, 1	322(7)	-1(1)	0(3)		
Cu[1]	0	9976(8)	5000	5112(3)	1	17(1)
	sin, 1	-70(15)	1(1)	13(6)		
	cos, 1	3(1)	25(11)	0(1)		
Cu[2]	0	4985(8)	0	5108(3)	1	21(1)
	sin, 1	-68(15)	1(1)	11(6)		
	cos, 1	2(1)	27(13)	0(1)		
K	0	5004(13)	5000	7751(6)	1	13(1)
	sin, 1	-4(19)	8(15)	15(6)		
	cos, 1	5(20)	7(13)	-18(7)		

Table 6.19. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0	9(1)	7(1)	17(1)	0	0(1)	0
	sin, 1	-1(1)	1(1)	0(1)	0(1)	-1(1)	0(1)
	cos, 1	-1(1)	1(1)	0(1)	0(1)	0(1)	0(1)
Te[1]	0	9(1)	6(1)	18(1)	0	1(1)	0
	sin, 1	-1(1)	-1(1)	0(1)	0(1)	-2(1)	-1(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	-1(1)	2(1)
Te[2]	0	11(1)	8(1)	17(1)	0	1(1)	0
	sin, 1	0(1)	-1(1)	2(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	1(1)	-1(1)	0(1)	0(1)	1(1)
Te[3]	0	12(1)	6(1)	17(1)	0	1(1)	0
	sin, 1	0(1)	0(1)	1(1)	2(1)	0(1)	2(1)
	cos, 1	-3(2)	0(1)	9(2)	0(1)	0(2)	0(1)
Te[4]	0	13(1)	10(1)	15(1)	0	2(1)	0
	sin, 1	1(1)	0(1)	0(1)	-1(1)	0(1)	1(1)
	cos, 1	5(2)	2(1)	-1(2)	0(1)	-1(2)	0(1)
Cu[1]	0	26(2)	9(1)	17(2)	0	0(1)	0
	sin, 1	-3(4)	2(2)	10(4)	0(1)	-5(3)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(2)	0(1)	7(2)
Cu[2]	0	14(2)	32(1)	16(2)	0	0(1)	0
	sin, 1	0(3)	3(3)	7(4)	0(1)	-2(3)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(2)	0(1)	11(2)
K	0	14(2)	11(1)	14(2)	0	1(1)	0
	sin, 1	3(3)	4(2)	-3(3)	1(2)	1(2)	-3(2)
	cos, 1	-4(3)	-5(3)	3(4)	1(2)	-1(2)	-2(2)

Table 6.20. Bond lengths distributions [$\text{\AA}$] for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu - Te[1] x 4	3.281(2)	3.259(2)	3.304(2)
Eu - Te[3] x 2	3.420(3)	3.366(4)	3.474(4)
Eu - Te[4] x 2	3.431(3)	3.428(3)	3.436(3)
Eu - Cu[1] x 2	3.491(4)	3.478(5)	3.504(5)
Eu - Cu[2] x 2	3.484(5)	3.479(7)	3.489(7)
Te[1] - Cu[1]	2.757(6)	2.733(8)	2.780(8)
Te[1] - Cu[1]	2.737(6)	2.730(8)	2.744(8)
Te[1] - Cu[2] x 2	2.752(4)	2.740(4)	2.764(4)
Te[2] - Cu[1] x 2	2.619(4)	2.608(4)	2.630(4)
Te[2] - Cu[2] x 2	2.616(6)	2.616(5)	2.616(8)
Te[2] - K x 4	3.470(9)	3.455(9)	3.484(9)
Te[3] - Te[4] x 2	3.105(4)	2.934(4)	3.284(4)
Te[3] - Te[4] x 2	3.118(4)	2.948(4)	3.290(4)
Cu[1] - Cu[2] x 4	3.106(6)	3.086(6)	3.127(6)

Table 6.21. Bond angles distributions [$^\circ$] for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu - Te[1] x 4	84.38(6)	83.68(6)	85.07(6)
Te[1] - Eu - Te[1] x 4	83.83(5)	83.77(5)	83.89(5)
Te[1] - Eu - Te[1] x 4	142.55(8)	142.37(8)	142.72(8)
Te[1] - Eu - Te[3] x 4	79.53(7)	79.08(7)	80.00(7)
Te[1] - Eu - Te[3] x 4	132.42(8)	131.87(8)	132.98(8)
Te[1] - Eu - Te[4] x 4	79.41(7)	77.43(7)	81.36(7)
Te[1] - Eu - Te[4] x 4	132.79(8)	129.72(8)	135.79(8)
Te[1] - Eu - Cu[1] x 4	47.55(12)	47.31(13)	47.78(13)
Te[1] - Eu - Cu[1] x 4	99.96(11)	99.69(12)	100.23(12)
Te[1] - Eu - Cu[2] x 4	47.89(7)	47.57(6)	48.21(6)
Te[1] - Eu - Cu[2] x 4	99.81(11)	99.41(10)	100.21(10)
Te[3] - Eu - Te[3] x 2	79.77(7)	79.71(8)	79.80(7)
Te[3] - Eu - Te[4] x 4	54.14(7)	51.32(7)	56.96(7)
Te[3] - Eu - Cu[1] x 4	126.38(12)	125.92(13)	126.84(13)

Table 6.21. (Cont'd) Bond angles distributions [°] for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Te[3] - Eu - Cu[2] x 2	100.97(14)	100.20(14)	101.77(14)
Te[3] - Eu - Cu[2] x 2	178.98(13)	177.97(15)	179.82(7)
Te[4] - Eu - Te[4] x 2	79.98(8)	79.76(8)	80.09(9)
Te[4] - Eu - Cu[1] x 2	100.86(9)	100.64(9)	101.05(9)
Te[4] - Eu - Cu[1] x 2	177.59(14)	176.46(15)	179.44(10)
Te[4] - Eu - Cu[2] x 4	126.56(10)	124.20(11)	128.84(10)
Cu[1] - Eu - Cu[1] x 2	78.28(10)	77.80(10)	78.78(10)
Cu[1] - Eu - Cu[2] x 4	52.89(11)	52.42(11)	53.36(12)
Cu[2] - Eu - Cu[2] x 2	78.13(15)	77.78(17)	78.48(18)
Eu - Te[1] - Eu x 4	84.30(6)	83.90(6)	84.69(6)
Eu - Te[1] - Eu x 4	83.83(5)	83.77(5)	83.89(5)
Eu - Te[1] - Eu x 4	142.55(9)	142.26(8)	142.85(8)
Eu - Te[1] - Cu[1] x 4	69.98(12)	69.51(12)	70.47(12)
Eu - Te[1] - Cu[1] x 4	136.59(6)	136.49(6)	136.68(6)
Eu - Te[1] - Cu[2] x 4	69.68(14)	69.46(14)	69.91(15)
Eu - Te[1] - Cu[2] x 4	136.68(17)	136.30(17)	137.05(17)
Cu[1] - Te[1] - Cu[1] x 2	106.0(2)	105.5(2)	106.4(2)
Cu[1] - Te[1] - Cu[2] x 4	68.79(17)	68.11(18)	69.48(18)
Cu[2] - Te[1] - Cu[2] x 2	106.41(17)	105.94(17)	106.88(17)
Cu[1] - Te[2] - Cu[1] x 2	114.59(18)	114.54(18)	114.64(18)
Cu[1] - Te[2] - Cu[2] x 4	72.79(14)	72.23(12)	73.35(12)
Cu[1] - Te[2] - K x 4	72.81(17)	72.46(16)	73.16(16)
Cu[1] - Te[2] - K x 4	140.7(2)	139.92(18)	141.38(18)
Cu[2] - Te[2] - Cu[2] x 2	114.1(2)	113.8(2)	114.5(2)
Cu[2] - Te[2] - K x 4	73.28(19)	73.07(19)	73.48(19)
Cu[2] - Te[2] - K x 4	140.59(16)	140.26(14)	140.92(14)
K - Te[2] - K x 8	78.86(19)	78.76(19)	78.95(19)
K - Te[2] - K x 4	127.1(2)	126.6(2)	127.6(2)
Eu - Te[3] - Eu x 2	79.77(7)	79.71(9)	79.80(7)
Eu - Te[3] - Te[4] x 4	63.27(8)	61.04(7)	65.55(8)
Eu - Te[3] - Te[4] x 4	116.93(9)	115.68(9)	118.07(9)
Te[4] - Te[3] - Te[4] x 4	90.69(12)	84.92(12)	96.57(14)
Te[4] - Te[3] - Te[4] x 4	89.54(10)	89.25(11)	90.04(11)
Te[4] - Te[3] - Te[4] x 4	176.31(13)	174.08(13)	179.81(12)

Table 6.21. (Cont'd) Bond angles distributions [°] for $\text{KCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Eu - Te[4] - Eu x 2	79.92(7)	79.85(8)	79.98(6)
Eu - Te[4] - Te[3] x 4	62.71(7)	61.98(7)	63.40(7)
Eu - Te[4] - Te[3] x 4	116.85(10)	113.09(12)	120.58(13)
Eu - Te[4] - K x 4	127.63(15)	124.56(15)	130.68(15)
Te[3] - Te[4] - Te[3] x 4	90.24(11)	84.35(12)	96.43(14)
Te[3] - Te[4] - Te[3] x 4	89.54(10)	89.25(8)	90.04(11)
Te[3] - Te[4] - Te[3] x 4	176.26(13)	173.94(13)	179.82(12)
Te[3] - Te[4] - K x 4	64.98(15)	62.59(15)	67.48(15)
Te[3] - Te[4] - K x 4	114.98(16)	114.42(16)	115.60(16)
Eu - Cu[1] - Eu x 2	78.29(10)	77.90(15)	78.68(15)
Eu - Cu[1] - Te[1] x 4	62.21(10)	61.68(9)	62.75(9)
Eu - Cu[1] - Te[2] x 2	83.56(10)	83.25(13)	83.86(13)
Eu - Cu[1] - Te[2] x 2	161.84(17)	161.33(16)	162.36(16)
Eu - Cu[1] - Cu[2] x 4	63.44(14)	63.39(15)	63.49(15)
Eu - Cu[1] - Cu[2] x 4	116.65(19)	116.12(16)	117.19(16)
Te[1] - Cu[1] - Te[1] x 2	105.96(17)	105.5(2)	106.4(2)
Te[1] - Cu[1] - Te[2] x 4	109.20(16)	108.80(19)	109.59(19)
Te[1] - Cu[1] - Cu[2] x 4	55.76(15)	55.56(16)	55.96(16)
Te[1] - Cu[1] - Cu[2] x 4	124.16(18)	123.96(17)	124.36(17)
Te[2] - Cu[1] - Te[2] x 2	114.59(18)	114.2(3)	115.0(3)
Te[2] - Cu[1] - Cu[2] x 4	53.57(14)	53.27(14)	53.86(14)
Te[2] - Cu[1] - Cu[2] x 4	126.9(2)	126.4(3)	127.4(3)
Cu[2] - Cu[1] - Cu[2] x 8	90.38(19)	90.3(2)	90.4(2)
Cu[2] - Cu[1] - Cu[2] x 4	179.7(2)	179.4(3)	180
Eu - Cu[2] - Eu x 2	78.13(11)	77.78(15)	78.48(15)
Eu - Cu[2] - Te[1] x 4	62.38(11)	62.18(13)	62.57(13)
Eu - Cu[2] - Te[2] x 2	84.00(15)	83.9(2)	84.1(2)
Eu - Cu[2] - Te[2] x 2	161.9(2)	161.6(3)	162.1(3)
Eu - Cu[2] - Cu[1] x 4	63.72(15)	63.59(14)	63.85(14)
Eu - Cu[2] - Cu[1] x 4	116.40(18)	116.21(17)	116.60(17)
Te[1] - Cu[2] - Te[1] x 2	106.40(17)	106.0(2)	106.8(2)
Te[1] - Cu[2] - Te[2] x 4	109.18(17)	108.73(19)	109.63(19)
Te[1] - Cu[2] - Cu[1] x 4	55.67(14)	55.14(14)	56.21(14)
Te[1] - Cu[2] - Cu[1] x 4	124.8(2)	124.5(3)	125.1(3)

Table 6.22. Crystal data and structure refinement for $K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$ at 100 K.

Empirical formula	$K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$
Formula weight	921.7
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	$Pm(0\beta 1/2)0$
Unit cell dimensions	$a = 4.4641(5)$ Å, $\alpha = 90^\circ$ $b = 4.4964(8)$ Å, $\beta = 90^\circ$ $c = 11.3501(17)$ Å, $\gamma = 90^\circ$
q-vector	$0.2853(5)b^* + 1/2c^*$
Volume	$227.82(6)$ Å ³
Z	1
Density (calculated)	6.7159 g/cm ³
Absorption coefficient	24.129 mm ⁻¹
F(000)	385
Crystal size	$0.25 \times 0.15 \times 0.01$ mm ³
Theta range for data collection	2.98 to 29.04°
Index ranges	$-5 \leq h \leq 6$, $-6 \leq k \leq 6$, $-15 \leq l \leq 15$, $-1 \leq m \leq 1$
Reflections collected	4663 (1419 main + 3244 satellites)
Independent reflections	2952 (981 main + 1971 satellites) [$R_{int} = 0.0602$]
Completeness to $\theta = 29.04^\circ$	95%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2952 / 28 / 123
Goodness-of-fit on F^2	2.85
Final R indices [$I > 2\sigma(I)$]	$R_{obs} = 0.0754$, $wR_{obs} = 0.1999$
R indices (all data)	$R_{all} = 0.1113$, $wR_{all} = 0.2113$
Final R main indices [$I > 2\sigma(I)$]	$R_{obs} = 0.0577$, $wR_{obs} = 0.1541$
R main indices (all data)	$R_{all} = 0.0613$, $wR_{all} = 0.1554$
Final R 1 st order satellites [$I > 2\sigma(I)$]	$R_{obs} = 0.1497$, $wR_{obs} = 0.3067$
R 1 st order satellites (all data)	$R_{all} = 0.2799$, $wR_{all} = 0.3353$
Extinction coefficient	$0.00054(10)$
T_{min} and T_{max} coefficients	0.0439 and 0.8501
Largest diff. peak and hole	6.86 and -6.18 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o $, $wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.23. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{K}_{0.97(2)}\text{Ag}_2\text{Eu}_{1.03(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu[1]	0	0	0	2749	0.678(11)	13(1)
	sin, 1	-70(8)	14(5)	0(3)		
	cos, 1	-62(7)	-16(5)	0(2)		
Eu[2]	0	4991(7)	5000	7970(3)	0.347(11)	13(1)
	sin, 1	-98(10)	-25(10)	-3(3)		
	cos, 1	132(14)	-19(7)	4(4)		
Te[1]	0	5011(8)	5000	3668(3)	1	15(1)
	sin, 1	-48(9)	8(3)	0(3)		
	cos, 1	-21(4)	-18(6)	0(1)		
Te[2]	0	19(8)	0	6870(3)	1	20(1)
	sin, 1	-44(8)	-9(4)	0(3)		
	cos, 1	30(5)	-14(6)	0(2)		
Te[3]	0	4986(10)	0	393(3)	1	21(1)
	sin, 1	-47(1)	-30(10)	3(1)		
	cos, 1	-383(10)	4(1)	23(4)		
Te[4]	0	10009(9)	5000	379(3)	1	17(1)
	sin, 1	49(1)	5(10)	2(1)		
	cos, 1	410(10)	-1(1)	19(4)		
Ag[1]	0	9964(7)	5000	5333(3)	1	20(1)
	sin, 1	-85(30)	0(1)	28(5)		
	cos, 1	10(3)	-3(9)	-3(1)		
Ag[2]	0	4969(6)	0	5319(3)	1	16(1)
	sin, 1	-25(20)	0(1)	18(5)		
	cos, 1	3(2)	-4(8)	-2(1)		
K[1]	0	0	0	2749	0.322(11)	13(1)
	sin, 1	-70(8)	14(5)	0(3)		
	cos, 1	-62(7)	-16(5)	0(2)		
K[2]	0	4991	5000	7970	0.653(11)	13(1)
	sin, 1	-98(10)	-25(10)	-3(3)		
	cos, 1	132(14)	-19(7)	4(4)		

Table 6.24. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{K}_{0.97(2)}\text{Ag}_2\text{Eu}_{1.03(2)}\text{Te}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu[1]	0	8(1)	6(1)	24(1)	0	-1(1)	0
	sin, 1	-1(2)	0(1)	2(1)	0(1)	1(1)	-1(1)
	cos, 1	-1(1)	0(1)	2(1)	0(1)	1(1)	1(1)
Eu[2]	0	12(2)	16(1)	10(2)	0	2(1)	0
	sin, 1	-1(2)	0(1)	0(1)	-1(1)	-1(1)	-3(2)
	cos, 1	1(3)	0(2)	0(2)	-1(1)	1(2)	-2(1)
Te[1]	0	12(1)	10(1)	24(1)	0	1(1)	0
	sin, 1	-5(2)	1(1)	4(2)	0(1)	-2(1)	0(1)
	cos, 1	-2(1)	0(1)	2(1)	-1(1)	-1(1)	0(1)
Te[2]	0	13(1)	13(1)	36(1)	0	0(1)	0
	sin, 1	-4(1)	1(1)	0(2)	0(1)	0(1)	-2(1)
	cos, 1	2(1)	-1(1)	0(1)	0(1)	0(1)	-2(1)
Te[3]	0	24(2)	16(1)	25(1)	0	1(1)	0
	sin, 1	-3(1)	0(1)	2(1)	7(1)	0(1)	-2(1)
	cos, 1	-23(3)	1(2)	16(2)	-1(1)	-4(2)	0(1)
Te[4]	0	16(2)	8(1)	27(1)	0	-3(1)	0
	sin, 1	2(1)	0(1)	-1(1)	-3(1)	0(1)	-2(1)
	cos, 1	20(2)	0(2)	-8(2)	0(1)	1(2)	0(1)
Ag[1]	0	19(2)	19(1)	22(1)	0	-2(1)	0
	sin, 1	-8(3)	2(2)	12(2)	0(1)	-6(2)	0(1)
	cos, 1	1(1)	0(1)	-1(1)	-1(2)	1(1)	-4(2)
Ag[2]	0	14(1)	10(1)	25(1)	0	-1(1)	0
	sin, 1	-4(2)	2(2)	10(2)	0(1)	-4(2)	0(1)
	cos, 1	1(1)	0(1)	-1(1)	-1(1)	0(1)	0(2)
K[1]	0	8(1)	6(1)	24(1)	0	-1(1)	0
	sin, 1	-1(2)	0(1)	2(1)	0(1)	1(1)	-1(1)
	cos, 1	-1(1)	0(1)	2(1)	0(1)	1(1)	1(1)
K[2]	0	12(2)	16(1)	10(2)	0	2(1)	0
	sin, 1	-1(2)	0(1)	0(1)	-1(1)	-1(1)	-3(2)
	cos, 1	1(3)	0(2)	0(2)	-1(1)	1(2)	-2(1)

Table 6.25. Bond lengths distributions [Å] for $K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu[1] - Te[1] x 4	3.350(5)	3.330(4)	3.370(5)
Eu[1] - Te[3] x 2	3.446(6)	3.383(7)	3.511(7)
Eu[1] - Te[4] x 2	3.466(5)	3.457(5)	3.481(5)
Eu[2] - Te[2] x 2	3.397(6)	3.357(6)	3.438(6)
Eu[2] - Te[2] x 2	3.414(6)	3.373(6)	3.455(7)
Eu[2] - Te[4] x 2	3.526(7)	3.468(8)	3.584(8)
Te[1] - Ag[1]	2.940(8)	2.905(12)	2.975(12)
Te[1] - Ag[1]	2.908(8)	2.902(12)	2.915(11)
Te[1] - Ag[2] x 2	2.927(5)	2.908(5)	2.945(5)
Te[1] - K[1] x 4	3.357(5)	3.332(5)	3.381(5)
Te[2] - Ag[1] x 2	2.846(5)	2.831(5)	2.861(5)
Te[2] - Ag[2]	2.860(8)	2.839(11)	2.881(11)
Te[2] - Ag[2]	2.825(8)	2.820(11)	2.830(11)
Te[2] - K[2] x 2	3.414(6)	3.373(6)	3.455(6)
Te[2] - K[2] x 2	3.397(6)	3.357(6)	3.438(6)
Te[3] - Te[4] x 2	3.163(6)	2.940(5)	3.398(6)
Te[3] - Te[4] x 2	3.181(6)	2.961(5)	3.407(6)
Te[3] - K[1] x 2	3.436(6)	3.333(7)	3.543(7)
Te[4] - K[1] x 2	3.466(5)	3.457(5)	3.481(5)
Te[4] - K[2] x 2	3.536(7)	3.453(8)	3.619(8)
Ag[1] - Ag[2] x 4	3.166(8)	3.143(9)	3.190(9)

Table 6.26. Bond angles distributions [°] for $K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu[1] - Te[1] x 4	84.31(11)	83.58(11)	85.03(11)
Te[1] - Eu[1] - Te[1] x 4	83.46(11)	83.29(11)	83.63(11)
Te[1] - Eu[1] - Te[1] x 4	141.73(14)	141.59(15)	141.88(15)
Te[1] - Eu[1] - Te[3] x 4	79.49(12)	78.30(12)	80.73(12)
Te[1] - Eu[1] - Te[3] x 4	132.87(12)	132.07(12)	133.66(12)
Te[1] - Eu[1] - Te[4] x 4	79.34(11)	77.26(11)	81.40(11)
Te[1] - Eu[1] - Te[4] x 4	133.34(14)	129.61(13)	137.01(14)

Table 6.26. (Cont'd) Bond angles distributions [°] for $K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$ at 100 K with e.s.d.'s in parentheses.

Te[3] - Eu[1] - Te[3] x 2	80.85(12)	80.23(14)	81.39(14)
Te[3] - Eu[1] - Te[4] x 4	54.80(10)	51.05(10)	58.59(10)
Te[4] - Eu[1] - Te[4] x 2	80.97(11)	80.52(11)	81.21(11)
Te[2] - Eu[2] - Te[2] x 4	82.89(16)	81.55(16)	84.23(17)
Te[2] - Eu[2] - Te[2] x 4	81.90(13)	81.72(13)	82.10(13)
Te[2] - Eu[2] - Te[2] x 4	137.0(2)	136.7(2)	137.2(2)
Te[2] - Eu[2] - Te[3] x 4	82.27(14)	80.34(14)	84.16(14)
Te[2] - Eu[2] - Te[3] x 4	134.7(2)	130.61(19)	138.7(2)
Te[2] - Eu[2] - Te[4] x 4	82.71(16)	81.97(17)	83.49(18)
Te[2] - Eu[2] - Te[4] x 4	134.29(16)	133.41(16)	135.17(15)
Te[4] - Eu[2] - Te[4] x 2	78.42(15)	78.05(16)	78.72(16)
Eu[1] - Te[1] - Eu[1] x 8	84.11(12)	83.98(13)	84.23(13)
Eu[1] - Te[1] - Eu[1] x 4	141.73(15)	141.47(14)	141.99(14)
Eu[1] - Te[1] - Ag[1] x 4	72.52(17)	72.07(16)	72.98(16)
Eu[1] - Te[1] - Ag[1] x 4	136.00(11)	135.75(11)	136.26(11)
Eu[1] - Te[1] - Ag[2] x 4	71.99(19)	71.71(18)	72.27(18)
Eu[1] - Te[1] - Ag[2] x 4	136.1(3)	135.8(3)	136.3(3)
Ag[1] - Te[1] - Ag[1] x 2	99.5(3)	98.6(3)	100.5(3)
Ag[1] - Te[1] - Ag[2] x 4	65.4(2)	65.0(2)	65.8(2)
Ag[2] - Te[1] - Ag[2] x 2	100.38(18)	100.04(18)	100.73(18)
Eu[2] - Te[2] - Eu[2] x 8	82.40(15)	82.28(15)	82.50(16)
Eu[2] - Te[2] - Eu[2] x 4	136.98(18)	136.44(18)	137.50(18)
Eu[2] - Te[2] - Ag[1] x 4	72.4(2)	71.7(2)	73.2(2)
Eu[2] - Te[2] - Ag[1] x 4	137.6(3)	137.4(3)	137.9(3)
Eu[2] - Te[2] - Ag[2] x 4	72.95(18)	72.13(18)	73.78(18)
Eu[2] - Te[2] - Ag[2] x 4	137.92(13)	137.62(13)	138.21(13)
Ag[1] - Te[2] - Ag[1] x 2	104.4(2)	103.70(20)	105.0(2)
Ag[1] - Te[2] - Ag[2] x 4	67.42(19)	66.94(15)	67.89(15)
Ag[2] - Te[2] - Ag[2] x 2	103.5(3)	102.8(3)	104.2(3)
Eu[1] - Te[3] - Eu[1] x 2	80.85(13)	80.23(15)	81.39(15)
Eu[1] - Te[3] - Eu[2] x 4	126.19(16)	122.11(16)	130.14(15)
Eu[1] - Te[3] - Te[4] x 4	63.28(12)	60.22(12)	66.45(14)
Eu[1] - Te[3] - Te[4] x 4	117.31(15)	115.49(14)	118.87(14)
Te[4] - Te[3] - Te[4] x 4	91.04(17)	83.67(17)	98.6(2)

Table 6.26. (Cont'd) Bond angles distributions [°] for $K_{0.97(2)}Ag_2Eu_{1.03(2)}Te_4$ at 100 K with e.s.d.'s in parentheses.

Te[4] - Te[3] - Te[4] x 4	89.29(13)	88.85(13)	89.96(14)
Te[4] - Te[3] - Te[4] x 4	175.19(19)	172.27(19)	179.47(17)
Eu[1] - Te[4] - Eu[1] x 2	80.88(12)	80.15(14)	81.42(14)
Eu[1] - Te[4] - Eu[2] x 4	125.93(15)	122.22(15)	129.63(15)
Eu[1] - Te[4] - Te[3] x 4	62.23(11)	61.27(11)	63.07(11)
Eu[1] - Te[4] - Te[3] x 4	117.01(17)	112.47(18)	121.5(2)
Eu[2] - Te[4] - Eu[2] x 2	78.41(16)	78.05(18)	78.72(18)
Eu[2] - Te[4] - Te[3] x 4	63.72(13)	60.95(13)	66.67(15)
Eu[2] - Te[4] - Te[3] x 4	116.54(16)	115.00(15)	117.86(15)
Te[3] - Te[4] - Te[3] x 4	90.40(17)	82.89(17)	98.4(2)
Te[3] - Te[4] - Te[3] x 4	89.29(13)	88.85(11)	89.96(14)
Te[3] - Te[4] - Te[3] x 4	175.16(18)	172.18(19)	179.44(17)
Te[1] - Ag[1] - Te[1] x 2	99.5(2)	98.6(2)	100.5(2)
Te[1] - Ag[1] - Te[2] x 4	113.9(2)	113.4(3)	114.4(3)
Te[1] - Ag[1] - Ag[2] x 4	57.42(19)	56.92(19)	57.90(19)
Te[1] - Ag[1] - Ag[2] x 4	122.19(19)	121.71(19)	122.67(19)
Te[2] - Ag[1] - Te[2] x 2	104.38(19)	103.2(2)	105.5(2)
Te[2] - Ag[1] - Ag[2] x 4	56.50(18)	56.06(17)	56.94(17)
Te[2] - Ag[1] - Ag[2] x 4	124.8(3)	123.4(4)	126.1(4)
Ag[2] - Ag[1] - Ag[2] x 8	90.5(3)	89.6(4)	91.4(4)
Ag[2] - Ag[1] - Ag[2] x 4	179.1(3)	178.4(3)	179.6(2)
Te[1] - Ag[2] - Te[1] x 2	100.38(18)	99.9(2)	100.8(2)
Te[1] - Ag[2] - Te[2] x 4	113.8(2)	113.57(18)	114.05(17)
Te[1] - Ag[2] - Ag[1] x 4	57.50(18)	57.11(18)	57.88(18)
Te[1] - Ag[2] - Ag[1] x 4	123.5(3)	123.1(2)	124.0(2)
Te[2] - Ag[2] - Te[2] x 2	103.5(2)	102.8(2)	104.2(2)
Te[2] - Ag[2] - Ag[1] x 4	56.33(19)	55.72(17)	56.94(17)
Te[2] - Ag[2] - Ag[1] x 4	123.2(2)	122.66(19)	123.76(19)
Ag[1] - Ag[2] - Ag[1] x 8	90.4(3)	90.0(3)	90.7(3)
Ag[1] - Ag[2] - Ag[1] x 4	179.4(2)	179.3(3)	179.44(19)

Table 6.27. Crystal data and structure refinement for RbCu₂EuTe₄ at 100 K.

Empirical formula	RbCu ₂ EuTe ₄
Formula weight	874.9
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.3984(7) Å, α = 90° b = 4.4281(7) Å, β = 90° c = 11.5510(17) Å, γ = 90°
q-vector	0.2656(8)b* + 1/2c*
Volume	224.97(6) Å ³
Z	1
Density (calculated)	6.4557 g/cm ³
Absorption coefficient	29.389 mm ⁻¹
F(000)	366
Crystal size	0.50 x 0.10 x 0.01 mm ³
Theta range for data collection	2.91 to 28.98°
Index ranges	-6<=h<=5, -6<=k<=6, -16<=l<=15, -1<=m<=1
Reflections collected	4345 (1320 main + 3025 satellites)
Independent reflections	2900 (947 main + 1953 satellites) [R _{int} = 0.0817]
Completeness to θ = 28.98°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2900 / 0 / 109
Goodness-of-fit on F ²	1.87
Final R indices [I>2σ(I)]	R _{obs} = 0.0656, wR _{obs} = 0.1430
R indices (all data)	R _{all} = 0.1077, wR _{all} = 0.1512
Final R main indices [I>2σ(I)]	R _{obs} = 0.0509, wR _{obs} = 0.1352
R main indices (all data)	R _{all} = 0.0528, wR _{all} = 0.1356
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1501, wR _{obs} = 0.2131
R 1 st order satellites (all data)	R _{all} = 0.3162, wR _{all} = 0.2697
Extinction coefficient	0.00025(4)
T _{min} and T _{max} coefficients	0.0496 and 0.9057
Largest diff. peak and hole	5.53 and -4.38 e.Å ⁻³
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{ \Sigma [w(F_o ^2 - F_c ^2)^2] / \Sigma [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.28. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{RbCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu	0	0	0	2749	1	9(1)
	sin, 1	-72(5)	16(4)	-1(2)		
	cos, 1	-63(4)	-18(5)	-1(2)		
Te[1]	0	5002(5)	5000	3594(2)	1	10(1)
	sin, 1	-53(5)	3(3)	-2(3)		
	cos, 1	-25(3)	-7(7)	-1(2)		
Te[2]	0	10001(4)	0	6238(2)	1	11(1)
	sin, 1	-64(5)	-1(3)	5(3)		
	cos, 1	26(2)	-2(6)	-2(1)		
Te[3]	0	5033(7)	0	430(2)	1	11(1)
	sin, 1	-48(1)	42(13)	0(1)		
	cos, 1	-354(10)	-6(2)	1(4)		
Te[4]	0	34(7)	5000	429(2)	1	13(1)
	sin, 1	43(1)	-43(14)	0(1)		
	cos, 1	318(10)	6(2)	-2(4)		
Cu[1]	0	36(9)	5000	5025(3)	1	17(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Cu[2]	0	5018(9)	0	5021(3)	1	20(1)
	sin, 1	-29(11)	0	5(6)		
	cos, 1	0(1)	0	0(1)		
Rb	0	5009(7)	5000	7776(3)	1	11(1)
	sin, 1	-86(10)	-27(11)	-6(4)		
	cos, 1	103(12)	-23(9)	7(4)		

Table 6.29. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{RbCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0	7(1)	8(1)	12(1)	0	-3(1)	0
	sin, 1	-1(1)	1(1)	-2(1)	0(1)	0(1)	2(1)
	cos, 1	0(1)	1(1)	-2(1)	0(1)	0(1)	-2(1)
Te[1]	0	8(1)	8(1)	14(1)	0	-2(1)	0
	sin, 1	-4(1)	0(1)	10(2)	0(1)	1(1)	-1(1)
	cos, 1	-2(1)	0(1)	5(1)	0(1)	0(1)	1(1)
Te[2]	0	8(1)	11(1)	14(1)	0	-4(1)	0
	sin, 1	-3(1)	0(1)	1(2)	0(1)	1(1)	1(1)
	cos, 1	1(1)	0(1)	0(1)	-1(1)	0(1)	1(1)
Te[3]	0	8(1)	11(1)	15(1)	0	-3(1)	0
	sin, 1	-1(1)	-1(1)	-1(1)	0(2)	0(1)	-5(2)
	cos, 1	-5(2)	-5(2)	-4(2)	0(1)	-2(2)	1(1)
Te[4]	0	13(1)	12(1)	14(1)	0	-2(1)	0
	sin, 1	1(1)	0(1)	1(1)	-6(2)	0(1)	-5(2)
	cos, 1	5(2)	-1(2)	8(3)	1(1)	0(2)	1(1)
Cu[1]	0	24(2)	17(1)	9(1)	0	1(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Cu[2]	0	12(2)	39(2)	9(2)	0	1(1)	0
	sin, 1	2(2)	-8(5)	-5(4)	0	-3(3)	0
	cos, 1	0(1)	0(1)	0(1)	0	0(1)	0
Rb	0	11(1)	14(1)	9(1)	0	-4(1)	0
	sin, 1	0(2)	0(2)	4(2)	1(1)	2(1)	-2(2)
	cos, 1	0(2)	0(2)	-4(2)	0(1)	-3(2)	-2(2)

Table 6.30. Bond lengths distributions [$\text{\AA}$] for $\text{RbCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu - Te[1] x 4	3.286(3)	3.263(3)	3.310(3)
Eu - Te[3]	3.414(4)	3.342(6)	3.486(6)
Eu - Te[3]	3.431(4)	3.356(6)	3.509(6)
Eu - Te[4] x 2	3.435(4)	3.414(5)	3.453(5)
Eu - Cu[1] x 2	3.481(4)	3.474(4)	3.488(4)
Eu - Cu[2] x 2	3.463(6)	3.450(8)	3.475(7)
Te[1] - Cu[1]	2.740(5)	2.720(5)	2.759(5)
Te[1] - Cu[1]	2.763(5)	2.741(5)	2.785(5)
Te[1] - Cu[2] x 2	2.760(4)	2.754(5)	2.767(5)
Te[2] - Cu[1] x 2	2.620(3)	2.617(3)	2.624(3)
Te[2] - Cu[2]	2.604(6)	2.589(7)	2.619(7)
Te[2] - Cu[2]	2.616(6)	2.601(7)	2.632(7)
Te[2] - Rb x 4	3.589(6)	3.571(6)	3.607(6)
Te[3] - Te[4] x 4	3.122(6)	2.932(5)	3.320(5)
Te[3] - Rb x 2	3.784(7)	3.767(6)	3.801(7)
Te[4] - Rb x 2	3.779(7)	3.742(8)	3.816(8)
Cu[1] - Cu[2] x 2	3.126(4)	3.117(5)	3.135(5)
Cu[1] - Cu[2] x 2	3.115(4)	3.106(5)	3.124(5)

Table 6.31. Bond angles distributions [$^\circ$] for $\text{RbCu}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu - Te[1] x 4	84.71(8)	84.12(8)	85.29(8)
Te[1] - Eu - Te[1] x 4	83.98(8)	83.81(8)	84.16(8)
Te[1] - Eu - Te[1] x 4	143.37(12)	143.23(13)	143.52(13)
Te[1] - Eu - Te[3] x 4	79.24(10)	78.40(10)	80.13(10)
Te[1] - Eu - Te[3] x 4	132.18(13)	131.43(12)	132.91(12)
Te[1] - Eu - Te[4] x 4	78.98(10)	77.11(10)	80.82(10)
Te[1] - Eu - Te[4] x 4	132.67(10)	129.69(10)	135.59(10)
Te[1] - Eu - Cu[1] x 4	48.09(9)	47.71(9)	48.47(9)
Te[1] - Eu - Cu[1] x 4	100.90(10)	100.37(9)	101.42(9)
Te[1] - Eu - Cu[2] x 4	48.20(8)	47.84(8)	48.54(8)

Table 6.31. (Cont'd) Bond angles distributions [°] for RbCu₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Eu - Cu[2] x 4	100.51(12)	100.45(12)	100.57(12)
Te[3] - Eu - Te[3] x 2	79.95(10)	79.84(11)	80.00(9)
Te[3] - Eu - Te[4] x 4	54.29(10)	51.20(9)	57.38(9)
Te[3] - Eu - Cu[1] x 2	126.57(10)	126.22(10)	126.94(10)
Te[3] - Eu - Cu[2] x 2	100.94(14)	99.91(15)	102.03(15)
Te[3] - Eu - Cu[2] x 2	179.18(14)	178.46(16)	180
Te[3] - Eu - Cu[1] x 2	125.94(10)	125.59(10)	126.30(10)
Te[4] - Eu - Te[4] x 2	80.31(11)	79.86(11)	80.62(11)
Te[4] - Eu - Cu[1] x 2	100.32(9)	99.88(10)	100.81(10)
Te[4] - Eu - Cu[1] x 2	177.61(11)	175.98(13)	179.79(11)
Te[4] - Eu - Cu[2] x 4	126.48(11)	124.03(12)	128.85(11)
Cu[1] - Eu - Cu[1] x 2	78.99(7)	78.94(7)	79.04(7)
Cu[1] - Eu - Cu[2] x 4	53.52(10)	53.25(9)	53.77(10)
Cu[2] - Eu - Cu[2] x 2	78.72(15)	78.55(17)	78.88(17)
Eu - Te[1] - Eu x 4	84.67(9)	84.49(9)	84.83(9)
Eu - Te[1] - Eu x 4	83.98(8)	83.81(8)	84.16(8)
Eu - Te[1] - Eu x 4	143.38(13)	143.12(13)	143.63(13)
Eu - Te[1] - Cu[1] x 4	69.88(9)	69.42(9)	70.33(9)
Eu - Te[1] - Cu[1] x 4	136.40(10)	136.16(11)	136.63(11)
Eu - Te[1] - Cu[2] x 4	69.46(15)	69.20(14)	69.71(14)
Eu - Te[1] - Cu[2] x 4	136.84(17)	136.42(17)	137.25(17)
Cu[1] - Te[1] - Cu[1] x 2	106.13(16)	106.04(17)	106.21(17)
Cu[1] - Te[1] - Cu[2] x 4	69.00(15)	68.74(15)	69.25(15)
Cu[2] - Te[1] - Cu[2] x 2	106.7(2)	106.5(2)	106.9(2)
Cu[1] - Te[2] - Cu[1] x 2	115.34(15)	115.10(16)	115.58(16)
Cu[1] - Te[2] - Cu[2] x 4	73.52(13)	73.08(13)	73.94(14)
Cu[1] - Te[2] - Rb x 4	75.34(12)	75.06(12)	75.62(12)
Cu[1] - Te[2] - Rb x 4	142.15(15)	141.23(14)	143.05(14)
Cu[2] - Te[2] - Cu[2] x 2	114.8(2)	114.8(3)	114.8(3)
Cu[2] - Te[2] - Rb x 4	75.65(14)	75.03(12)	76.28(12)
Cu[2] - Te[2] - Rb x 4	141.52(11)	141.10(13)	141.95(12)
Rb - Te[2] - Rb x 8	76.19(12)	75.86(13)	76.51(13)
Rb - Te[2] - Rb x 4	120.71(15)	120.00(14)	121.41(14)
Eu - Te[3] - Eu x 2	79.95(9)	79.84(12)	80.00(8)

Table 6.31. (Cont'd) Bond angles distributions [°] for RbCu₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Eu - Te[3] - Te[4] x 4	63.08(10)	60.46(10)	65.75(11)
Eu - Te[3] - Te[4] x 4	116.96(13)	115.79(12)	117.89(12)
Eu - Te[3] - Rb x 4	128.16(14)	124.65(14)	131.57(14)
Te[4] - Te[3] - Te[4] x 4	90.68(16)	84.56(16)	96.98(19)
Te[4] - Te[3] - Te[4] x 4	89.40(15)	88.72(14)	90.52(17)
Te[4] - Te[3] - Te[4] x 4	175.76(18)	173.31(17)	180
Te[4] - Te[3] - Rb x 4	65.23(12)	64.16(11)	66.36(11)
Te[4] - Te[3] - Rb x 4	114.40(15)	110.72(17)	117.94(18)
Rb - Te[3] - Rb x 2	71.61(12)	71.40(14)	71.73(12)
Eu - Te[4] - Eu x 2	80.26(9)	80.05(12)	80.37(8)
Eu - Te[4] - Te[3] x 4	62.47(10)	61.43(9)	63.64(9)
Eu - Te[4] - Te[3] x 4	116.96(13)	113.17(16)	120.76(17)
Eu - Te[4] - Rb x 4	128.07(14)	125.25(13)	130.87(13)
Te[3] - Te[4] - Te[3] x 4	90.55(15)	84.65(16)	96.81(19)
Te[3] - Te[4] - Te[3] x 4	89.40(15)	88.72(18)	90.52(17)
Te[3] - Te[4] - Te[3] x 4	175.86(18)	173.48(17)	180
Te[3] - Te[4] - Rb x 4	65.71(12)	63.57(13)	67.98(14)
Te[3] - Te[4] - Rb x 4	114.13(15)	112.78(16)	115.33(15)
Rb - Te[4] - Rb x 2	71.32(14)	71.07(15)	71.55(15)
Eu - Cu[1] - Eu x 2	79.00(9)	78.82(9)	79.16(9)
Eu - Cu[1] - Te[1] x 4	62.26(9)	61.78(9)	62.76(10)
Eu - Cu[1] - Te[2] x 2	82.82(9)	82.62(9)	83.02(9)
Eu - Cu[1] - Te[2] x 2	161.80(13)	161.57(13)	162.04(13)
Eu - Cu[1] - Cu[2] x 4	62.94(14)	62.57(14)	63.31(14)
Eu - Cu[1] - Cu[2] x 4	116.48(17)	115.92(17)	117.06(17)
Eu - Cu[1] - Rb x 2	129.66(11)	128.75(11)	130.55(11)
Te[1] - Cu[1] - Te[1] x 2	106.13(16)	106.04(17)	106.21(17)
Te[1] - Cu[1] - Te[2] x 4	108.37(13)	107.82(12)	108.94(12)
Te[1] - Cu[1] - Cu[2] x 4	55.48(14)	55.31(14)	55.66(14)
Te[1] - Cu[1] - Cu[2] x 4	124.24(15)	124.11(15)	124.36(15)
Te[1] - Cu[1] - Rb	161.29(17)	160.38(17)	162.21(17)
Te[1] - Cu[1] - Rb	92.58(15)	91.59(15)	93.58(15)
Te[2] - Cu[1] - Te[2] x 2	115.35(17)	115.20(17)	115.49(17)
Te[2] - Cu[1] - Cu[2] x 4	53.00(13)	52.53(13)	53.49(13)

Table 6.31. (Cont'd) Bond angles distributions [°] for RbCu₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Te[2] - Cu[1] - Cu[2] x 4	126.53(19)	125.88(19)	127.18(19)
Te[2] - Cu[1] - Rb x 2	64.08(12)	63.62(12)	64.54(12)
Cu[2] - Cu[1] - Cu[2] x 8	90.18(14)	89.96(14)	90.40(14)
Cu[2] - Cu[1] - Cu[2] x 4	179.67(18)	179.57(14)	179.74(19)
Cu[2] - Cu[1] - Rb x 2	113.68(14)	113.23(13)	114.12(13)
Cu[2] - Cu[1] - Rb x 2	66.58(14)	66.16(15)	66.99(15)
Eu - Cu[2] - Eu x 2	78.72(12)	78.55(17)	78.88(17)
Eu - Cu[2] - Te[1] x 4	62.44(13)	62.28(11)	62.61(11)
Eu - Cu[2] - Te[2] x 2	83.04(15)	82.55(18)	83.54(19)
Eu - Cu[2] - Te[2] x 2	162.1(2)	161.6(3)	162.6(3)
Eu - Cu[2] - Cu[1] x 4	63.52(11)	63.29(11)	63.76(12)
Eu - Cu[2] - Cu[1] x 4	116.74(14)	116.51(14)	116.96(14)
Te[1] - Cu[2] - Te[1] x 2	106.7(2)	106.5(3)	106.8(3)
Te[1] - Cu[2] - Te[2] x 4	108.59(14)	108.24(13)	108.94(13)
Te[1] - Cu[2] - Cu[1] x 4	55.19(10)	54.80(10)	55.58(10)
Te[1] - Cu[2] - Cu[1] x 4	124.7(2)	124.32(16)	125.09(16)
Te[2] - Cu[2] - Te[2] x 2	114.8(2)	114.8(3)	114.8(3)
Te[2] - Cu[2] - Cu[1] x 4	53.55(11)	53.45(12)	53.65(12)
Te[2] - Cu[2] - Cu[1] x 4	126.48(14)	126.19(18)	126.77(18)
Cu[1] - Cu[2] - Cu[1] x 4	90.60(15)	90.26(18)	90.92(18)
Cu[1] - Cu[2] - Cu[1] x 4	89.61(7)	89.61(7)	89.61(7)
Cu[1] - Cu[2] - Cu[1] x 4	179.62(18)	179.46(18)	179.74(16)
Te[2] - Rb - Te[2] x 8	76.09(12)	75.29(12)	76.89(13)
Te[2] - Rb - Te[2] x 4	120.70(18)	120.19(19)	121.20(19)
Te[2] - Rb - Te[3] x 4	92.40(13)	90.71(13)	94.03(13)
Te[2] - Rb - Te[3] x 4	139.74(18)	136.47(17)	143.00(17)
Te[2] - Rb - Te[4] x 4	92.64(15)	92.07(15)	93.23(15)
Te[2] - Rb - Te[4] x 4	139.42(17)	138.76(17)	140.07(16)
Te[2] - Rb - Cu[1] x 2	40.99(8)	40.50(7)	41.48(8)
Te[2] - Rb - Cu[1] x 2	86.51(13)	86.21(13)	86.82(13)
Te[3] - Rb - Te[3] x 2	71.66(14)	71.05(14)	72.13(14)
Te[3] - Rb - Te[4] x 4	48.89(12)	46.05(12)	51.72(13)
Te[3] - Rb - Cu[1] x 2	132.01(15)	129.34(16)	134.58(15)
Te[4] - Rb - Te[4] x 2	71.32(13)	71.07(13)	71.55(14)

Table 6.32. Crystal data and structure refinement for RbAg₂EuTe₄ at 100 K.

Empirical formula	RbAg ₂ EuTe ₄
Formula weight	963.6
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.4814(7) Å, α = 90° b = 4.4928(8) Å, β = 90° c = 11.9199(19) Å, γ = 90°
q-vector	0.2625(7)b* + 1/2c*
Volume	240.00(7) Å ³
Z	1
Density (calculated)	6.6648 g/cm ³
Absorption coefficient	27.14 mm ⁻¹
F(000)	402
Crystal size	0.20 x 0.16 x 0.02 mm ³
Theta range for data collection	2.82 to 29.13°
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 5, -16 ≤ l ≤ 16, -1 ≤ m ≤ 1
Reflections collected	5578 (1738 main + 3840 satellites)
Independent reflections	3354 (1155 main + 2199 satellites) [R _{int} = 0.0368]
Completeness to θ = 29.13°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3354 / 0 / 121
Goodness-of-fit on F ²	2.26
Final R indices [I > 2σ(I)]	R _{obs} = 0.0533, wR _{obs} = 0.1427
R indices (all data)	R _{all} = 0.0755, wR _{all} = 0.1522
Final R main indices [I > 2σ(I)]	R _{obs} = 0.0369, wR _{obs} = 0.1141
R main indices (all data)	R _{all} = 0.0374, wR _{all} = 0.1143
Final R 1 st order satellites [I > 2σ(I)]	R _{obs} = 0.1389, wR _{obs} = 0.2338
R 1 st order satellites (all data)	R _{all} = 0.2355, wR _{all} = 0.2643
Extinction coefficient	0.00060(7)
T _{min} and T _{max} coefficients	0.0304 and 0.5411
Largest diff. peak and hole	5.16 and -8.53 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.33. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{RbAg}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu	0	0	0	2749	1	9(1)
	sin, 1	92(3)	-13(2)	-4(1)		
	cos, 1	81(2)	15(2)	-3(1)		
Te[1]	0	5000(4)	5000	3530(1)	1	10(1)
	sin, 1	24(3)	-2(2)	2(2)		
	cos, 1	12(2)	5(3)	1(1)		
Te[2]	0	-2(3)	0	6550(1)	1	11(1)
	sin, 1	47(3)	5(2)	1(2)		
	cos, 1	-25(2)	9(3)	0(1)		
Te[3]	0	4998(4)	0	507(1)	1	17(1)
	sin, 1	0(1)	-9(5)	0(1)		
	cos, 1	1(5)	1(1)	-2(2)		
Te[4]	0	-7(4)	5000	503(1)	1	18(1)
	sin, 1	-4(1)	-7(5)	0(1)		
	cos, 1	-28(6)	1(1)	-2(2)		
Ag[1]	0	3(5)	5000	5146(2)	1	12(1)
	sin, 1	-311(5)	-2(1)	-4(2)		
	cos, 1	14(1)	-39(6)	0(1)		
Ag[2]	0	5001(6)	0	5146(2)	1	10(1)
	sin, 1	406(5)	5(1)	-1(2)		
	cos, 1	-19(1)	105(6)	0(1)		
Rb	0	5002(5)	5000	7932(2)	1	11(1)
	sin, 1	32(5)	12(4)	-2(2)		
	cos, 1	-42(6)	9(3)	3(2)		

Table 6.34. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{RbAg}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0	7(1)	6(1)	14(1)	0	-1(1)	0
	sin, 1	0(1)	1(1)	2(1)	0(1)	3(1)	0(1)
	cos, 1	0(1)	1(1)	2(1)	0(1)	3(1)	0(1)
Te[1]	0	8(1)	6(1)	14(1)	0	0(1)	0
	sin, 1	1(1)	1(1)	-2(1)	0(1)	6(1)	-1(1)
	cos, 1	1(1)	0(1)	-1(1)	-1(1)	3(1)	1(1)
Te[2]	0	9(1)	7(1)	16(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	3(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	-1(1)	0(1)
Te[3]	0	23(1)	14(1)	13(1)	0	-1(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	0(1)	1(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	1(1)	0(1)
Te[4]	0	26(1)	14(1)	13(1)	0	-1(1)	0
	sin, 1	0(1)	0(1)	0(1)	-1(1)	0(1)	0(1)
	cos, 1	-1(1)	0(1)	1(1)	0(1)	3(1)	0(1)
Ag[1]	0	12(1)	8(1)	15(1)	0	-1(1)	0
	sin, 1	-1(2)	-1(1)	9(2)	0(1)	0(2)	0(1)
	cos, 1	0(1)	0(1)	0(1)	-5(1)	0(1)	2(1)
Ag[2]	0	2(1)	12(1)	15(1)	0	-1(1)	0
	sin, 1	-1(2)	-1(1)	0(2)	0(1)	2(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	4(1)	0(1)	3(1)
Rb	0	12(1)	10(1)	13(1)	0	-1(1)	0
	sin, 1	-1(1)	0(1)	4(1)	1(1)	0(1)	-1(1)
	cos, 1	1(1)	0(1)	-6(1)	1(1)	0(1)	0(1)

Table 6.35. Bond lengths distributions [Å] for RbAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu - Te[1] x 4	3.324(2)	3.286(2)	3.361(2)
Eu - Te[3] x 2	3.445(3)	3.415(3)	3.474(3)
Eu - Te[4] x 2	3.451(2)	3.445(2)	3.456(2)
Eu - Ag[1] x 2	3.683(3)	3.664(3)	3.698(3)
Eu - Ag[2] x 2	3.677(3)	3.600(4)	3.756(4)
Te[1] - Ag[1] x 2	2.957(3)	2.851(4)	3.063(4)
Te[1] - Ag[2] x 2	2.960(3)	2.934(3)	2.982(3)
Te[2] - Ag[1] x 2	2.803(3)	2.779(3)	2.823(3)
Te[2] - Ag[2] x 2	2.799(4)	2.679(4)	2.922(4)
Te[2] - Rb x 4	3.574(3)	3.558(3)	3.590(3)
Te[3] - Te[4] x 4	3.174(3)	3.164(3)	3.185(3)
Te[3] - Rb x 2	3.803(4)	3.797(4)	3.808(4)
Te[4] - Rb x 2	3.794(4)	3.788(5)	3.799(5)
Ag[1] - Ag[2] x 4	3.176(4)	2.970(3)	3.391(4)

Table 6.36. Bond angles distributions [°] for RbAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu - Te[1] x 8	85.04(5)	84.12(5)	85.99(5)
Te[1] - Eu - Te[1] x 4	145.34(7)	145.13(7)	145.55(7)
Te[1] - Eu - Te[3] x 4	77.71(5)	76.90(5)	78.55(5)
Te[1] - Eu - Te[3] x 4	131.65(6)	131.48(6)	131.83(6)
Te[1] - Eu - Te[4] x 4	77.60(5)	76.97(5)	78.23(5)
Te[1] - Eu - Te[4] x 4	131.70(6)	130.43(6)	133.00(6)
Te[1] - Eu - Ag[1] x 4	49.56(6)	47.20(6)	51.96(6)
Te[1] - Eu - Ag[1] x 4	100.14(6)	98.07(6)	102.22(6)
Te[1] - Eu - Ag[2] x 4	49.70(4)	49.04(5)	50.35(5)
Te[1] - Eu - Ag[2] x 4	100.07(6)	98.60(6)	101.48(6)
Te[3] - Eu - Te[3] x 2	81.18(5)	81.04(6)	81.30(6)
Te[3] - Eu - Te[4] x 4	54.76(5)	54.41(5)	55.12(5)
Te[3] - Eu - Ag[1] x 4	126.93(6)	124.17(6)	129.71(6)
Te[3] - Eu - Ag[2] x 2	101.84(7)	101.02(8)	102.68(8)

Table 6.36. (Cont'd) Bond angles distributions [°] for RbAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Eu - Ag[2] x 2	176.93(8)	176.06(8)	177.76(8)
Te[4] - Eu - Te[4] x 2	81.23(5)	81.05(5)	81.40(5)
Te[4] - Eu - Ag[1] x 2	101.74(5)	101.23(5)	102.30(5)
Te[4] - Eu - Ag[1] x 2	176.06(6)	175.14(6)	177.59(6)
Te[4] - Eu - Ag[2] x 4	126.95(6)	126.74(6)	127.14(6)
Ag[1] - Eu - Ag[1] x 2	75.21(5)	74.73(5)	75.57(5)
Ag[1] - Eu - Ag[2] x 4	51.12(5)	48.18(5)	54.15(6)
Ag[2] - Eu - Ag[2] x 2	75.10(8)	75.04(8)	75.13(7)
Eu - Te[1] - Eu x 8	85.06(6)	84.38(6)	85.72(6)
Eu - Te[1] - Eu x 4	145.35(8)	145.01(8)	145.70(8)
Eu - Te[1] - Ag[1] x 4	71.53(6)	70.47(6)	72.67(7)
Eu - Te[1] - Ag[1] x 4	134.83(5)	133.74(5)	135.94(5)
Eu - Te[1] - Ag[2] x 4	71.34(7)	69.16(7)	73.48(7)
Eu - Te[1] - Ag[2] x 4	134.96(10)	131.71(10)	138.18(10)
Ag[1] - Te[1] - Ag[1] x 2	98.56(10)	98.11(11)	98.88(11)
Ag[1] - Te[1] - Ag[2] x 4	64.93(9)	61.36(8)	68.47(9)
Ag[2] - Te[1] - Ag[2] x 2	98.86(9)	97.80(10)	99.70(10)
Ag[1] - Te[2] - Ag[1] x 2	106.60(10)	105.80(10)	107.21(10)
Ag[1] - Te[2] - Ag[2] x 4	69.04(8)	65.60(8)	72.57(8)
Ag[1] - Te[2] - Rb x 4	76.78(7)	74.78(8)	78.84(8)
Ag[1] - Te[2] - Rb x 4	141.20(9)	137.86(9)	144.61(10)
Ag[2] - Te[2] - Ag[2] x 2	106.34(12)	106.02(13)	106.51(12)
Ag[2] - Te[2] - Rb x 4	77.01(8)	75.46(8)	78.58(8)
Ag[2] - Te[2] - Rb x 4	141.07(7)	140.16(8)	142.00(8)
Rb - Te[2] - Rb x 8	77.89(7)	77.82(7)	77.95(7)
Rb - Te[2] - Rb x 4	125.11(9)	124.84(10)	125.36(9)
Eu - Te[3] - Eu x 2	81.18(6)	81.04(7)	81.30(7)
Eu - Te[3] - Te[4] x 4	62.71(5)	62.39(6)	63.02(6)
Eu - Te[3] - Te[4] x 4	117.39(7)	116.96(8)	117.83(8)
Eu - Te[3] - Rb x 4	127.82(7)	127.55(7)	128.09(7)
Te[4] - Te[3] - Te[4] x 8	90.09(8)	89.89(9)	90.29(9)
Te[4] - Te[3] - Te[4] x 4	179.77(9)	179.66(10)	179.85(8)
Te[4] - Te[3] - Rb x 4	65.25(7)	65.00(7)	65.50(7)
Te[4] - Te[3] - Rb x 4	114.67(9)	114.35(10)	114.99(10)

Table 6.36. (Cont'd) Bond angles distributions [°] for RbAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Rb - Te[3] - Rb x 2	72.41(6)	72.29(7)	72.54(7)
Eu - Te[4] - Eu x 2	81.24(6)	80.93(7)	81.53(7)
Eu - Te[4] - Te[3] x 4	62.52(5)	61.83(5)	63.20(5)
Eu - Te[4] - Te[3] x 4	117.45(8)	116.46(8)	118.41(8)
Eu - Te[4] - Rb x 4	127.86(7)	127.31(7)	128.39(7)
Te[3] - Te[4] - Te[3] x 8	90.20(8)	89.84(10)	90.56(10)
Te[3] - Te[4] - Te[3] x 4	179.74(9)	179.62(10)	179.85(8)
Te[3] - Te[4] - Rb x 4	65.47(7)	65.37(7)	65.58(7)
Te[3] - Te[4] - Rb x 4	114.72(8)	114.50(8)	114.95(8)
Rb - Te[4] - Rb x 2	72.35(8)	72.31(9)	72.39(9)
Eu - Ag[1] - Eu x 2	75.18(5)	74.83(7)	75.43(7)
Eu - Ag[1] - Te[1] x 4	58.90(6)	57.34(6)	60.40(6)
Eu - Ag[1] - Te[2] x 2	88.99(6)	88.29(8)	89.83(9)
Eu - Ag[1] - Te[2] x 2	163.74(9)	162.84(10)	165.09(10)
Eu - Ag[1] - Ag[2] x 4	64.30(7)	63.81(7)	64.63(8)
Eu - Ag[1] - Ag[2] x 4	115.57(10)	111.41(10)	119.61(12)
Te[1] - Ag[1] - Te[1] x 2	98.56(10)	98.11(12)	98.88(12)
Te[1] - Ag[1] - Te[2] x 4	112.92(9)	109.19(9)	116.58(8)
Te[1] - Ag[1] - Ag[2] x 4	57.69(8)	54.19(7)	61.32(9)
Te[1] - Ag[1] - Ag[2] x 4	122.19(10)	119.88(10)	124.38(10)
Te[2] - Ag[1] - Te[2] x 2	106.53(10)	106.12(12)	106.73(9)
Te[2] - Ag[1] - Ag[2] x 4	55.34(8)	55.08(7)	55.68(7)
Te[2] - Ag[1] - Ag[2] x 4	124.63(11)	119.40(12)	129.74(14)
Ag[2] - Ag[1] - Ag[2] x 4	90.39(10)	83.04(9)	97.94(12)
Ag[2] - Ag[1] - Ag[2] x 4	89.62(8)	88.38(9)	91.37(9)
Ag[2] - Ag[1] - Ag[2] x 4	175.64(11)	173.00(11)	180
Eu - Ag[2] - Eu x 2	75.10(6)	75.04(7)	75.13(5)
Eu - Ag[2] - Te[1] x 4	58.94(7)	57.41(7)	60.46(7)
Eu - Ag[2] - Te[2] x 2	89.28(9)	85.98(10)	92.77(11)
Eu - Ag[2] - Te[2] x 2	164.35(12)	160.74(13)	167.99(14)
Eu - Ag[2] - Ag[1] x 4	64.59(8)	61.79(8)	67.57(9)
Eu - Ag[2] - Ag[1] x 4	115.39(9)	113.83(9)	116.97(9)
Te[1] - Ag[2] - Te[1] x 2	98.73(9)	98.24(11)	99.01(10)
Te[1] - Ag[2] - Te[2] x 4	112.92(10)	108.87(10)	117.06(10)

Table 6.36. (Cont'd) Bond angles distributions [°] for RbAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Te[1] - Ag[2] - Ag[1] x 4	57.42(8)	56.81(7)	57.96(7)
Te[1] - Ag[2] - Ag[1] x 4	122.54(12)	117.41(13)	127.74(14)
Te[2] - Ag[2] - Te[2] x 2	106.34(11)	106.02(13)	106.51(11)
Te[2] - Ag[2] - Ag[1] x 4	55.60(8)	52.09(7)	59.38(9)
Te[2] - Ag[2] - Ag[1] x 4	124.23(10)	121.83(9)	126.57(10)
Ag[1] - Ag[2] - Ag[1] x 4	90.35(10)	83.07(10)	98.17(12)
Ag[1] - Ag[2] - Ag[1] x 4	89.62(8)	88.38(9)	91.37(9)
Ag[1] - Ag[2] - Ag[1] x 4	175.38(11)	172.75(11)	179.90(11)
Te[2] - Rb - Te[2] x 8	77.82(7)	77.80(7)	77.83(7)
Te[2] - Rb - Te[2] x 4	125.10(10)	124.85(10)	125.35(10)
Te[2] - Rb - Te[3] x 4	90.02(6)	89.68(6)	90.37(6)
Te[2] - Rb - Te[3] x 4	137.94(10)	137.42(10)	138.46(10)
Te[2] - Rb - Te[4] x 4	90.06(8)	89.83(8)	90.29(8)
Te[2] - Rb - Te[4] x 4	137.89(7)	137.56(7)	138.22(7)
Te[3] - Rb - Te[3] x 2	72.41(7)	72.31(7)	72.52(7)
Te[3] - Rb - Te[4] x 4	49.36(6)	49.12(6)	49.62(6)
Te[4] - Rb - Te[4] x 2	72.35(7)	72.31(8)	72.39(8)

Table 6.37. Crystal data and structure refinement for CsAg₂EuTe₄ at 100 K.

Empirical formula	CsAg ₂ EuTe ₄
Formula weight	1011
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.4911(6) Å, α = 90° b = 4.5068(7) Å, β = 90° c = 12.3484(18) Å, γ = 90°
q-vector	0.2631(6)b* + 1/2c*
Volume	249.94(6) Å ³
Z	1
Density (calculated)	6.7147 g/cm ³
Absorption coefficient	24.895 mm ⁻¹
F(000)	420
Crystal size	0.19 x 0.11 x 0.02 mm ³
Theta range for data collection	2.74 to 29.07°
Index ranges	-6<=h<=5, -6<=k<=6, -17<=l<=17, -1<=m<=1
Reflections collected	4892 (1398 main + 3494 satellites)
Independent reflections	3317 (1065 main + 2252 satellites) [R _{int} = 0.0313]
Completeness to θ = 29.07°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3317 / 0 / 103
Goodness-of-fit on F ²	1.74
Final R indices [I>2σ(I)]	R _{obs} = 0.0415, wR _{obs} = 0.1094
R indices (all data)	R _{all} = 0.0624, wR _{all} = 0.1170
Final R main indices [I>2σ(I)]	R _{obs} = 0.0248, wR _{obs} = 0.0743
R main indices (all data)	R _{all} = 0.0258, wR _{all} = 0.0748
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.1005, wR _{obs} = 0.1720
R 1 st order satellites (all data)	R _{all} = 0.1733, wR _{all} = 0.1888
Extinction coefficient	0.00056(7)
T _{min} and T _{max} coefficients	0.0721 and 0.5240
Largest diff. peak and hole	4.42 and -4.59 e.Å ⁻³
R = Σ F _o - F _c / Σ F _o , wR = {Σ[w(F _o ² - F _c ²)] / Σ[w(F _o ⁴)]} ^{1/2} and w=1/(σ ² (I)+0.0016I ²)	

Table 6.38. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$), occupancies and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{CsAg}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu	0	0	0	2749	1	6(1)
	sin, 1	89(1)	-9(2)	-1(1)		
	cos, 1	79(1)	10(2)	-1(1)		
Te[1]	0	5002(3)	5000	3494(1)	1	6(1)
	sin, 1	35(2)	-1(1)	-4(1)		
	cos, 1	18(1)	2(3)	-2(1)		
Te[2]	0	2(2)	0	6388(1)	1	6(1)
	sin, 1	60(2)	2(1)	-1(1)		
	cos, 1	-28(1)	5(2)	0(1)		
Te[3]	0	4999(5)	0	578(1)	1	6(1)
	sin, 1	89(1)	-52(5)	0(1)		
	cos, 1	485(3)	10(1)	2(2)		
Te[4]	0	4(4)	5000	580(1)	1	10(1)
	sin, 1	-68(1)	33(5)	1(1)		
	cos, 1	-371(3)	-6(1)	5(1)		
Ag[1]	0	-4(4)	5000	5053(1)	1	12(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Ag[2]	0	4996(3)	0	5048(1)	1	12(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Cs	0	4998(3)	5000	7945(1)	1	8(1)
	sin, 1	62(2)	11(3)	-3(1)		
	cos, 1	-82(2)	9(2)	4(1)		

Table 6.39. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{CsAg}_2\text{EuTe}_4$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0	3(1)	4(1)	10(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	3(1)	-1(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	2(1)	1(1)
Te[1]	0	4(1)	5(1)	7(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)
Te[2]	0	4(1)	4(1)	8(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	1(1)	0(1)	1(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
Te[3]	0	1(1)	7(1)	9(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	-6(1)	0(1)	2(1)
	cos, 1	1(1)	-2(1)	2(1)	1(1)	-2(1)	0(1)
Te[4]	0	15(1)	8(1)	7(1)	0	1(1)	0
	sin, 1	0(1)	0(1)	-1(1)	5(1)	-3(1)	3(1)
	cos, 1	0(1)	0(1)	-5(1)	-1(1)	-15(1)	-1(1)
Ag[1]	0	19(1)	9(1)	7(1)	0	0(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Ag[2]	0	9(1)	16(1)	10(1)	0	0(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Cs	0	9(1)	9(1)	5(1)	0	0(1)	0
	sin, 1	0(1)	1(1)	2(1)	0(1)	1(1)	1(1)
	cos, 1	1(1)	-1(1)	-2(1)	0(1)	-2(1)	1(1)

Table 6.40. Bond lengths distributions [Å] for CsAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu - Te[1] x 4	3.3288(16)	3.2984(16)	3.3588(16)
Eu - Te[3] x 2	3.451(2)	3.341(3)	3.566(3)
Eu - Te[4] x 2	3.4576(19)	3.441(2)	3.4708(18)
Eu - Ag[1] x 2	3.6767(15)	3.6726(15)	3.6805(15)
Eu - Ag[2] x 2	3.6689(18)	3.6344(18)	3.7028(18)
Te[1] - Ag[1]	2.960(2)	2.942(3)	2.977(3)
Te[1] - Ag[1]	2.955(2)	2.946(3)	2.965(3)
Te[1] - Ag[2] x 2	2.9599(17)	2.9558(17)	2.9639(17)
Te[2] - Ag[1] x 2	2.7923(14)	2.7901(15)	2.7943(15)
Te[2] - Ag[2]	2.791(2)	2.768(2)	2.815(2)
Te[2] - Ag[2]	2.787(2)	2.763(2)	2.812(2)
Te[2] - Cs x 4	3.7182(18)	3.6960(18)	3.7407(18)
Te[3] - Te[4] x 4	3.187(3)	2.937(2)	3.442(3)
Te[3] - Cs x 2	3.960(2)	3.936(2)	3.976(2)
Te[4] - Cs x 2	3.955(3)	3.885(3)	4.027(3)
Ag[1] - Ag[2] x 4	3.1811(16)	3.1811(16)	3.1811(16)

Table 6.41. Bond angles distributions [°] for CsAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu - Te[1] x 4	85.22(4)	84.35(4)	86.10(4)
Te[1] - Eu - Te[1] x 4	84.84(4)	84.68(4)	85.00(4)
Te[1] - Eu - Te[1] x 4	145.73(5)	145.62(5)	145.86(5)
Te[1] - Eu - Te[3] x 4	77.61(5)	76.53(5)	78.74(5)
Te[1] - Eu - Te[3] x 4	131.48(5)	130.31(5)	132.60(5)
Te[1] - Eu - Te[4] x 4	77.38(4)	74.99(4)	79.81(4)
Te[1] - Eu - Te[4] x 4	131.66(5)	128.17(4)	135.17(5)
Te[1] - Eu - Ag[1] x 4	49.60(4)	49.31(4)	49.89(4)
Te[1] - Eu - Ag[1] x 4	100.47(4)	99.82(4)	101.12(4)
Te[1] - Eu - Ag[2] x 4	49.76(3)	49.30(3)	50.22(3)
Te[1] - Eu - Ag[2] x 4	100.35(4)	100.24(4)	100.45(4)
Te[3] - Eu - Te[3] x 2	81.12(5)	80.97(6)	81.20(5)

Table 6.41. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Te[3] - Eu - Te[4] x 4	54.89(4)	51.08(4)	58.83(4)
Te[3] - Eu - Ag[1] x 4	126.87(4)	126.19(4)	127.58(4)
Te[3] - Eu - Ag[2] x 2	101.68(5)	100.26(5)	103.13(5)
Te[3] - Eu - Ag[2] x 2	177.18(5)	175.80(5)	178.60(5)
Te[4] - Eu - Te[4] x 2	81.42(5)	80.92(4)	81.72(4)
Te[4] - Eu - Ag[1] x 2	101.45(4)	101.18(4)	101.78(4)
Te[4] - Eu - Ag[1] x 2	175.92(4)	174.87(5)	177.39(4)
Te[4] - Eu - Ag[2] x 4	126.77(4)	123.79(4)	129.75(4)
Ag[1] - Eu - Ag[1] x 2	75.60(3)	75.56(3)	75.63(3)
Ag[1] - Eu - Ag[2] x 4	51.32(3)	51.06(3)	51.59(3)
Ag[2] - Eu - Ag[2] x 2	75.51(4)	75.47(4)	75.54(4)
Eu - Te[1] - Eu x 4	85.20(4)	84.87(5)	85.52(5)
Eu - Te[1] - Eu x 4	84.84(3)	84.68(3)	85.00(3)
Eu - Te[1] - Eu x 4	145.74(6)	145.43(5)	146.05(5)
Eu - Te[1] - Ag[1] x 4	71.28(4)	70.85(4)	71.71(4)
Eu - Te[1] - Ag[1] x 4	134.73(4)	134.37(4)	135.09(4)
Eu - Te[1] - Ag[2] x 4	71.04(4)	70.72(4)	71.37(4)
Eu - Te[1] - Ag[2] x 4	134.89(7)	134.34(6)	135.43(6)
Ag[1] - Te[1] - Ag[1] x 2	98.80(7)	98.62(7)	98.98(7)
Ag[1] - Te[1] - Ag[2] x 4	65.02(5)	64.76(5)	65.29(5)
Ag[2] - Te[1] - Ag[2] x 2	99.16(6)	98.98(6)	99.34(7)
Ag[1] - Te[2] - Ag[1] x 2	107.61(6)	107.57(6)	107.64(6)
Ag[1] - Te[2] - Ag[2] x 4	69.46(5)	69.14(5)	69.78(5)
Ag[1] - Te[2] - Cs x 4	79.38(4)	78.99(4)	79.77(4)
Ag[1] - Te[2] - Cs x 4	142.55(6)	141.79(6)	143.31(6)
Ag[2] - Te[2] - Ag[2] x 2	107.24(7)	107.20(7)	107.27(7)
Ag[2] - Te[2] - Cs x 4	79.62(4)	79.14(4)	80.10(5)
Ag[2] - Te[2] - Cs x 4	142.47(3)	142.18(4)	142.75(4)
Cs - Te[2] - Cs x 4	74.61(4)	74.55(4)	74.67(4)
Cs - Te[2] - Cs x 4	74.32(4)	74.22(4)	74.43(4)
Cs - Te[2] - Cs x 4	117.69(5)	117.31(5)	118.08(5)
Eu - Te[3] - Eu x 2	81.12(5)	80.97(5)	81.20(4)
Eu - Te[3] - Te[4] x 4	62.70(5)	59.22(5)	66.41(6)
Eu - Te[3] - Te[4] x 4	117.09(6)	115.76(6)	118.05(6)

Table 6.41. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Eu - Te[3] - Cs x 4	128.53(6)	123.99(6)	133.09(6)
Te[4] - Te[3] - Te[4] x 4	90.54(8)	82.56(7)	99.24(9)
Te[4] - Te[3] - Te[4] x 4	89.43(6)	88.76(7)	90.71(7)
Te[4] - Te[3] - Te[4] x 4	174.46(9)	171.24(8)	179.77(9)
Te[4] - Te[3] - Cs x 4	66.08(5)	64.86(5)	67.44(5)
Te[4] - Te[3] - Cs x 4	113.74(7)	109.19(7)	118.27(8)
Cs - Te[3] - Cs x 2	69.37(4)	69.14(5)	69.49(4)
Eu - Te[4] - Eu x 2	81.35(4)	81.22(5)	81.45(4)
Eu - Te[4] - Te[3] x 4	62.38(5)	61.28(4)	63.72(5)
Eu - Te[4] - Te[3] x 4	117.54(7)	112.68(7)	122.28(8)
Eu - Te[4] - Cs x 4	128.53(5)	125.19(5)	131.72(5)
Te[3] - Te[4] - Te[3] x 4	90.56(8)	82.99(7)	98.45(9)
Te[3] - Te[4] - Te[3] x 4	89.43(7)	88.76(6)	90.71(7)
Te[3] - Te[4] - Te[3] x 4	174.76(9)	171.77(8)	179.88(8)
Te[3] - Te[4] - Cs x 4	66.40(5)	63.69(5)	69.19(6)
Te[3] - Te[4] - Cs x 4	113.42(6)	111.90(7)	114.81(6)
Cs - Te[4] - Cs x 2	69.20(4)	69.16(5)	69.23(4)
Eu - Ag[1] - Eu x 2	75.60(3)	75.46(3)	75.73(3)
Eu - Ag[1] - Te[1] x 4	59.07(4)	58.46(4)	59.66(4)
Eu - Ag[1] - Te[2] x 2	88.39(3)	88.29(3)	88.50(3)
Eu - Ag[1] - Te[2] x 2	163.98(5)	163.89(5)	164.08(5)
Eu - Ag[1] - Ag[2] x 4	64.21(4)	63.54(4)	64.87(4)
Eu - Ag[1] - Ag[2] x 4	115.68(6)	115.03(5)	116.31(6)
Te[1] - Ag[1] - Te[1] x 2	98.80(7)	98.62(7)	98.98(7)
Te[1] - Ag[1] - Te[2] x 4	112.67(5)	112.06(5)	113.26(5)
Te[1] - Ag[1] - Ag[2] x 4	57.54(4)	57.36(4)	57.71(4)
Te[1] - Ag[1] - Ag[2] x 4	122.32(5)	122.14(5)	122.49(5)
Te[2] - Ag[1] - Te[2] x 2	107.61(6)	107.59(7)	107.63(6)
Te[2] - Ag[1] - Ag[2] x 4	55.26(4)	54.74(4)	55.77(4)
Te[2] - Ag[1] - Ag[2] x 4	124.99(7)	124.45(7)	125.52(7)
Ag[2] - Ag[1] - Ag[2] x 4	90.21(5)	90.21(5)	90.21(5)
Ag[2] - Ag[1] - Ag[2] x 4	89.80(3)	89.80(3)	89.80(3)
Ag[2] - Ag[1] - Ag[2] x 4	179.80(7)	179.80(7)	179.80(7)
Eu - Ag[2] - Eu x 2	75.51(4)	75.47(4)	75.54(4)

Table 6.41. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 100 K with e.s.d.'s in parentheses.

Eu - Ag[2] - Te[1] x 4	59.18(4)	58.98(4)	59.39(5)
Eu - Ag[2] - Te[2] x 2	88.69(5)	87.66(5)	89.71(5)
Eu - Ag[2] - Te[2] x 2	164.07(7)	163.02(7)	165.14(7)
Eu - Ag[2] - Ag[1] x 4	64.50(4)	64.07(4)	64.92(4)
Eu - Ag[2] - Ag[1] x 4	115.67(5)	115.25(5)	116.10(5)
Te[1] - Ag[2] - Te[1] x 2	99.16(6)	99.02(6)	99.30(6)
Te[1] - Ag[2] - Te[2] x 4	112.68(5)	112.19(5)	113.15(5)
Te[1] - Ag[2] - Ag[1] x 4	57.48(4)	57.14(5)	57.82(5)
Te[1] - Ag[2] - Ag[1] x 4	122.75(7)	122.51(7)	122.99(7)
Te[2] - Ag[2] - Te[2] x 2	107.24(7)	107.20(7)	107.27(7)
Te[2] - Ag[2] - Ag[1] x 4	55.31(4)	55.13(4)	55.49(4)
Te[2] - Ag[2] - Ag[1] x 4	124.54(5)	124.36(5)	124.72(5)
Ag[1] - Ag[2] - Ag[1] x 4	90.19(5)	90.19(5)	90.19(5)
Ag[1] - Ag[2] - Ag[1] x 4	89.80(3)	89.80(3)	89.80(3)
Ag[1] - Ag[2] - Ag[1] x 4	179.80(7)	179.80(7)	179.80(7)
Te[2] - Cs - Te[2] x 4	74.65(4)	74.31(4)	74.99(4)
Te[2] - Cs - Te[2] x 4	74.32(4)	74.22(4)	74.43(4)
Te[2] - Cs - Te[2] x 4	117.69(5)	117.42(5)	117.97(5)
Te[2] - Cs - Te[3] x 4	94.56(4)	92.34(4)	96.81(4)
Te[2] - Cs - Te[3] x 4	140.41(6)	136.48(5)	144.33(6)
Te[2] - Cs - Te[4] x 4	94.80(5)	93.93(5)	95.68(5)
Te[2] - Cs - Te[4] x 4	140.25(5)	139.74(5)	140.75(5)
Te[3] - Cs - Te[3] x 2	69.47(5)	69.02(5)	69.71(5)
Te[3] - Cs - Te[4] x 4	47.43(5)	43.86(5)	51.16(5)
Te[4] - Cs - Te[4] x 2	69.20(5)	69.16(5)	69.23(4)

Table 6.42. Crystal data and structure refinement for CsAg₂EuTe₄ at 300 K.

Empirical formula	CsAg ₂ EuTe ₄
Formula weight	1011
Temperature	300.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	Pm(0β1/2)0
Unit cell dimensions	a = 4.5094(4) Å, α = 90° b = 4.5226(4) Å, β = 90° c = 12.3962(13) Å, γ = 90°
q-vector(1)	0.2650(4)b* + 1/2c*
Volume	252.81(4) Å ³
Z	2
Density (calculated)	13.277 g/cm ³
Absorption coefficient	49.225 mm ⁻¹
F(000)	420
Crystal size	0.19 x 0.11 x 0.02 mm ³
Theta range for data collection	3.40 to 29.11°
Index ranges	-5<=h<=6, -6<=k<=6, -17<=l<=17, -1<=m<=1
Reflections collected	7087 (2308 main + 4779 satellites)
Independent reflections	3846 (1350 main + 2496 satellites) [R _{int} = 0.0240]
Completeness to θ = 29.11°	99%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3846 / 0 / 103
Goodness-of-fit on F ²	2.06
Final R indices [I>2σ(I)]	R _{obs} = 0.0403, wR _{obs} = 0.1220
R indices (all data)	R _{all} = 0.0524, wR _{all} = 0.1275
Final R main indices [I>2σ(I)]	R _{obs} = 0.0280, wR _{obs} = 0.0841
R main indices (all data)	R _{all} = 0.0288, wR _{all} = 0.0876
Final R 1 st order satellites [I>2σ(I)]	R _{obs} = 0.0941, wR _{obs} = 0.1859
R 1 st order satellites (all data)	R _{all} = 0.1431, wR _{all} = 0.1945
Extinction coefficient	0.00089(7)
T _{min} and T _{max} coefficients	0.0721 and 0.5240
Largest diff. peak and hole	3.32 and -3.87 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o , wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2} \text{ and } w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.43. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{CsAg}_2\text{EuTe}_4$ at 300 K with e.s.d.'s.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu	0	0	0	2749	1	18(1)
	sin, 1	83(1)	-7(1)	2(1)		
	cos, 1	73(1)	8(1)	1(1)		
Te[1]	0	4999(3)	5000	3489(1)	1	17(1)
	sin, 1	26(2)	0(1)	3(1)		
	cos, 1	13(1)	1(2)	2(1)		
Te[2]	0	0(2)	0	6376(1)	1	20(1)
	sin, 1	56(2)	2(1)	1(1)		
	cos, 1	-26(1)	5(2)	-1(1)		
Te[3]	0	5010(5)	0	575(1)	1	21(1)
	sin, 1	86(1)	-34(4)	-1(1)		
	cos, 1	469(3)	6(1)	-3(1)		
Te[4]	0	7(4)	5000	578(1)	1	24(1)
	sin, 1	-69(1)	26(4)	-1(1)		
	cos, 1	-377(3)	-5(1)	-3(1)		
Ag[1]	0	-10(4)	5000	5049(2)	1	35(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Ag[2]	0	4995(3)	0	5045(2)	1	35(1)
	sin, 1	0	0	0		
	cos, 1	0	0	0		
Cs	0	4997(3)	5000	7943(1)	1	25(1)
	sin, 1	53(2)	10(2)	2(1)		
	cos, 1	-71(2)	8(2)	-3(1)		

Table 6.44. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{CsAg}_2\text{EuTe}_4$ at 300 K with e.s.d.'s.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0	15(1)	15(1)	25(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	1(1)	0(1)	1(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	1(1)	0(1)
Te[1]	0	14(1)	14(1)	22(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	-1(1)	0(1)	0(1)	0(1)
Te[2]	0	19(1)	17(1)	25(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
Te[3]	0	21(1)	20(1)	24(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	1(1)	-8(1)	-1(1)	2(1)
	cos, 1	1(1)	-1(1)	3(1)	1(1)	-4(1)	0(1)
Te[4]	0	30(1)	22(1)	20(1)	0	-1(1)	0
	sin, 1	0(1)	0(1)	0(1)	8(1)	-1(1)	2(1)
	cos, 1	-1(1)	1(1)	2(1)	-1(1)	-8(1)	0(1)
Ag[1]	0	53(1)	25(1)	27(1)	0	-1(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Ag[2]	0	26(1)	50(1)	30(1)	0	-1(1)	0
	sin, 1	0	0	0	0	0	0
	cos, 1	0	0	0	0	0	0
Cs	0	27(1)	27(1)	20(1)	0	-1(1)	0
	sin, 1	0(1)	0(1)	-1(1)	0(1)	1(1)	1(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	-2(1)	0(1)

Table 6.45. Bond lengths distributions [Å] for CsAg₂EuTe₄ at 300 K with e.s.d.'s.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu - Te[1] x 4	3.3402(12)	3.3113(12)	3.3687(13)
Eu - Te[3]	3.464(2)	3.364(2)	3.569(2)
Eu - Te[3]	3.472(2)	3.359(2)	3.585(2)
Eu - Te[4] x 2	3.4725(16)	3.4581(17)	3.4829(16)
Eu - Ag[1] x 2	3.6873(16)	3.6838(16)	3.6907(16)
Eu - Ag[2] x 2	3.6810(19)	3.6523(19)	3.7093(19)
Te[1] - Ag[1]	2.974(2)	2.967(2)	2.981(2)
Te[1] - Ag[1]	2.968(2)	2.955(2)	2.980(2)
Te[1] - Ag[2] x 2	2.9728(17)	2.9702(17)	2.9754(17)
Te[2] - Ag[1] x 2	2.7958(14)	2.7934(14)	2.7981(14)
Te[2] - Ag[2]	2.795(2)	2.772(2)	2.818(2)
Te[2] - Ag[2]	2.791(2)	2.770(2)	2.813(2)
Te[2] - Cs x 4	3.7387(17)	3.7233(17)	3.7542(17)
Te[3] - Te[4] x 2	3.202(2)	2.954(2)	3.455(2)
Te[3] - Te[4] x 2	3.195(2)	2.951(2)	3.453(2)
Te[3] - Cs x 2	3.974(2)	3.962(2)	3.981(2)
Te[4] - Cs	3.971(2)	3.897(3)	4.048(3)
Te[4] - Cs	3.967(2)	3.892(3)	4.043(3)
Ag[1] - Ag[2] x 4	3.1917(17)	3.1917(17)	3.1917(17)

Table 6.46. Bond angles distributions [°] for CsAg₂EuTe₄ at 300 K with e.s.d.'s.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - Eu - Te[1] x 4	85.22(3)	84.36(3)	86.11(3)
Te[1] - Eu - Te[1] x 4	84.92(3)	84.86(3)	85.00(3)
Te[1] - Eu - Te[1] x 4	145.94(5)	145.88(5)	146.02(5)
Te[1] - Eu - Te[3] x 4	77.57(4)	76.40(4)	78.78(4)
Te[1] - Eu - Te[3] x 4	131.43(4)	130.34(4)	132.46(4)
Te[1] - Eu - Te[4] x 4	77.35(4)	75.15(4)	79.58(4)
Te[1] - Eu - Te[4] x 4	131.56(4)	128.03(4)	135.13(4)
Te[1] - Eu - Ag[1] x 4	49.66(4)	49.35(4)	49.97(4)
Te[1] - Eu - Ag[1] x 4	100.55(4)	99.94(4)	101.16(4)
Te[1] - Eu - Ag[2] x 4	49.81(3)	49.35(3)	50.28(3)

Table 6.46. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 300 K with e.s.d.'s.

Te[1] - Eu - Ag[2] x 4	100.49(4)	100.38(4)	100.59(4)
Te[3] - Eu - Te[3] x 2	81.07(5)	80.85(5)	81.18(5)
Te[3] - Eu - Te[4] x 4	54.83(4)	50.96(4)	58.85(4)
Te[3] - Eu - Ag[1] x 4	126.88(4)	126.14(4)	127.64(4)
Te[3] - Eu - Ag[2] x 2	101.72(4)	100.22(5)	103.26(5)
Te[3] - Eu - Ag[2] x 2	177.30(5)	175.75(5)	178.88(5)
Te[4] - Eu - Te[4] x 2	81.35(4)	81.13(4)	81.46(4)
Te[4] - Eu - Ag[1] x 2	101.46(3)	101.23(3)	101.76(4)
Te[4] - Eu - Ag[1] x 2	176.00(4)	174.96(4)	177.38(4)
Te[4] - Eu - Ag[2] x 4	126.79(4)	123.92(4)	129.67(4)
Ag[1] - Eu - Ag[1] x 2	75.65(3)	75.60(3)	75.69(3)
Ag[1] - Eu - Ag[2] x 4	51.34(3)	51.14(3)	51.54(3)
Ag[2] - Eu - Ag[2] x 2	75.58(4)	75.53(4)	75.62(4)
Eu - Te[1] - Eu x 4	85.25(3)	84.92(4)	85.57(4)
Eu - Te[1] - Eu x 4	84.92(3)	84.86(3)	85.00(3)
Eu - Te[1] - Eu x 4	145.95(6)	145.67(6)	146.23(6)
Eu - Te[1] - Ag[1] x 4	71.20(4)	70.85(4)	71.56(4)
Eu - Te[1] - Ag[1] x 4	134.65(4)	134.34(4)	134.96(4)
Eu - Te[1] - Ag[2] x 4	71.00(4)	70.70(4)	71.31(4)
Eu - Te[1] - Ag[2] x 4	134.81(6)	134.39(5)	135.23(5)
Ag[1] - Te[1] - Ag[1] x 2	98.74(7)	98.62(7)	98.85(7)
Ag[1] - Te[1] - Ag[2] x 4	64.99(5)	64.93(5)	65.05(5)
Ag[2] - Te[1] - Ag[2] x 2	99.05(6)	98.93(6)	99.16(6)
Ag[1] - Te[2] - Ag[1] x 2	107.96(6)	107.90(6)	108.02(6)
Ag[1] - Te[2] - Ag[2] x 4	69.62(5)	69.27(5)	69.97(5)
Ag[1] - Te[2] - Cs x 4	79.36(4)	79.10(4)	79.63(4)
Ag[1] - Te[2] - Cs x 4	142.54(6)	141.84(5)	143.26(5)
Ag[2] - Te[2] - Ag[2] x 2	107.64(7)	107.58(7)	107.70(7)
Ag[2] - Te[2] - Cs x 4	79.59(4)	79.13(4)	80.05(4)
Ag[2] - Te[2] - Cs x 4	142.52(3)	142.22(3)	142.81(3)
Cs - Te[2] - Cs x 4	74.44(3)	74.30(3)	74.57(3)
Cs - Te[2] - Cs x 4	74.20(3)	74.12(3)	74.27(3)
Cs - Te[2] - Cs x 4	117.36(5)	117.02(5)	117.70(5)
Eu - Te[3] - Eu x 2	81.07(4)	80.85(5)	81.18(4)

Table 6.46. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 300 K with e.s.d.'s.

Eu - Te[3] - Te[4] x 4	62.64(5)	59.30(4)	66.21(5)
Eu - Te[3] - Te[4] x 4	117.10(6)	115.71(5)	118.14(5)
Eu - Te[3] - Cs x 4	128.46(6)	124.17(5)	132.77(5)
Te[4] - Te[3] - Te[4] x 4	90.40(7)	82.53(6)	98.96(8)
Te[4] - Te[3] - Te[4] x 4	89.48(5)	88.98(4)	90.48(6)
Te[4] - Te[3] - Te[4] x 4	174.58(8)	171.51(7)	179.90(7)
Te[4] - Te[3] - Cs x 4	66.07(5)	64.99(4)	67.25(4)
Te[4] - Te[3] - Cs x 4	113.67(6)	109.24(7)	118.08(7)
Cs - Te[3] - Cs x 2	69.37(4)	69.17(4)	69.47(4)
Eu - Te[4] - Eu x 2	81.27(4)	80.98(4)	81.42(4)
Eu - Te[4] - Te[3] x 4	62.38(4)	61.40(4)	63.56(4)
Eu - Te[4] - Te[3] x 4	117.50(6)	112.77(6)	122.10(7)
Eu - Te[4] - Cs x 4	128.52(5)	125.03(5)	131.87(4)
Te[3] - Te[4] - Te[3] x 4	90.61(7)	82.97(6)	98.58(8)
Te[3] - Te[4] - Te[3] x 4	89.48(6)	88.98(6)	90.48(6)
Te[3] - Te[4] - Te[3] x 4	174.82(7)	171.79(7)	179.89(7)
Te[3] - Te[4] - Cs x 4	66.39(5)	63.55(5)	69.30(6)
Te[3] - Te[4] - Cs x 4	113.39(6)	111.98(6)	114.72(6)
Cs - Te[4] - Cs x 2	69.21(4)	69.17(4)	69.24(4)
Eu - Ag[1] - Eu x 2	75.66(4)	75.60(4)	75.71(4)
Eu - Ag[1] - Te[1] x 4	59.08(4)	58.43(4)	59.71(4)
Eu - Ag[1] - Te[2] x 2	88.18(3)	88.10(3)	88.28(3)
Eu - Ag[1] - Te[2] x 2	163.83(6)	163.78(6)	163.90(6)
Eu - Ag[1] - Ag[2] x 4	64.23(4)	63.63(4)	64.82(4)
Eu - Ag[1] - Ag[2] x 4	115.74(6)	115.11(6)	116.35(6)
Te[1] - Ag[1] - Te[1] x 2	98.74(7)	98.62(7)	98.85(7)
Te[1] - Ag[1] - Te[2] x 4	112.62(5)	112.10(5)	113.13(5)
Te[1] - Ag[1] - Ag[2] x 4	57.58(5)	57.52(5)	57.64(5)
Te[1] - Ag[1] - Ag[2] x 4	122.32(5)	122.26(5)	122.38(5)
Te[2] - Ag[1] - Te[2] x 2	107.97(7)	107.88(7)	108.05(7)
Te[2] - Ag[1] - Ag[2] x 4	55.18(4)	54.67(4)	55.68(4)
Te[2] - Ag[1] - Ag[2] x 4	125.11(7)	124.63(7)	125.58(7)
Ag[2] - Ag[1] - Ag[2] x 4	90.22(5)	90.22(5)	90.22(5)
Ag[2] - Ag[1] - Ag[2] x 4	89.83(3)	89.83(3)	89.83(3)

Table 6.46. (Cont'd) Bond angles distributions [°] for CsAg₂EuTe₄ at 300 K with e.s.d.'s.

Ag[2] - Ag[1] - Ag[2] x 4	179.82(8)	179.82(8)	179.82(8)
Eu - Ag[2] - Eu x 2	75.58(4)	75.53(4)	75.62(4)
Eu - Ag[2] - Te[1] x 4	59.15(4)	58.99(4)	59.31(4)
Eu - Ag[2] - Te[2] x 2	88.45(5)	87.49(5)	89.40(5)
Eu - Ag[2] - Te[2] x 2	163.91(7)	163.02(7)	164.81(7)
Eu - Ag[2] - Ag[1] x 4	64.45(4)	64.08(4)	64.81(4)
Eu - Ag[2] - Ag[1] x 4	115.68(5)	115.31(5)	116.05(5)
Te[1] - Ag[2] - Te[1] x 2	99.05(7)	98.98(7)	99.12(7)
Te[1] - Ag[2] - Te[2] x 4	112.58(5)	112.22(5)	112.93(5)
Te[1] - Ag[2] - Ag[1] x 4	57.52(4)	57.34(4)	57.70(4)
Te[1] - Ag[2] - Ag[1] x 4	122.67(7)	122.43(7)	122.92(7)
Te[2] - Ag[2] - Te[2] x 2	107.64(7)	107.58(7)	107.70(7)
Te[2] - Ag[2] - Ag[1] x 4	55.19(4)	55.00(4)	55.38(4)
Te[2] - Ag[2] - Ag[1] x 4	124.65(5)	124.46(5)	124.84(5)
Ag[1] - Ag[2] - Ag[1] x 4	90.11(5)	90.11(5)	90.11(5)
Ag[1] - Ag[2] - Ag[1] x 4	89.83(3)	89.83(3)	89.83(3)
Ag[1] - Ag[2] - Ag[1] x 4	179.82(8)	179.82(8)	179.82(8)
Te[2] - Cs - Te[2] x 4	74.47(3)	74.09(3)	74.85(3)
Te[2] - Cs - Te[2] x 4	74.20(3)	74.12(3)	74.27(3)
Te[2] - Cs - Te[2] x 4	117.36(5)	117.11(5)	117.62(5)
Te[2] - Cs - Te[3] x 4	94.77(4)	92.73(4)	96.84(4)
Te[2] - Cs - Te[3] x 4	140.60(5)	136.96(5)	144.23(5)
Te[2] - Cs - Te[4] x 4	94.95(4)	93.86(4)	96.06(4)
Te[2] - Cs - Te[4] x 4	140.40(4)	139.77(4)	140.99(4)
Te[3] - Cs - Te[3] x 2	69.46(4)	69.05(4)	69.68(5)
Te[3] - Cs - Te[4] x 4	47.48(4)	44.00(4)	51.11(4)
Te[4] - Cs - Te[4] x 2	69.21(4)	69.17(5)	69.24(4)

Table 6.47. Crystal data and structure refinement for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K.

Empirical formula	$\text{Cu}_{0.63(2)}\text{EuTe}_2$
Formula weight	449.1
Temperature	100.0(3) K
Crystal system	Monoclinic
Space group	$\text{Xm}(0\beta_10)(0\beta_20)0$
Centering vector	$(0\ 0\ \frac{1}{2}\ \frac{1}{2}\ 0)$
Unit cell dimensions	$a = 4.4536(2)\ \text{\AA}, \alpha = 90^\circ$ $b = 4.4723(2)\ \text{\AA}, \beta = 90^\circ$ $c = 20.2982(6)\ \text{\AA}, \gamma = 90^\circ$
q-vector(1)	$0.2910(2)b^*$
q-vector(2)	$0.3557(3)b^*$
Volume	$404.30(3)\ \text{\AA}^3$
Z	4
Density (calculated)	$7.3758\ \text{g/cm}^3$
Absorption coefficient	$32.735\ \text{mm}^{-1}$
Crystal size	$0.14 \times 0.11 \times 0.02\ \text{mm}^3$
Theta range for data collection	1.62 to 29.21°
Index ranges	$-6 \leq h \leq 6, -6 \leq k \leq 6, -27 \leq l \leq 27, -1 \leq m \leq 1$
Reflections collected	17326 (1621 main + 15705 satellites)
Independent reflections	9015 (947 main + 4028 satellites) [$R_{\text{int}} = 0.0491$]
Completeness to $\theta = 29.21^\circ$	97%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9015 / 0 / 347
Goodness-of-fit on F^2	2.46
Final R indices [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0622, wR_{\text{obs}} = 0.2085$
R indices (all data)	$R_{\text{all}} = 0.1081, wR_{\text{all}} = 0.2267$
Final R main indices [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0380, wR_{\text{obs}} = 0.1332$
R main indices (all data)	$R_{\text{all}} = 0.0384, wR_{\text{all}} = 0.1342$
Final R 1 st order satellites [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.0963, wR_{\text{obs}} = 0.2237$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.1569, wR_{\text{all}} = 0.2416$
Final R 2 nd order satellites [$I > 3\sigma(I)$]	$R_{\text{obs}} = 0.1453, wR_{\text{obs}} = 0.3105$
R 2 nd order satellites (all data)	$R_{\text{all}} = 0.2931, wR_{\text{all}} = 0.3478$
T_{min} and T_{max} coefficients	0.0531 and 0.4664
Largest diff. peak and hole	3.54 and $-3.65\ \text{e.\AA}^{-3}$
$R = \Sigma F_o - F_c / \Sigma F_o , wR = \{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 6.48. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
Eu[1a]	0	2549	7549	1297	1	16(1)
	sin, 1	0	-17(2)	0		
	cos, 1	-2(2)	0	20(1)		
	sin, 2	0	-10(2)	0		
	cos, 2	-22(2)	0	0(1)		
	sin, 3	0	-1(2)	0		
	cos, 3	-44(2)	0	-2(1)		
	sin, 4	0	2(4)	0		
	cos, 4	-1(4)	0	0(1)		
Eu[1b]	0	-2500(2)	-7451	-1300(1)	1	17(1)
	sin, 1	0	2(2)	0		
	cos, 1	3(2)	0	25(1)		
	sin, 2	0	5(2)	0		
	cos, 2	36(2)	0	0(1)		
	sin, 3	0	11(2)	0		
	cos, 3	-39(2)	0	2(1)		
	sin, 4	0	1(4)	0		
	cos, 4	-2(3)	0	1(1)		
Te[1a]	0	2522(3)	7549	3211(1)	1	13(1)
	sin, 1	0	42(2)	0		
	cos, 1	2(2)	0	-8(1)		
	sin, 2	0	-1(5)	0		
	cos, 2	-1(8)	0	0(2)		
	sin, 3	0	-1(2)	0		
	cos, 3	-7(2)	0	0(1)		
	sin, 4	0	1(4)	0		
	cos, 4	2(4)	0	1(1)		

Table 6.48. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Te[1b]	0	-2479(3)	-7451	-3213(1)	1	12(1)
	sin, 1	0	-40(2)	0		
	cos, 1	-2(2)	0	-9(1)		
	sin, 2	0	1(4)	0		
	cos, 2	0(4)	0	0(1)		
	sin, 3	0	1(2)	0		
	cos, 3	-5(2)	0	0(1)		
	sin, 4	0	5(4)	0		
	cos, 4	-3(3)	0	-2(1)		
Te[2a]	0	2476(5)	2549	2(1)	1	16(1)
	sin, 1	0	-75(2)	0		
	cos, 1	6(4)	0	16(1)		
	sin, 2	0	-2(3)	0		
	cos, 2	125(3)	0	-2(1)		
	sin, 3	0	-31(2)	0		
	cos, 3	-152(3)	0	6(1)		
	sin, 4	0	4(5)	0		
	cos, 4	-12(4)	0	0(1)		
Te[2b]	0	-2516(6)	-2451	5(1)	1	17(1)
	sin, 1	0	102(3)	0		
	cos, 1	-8(4)	0	11(1)		
	sin, 2	0	14(3)	0		
	cos, 2	-158(3)	0	-1(1)		
	sin, 3	0	-40(2)	0		
	cos, 3	-173(4)	0	-7(1)		
	sin, 4	0	-9(5)	0		
	cos, 4	-13(4)	0	-5(1)		

Table 6.48. (Cont'd) Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Cu[1a]	0	2536(19)	2549	2502(4)	0.562(9)	30(1)
	sin, 1	0	94(13)	0		
	cos, 1	-8(12)	0	-4(3)		
	sin, 2	0	10(13)	0		
	cos, 2	30(11)	0	-12(3)		
	sin, 3	0	52(11)	0		
	cos, 3	195(30)	0	-22(3)		
	sin, 4	0	14(19)	0		
	cos, 4	-54(16)	0	8(5)		
Cu[1b]	0	-2464(11)	-2451	-2501(2)	0.700(8)	10(1)
	sin, 1	0	-40(8)	0		
	cos, 1	-6(7)	0	3(2)		
	sin, 2	0	41(8)	0		
	cos, 2	11(6)	0	-6(1)		
	sin, 3	0	-21(7)	0		
	cos, 3	-95(16)	0	4(2)		
	sin, 4	0	-18(11)	0		
	cos, 4	41(10)	0	-2(2)		

Table 6.49. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu[1a]	0	12(1)	11(1)	26(1)	0	-2(1)	0
	sin, 1	0	0	0	0(1)	0	0(1)
	cos, 1	0(1)	-1(1)	5(1)	0	-3(1)	0
	sin, 2	0	0	0	1(1)	0	0(1)
	cos, 2	1(1)	1(1)	-2(1)	0	0(1)	0
	sin, 3	0	0	0	1(1)	0	-2(1)
	cos, 3	0(1)	-1(1)	0(1)	0	-2(1)	0
	sin, 4	0	0	0	1(1)	0	0(1)
	cos, 4	0(1)	2(1)	2(1)	0	-1(1)	0

Table 6.49. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Eu[1b]	0	15(1)	10(1)	26(1)	0	2(1)	0
	sin, 1	0	0	0	0(1)	0	-2(1)
	cos, 1	-2(1)	-2(1)	4(1)	0	-3(1)	0
	sin, 2	0	0	0	1(1)	0	1(1)
	cos, 2	0(1)	-1(1)	1(1)	0	-1(1)	0
	sin, 3	0	0	0	-1(1)	0	2(1)
	cos, 3	0(1)	0(1)	0(1)	0	0(1)	0
	sin, 4	0	0	0	1(1)	0	0(1)
	cos, 4	0(1)	0(1)	1(1)	0	0(1)	0
Te[1a]	0	10(1)	9(1)	20(1)	0	1(1)	0
	sin, 1	0	0	0	-1(1)	0	1(1)
	cos, 1	0(1)	1(1)	-1(1)	0	1(1)	0
	sin, 2	0	0	0	0(1)	0	0(1)
	cos, 2	-1(1)	0(1)	1(1)	0	0(1)	0
	sin, 3	0	0	0	1(1)	0	1(1)
	cos, 3	1(1)	-1(1)	-1(1)	0	1(1)	0
	sin, 4	0	0	0	0(1)	0	0(1)
	cos, 4	0(1)	0(1)	0(1)	0	0(1)	0
Te[1b]	0	12(1)	9(1)	15(1)	0	-1(1)	0
	sin, 1	0	0	0	1(1)	0	0(1)
	cos, 1	0(1)	-1(1)	-1(1)	0	1(1)	0
	sin, 2	0	0	0	0(1)	0	0(1)
	cos, 2	1(1)	0(1)	0(1)	0	0(1)	0
	sin, 3	0	0	0	1(1)	0	0(1)
	cos, 3	1(1)	-1(1)	-1(1)	0	0(1)	0
	sin, 4	0	0	0	0(1)	0	-1(1)
	cos, 4	0(1)	0(1)	1(1)	0	-1(1)	0

Table 6.49. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Te[2a]	0	15(1)	19(1)	13(1)	0	1(1)	0
sin, 1	0	0	0	0	-1(1)	0	1(1)
cos, 1	-11(1)	-2(1)	-1(1)	0	1(1)	0	0
sin, 2	0	0	0	1(1)	0	1(1)	0
cos, 2	2(1)	1(1)	-2(1)	0	-2(1)	0	0
sin, 3	0	0	0	0(1)	0	0(1)	0
cos, 3	0(1)	-2(1)	-1(1)	0	1(1)	0	0
sin, 4	0	0	0	2(1)	0	0(1)	0
cos, 4	-1(1)	0(1)	4(1)	0	2(1)	0	0
Te[2b]	0	21(1)	17(1)	15(1)	0	0(1)	0
sin, 1	0	0	0	0(1)	0	-2(1)	0
cos, 1	12(1)	-1(1)	-1(1)	0	1(1)	0	0
sin, 2	0	0	0	1(1)	0	1(1)	0
cos, 2	-2(1)	0(1)	-1(1)	0	-2(1)	0	0
sin, 3	0	0	0	1(1)	0	0(1)	0
cos, 3	0(1)	-2(1)	-1(1)	0	-3(1)	0	0
sin, 4	0	0	0	3(1)	0	1(1)	0
cos, 4	1(1)	3(1)	1(1)	0	-2(1)	0	0
Cu[1a]	0	30(3)	22(2)	32(2)	0	0(1)	0
sin, 1	0	0	0	0(2)	0	2(2)	0
cos, 1	5(3)	-8(3)	3(3)	0	0(2)	0	0
sin, 2	0	0	0	4(2)	0	-3(2)	0
cos, 2	-21(4)	-13(3)	20(3)	0	0(3)	0	0
sin, 3	0	0	0	6(2)	0	5(2)	0
cos, 3	-15(3)	-6(2)	1(2)	0	2(2)	0	0
sin, 4	0	0	0	0(3)	0	-2(3)	0
cos, 4	13(4)	1(4)	2(5)	0	5(3)	0	0

Table 6.49. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Cu[1b]	0	16(1)	11(1)	4(1)	0	1(1)	0
	sin, 1	0	0	0	-1(1)	0	-1(1)
	cos, 1	4(2)	-5(2)	1(1)	0	1(1)	0
	sin, 2	0	0	0	1(1)	0	-1(1)
	cos, 2	7(2)	5(2)	-3(2)	0	-2(1)	0
	sin, 3	0	0	0	-5(1)	0	4(1)
	cos, 3	-1(2)	-4(1)	-2(1)	0	-1(1)	0
	sin, 4	0	0	0	1(2)	0	-2(1)
	cos, 4	5(2)	7(2)	4(2)	0	0(2)	0

Table 6.50. Fourier components of the occupational modulation for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Cu[1a]	sin, 1	0
	cos, 1	-0.065(14)
Cu[1a]	sin, 2	0
	cos, 2	-0.003(18)
Cu[1a]	sin, 3	0
	cos, 3	-0.060(9)
Cu[1a]	sin, 4	0
	cos, 4	0.02(3)
Cu[1b]	sin, 1	0
	cos, 1	0.026(12)
Cu[1b]	sin, 2	0
	cos, 2	-0.019(16)
Cu[1b]	sin, 3	0
	cos, 3	-0.046(8)
Cu[1b]	sin, 4	0
	cos, 4	0.02(2)

Table 6.51. Bond lengths distributions [Å] for Cu_{0.63(2)}EuTe₂ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
Eu[1a] - Te[1a] x 2	3.303(4)	3.283(4)	3.329(4)
Eu[1a] - Te[1b] x 2	3.315(4)	3.289(4)	3.340(4)
Eu[1a] - Te[2a] x 2	3.451(4)	3.425(4)	3.479(4)
Eu[1a] - Te[2b] x 2	3.444(5)	3.364(8)	3.556(8)
Eu[1a] - Cu[1a] x 2	3.311(16)	3.233(15)	3.372(15)
Eu[1a] - Cu[1b]	3.294(9)	3.209(13)	3.364(10)
Eu[1a] - Cu[1b]	3.313(9)	3.252(11)	3.375(11)
Eu[1b] - Te[1a] x 2	3.302(4)	3.280(4)	3.324(4)
Eu[1b] - Te[1a] x 2	3.315(4)	3.286(4)	3.340(5)
Eu[1b] - Te[1b]	3.882(4)	3.801(7)	3.959(7)
Eu[1b] - Te[2a]	3.463(5)	3.412(8)	3.543(8)
Eu[1b] - Te[2a]	3.450(5)	3.408(8)	3.517(8)
Eu[1b] - Te[2b] x 2	3.469(5)	3.443(5)	3.500(5)
Eu[1b] - Cu[1a] x 2	3.289(17)	3.250(17)	3.35(3)
Eu[1b] - Cu[1b] x 2	3.308(9)	3.268(8)	3.355(8)
Te[1a] - Cu[1a] x 2	2.662(15)	2.607(15)	2.728(16)
Te[1a] - Cu[1b] x 2	2.651(10)	2.603(12)	2.699(12)
Te[1b] - Cu[1a] x 2	2.651(17)	2.526(18)	2.773(19)
Te[1b] - Cu[1b] x 2	2.663(8)	2.636(8)	2.690(9)
Te[2a] - Te[2b] x 4	3.159(5)	2.935(5)	3.280(5)
Cu[1a] - Cu[1b] x 4	3.159(18)	3.050(19)	3.271(18)

Table 6.52. Bond angles distributions [°] for Cu_{0.63(2)}EuTe₂ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1a] - Eu[1a] - Te[1b] x 4	72.55(7)	71.92(10)	73.15(11)
Te[1a] - Eu[1a] - Te[2a] x 2	139.60(11)	138.78(13)	140.40(11)
Te[1a] - Eu[1a] - Te[2b] x 2	139.71(10)	138.95(8)	140.85(17)
Te[1a] - Eu[1a] - Cu[1a] x 2	42.5(3)	40.9(3)	44.3(3)
Te[1a] - Eu[1a] - Cu[1b] x 2	42.34(10)	41.37(9)	43.20(9)
Te[1b] - Eu[1a] - Te[1b] x 4	85.22(10)	84.41(13)	86.47(13)

Table 6.52. (Cont'd) Bond angles distributions [°] for Cu_{0.63(2)}EuTe₂ at 100 K with e.s.d.'s in parentheses.

Te[1b] - Eu[1a] - Te[1b] x 4	84.59(9)	84.21(9)	84.93(9)
Te[1b] - Eu[1a] - Te[1b] x 4	144.97(10)	143.67(17)	146.21(17)
Te[1b] - Eu[1a] - Te[2a] x 4	77.84(9)	75.96(9)	79.55(11)
Te[1b] - Eu[1a] - Te[2a] x 4	131.73(10)	129.34(8)	134.18(9)
Te[1b] - Eu[1a] - Te[2b] x 4	78.17(10)	76.95(10)	79.78(9)
Te[1b] - Eu[1a] - Te[2b] x 4	131.67(13)	129.85(13)	133.75(13)
Te[1b] - Eu[1a] - Cu[1a] x 4	47.5(2)	45.9(2)	49.0(2)
Te[1b] - Eu[1a] - Cu[1a] x 4	103.7(3)	100.9(3)	106.7(3)
Te[1b] - Eu[1a] - Cu[1b] x 4	47.6(2)	46.7(2)	48.4(2)
Te[1b] - Eu[1a] - Cu[1b] x 4	103.4(2)	102.1(2)	104.6(2)
Te[2a] - Eu[1a] - Te[2a] x 2	80.79(11)	79.21(14)	82.21(14)
Te[2a] - Eu[1a] - Te[2b] x 4	54.51(11)	50.75(11)	56.54(11)
Te[2a] - Eu[1a] - Cu[1a] x 2	97.1(4)	96.0(4)	98.4(4)
Te[2a] - Eu[1a] - Cu[1a] x 2	177.2(3)	175.2(3)	179.4(3)
Te[2a] - Eu[1a] - Cu[1b] x 4	124.2(2)	121.4(2)	126.8(2)
Te[2b] - Eu[1a] - Te[2b] x 2	80.67(10)	79.75(16)	81.48(16)
Te[2b] - Eu[1a] - Cu[1a] x 4	124.4(3)	122.2(2)	126.0(3)
Te[2b] - Eu[1a] - Cu[1b] x 2	97.37(12)	96.35(18)	98.37(18)
Te[2b] - Eu[1a] - Cu[1b] x 2	177.59(17)	176.7(2)	179.0(2)
Cu[1a] - Eu[1a] - Cu[1a] x 2	84.9(4)	82.3(4)	86.9(4)
Cu[1a] - Eu[1a] - Cu[1b] x 4	57.1(4)	54.4(4)	60.1(4)
Cu[1b] - Eu[1a] - Cu[1b] x 2	84.76(19)	83.4(3)	86.1(3)
Te[1a] - Eu[1b] - Te[1a] x 6	85.25(11)	84.36(10)	86.68(14)
Te[1a] - Eu[1b] - Te[1a] x 4	145.06(11)	143.44(16)	146.79(17)
Te[1a] - Eu[1b] - Te[1b] x 4	72.59(10)	71.72(12)	73.41(9)
Te[1a] - Eu[1b] - Te[2a] x 4	78.24(11)	77.23(11)	79.26(11)
Te[1a] - Eu[1b] - Te[2a] x 4	131.48(13)	129.80(13)	133.23(12)
Te[1a] - Eu[1b] - Te[2b] x 4	78.01(11)	75.84(12)	80.23(14)
Te[1a] - Eu[1b] - Te[2b] x 4	131.64(12)	128.71(10)	134.63(9)
Te[1a] - Eu[1b] - Cu[1a] x 4	47.6(4)	46.3(4)	48.9(4)
Te[1a] - Eu[1b] - Cu[1a] x 4	103.5(3)	101.9(3)	105.0(3)
Te[1a] - Eu[1b] - Cu[1b] x 4	47.43(14)	46.29(12)	48.81(13)
Te[1a] - Eu[1b] - Cu[1b] x 4	103.82(18)	101.92(18)	105.7(2)
Te[1a] - Eu[1b] - Te[1a] x 2	84.60(10)	84.30(11)	84.93(10)

Table 6.52. (Cont'd) Bond angles distributions [°] for $\text{Cu}_{0.63(2)}\text{EuTe}_2$ at 100 K with e.s.d.'s in parentheses.

Te[1b] - Eu[1b] - Te[2a] x 2	139.89(9)	139.46(15)	140.77(16)
Te[1b] - Eu[1b] - Te[2b] x 2	139.80(11)	138.75(13)	140.85(10)
Te[1b] - Eu[1b] - Cu[1a] x 2	42.38(16)	40.23(16)	44.71(16)
Te[1b] - Eu[1b] - Cu[1b] x 2	42.5(2)	41.4(2)	43.7(2)
Te[2a] - Eu[1b] - Te[2a] x 2	80.21(9)	79.66(14)	80.65(8)
Te[2a] - Eu[1b] - Te[2b] x 4	54.32(9)	50.80(9)	56.80(9)
Te[2a] - Eu[1b] - Cu[1a] x 2	97.51(18)	94.89(17)	99.92(17)
Te[2a] - Eu[1b] - Cu[1a] x 2	177.3(2)	175.8(2)	179.0(2)
Te[2a] - Eu[1b] - Cu[1b] x 4	124.45(17)	122.55(16)	126.18(17)
Te[2b] - Eu[1b] - Te[2b] x 2	80.34(11)	78.30(14)	82.22(11)
Te[2b] - Eu[1b] - Cu[1a] x 4	124.4(4)	121.8(4)	126.3(4)
Te[2b] - Eu[1b] - Cu[1b] x 2	97.3(2)	96.3(2)	98.3(2)
Te[2b] - Eu[1b] - Cu[1b] x 2	177.2(2)	175.0(2)	179.3(2)
Cu[1a] - Eu[1b] - Cu[1a] x 2	84.9(3)	83.2(3)	87.0(4)
Cu[1a] - Eu[1b] - Cu[1b] x 4	57.2(3)	54.7(3)	59.6(3)
Cu[1b] - Eu[1b] - Cu[1b] x 2	85.1(2)	83.4(3)	87.4(3)
Eu[1a] - Te[1a] - Eu[1b] x 4	107.28(10)	106.13(11)	108.43(10)
Eu[1a] - Te[1a] - Cu[1a] x 2	57.2(3)	55.1(4)	59.2(3)
Eu[1a] - Te[1a] - Cu[1b] x 2	56.82(13)	55.53(12)	58.18(11)
Eu[1b] - Te[1a] - Eu[1b] x 8	84.85(11)	84.38(17)	85.21(10)
Eu[1b] - Te[1a] - Eu[1b] x 4	145.08(14)	144.56(9)	145.80(10)
Eu[1b] - Te[1a] - Cu[1a] x 4	66.2(3)	63.4(3)	68.7(3)
Eu[1b] - Te[1a] - Cu[1a] x 4	136.9(2)	134.8(3)	139.3(3)
Eu[1b] - Te[1a] - Cu[1b] x 4	66.3(3)	65.1(3)	67.8(3)
Eu[1b] - Te[1a] - Cu[1b] x 4	136.8(3)	136.1(3)	138.0(3)
Cu[1a] - Te[1a] - Cu[1a] x 2	114.4(5)	111.2(6)	116.8(5)
Cu[1a] - Te[1a] - Cu[1b] x 4	73.0(5)	71.0(5)	75.3(5)
Cu[1b] - Te[1a] - Cu[1b] x 2	114.0(3)	113.3(3)	115.1(4)
Eu[1a] - Te[1b] - Eu[1a] x 8	84.83(10)	84.52(10)	85.22(13)
Eu[1a] - Te[1b] - Eu[1a] x 4	144.95(10)	144.68(8)	145.36(10)
Eu[1a] - Te[1b] - Eu[1b] x 4	107.35(10)	106.32(8)	108.40(9)
Eu[1a] - Te[1b] - Cu[1a] x 4	66.4(4)	65.5(4)	67.3(4)
Eu[1a] - Te[1b] - Cu[1a] x 4	136.8(6)	135.7(6)	138.0(6)
Eu[1a] - Te[1b] - Cu[1b] x 4	66.26(17)	64.88(17)	67.90(17)

Table 6.52. (Cont'd) Bond angles distributions [°] for Cu_{0.63(2)}EuTe₂ at 100 K with e.s.d.'s in parentheses.

Eu[1a] - Te[1b] - Cu[1b] x 4	136.96(16)	135.26(17)	138.50(17)
Eu[1b] - Te[1b] - Cu[1a] x 2	56.7(2)	55.8(2)	58.0(2)
Eu[1b] - Te[1b] - Cu[1b] x 2	57.1(2)	56.2(2)	58.17(19)
Cu[1a] - Te[1b] - Cu[1a] x 2	113.9(4)	111.6(4)	117.0(7)
Cu[1a] - Te[1b] - Cu[1b] x 4	72.9(3)	70.8(3)	75.2(4)
Cu[1b] - Te[1b] - Cu[1b] x 2	114.3(3)	112.5(3)	116.0(3)
Eu[1a] - Te[2a] - Eu[1a] x 2	80.77(11)	80.36(15)	81.06(10)
Eu[1a] - Te[2a] - Eu[1b] x 4	125.80(13)	123.09(12)	128.85(13)
Eu[1a] - Te[2a] - Te[2b] x 4	62.66(9)	61.10(9)	63.99(10)
Eu[1a] - Te[2a] - Te[2b] x 4	117.36(14)	113.54(19)	120.3(2)
Eu[1b] - Te[2a] - Eu[1b] x 2	80.23(9)	79.67(15)	80.65(7)
Eu[1b] - Te[2a] - Te[2b] x 4	63.15(10)	61.56(9)	65.58(10)
Eu[1b] - Te[2a] - Te[2b] x 4	117.04(13)	115.74(12)	118.97(12)
Te[2b] - Te[2a] - Te[2b] x 8	90.35(15)	85.40(18)	94.1(2)
Te[2b] - Te[2a] - Te[2b] x 4	177.73(17)	174.39(17)	180
Eu[1a] - Te[2b] - Eu[1a] x 2	80.66(10)	79.75(16)	81.48(16)
Eu[1a] - Te[2b] - Eu[1b] x 4	125.84(13)	122.01(12)	129.40(13)
Eu[1a] - Te[2b] - Te[2a] x 4	63.02(10)	60.86(11)	65.85(10)
Eu[1a] - Te[2b] - Te[2a] x 4	117.20(13)	115.39(12)	119.26(13)
Eu[1b] - Te[2b] - Eu[1b] x 2	80.30(11)	79.60(15)	81.06(15)
Eu[1b] - Te[2b] - Te[2a] x 4	62.82(10)	60.95(9)	63.89(10)
Eu[1b] - Te[2b] - Te[2a] x 4	117.21(14)	113.2(2)	121.0(2)
Te[2a] - Te[2b] - Te[2a] x 8	90.29(16)	84.96(20)	94.7(2)
Te[2a] - Te[2b] - Te[2a] x 4	177.56(18)	173.58(17)	180
Eu[1a] - Cu[1a] - Eu[1a] x 2	85.0(4)	83.4(4)	86.7(5)
Eu[1a] - Cu[1a] - Eu[1b] x 4	122.6(5)	119.2(5)	126.2(5)
Eu[1a] - Cu[1a] - Te[1a] x 2	80.3(3)	78.1(3)	82.9(5)
Eu[1a] - Cu[1a] - Te[1a] x 2	165.1(6)	161.4(6)	168.4(6)
Eu[1a] - Cu[1a] - Te[1b] x 4	66.1(4)	65.1(4)	67.3(4)
Eu[1a] - Cu[1a] - Cu[1b] x 4	61.1(3)	59.1(3)	63.2(3)
Eu[1a] - Cu[1a] - Cu[1b] x 4	118.3(5)	116.8(6)	119.5(6)
Eu[1b] - Cu[1a] - Eu[1b] x 2	84.9(4)	83.2(4)	87.0(5)
Eu[1b] - Cu[1a] - Te[1a] x 4	66.4(4)	63.8(4)	69.1(4)
Eu[1b] - Cu[1a] - Te[1b] x 2	80.3(4)	77.3(4)	83.2(5)

Table 6.52. (Cont'd) Bond angles distributions [°] for Cu_{0.63(2)}EuTe₂ at 100 K with e.s.d.'s in parentheses.

Eu[1b] - Cu[1a] - Te[1b] x 2	165.7(6)	164.6(5)	166.8(7)
Eu[1b] - Cu[1a] - Cu[1b] x 4	61.5(3)	59.2(3)	63.6(4)
Eu[1b] - Cu[1a] - Cu[1b] x 4	118.6(5)	116.0(5)	120.8(5)
Te[1a] - Cu[1a] - Te[1a] x 2	114.3(6)	112.0(6)	116.8(6)
Te[1a] - Cu[1a] - Te[1b] x 4	107.0(6)	103.5(5)	110.5(6)
Te[1a] - Cu[1a] - Cu[1b] x 4	53.3(3)	51.1(3)	55.2(3)
Te[1a] - Cu[1a] - Cu[1b] x 4	126.5(6)	122.2(7)	131.1(7)
Te[1b] - Cu[1a] - Te[1b] x 2	114.0(6)	111.6(6)	117.0(10)
Te[1b] - Cu[1a] - Cu[1b] x 4	53.6(3)	52.2(3)	55.4(4)
Te[1b] - Cu[1a] - Cu[1b] x 4	126.2(5)	124.5(5)	127.9(6)
Cu[1b] - Cu[1a] - Cu[1b] x 8	90.3(5)	87.3(7)	92.9(5)
Cu[1b] - Cu[1a] - Cu[1b] x 4	177.8(6)	175.6(6)	179.8(6)
Eu[1a] - Cu[1b] - Eu[1a] x 2	84.7(2)	83.4(3)	86.1(3)
Eu[1a] - Cu[1b] - Eu[1b] x 4	122.7(3)	120.4(3)	125.3(3)
Eu[1a] - Cu[1b] - Te[1a] x 2	80.4(3)	78.4(3)	82.2(3)
Eu[1a] - Cu[1b] - Te[1a] x 2	165.6(4)	163.4(4)	167.9(3)
Eu[1a] - Cu[1b] - Te[1b] x 4	66.3(2)	65.5(2)	67.43(18)
Eu[1a] - Cu[1b] - Cu[1a] x 4	61.6(3)	60.6(3)	63.3(3)
Eu[1a] - Cu[1b] - Cu[1a] x 4	118.6(3)	117.2(3)	119.9(3)
Eu[1b] - Cu[1b] - Eu[1b] x 2	85.0(2)	84.27(18)	86.1(3)
Eu[1b] - Cu[1b] - Te[1a] x 4	66.1(2)	65.0(2)	67.4(2)
Eu[1b] - Cu[1b] - Te[1b] x 2	80.3(2)	78.3(2)	82.1(2)
Eu[1b] - Cu[1b] - Te[1b] x 2	165.3(3)	163.5(3)	167.1(3)
Eu[1b] - Cu[1b] - Cu[1a] x 4	61.1(3)	59.8(3)	62.1(3)
Eu[1b] - Cu[1b] - Cu[1a] x 4	118.4(4)	115.9(3)	120.8(3)
Te[1a] - Cu[1b] - Te[1a] x 2	114.0(3)	113.3(3)	115.1(5)
Te[1a] - Cu[1b] - Te[1b] x 4	107.1(3)	105.2(3)	109.3(4)
Te[1a] - Cu[1b] - Cu[1a] x 4	53.7(3)	51.8(4)	55.6(3)
Te[1a] - Cu[1b] - Cu[1a] x 4	126.3(4)	124.3(4)	128.1(4)
Te[1b] - Cu[1b] - Te[1b] x 2	114.3(3)	113.1(5)	115.9(5)
Te[1b] - Cu[1b] - Cu[1a] x 4	53.4(3)	50.8(3)	55.5(3)
Te[1b] - Cu[1b] - Cu[1a] x 4	126.5(4)	124.7(5)	128.4(5)
Cu[1a] - Cu[1b] - Cu[1a] x 8	90.3(5)	87.8(6)	92.6(6)
Cu[1a] - Cu[1b] - Cu[1a] x 4	178.4(5)	177.2(6)	179.9(4)

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Chapter 7

Cu_xUTe_3 ($0 \leq x < 0.5$): Evolution of the Incommensurate Charge Density Wave

Modulations in the Linear Chains of Tellurium and Stripes of Copper

via Successive Intercalation of Copper in $\alpha\text{-UTe}_3$

7.1. Introduction

Actinide polychalcogenides have been fascinated because of the numerous structural motifs they can adopt.¹ Uranium in particular, because of its ability to be stable in several oxidation states (3, 4, 5 and 6+) has shown a plethora of different structures within the polychalcogenide family. A few representative examples of Uranium or Thorium containing polychalcogenide phases include the sulfides $K_6Cu_{12}U_2S_{15}$,² RbU_2SbS_8 ,³ and $AMUQ_3$ (A = alkali or alkaline earth metal, M = 3d metal, Q = S, Se, Te),⁴ the selenides, $K_2UP_3Se_9$,⁵ $K_2ThP_3Se_9$,⁶ $Cs_4Th_2P_5Se_{17}$,⁶ and $Rb_4U_4P_4Se_{26}$,⁷ KU_2SbSe_8 ,³ and tellurides $CsUTe_6$,^{4,8} $Cs_8Hf_3UTe_{30.6}$,^{4,8} $CsTiUTe_5$,⁴ $Tl_{0.56}UTe_3$.⁹ Tellurium from the other hand has the tendency to form hypervalent $Te \cdots Te$ interaction¹⁰ and distort, especially when found in planar arrangements, in a variety of $(Te_x)^{2-}$ oligomeric patterns.¹¹ Modulations are created because of instabilities on the Fermi surface and this so-called Peierls distortion is thermodynamically favorable due to phonon-electron interactions. The result of these interactions is a spatial modulation of the diffuse electron density into charge density waves (CDWs).

The short list of actinide-containing phases with planar nets of chalcogen that possess CDW-type distortions include ATh_2Se_6 (A = K, Rb)¹² and Cu_xUTe_3 (x = 0.25, 0.33).¹³ Nevertheless the detailed CDW structures of these compounds remain unknown. The telluride member Cu_xUTe_3 can be seen as a Cu-intercalated product of the layered α - UTe_3 parent compound. The UTe_3 phase crystallizes into two possible forms. The so-called α - UTe_3 adopts the $ZrSe_3$ structure type¹⁴ and the β - UTe_3 phase crystallizes in the $NdTe_3$ structure type,¹⁵ Figure 7.2. The Cu atoms intercalate between the layers of α - UTe_3 . Since the CDW distortions are sensitive to the Fermi surface topology, a

successive incorporation of Cu^+ ions into the structure will continuously change the Fermi level thus the CDW modulations.

In this work we succeeded in solving the incommensurate CDW modulated structures of three different distorted Cu_xUTe_3 phases with $x = 0.14(1)$, $0.18(1)$ and $0.40(1)$. Surprisingly, besides the distorted linear chains of Te found in these compounds we observed an unusual ordering of the Cu ions into clusters with a reasonable average Cu-Cu distance of $\sim 2.6 \text{ \AA}$. This unique arrangement of Cu atoms seems to be correlated to the observed distortions in the planar Te nets. In the Cu-rich intercalated compound the clusters of Cu atoms and distorted pairs of Te were found to form stripes as a result of a modulation wave that is orientated along the three-dimensions.

7.2. Experimental Section

7.2.1. Reagents

The following reagents were used as obtained. Uranium metal, $\sim 1 \text{ mm}$ turnings, Cerac, Milwaukee, WI; Tellurium chunks, Tellurex Corp, Traverse City, MI; Tellurium (IV) bromide, Alfa Aesar, Ward Hill, MA.

Activated Copper – Copper metal (40 mesh, Cerac, Milwaukee, WI) was first activated by washing it with copious amounts of dilute hydrochloric acid. This step was necessary to remove the oxide layer from the fine particles (powder) and to ensure stoichiometric reaction of Cu.

7.2.2. Synthesis

α - UTe_3 – α - UTe_3 was synthesized from a stoichiometric mixture of uranium (1.0 mmol) and tellurium (3.0 mmol) metal that was sealed under vacuum in a quartz tube and heated to 800 °C for 5 days. The tube was then cooled to 300 °C at a rate of 4 °C/h, followed by quenching to room temperature at a rate of 10 °C/h. The majority of the reaction product was polycrystalline powder and a few relative big ($\sim 250 \mu\text{m}$) single crystals of the target phase.

β - UTe_3 – Although β - UTe_3 is thermodynamically more stable from the α -phase and an extended heating / annealing temperature profile from the one used for the synthesis of α - UTe_3 could be used, a vapor transport synthetic procedure was preferred to obtain single crystals of good quality. Stoichiometric mixture of uranium (1.0 mmol) and tellurium (3.0 mmol) metal together with a small amount of TeBr_4 (~ 40 times less the total mass of the reactants) was sealed under vacuum in a 9 mm quartz tube (~ 25 cm length). The tube was placed in a dual-zone furnace with the side of the reactants to be at 950 °C. The temperature difference between the two zones was 150 °C ($T_{\text{cold}} = 800$ °C) and the reaction was kept at this temperature for 2 days. The tube was then cooled to room temperature in ~ 10 h. High quality plate-like single crystals up to ~ 3 mm in size were grown on the side of the tube that was at 800 °C, Figure 7.1. The crystals were soaked in acetone to wash off traces of TeBr_4 from the surface.

Cu_xUTe_3 – The procedure for the synthesis of Cu_xUTe_3 was the same as described above for β - UTe_3 . In addition, an amount of activated copper (depended on the target x -value) was mixed with the reactants. For low concentration of Cu ($x \sim 0.1 - 0.2$) the

product was found to contain single crystals with different superstructures due to small variations in the atomic fraction of the intercalated atoms of Cu.

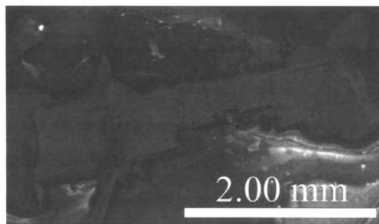


Figure 7.1. SEM image of a single crystal of $\text{Cu}_{0.14(1)}\text{UTe}_3$ used for resistivity measurement. Typical crystal size is ~ 3 mm in length.

7.2.3. Physical Measurements

Semiquantitative Energy Dispersive Spectroscopy (EDS) – The analyses were performed with a JEOL JSM-35C scanning electron microscope equipped with a Noran Vantage EDS (Si:Li) detector. Crystals were mounted on an aluminum stage with carbon tape. Data were acquired on several crystals and different regions of each crystal using an accelerating voltage of 25 kV and accumulation time of 40s.

Single Crystal X-ray Diffraction – All the temperature dependent measurements were performed on the same single crystal for some of the Cu_xUTe_3 compounds. Single crystals were quenched from room temperature to 100 K. The heating rate for warming ramps was ~ 200 K/h. Typical acquisition time was ~ 24 h. Summary table of crystal data and detailed crystallographic table reports for each individual Cu_xUTe_3 analogue and temperature can be found in Tables 8.1-8.18. Intensity data were collected on a STOE IPDS II diffractometer equipped with a graphite monochromatized Mo radiation ($\lambda =$

0.71073 Å) and an Image Plate (IP) detector. The data were collected with an ω -scan technique from 0-180° and an arbitrary ϕ -angle. Data reduction was performed with the X-Area package.¹⁶ The length determination and refinement of the q-vectors was performed with the Peaklist 1.06 software part of the X-Area suite using a least square refinement algorithm. An analytical absorption correction was performed (X-Shape within X-Area) and all structures were refined with JANA2000 software.¹⁷ Direct methods of SHELXTL software¹⁸ were used to find the atomic positions in the subcell.

Satellite reflections of first order were observed and used for the refinement. A single modulation wave for positional and thermal parameters was used. Only the symmetry allowed Fourier terms were refined. Temperature was controlled by an Oxford Cryostream 700 Plus cryostat.

Magnetic Susceptibility Measurements – A MPMS Quantum Design SQUID magnetometer was used to measure the magnetic response of some of the Cu_xUTe_3 compounds over the range of 2-300 K. Single crystals of each sample were measured parallel and perpendicular to the applied magnetic field in respect to the plate geometry of the crystals. A perpendicular field corresponds to a magnetization direction along the c -axis. A parallel magnetic field corresponds to a random direction along the ab -plane. A field dependent magnetic susceptibility at 300 K was first investigated in the range of 0 – 1 T to ensure a linear response of the magnetization. Subsequent temperature dependent studies were then performed at a constant field of 3,000 G. The effective magnetic moment, μ_{eff} , was calculated from the following formula:

$$\mu_{\text{eff}} = 2.818 \times \sqrt{\chi_M \cdot T}$$

where χ_M is the inverse of the slope taken from the linear region of the $1/\chi_M$ vs T plot (χ_M is the molar magnetic susceptibility).

Charge transport measurements - Electrical contact for the resistivity measurement at low temperature (2-300 K) was made using silver paint and Cu wire directly on to the single crystal surface of Cu_xUTe_3 ($x = 0, 0.10, 0.40$). Measurements were made for arbitrary current directions in the ab-plane using a standard four point contact geometry (AC) in a Quantum Design Physical Property Measurement System (PPMS).

Electrical resistivity data at high temperature (300-700 K) were measured as a function of temperature on single crystals of Cu_xUTe_3 ($x = 0, 0.14(1), 0.18(1)$ and $0.40(1)$). Electrical contacts for the resistivity measurements were made using gold paint and Cu wire directly on the crystal surface. Measurements were made for arbitrary current directions in the ab-plane using a standard four point contact geometry (AC). We used a home made resistivity apparatus equipped with a Keithley 2182A Nanovoltmeter, 6220 Precision Current Source, and a high temperature vacuum chamber ($\sim 5 \cdot 10^{-3}$ torr) controlled by a K-20 MMR System.

7.3. Results and Discussion

Subcell Description of $\alpha\text{-UTe}_3$ – The structure of $\alpha\text{-UTe}_3$ crystallized in the ZrSe_3 structure type ($\text{P2}_1/\text{m}$). It is composed by two puckered layers of (UTe) that are sandwiched by planar nets of Te making an UTe_3 slab. The slabs then stack along the c -axis creating van der Waals gaps. The structure can be seen as a distorted version of the NdTe_3 structure type in which the NdTe_3 slabs have been shifted in respect to each

other in the *ab* plane as shown in Figure 7.2A. Furthermore, the planar nets of Te consist of dimers oriented along the *a*-axis with Te-Te distances of 2.750(2) Å, Figure 7.2B. The dimers are separated from each other in a distance of 3.061 Å (along *a*-axis). The vertical separation (along *b*-axis) of the linear chains is 4.205(1) Å. Each U atom is coordinated to eight Te atoms in a bicapped trigonal prismatic environment. These trigonal prisms stack along the *b*-axis to form wedge-shaped columns by sharing triangular faces. Layers are then formed when neighboring columns share both their capping and apex monotellurides, Figure 7.2A.

Subcell Description of β -UTe₃ – The average structure of β -UTe₃ crystallizes in the NdTe₃ structure type (Cmcm). It consists of puckered double layers of (UTe) that are sandwiched by square nets of Te making an UTe₃ slab. The slabs then stack along the *b*-axis creating van der Waals gaps. The formula can be more expressly written as (UTe)²⁺(Te₂)²⁻, Figure 7.2C. This gives an average oxidation state of the Te atoms in the net of 1- that is different from the average electron count of -0.5 found in the LnTe₃ (Ln = Lanthanide) family since U is in the 4+ oxidation state (verified by magnetic susceptibility measurements). The U atom is in a monocapped tetragonal antiprism of Te atoms. The Te atoms are surrounded by five U atoms in a tetragonal pyramidal geometry. The apparent Te-Te distances in the square net are 3.103(1) Å, Figure 7.2D.

Subcell Description of Cu_xUTe₃ – The average structure of Cu_xUTe₃ can be seen as an intercalation product of Cu into the van der Waals gaps of α -UTe₃. The Cu atoms interconnect the UTe₃ slabs creating a three-dimensionally connected structure, Figure 7.3A. The Cu atom is located in a distorted tetrahedral environment of Te atoms. The planar net of Te atoms does not contain discrete dimers any more like in α -UTe₃ but the

Te atoms form infinite linear chains along the a -axis. The shortest Te-Te distance in the chains is now 3.033(2) Å (2.750(2) Å in dimers of α -UTe₃) and the longest 3.061(2) Å (3.352(2) Å distance between dimers), Figure 7.3B. Interestingly, an unusual feature in the average Cu_xUTe₃ is the presence of zigzag chains of Cu atoms with Cu-Cu distances of 2.57(1) Å, Figure 7.3C. Although this short distance is reasonable for a Cu-Cu interaction (d^{10} - d^{10}) is not clear from this average disordered model if the two partially vacant sites of Cu generated by symmetry are occupied by Cu atoms at the same time.

Supercell Description of Cu_xUTe₃ Based on a Modulation q -vector – The CDW distortions in the Cu_xUTe₃ series found to be very sensitive to the average oxidation state on the Te atoms in the planar net. The electron count increases with the concentration of intercalated Cu atoms. For $x = 0.14(1)$ the average oxidation state on the Te atoms in the net becomes -1.07(1) with a modulation q -vector $0.1040(4)a^* - 0.0284(7)c^*$. With a small increase in x -value to 0.18(1) the q -vector changes significantly to $0.179(1)a^* - 0.086(3)c^*$ while the oxidation state is now -1.09(1). Finally, when the concentration of intercalated Cu atoms reaches 0.40(1) the CDW modulation vector becomes $0.2225(8)a^* + 0.2711(5)b^* + 0.513(1)c^*$.

The distorted patterns in Cu_xUTe₃ series can be seen as a sequence of dimers and monomers at a bonding threshold of 2.9 Å, Figure 7.7-7.8. The wide distribution of Te-Te distances for all three members is shown in Figure 7.4. In more details, the minimum Te-Te distance in Cu_{0.14(1)}UTe₃ at 100 K is 2.782(3) Å and the maximum 3.289(3) Å. For Cu_{0.18(1)}UTe₃ the minimum distance is 2.766(2) Å and the maximum 3.279(2) Å. In Cu_{0.40(1)}UTe₃ the minimum and maximum distances are 2.843(2) Å and 3.213(2) Å respectively. From Figure 7.4 is apparent that with increasing the electron count on the

Te net the distribution of Te-Te distances in the dimers compared to the distances found in the other oligomers gradually converges.

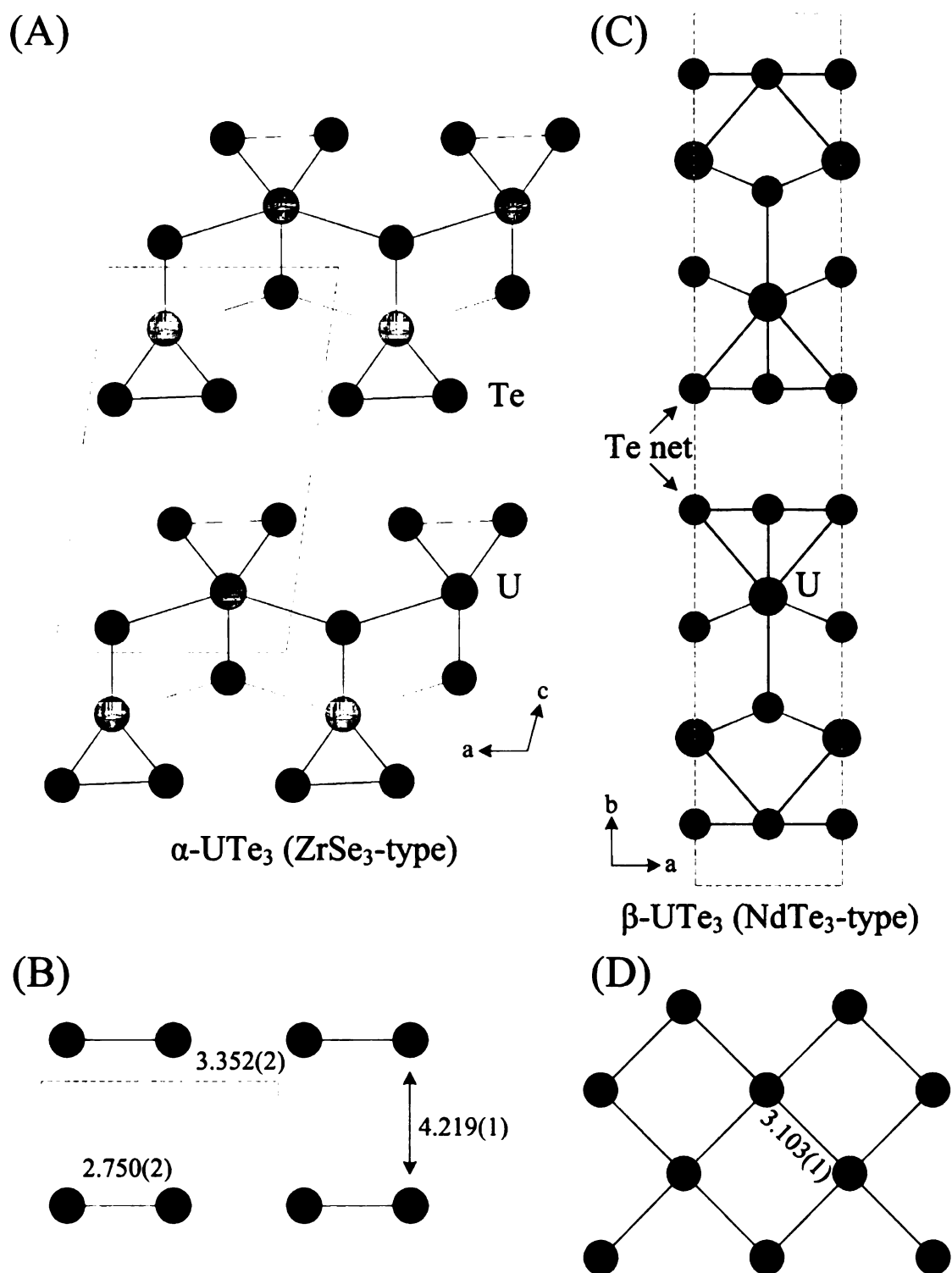


Figure 7.2. (A) Structure of $\alpha\text{-UTe}_3$ (ZrSe₃-type). (B) Linear chains of Te in $\alpha\text{-UTe}_3$ (bond lengths are indicated). (C) Structure of $\beta\text{-UTe}_3$ (NdTe₃-type). (D) Square net of Te in $\beta\text{-UTe}_3$ (bond lengths are indicated).

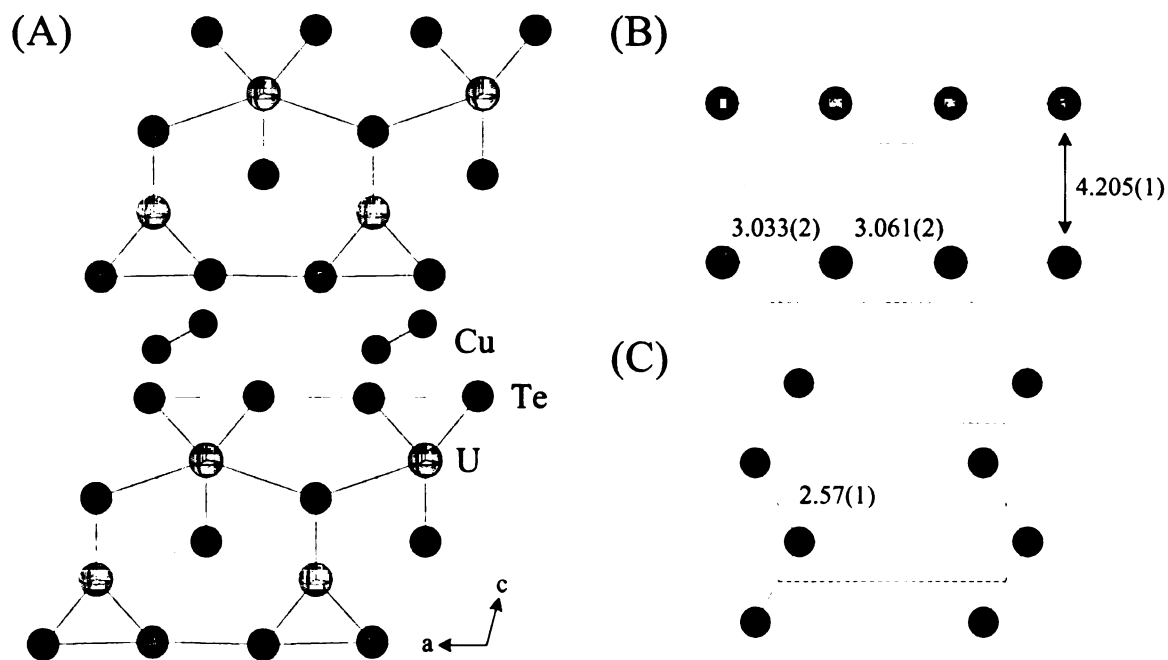


Figure 7.3. (A) Average undistorted structure of Cu_xUTe_3 . (B) Undistorted linear chains of Te in Cu_xUTe_3 . Bond lengths are indicated (C) Linear chains of Cu in the average Cu_xUTe_3 structure.

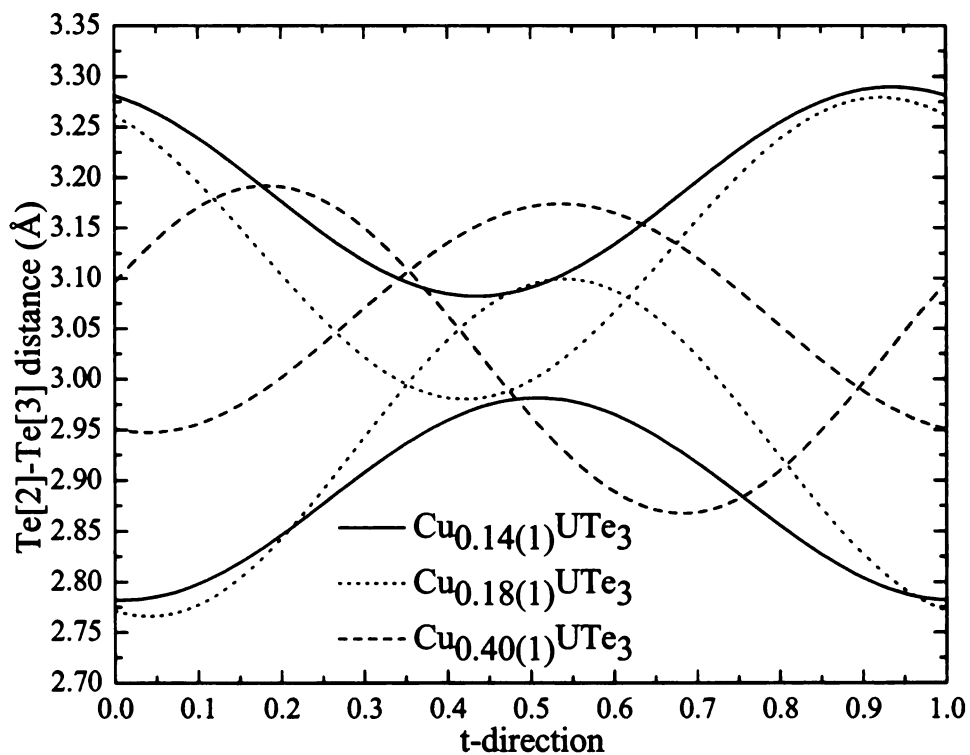


Figure 7.4. Te[2]-Te[3] distances found in the distorted net of Cu_xUTe_3 ($x = 0.14(1)$, $0.18(1)$ and $0.40(1)$) from the superspace analysis based on a q-vector as a function of t-direction.

Surprisingly, we found that the distorted Cu atoms are long range ordered and they form zigzag-shaped clusters of various lengths. The first attempt to model the Cu-site as a disordered one with a refined average occupancy equal to x was not acceptable. High residuals in the difference Fourier map with local maxima (peaks) and minima (holes) densities ($> 15 \text{ e} \cdot \text{\AA}^{-3}$) along the modulation t -director were observed. This suggested that an occupational modulation may be present. The application of a single occupational wave successfully described the electron residual intensity along the modulation. The occupancy of the Cu-site varies continuously between 0 and ~ 0.25 for $\text{Cu}_{0.14(1)}\text{UTe}_3$, and from 0 to ~ 0.45 for $\text{Cu}_{0.14(1)}\text{UTe}_3$. For the more Cu-rich $\text{Cu}_{0.14(1)}\text{UTe}_3$ phase the occupancy fraction changes from ~ 0.10 to ~ 0.75 , Figure 7.5. The Cu-Cu bond distribution within the clusters does not change significantly. The minimum Cu-Cu distance in $\text{Cu}_{0.14(1)}\text{UTe}_3$ is $2.57(5) \text{ \AA}$ and the maximum $2.67(6) \text{ \AA}$. The minimum and maximum distances in $\text{Cu}_{0.18(1)}\text{UTe}_3$ and $\text{Cu}_{0.40(1)}\text{UTe}_3$ are $2.52(4) \text{ \AA}$ to $2.57(5) \text{ \AA}$, and $2.473(2) \text{ \AA}$ to $2.548(2) \text{ \AA}$ respectively.

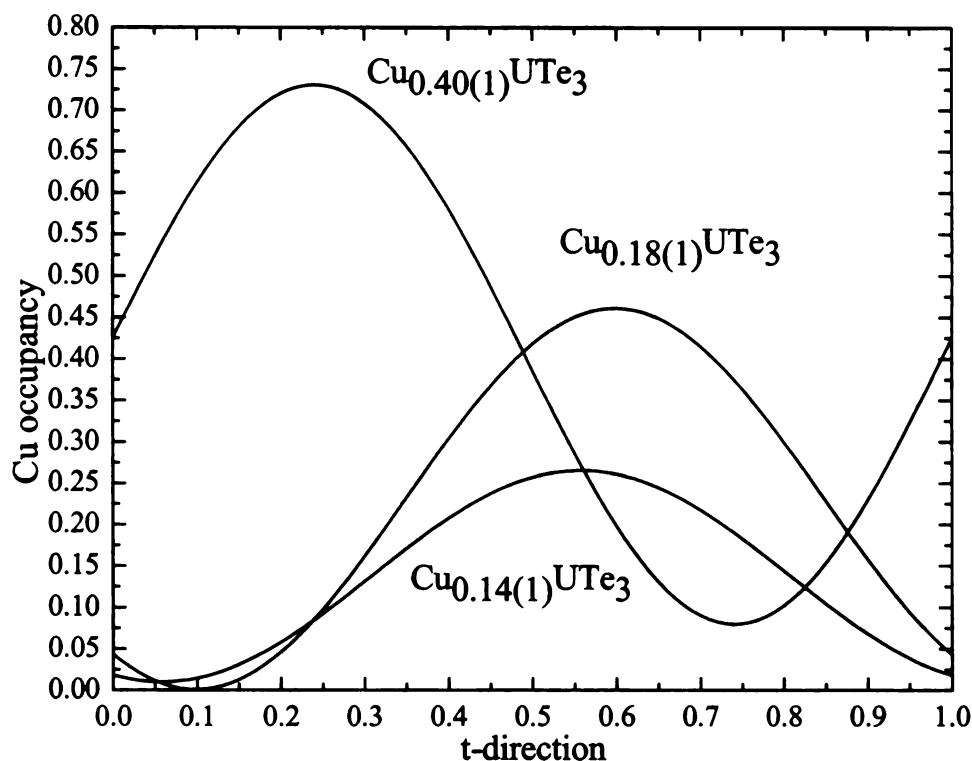


Figure 7.5. Occupational curves of Cu atoms found in Cu_xUTe_3 ($x = 0.14(1)$, $0.18(1)$ and $0.40(1)$) from the superspace analysis based on a q -vector as a function of t -direction.

The sequence of oligomers in the CDW distorted Te patterns and frequency of dimers is correlated to the occupational modulations found in the Cu plane. The average Te-Te distances of the atoms located above and below the regions with Cu vacancies are shorter than 2.9 Å, and when Cu atoms are present the corresponding distance are longer, Figure 7.6A. The short and long Te-Te bonding (linear distorted chains) occurs along the a -axis for the low Cu-loaded compounds, $\text{Cu}_{0.14(1)}\text{UTe}_3$ and $\text{Cu}_{0.18(1)}\text{UTe}_3$. The zigzag chains of Cu run along the b -axis perpendicular to the distorted Te chains, Figure 7.6B. The density of dimers increases with decreasing Cu concentration, Figure 7.7. In the high Cu-loaded phase $\text{Cu}_{0.40(1)}\text{UTe}_3$ the dimensionality of the CDW distortions increases and the modulations now propagate along the b -axis too. The orientation of the q -vector is along all three directions $(0.2225(8)a^* + 0.2711(5)b^* + 0.513(1)c^*)$. This situation result

in a more complex arrangement of Te monomers and Cu clusters, Figure 7.8. Surprisingly, the Cu oligomers that are mainly composed by tetramers and occasionally trimers and dimers seem to line in stripes along the diagonal of the ab-plane. At the same time, dimers of Te atoms lie between the Cu oligomers to form stripes too.

The correlation of Cu oligomers and presence of Te dimers can be rationalized using electron count. The more reduced Te is the longer the bonds become. The Te atoms coordinated on Cu atoms will be more reduced in respect with the Te atoms located above vacancies. Therefore the average Te-Te bonds of the later will be longer than the ones in the former species. It is amazing though how localized the electrons are juggling from the distorted patterns found in the Cu_xUTe_3 family. It seems that the undistorted one-dimensional framework of $\alpha\text{-UTe}_3$ favors the separation of Te oligomers and prevents the diffusion of electrons between linear chains of Te.

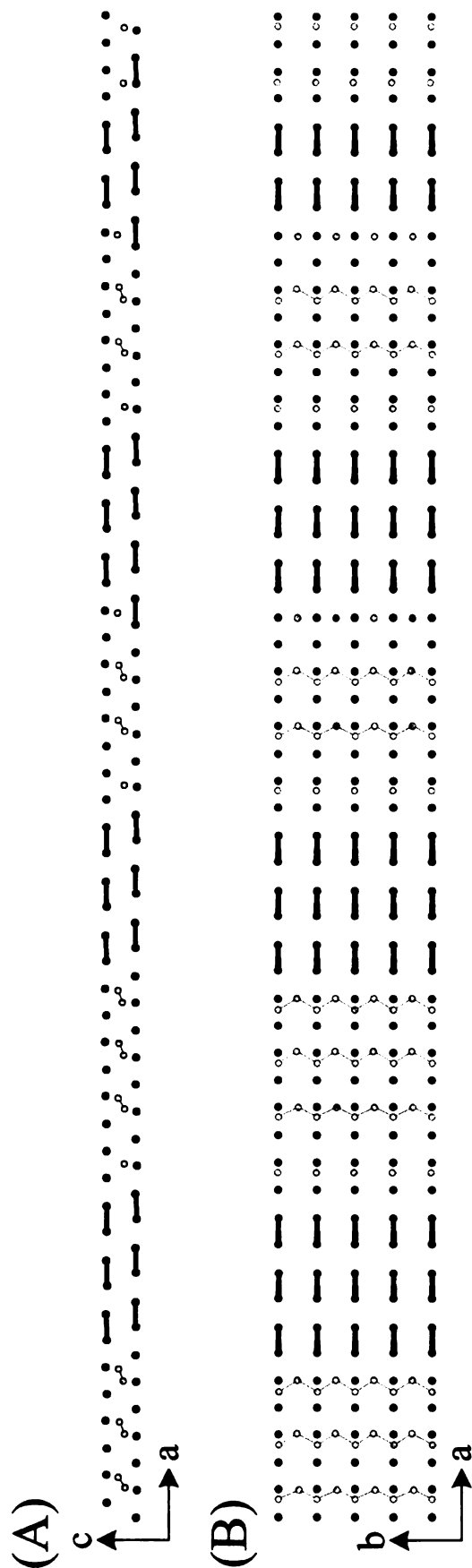


Figure 7.6. (A) Distorted Te pattern of $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with $q = 0.1040(4)a^* - 0.0284(7)c^*$ and 2.9 Å bonding threshold viewed down the b-axis. The formation of Te-Te dimers in the regions where there is no Cu atoms is apparent. (B) Distorted Te pattern of $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K viewed down the c-axis at a bonding threshold of 2.9 Å. The occupancy cutoff was set to the average value of 0.18.

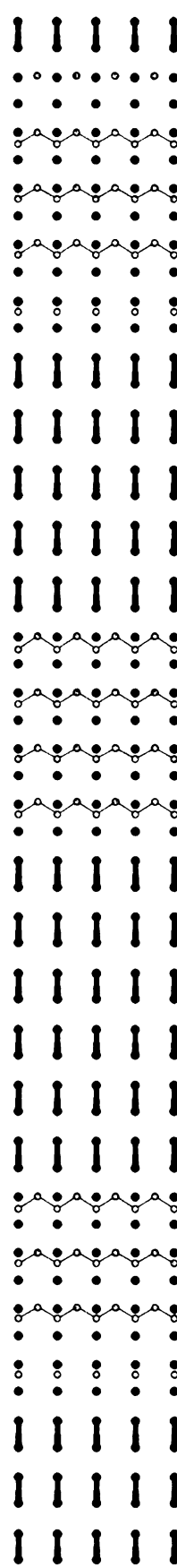


Figure 7.7. Distorted Te pattern of $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with $q = 0.1040(4)a^* - 0.0284(7)c^*$ and 2.9 Å bonding threshold. The occupancy cutoff was set to the average value of 0.14.

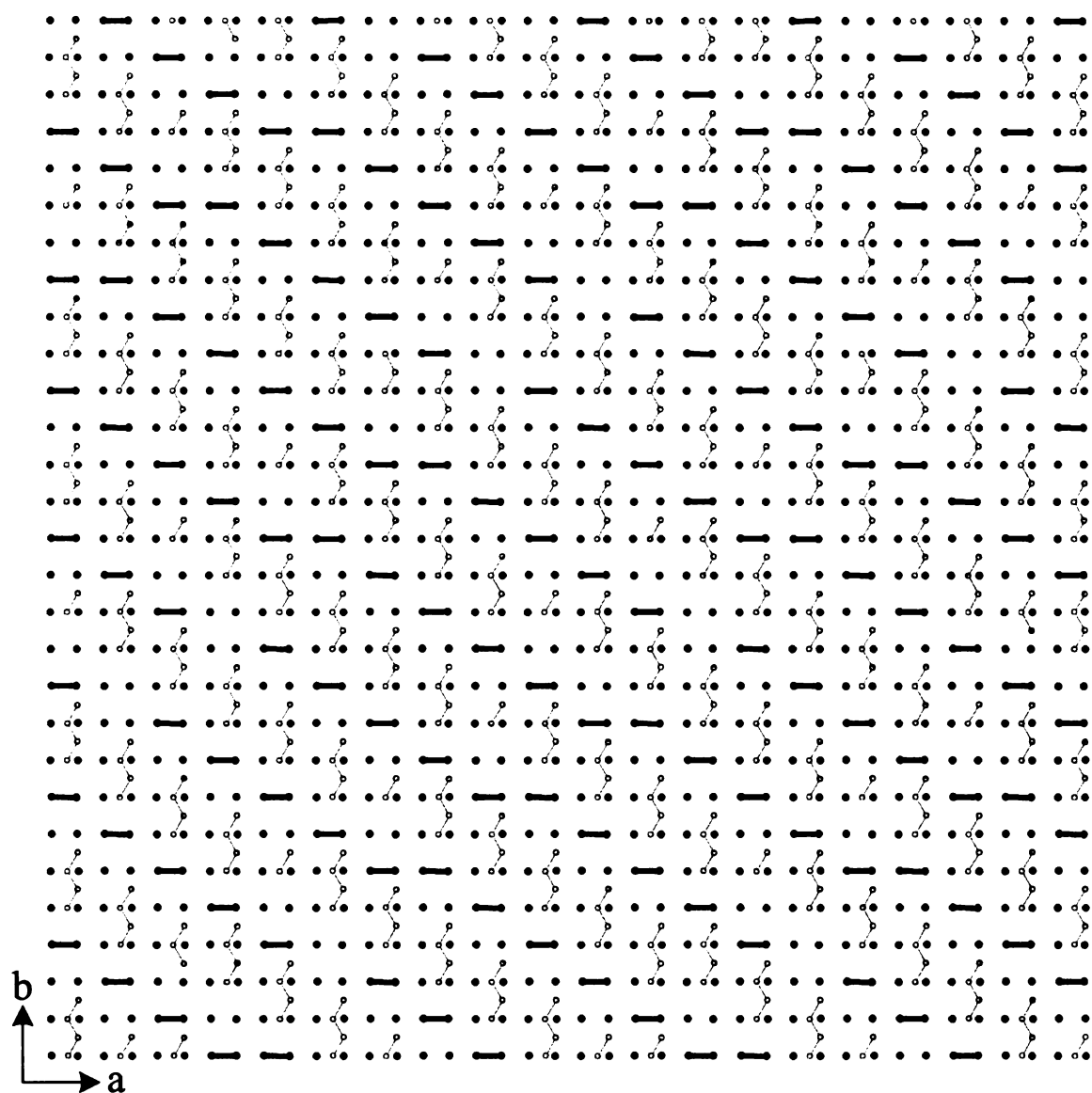


Figure 7.8. Distorted Te pattern of $\text{Cu}_{0.40(1)}\text{UTe}_3$ with $q = 0.1040(4)a^* - 0.0284(7)c^*$ at 100 K and 2.9 Å bonding threshold. The occupancy cutoff was set to the average value of 0.40.

Magnetic susceptibility measurements of $\beta\text{-UTe}_3$ and $\text{Cu}_{0.4}\text{UTe}_3$ – Variable temperature magnetic susceptibility data for $\beta\text{-UTe}_3$ and $\text{Cu}_{0.4}\text{UTe}_3$ were measured in the range of 2-300 K at 5000 G in both zero-field and field cooled modes. Both phases showed a maximum at 6 K and 3 K respectively. Above this temperature the data follow the Curie/Weiss law. A μ_{eff} value of $3.34 \mu_B$ and a Weiss constant of -51 K were

estimated by linear fitting of the $1/\chi_M$ vs T data for $\beta\text{-UTe}_3$, Figure 7.9. The data indicate antiferromagnetic ordering at low temperatures consistent with a U^{4+} configuration. No difference was observed between zero-field and field cooled data. A small difference at high fields in the field dependent curves was observed between the two orientations of the single crystals in respect to the magnetic field (parallel and perpendicular to the Te net), Figure 7.10.

The magnetic response of the Cu intercalated compound $\text{Cu}_{0.4}\text{UTe}_3$ showed similar behavior with the one observed for $\beta\text{-UTe}_3$. There is an antiferromagnetic transition at 3 K and a Weiss constant of -121 K, Figure 7.11. The transition remained the same at both crystal orientations with a relative small difference in the magnetization signal, Figure 7.12.

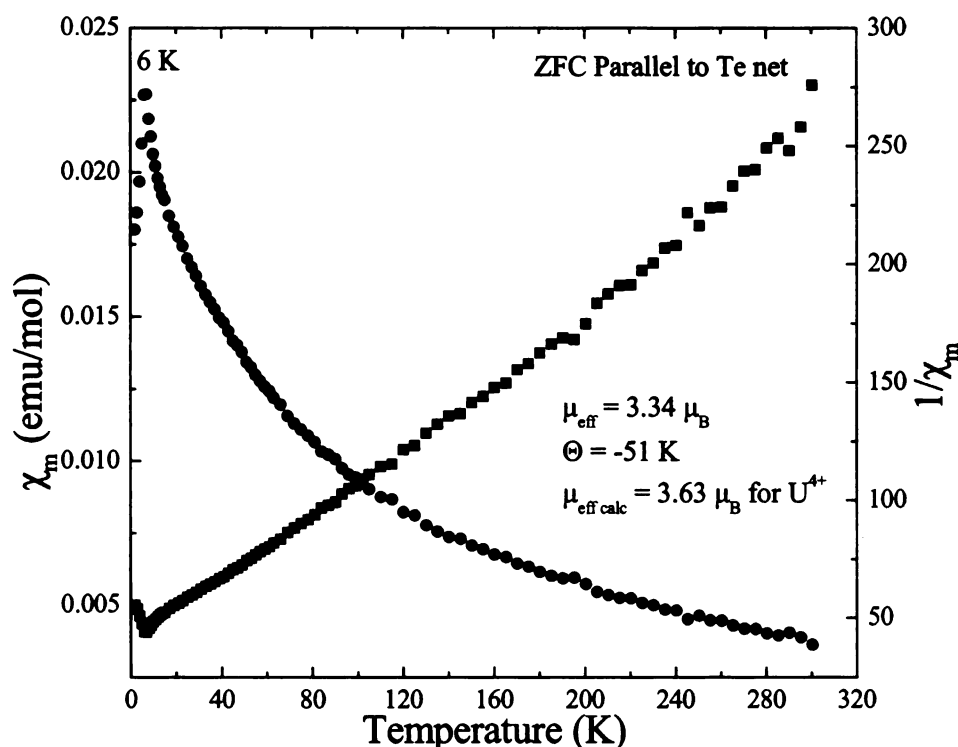


Figure 7.9. Temperature dependent magnetic susceptibility for $\beta\text{-UTe}_3$.

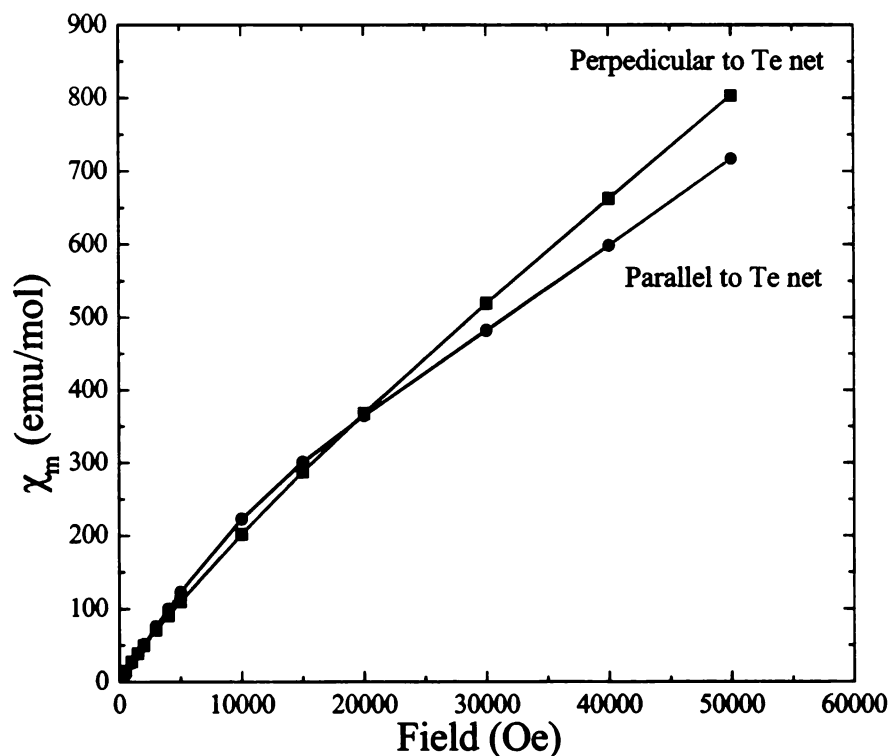


Figure 7.10. Field dependent magnetization curve for β - UTe_3 at 5 K.

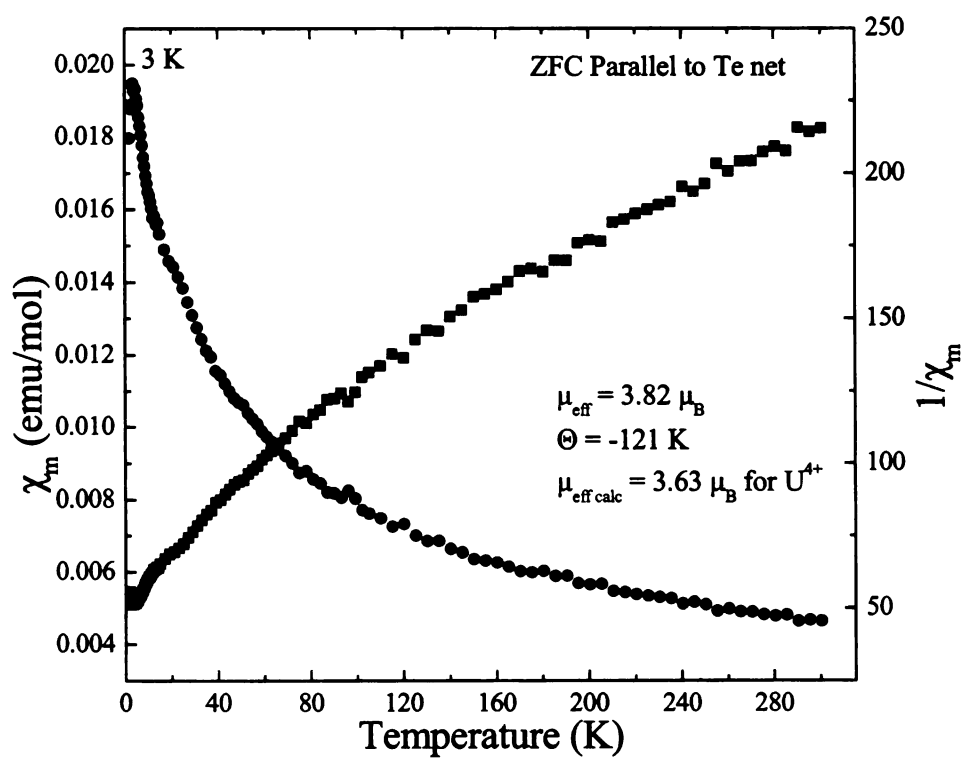


Figure 7.11. Temperature dependent magnetic susceptibility for $\text{Cu}_{0.4}\text{UTe}_3$.

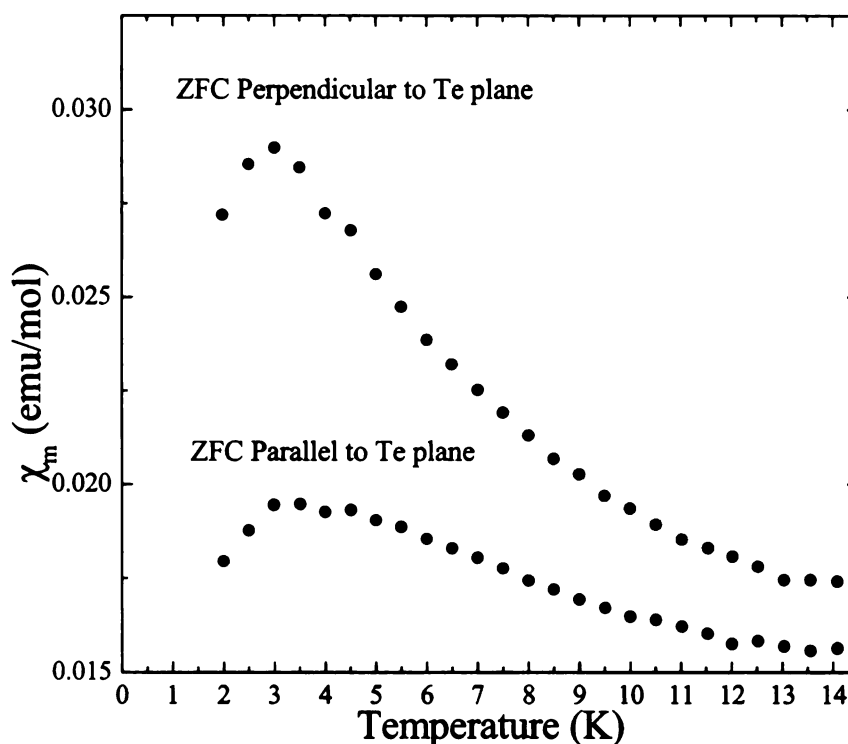


Figure 7.12. Field dependent magnetization curve for $\text{Cu}_{0.4}\text{UTe}_3$ at 5 K.

Resistivity measurements of $\alpha\text{-UTe}_3$, $\beta\text{-UTe}_3$ and Cu_xUTe_3 ($x = 0.10, 0.40$) –

Resistivity data for $\alpha\text{-UTe}_3$, $\beta\text{-UTe}_3$ and Cu_xUTe_3 ($x = 0.10, 0.40$) were collected in the range of 2-300 K. A qualitative difference between the members with different loading of Cu and between α and β -phase was observed. The $\alpha\text{-UTe}_3$ and $\text{Cu}_{0.2}\text{UTe}_3$ compounds showed a semiconducting behavior as seen in the resistivity vs temperature plot in Figure 7.13. The resistivity for $\text{Cu}_{0.2}\text{UTe}_3$ varies from 10 m Ω cm at 240 K to more than 1 M Ω cm at 2 K. The corresponding values for the resistivity of $\alpha\text{-UTe}_3$ were 100 m Ω cm to more than 1 M Ω cm (above the reading range of the instrument) respectively. The Arrhenius plot of $\text{Cu}_{0.2}\text{UTe}_3$ did not show a linear behavior suggesting that the carrier excitation does not follow a simple mechanism, Figure 7.14. The two apparent activation energies were ~ 3 meV and ~ 31 meV.

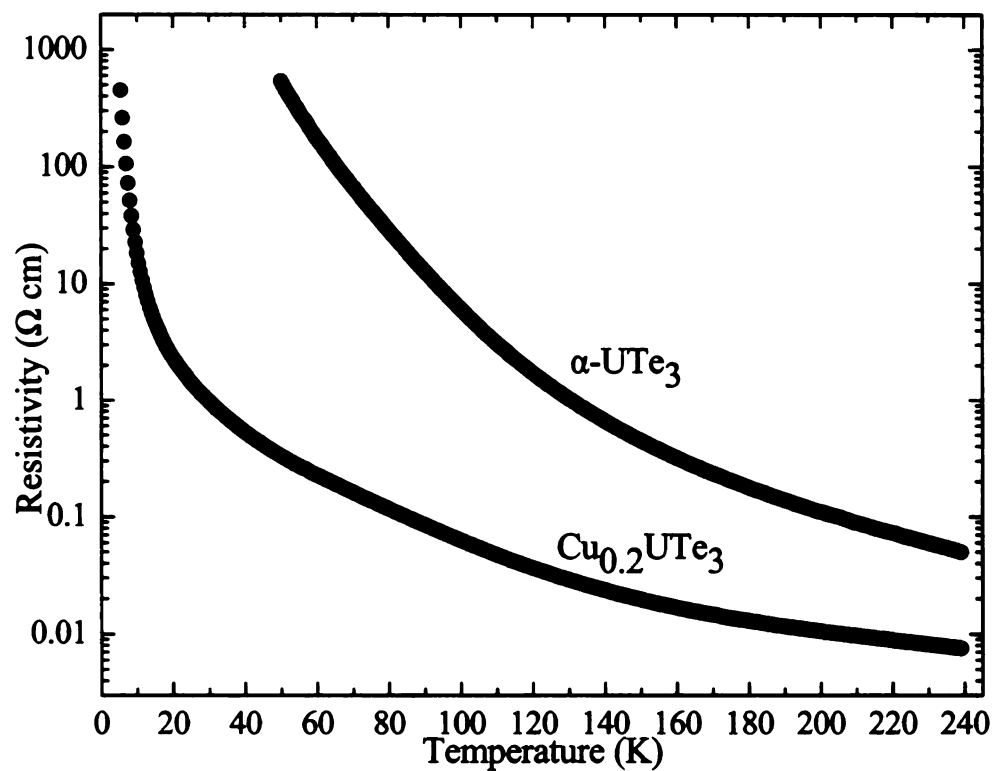


Figure 7.13. Resistivity vs. low temperature plot for $\alpha\text{-UTe}_3$ and $\text{Cu}_{0.2}\text{UTe}_3$.

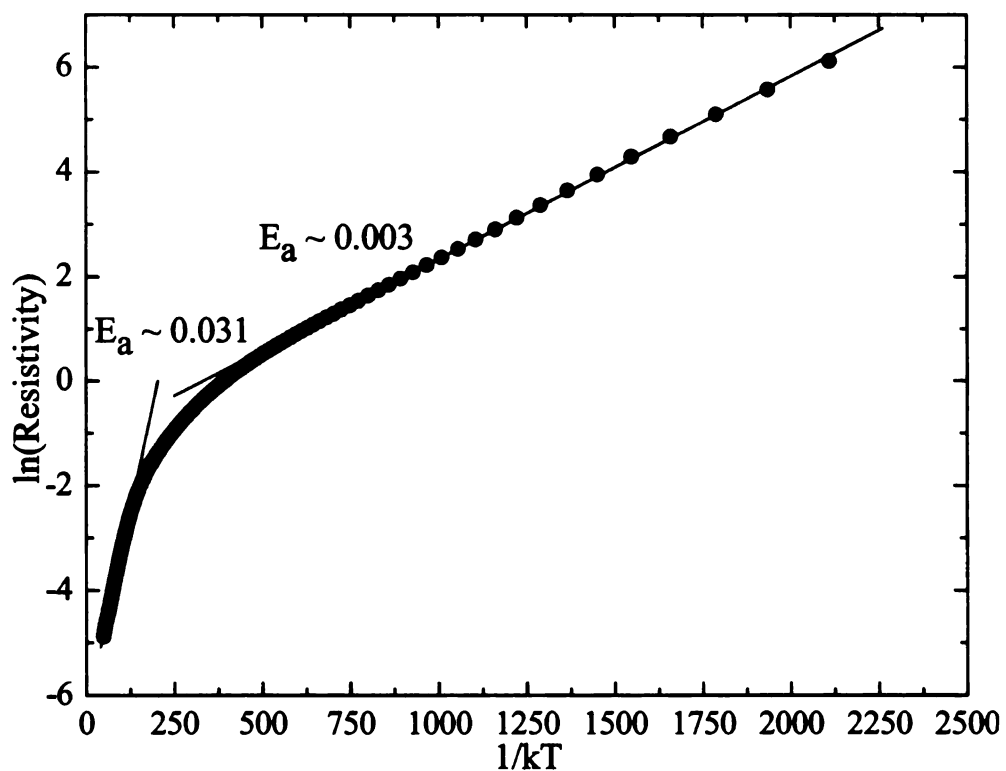


Figure 7.14. Arrhenius plot of the resistivity for $\text{Cu}_{0.2}\text{UTe}_3$.

The high temperature resistivity data in the range of 300-700 K did not show any discontinuities indicative of a CDW transition, Figure 7.15.

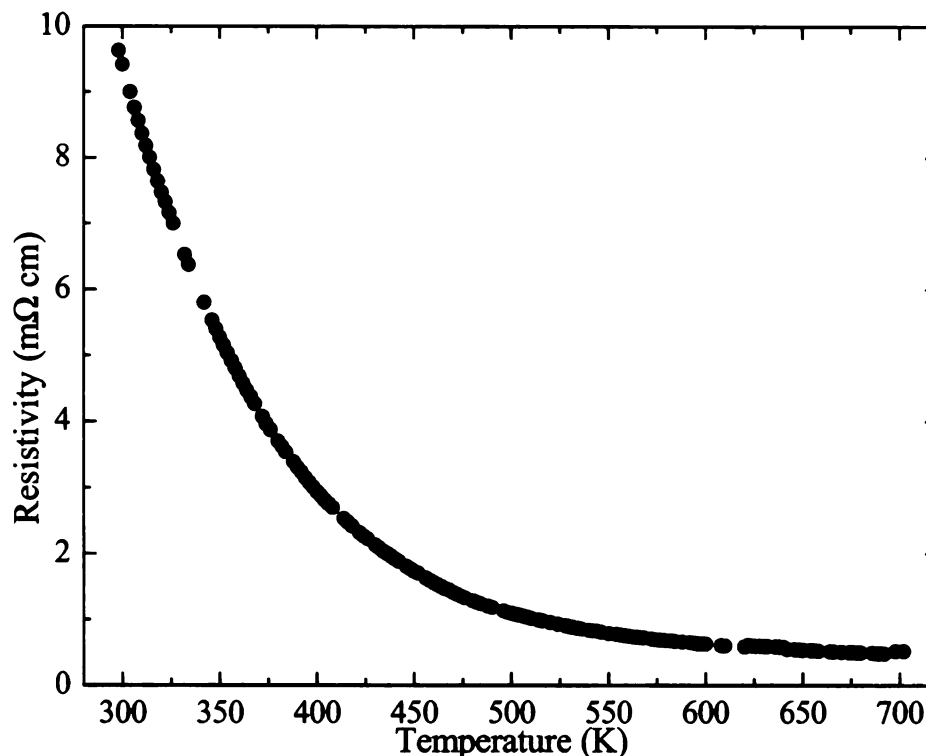


Figure 7.15. Resistivity vs. high temperature plot for $\text{Cu}_{0.2}\text{UTe}_3$.

The $\text{Cu}_{0.4}\text{UTe}_3$ phase showed a metallic behavior, Figure 7.16. The resistivity ranges from $\sim 1.5 \text{ m}\Omega \text{ cm}$ at 2 K to $\sim 4.5 \text{ m}\Omega \text{ cm}$ at 260 K. There is also a change in the slope of the resistivity vs temperature plot around 190 K. The single crystal X-ray diffraction experiment at 300 K and 100 K though did not show any change in the two superstructures. The temperature dependent resistivity measurement on $\beta\text{-UTe}_3$ revealed anomalies bellow 50 K as shown in Figure 7.17. Down to 100 K (limit of our low temperature device) the structure of $\beta\text{-UTe}_3$ (NdTe_3 -type) posses an ideal net of Te atoms. It would be surprising if an ideal square net of Te atoms with an average oxidation state of -1 really exists at the temperature range from 2-100 K. Although there is no

structural proof of the net distorts, we believe that the observed anomalies in the resistivity data correspond to CDW transitions.

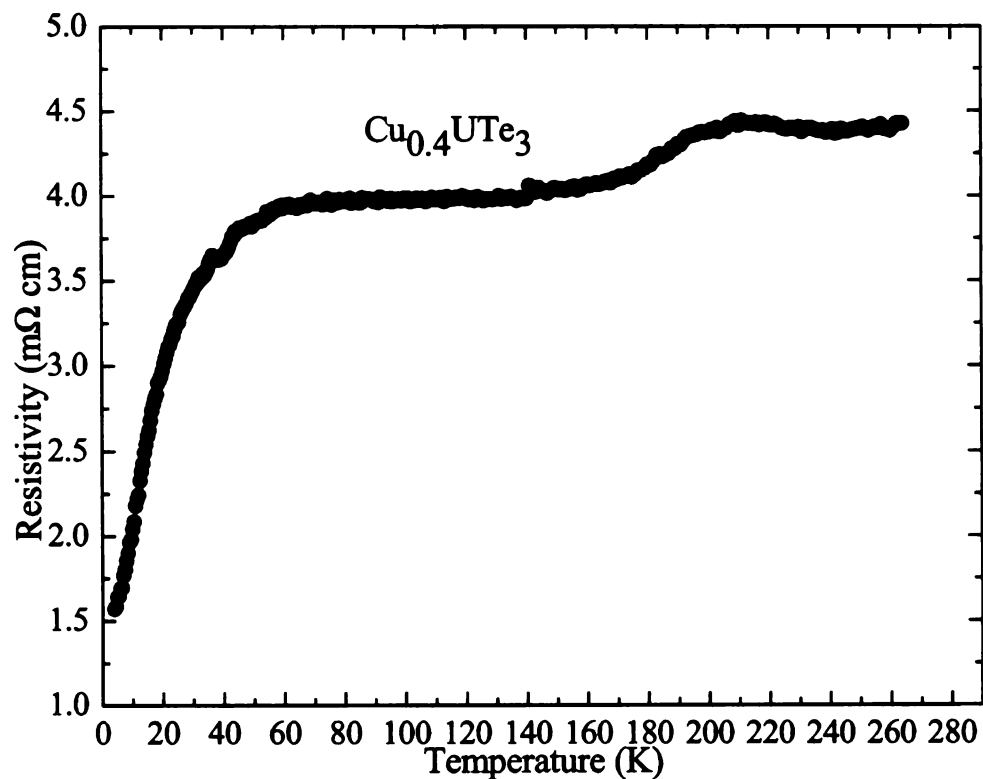


Figure 7.16. Resistivity vs. low temperature plot for $\text{Cu}_{0.4}\text{UTe}_3$.

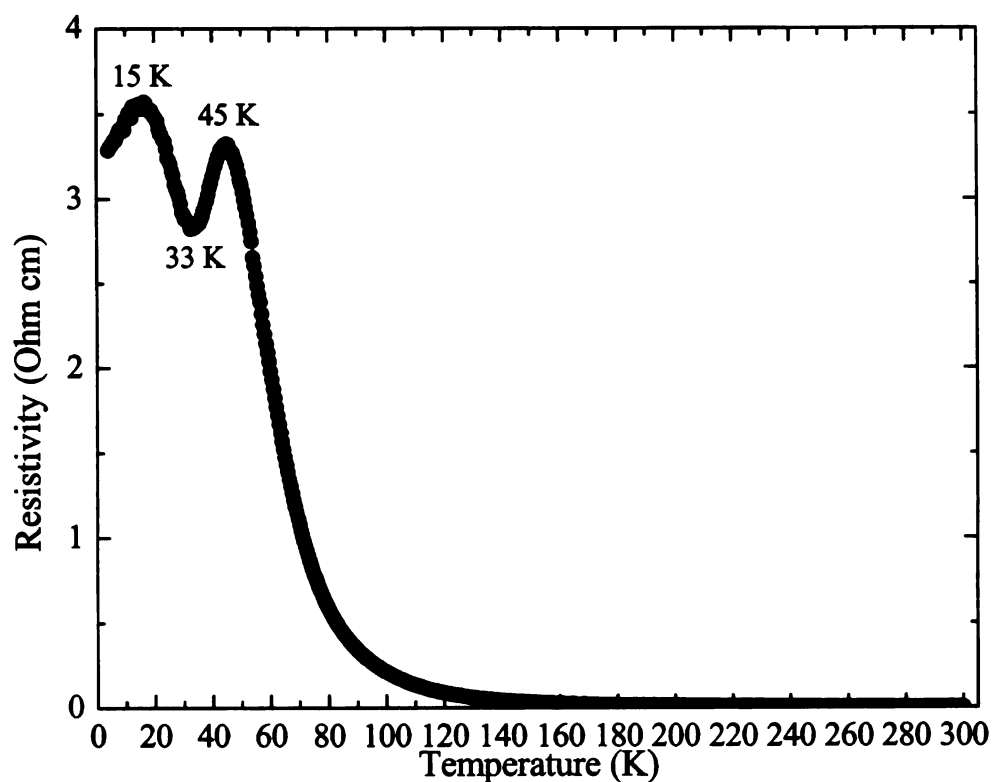


Figure 7.17. Resistivity vs. low temperature plot for $\beta\text{-UTe}_3$.

7.4. Conclusions

Intercalation of Cu atoms in the van der Waals gap of UTe_3 stabilizes the $\alpha\text{-UTe}_3$ phase. A successive increase in concentration of Cu gradually increases the Fermi level. This creates abrupt changes in the length and orientation of the modulation q -vector. The cross-plane interactions (along c -axis) increase with Cu since the empty space of the van der Waals gap is occupied by atoms. The orbital overlap between Cu and Te atoms increases the three-dimensional character of the structure while the concentration of intercalated atoms increases. This is apparent by the lengthening of the incommensurate component of the q -vector along c^* . In Cu_xUTe_3 for $x = 0.14(1)$ the absolute value of the component is $0.0284(7)c^*$. For $x = 0.18(1)$ and $0.40(1)$ the q -vector component becomes $0.086(3)c^*$ and $0.513(1)c^*$ respectively.

An interesting feature in these Cu_xUTe_3 compounds is the long range ordering of the Cu atoms and vacancies in a form of clusters with an average Cu-Cu distance of ~ 2.6 Å. To the best of our knowledge this is a unique arrangement that seems to be correlated to the CDW distortions. The Te-Te distances of the atoms located above or below the clusters of Cu are significantly elongated (more than 2.9 Å) in respect to the other Te atoms that lie on top of vacancies. This behavior can be explained by electron count arguments that predict a decrease of the Te-Te distance with oxidation. Interestingly, the extra electrons that are added in the system after the intercalation of Cu atoms are more localized in the distorted Te net. The quasi-one-dimensional character of the linearly distorted Te nets seems to promote this charge separation. Similar behavior was not observed for the quasi-two-dimensional RETe_3 ¹⁹ and AMRETe_4 ²⁰ members in which electrons are found to be delocalized in the planar distorted Te nets.

Table 7.1. Crystal data and structure refinement for Cu_{0.14(1)}UTe₃ at 100 K.

Empirical formula	Cu _{0.14(1)} UTe ₃
Formula weight	627.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	P2 ₁ /m($\alpha 0 \gamma$)00
Unit cell dimensions	a = 6.0603(10) Å, α = 90° b = 4.1992(3) Å, β = 98.428(6)° c = 10.2943(7) Å, γ = 90°
q-vector(1)	0.1040(4)a* - 0.0284(7)c*
Volume	259.35(3) Å ³
Z	2
Density (calculated)	8.0286 g/cm ³
Absorption coefficient	17.522 mm ⁻¹
F(000)	504
Crystal size	0.20 x 0.10 x 0.02 mm ³
Theta range for data collection	3.35 to 29.12°
Index ranges	-8 ≤ h ≤ 8, -5 ≤ k ≤ 5, -14 ≤ l ≤ 14, -1 ≤ m ≤ 1
Reflections collected	9550
Independent reflections	2265 [R _{int} = 0.0808]
Completeness to θ = 29.12°	95%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2265 / 0 / 83
Goodness-of-fit on F ²	16.21
Final R indices [I > 2 σ (I)]	R _{obs} = 0.0832, wR _{obs} = 0.1703
R indices (all data)	R _{all} = 0.0919, wR _{all} = 0.1716
Final R main indices [I > 2 σ (I)]	R _{obs} = 0.0513, wR _{obs} = 0.1072
R main indices (all data)	R _{all} = 0.0514, wR _{all} = 0.1072
Final R 1 st order satellites [I > 2 σ (I)]	R _{obs} = 0.2121, wR _{obs} = 0.4297
R 1 st order satellites (all data)	R _{all} = 0.2543, wR _{all} = 0.4402
Extinction coefficient	24.1(12)
T _{min} and T _{max} coefficients	0.0190 and 0.4759
Largest diff. peak and hole	8.04 and -7.02 e.Å ⁻³
R = $\sum F_o - F_c / \sum F_o $, wR = $\{\sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)]\}^{1/2}$ and w = $1/(\sigma^2(I) + 0.0016I^2)$	

Table 7.2. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with e.s.d.'s.

Atom	Wave	x	y	z	Occupancy	U_{eq}
U	0	7890(1)	2549	1615(1)	1	22(1)
	sin, 1	42(1)	0	55(1)		
	cos, 1	-17(1)	0	-20(1)		
Te[1]	0	2660(2)	2549	622(1)	1	22(1)
	sin, 1	35(2)	0	53(2)		
	cos, 1	2(2)	0	22(2)		
Te[2]	0	3969(2)	2549	6594(1)	1	25(1)
	sin, 1	19(3)	0	35(2)		
	cos, 1	-49(2)	0	-16(2)		
Te[3]	0	9240(2)	2549	6676(2)	1	29(1)
	sin, 1	24(3)	0	72(2)		
	cos, 1	121(3)	0	-9(2)		
Cu	0	915(70)	2549	4545(30)	0.138(7)	29
	sin, 1	35(50)	0	5(20)		
	cos, 1	-5(90)	0	-65(40)		

Table 7.3. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with e.s.d.'s.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
U	0	20(1)	17(1)	29(1)	0	6(1)	0
	sin, 1	0(1)	0(1)	0(1)	0	0(1)	0
	cos, 1	0(1)	0(1)	1(1)	0	0(1)	0
Te[1]	0	19(1)	20(1)	29(1)	0	5(1)	0
	sin, 1	0(1)	0(1)	1(1)	0	0(1)	0
	cos, 1	0(1)	-1(1)	1(1)	0	0(1)	0
Te[2]	0	25(1)	24(1)	29(1)	0	9(1)	0
	sin, 1	0(1)	0(1)	-1(1)	0	-1(1)	0
	cos, 1	-1(1)	0(1)	3(1)	0	1(1)	0
Te[3]	0	29(1)	23(1)	34(1)	0	0(1)	0
	sin, 1	0(1)	0(1)	0(1)	0	1(1)	0
	cos, 1	-5(1)	1(1)	0(1)	0	2(1)	0
Cu	0	47	38	2	0	0	0

Table 7.4. Fourier components of the occupational modulation for $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with e.s.d.'s.

Atom	Wave	Occupational component
Cu	sin, 1	-0.043(10)
	cos, 1	-0.120(10)

Table 7.5. Bond lengths distributions [$\text{\AA}$] for $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with e.s.d.'s.

Atom	Average Distance	Minimum Distance	Maximum Distance
U - Te[1]	3.1870(19)	3.1769(19)	3.1973(19)
U - Te[1]	3.207(2)	3.198(2)	3.216(2)
U - Te[1] x 2	3.0976(19)	3.0959(19)	3.0993(19)
U - Te[2] x 2	3.113(2)	3.105(2)	3.122(2)
U - Te[3] x 2	3.1048(18)	3.0933(18)	3.1163(18)
U - Cu	3.29(5)	3.23(4)	3.34(4)
Te[2] - Te[3]	2.881(3)	2.782(3)	2.981(3)
Te[2] - Te[3]	3.187(3)	3.082(3)	3.289(3)
Te[2] - Cu	2.60(5)	2.56(5)	2.64(5)
Te[3] - Cu	2.55(5)	2.49(5)	2.62(5)
Te[3] - Cu x 2	2.44(3)	2.38(2)	2.50(3)
Cu - Cu x 2	2.62(5)	2.57(5)	2.67(6)

Table 7.6. Bond angles distributions [$^\circ$] for $\text{Cu}_{0.14(1)}\text{UTe}_3$ at 100 K with e.s.d.'s.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - U - Te[1]	143.14(7)	141.65(7)	144.61(7)
Te[1] - U - Te[1] x 4	76.59(5)	76.12(5)	77.05(5)
Te[1] - U - Te[2] x 2	76.12(5)	75.51(5)	76.71(5)
Te[1] - U - Te[3] x 2	129.09(5)	127.83(5)	130.34(4)
Te[1] - U - Cu x 3	133.6(9)	133.2(9)	133.9(9)
Te[1] - U - Te[2] x 2	127.64(4)	126.50(4)	128.77(4)
Te[1] - U - Te[3] x 2	73.96(6)	73.23(6)	74.68(6)
Te[1] - U - Cu	83.3(9)	81.7(9)	84.9(9)
Te[1] - U - Te[1]	85.35(5)	85.29(5)	85.40(5)
Te[1] - U - Te[2] x 2	88.53(5)	87.94(5)	89.11(5)
Te[1] - U - Te[2] x 2	152.71(6)	151.67(6)	153.73(6)

Table 7.6. (Cont'd) Bond angles distributions [°] for Cu_{0.14(1)}UTe₃ at 100 K with e.s.d.'s.

Te[1] - U - Te[3] x 2	87.33(5)	86.78(5)	87.88(5)
Te[2] - U - Te[2]	84.82(5)	84.53(5)	85.10(5)
Te[2] - U - Te[3] x 2	55.20(5)	53.19(5)	57.24(5)
Te[2] - U - Cu x 2	70.1(6)	69.4(6)	70.8(6)
Te[3] - U - Te[3]	85.10(5)	84.71(5)	85.49(5)
Te[3] - U - Cu x 2	44.8(2)	44.2(2)	45.4(3)
U - Te[1] - U x 4	103.47(5)	102.88(5)	104.07(5)
U - Te[2] - U	84.82(6)	84.53(6)	85.10(6)
U - Te[2] - Te[3] x 2	62.24(5)	61.42(5)	63.07(5)
U - Te[2] - Te[3] x 2	115.68(6)	114.40(6)	116.99(6)
U - Te[2] - Cu x 2	101.8(8)	99.9(8)	103.7(8)
Te[3] - Te[2] - Te[3]	176.84(11)	175.49(11)	178.17(11)
Te[3] - Te[2] - Cu	55.2(11)	53.5(11)	57.0(11)
Te[3] - Te[2] - Cu	127.9(11)	127.3(11)	128.6(11)
U - Te[3] - U	85.10(6)	84.71(6)	85.49(6)
U - Te[3] - Te[2] x 2	119.46(7)	118.12(7)	120.83(7)
U - Te[3] - Te[2] x 2	62.55(5)	61.28(5)	63.82(5)
U - Te[3] - Cu x 2	103.2(7)	100.4(7)	105.9(7)
U - Te[3] - Cu x 2	71.6(9)	70.7(9)	72.5(9)
Te[2] - Te[3] - Te[2]	176.84(12)	175.33(12)	178.35(12)
Te[2] - Te[3] - Cu	120.1(10)	117.5(10)	122.8(10)
Te[2] - Te[3] - Cu x 4	91.3(12)	89.4(12)	93.3(12)
Cu - Te[3] - Cu x 2	63.2(11)	60.9(10)	65.6(11)
Cu - Te[3] - Cu	118.8(13)	114.4(13)	123.4(14)
U - Cu - Te[2]	169(2)	167(2)	171(2)
U - Cu - Te[3]	123(2)	122(2)	125(2)
U - Cu - Te[3] x 2	63.7(10)	62.2(9)	65.1(9)
U - Cu - Cu x 2	97.0(16)	94.8(17)	99.1(17)
Te[2] - Cu - Te[3]	68.0(12)	64.6(12)	71.5(14)
Te[2] - Cu - Te[3] x 2	112.7(13)	111.9(13)	113.6(12)
Te[2] - Cu - Cu x 2	89.7(15)	86.7(16)	92.8(17)
Te[3] - Cu - Te[3] x 3	116.8(13)	114.6(14)	118.9(14)
Te[3] - Cu - Cu x 4	56.3(13)	54.5(14)	58.2(15)
Te[3] - Cu - Cu x 2	153(3)	152(3)	153(2)

Table 7.7. Crystal data and structure refinement for Cu_{0.18(1)}UTe₃ at 100 K.

Empirical formula	Cu _{0.18(1)} UTe ₃
Formula weight	633.5
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	Monoclinic
Space group	P2 ₁ /m($\alpha\gamma$)00
Unit cell dimensions	a = 6.0603(10) Å, α = 90° b = 4.1980(8) Å, β = 98.171(14)° c = 10.2813(19) Å, γ = 90°
q-vector(1)	0.179(1)a* - 0.086(3)c*
Volume	258.91(8) Å ³
Z	2
Density (calculated)	8.124 g/cm ³
Absorption coefficient	17.953 mm ⁻¹
F(000)	506
Crystal size	0.15 x 0.09 x 0.02 mm ³
Theta range for data collection	3.10 to 29.32°
Index ranges	-8 ≤ h ≤ 8, -5 ≤ k ≤ 5, -14 ≤ l ≤ 14, -1 ≤ m ≤ 1
Reflections collected	12028 (3746 main + 8282 satellites)
Independent reflections	2346 (777 main + 1569 satellites) [R _{int} = 0.0559]
Completeness to θ = 29.32°	96%
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2346 / 0 / 95
Goodness-of-fit on F ²	2.75
Final R indices [I > 2 σ (I)]	R _{obs} = 0.0518, wR _{obs} = 0.1628
R indices (all data)	R _{all} = 0.0574, wR _{all} = 0.1646
Final R main indices [I > 2 σ (I)]	R _{obs} = 0.0385, wR _{obs} = 0.1000
R main indices (all data)	R _{all} = 0.0386, wR _{all} = 0.1002
Final R 1 st order satellites [I > 2 σ (I)]	R _{obs} = 0.1038, wR _{obs} = 0.2408
R 1 st order satellites (all data)	R _{all} = 0.1260, wR _{all} = 0.2441
Extinction coefficient	0.00355(13)
T _{min} and T _{max} coefficients	0.0243 and 0.4096
Largest diff. peak and hole	7.30 and -3.20 e.Å ⁻³
R = $\Sigma F_o - F_c / \Sigma F_o $, wR = $\{\Sigma[w(F_o ^2 - F_c ^2)^2] / \Sigma[w(F_o ^4)]\}^{1/2}$ and w = $1/(\sigma^2(I)+0.0016I^2)$	

Table 7.8. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
U	0	7905(1)	2549	1624(1)	1	15(1)
	sin, 1	31(1)	0	39(1)		
	cos, 1	-13(1)	0	-24(1)		
Te[1]	0	2659(1)	2549	610(1)	1	15(1)
	sin, 1	17(1)	0	37(1)		
	cos, 1	6(1)	0	30(1)		
Te[2]	0	3987(1)	2549	6602(1)	1	20(1)
	sin, 1	-23(1)	0	4(1)		
	cos, 1	-91(1)	0	-23(1)		
Te[3]	0	9169(1)	2549	6680(1)	1	21(1)
	sin, 1	-11(1)	0	69(1)		
	cos, 1	179(1)	0	-19(1)		
Cu	0	1065(60)	2549	4685(30)	0.180(7)	26(11)
	sin, 1	125(40)	0	45(20)		
	cos, 1	115(70)	0	15(40)		

Table 7.9. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
U	0	13(1)	14(1)	17(1)	0	3(1)	0
	sin, 1	0(1)	0(1)	0(1)	0	0(1)	0
	cos, 1	1(1)	0(1)	1(1)	0	0(1)	0
Te[1]	0	13(1)	17(1)	17(1)	0	3(1)	0
	sin, 1	0(1)	0(1)	0(1)	0	0(1)	0
	cos, 1	0(1)	0(1)	1(1)	0	1(1)	0
Te[2]	0	19(1)	20(1)	21(1)	0	7(1)	0
	sin, 1	-1(1)	-1(1)	0(1)	0	0(1)	0
	cos, 1	-1(1)	2(1)	1(1)	0	0(1)	0
Te[3]	0	20(1)	20(1)	22(1)	0	-1(1)	0
	sin, 1	-2(1)	1(1)	-1(1)	0	2(1)	0
	cos, 1	-4(1)	1(1)	1(1)	0	2(1)	0

Table 7.9. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Cu	0	24(13)	55(30)	13(13)	0	27(12)	0
	sin, 1	-6(9)	21(16)	-5(9)	0	14(8)	0
	cos, 1	-13(15)	35(30)	-7(16)	0	28(13)	0

Table 7.10. Fourier components of the occupational modulation for $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Cu	sin, 1	-0.107(7)
	cos, 1	-0.203(6)

Table 7.11. Bond lengths distributions [$\text{\AA}$] for $\text{Cu}_{0.20(2)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
U - Te[1] x 2	3.2016(11)	3.1892(11)	3.2139(11)
U - Te[1] x 2	3.0943(8)	3.0914(8)	3.0973(8)
U - Te[2] x 2	3.1056(9)	3.0936(9)	3.1170(9)
U - Te[3] x 2	3.1176(9)	3.0946(9)	3.1411(9)
U - Cu	3.42(4)	3.37(5)	3.50(5)
Te[2] - Te[3]	2.9313(16)	2.7660(16)	3.0995(16)
Te[2] - Te[3]	3.1315(16)	2.9803(16)	3.2792(16)
Te[2] - Cu	2.49(4)	2.37(4)	2.58(5)
Te[3] - Cu x 3	2.50(5)	2.41(5)	2.57(5)
Cu - Cu x 2	2.57(4)	2.52(5)	2.64(4)

Table 7.12. Bond angles distributions [$^\circ$] for $\text{Cu}_{0.18(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - U - Te[1] x 2	142.38(3)	140.60(3)	144.16(3)
Te[1] - U - Te[1] x 4	76.02(2)	75.56(2)	76.48(2)
Te[1] - U - Te[2] x 2	76.06(3)	74.95(3)	77.15(3)
Te[1] - U - Te[3] x 2	129.91(2)	127.96(2)	131.84(2)

Table 7.12. (Cont'd) Bond angles distributions [°] for Cu_{0.18(1)}UTe₃ at 100 K with e.s.d.'s in parentheses.

Te[1] - U - Cu x 3	133.9(8)	133.3(8)	134.7(7)
Te[1] - U - Te[1] x 4	76.57(2)	75.77(2)	77.38(2)
Te[1] - U - Te[2] x 2	128.00(2)	126.35(2)	129.62(2)
Te[1] - U - Te[3] x 2	73.47(3)	71.97(3)	74.93(3)
Te[1] - U - Cu	84.1(8)	81.6(7)	85.8(8)
Te[1] - U - Te[1] x 2	85.43(2)	85.33(2)	85.53(2)
Te[1] - U - Te[2] x 2	88.08(2)	87.23(2)	88.92(2)
Te[1] - U - Te[2] x 2	152.08(3)	150.55(3)	153.58(3)
Te[1] - U - Te[3] x 2	87.28(2)	86.39(2)	88.16(2)
Te[1] - U - Te[3] x 2	150.04(3)	147.86(3)	152.19(3)
Te[2] - U - Te[2] x 2	85.05(2)	84.66(2)	85.45(2)
Te[2] - U - Te[3] x 2	56.22(3)	52.94(3)	59.52(3)
Te[2] - U - Te[3] x 2	110.78(3)	108.22(3)	113.37(3)
Te[2] - U - Cu x 2	70.6(5)	69.4(5)	71.7(5)
Te[3] - U - Te[3] x 2	84.64(2)	83.86(2)	85.42(2)
Te[3] - U - Cu x 2	45.1(2)	43.94(18)	45.9(3)
U - Te[1] - U x 2	142.39(3)	140.53(3)	144.22(3)
U - Te[1] - U x 4	103.42(2)	102.61(2)	104.24(2)
U - Te[1] - U x 4	103.98(3)	103.49(3)	104.47(3)
U - Te[1] - U x 2	85.43(3)	85.33(3)	85.53(3)
U - Te[2] - U x 2	85.04(3)	84.66(3)	85.45(3)
U - Te[2] - Te[3] x 2	62.09(3)	60.73(3)	63.45(3)
U - Te[2] - Te[3] x 2	115.93(3)	113.78(3)	118.12(3)
U - Te[2] - Cu x 2	100.1(8)	97.9(7)	103.2(8)
Te[3] - Te[2] - Te[3] x 2	176.97(5)	174.75(5)	179.11(5)
Te[3] - Te[2] - Cu	53.7(11)	51.8(10)	56.7(11)
Te[3] - Te[2] - Cu	129.0(11)	127.9(11)	129.6(10)
U - Te[3] - U x 2	84.65(3)	83.86(3)	85.42(3)
U - Te[3] - Te[2] x 2	120.21(3)	117.71(3)	122.75(3)
U - Te[3] - Te[2] x 2	61.70(3)	59.67(2)	63.73(3)
U - Te[3] - Cu x 2	99.4(7)	97.4(7)	102.2(7)
U - Te[3] - Cu x 2	73.8(8)	71.9(8)	76.4(8)
U - Te[3] - Cu x 2	147.3(10)	142.6(10)	153.9(10)
Te[2] - Te[3] - Te[2] x 2	176.96(5)	174.49(5)	179.50(5)

Table 7.12. (Cont'd) Bond angles distributions [°] for Cu_{0.18(1)}UTe₃ at 100 K with e.s.d.'s in parentheses.

Te[2] - Te[3] - Cu	123.8(9)	123.0(9)	124.6(10)
Te[2] - Te[3] - Cu x 4	91.5(10)	86.8(10)	94.7(10)
Te[2] - Te[3] - Cu	53.3(9)	51.5(9)	54.9(9)
Cu - Te[3] - Cu x 4	61.2(10)	59.3(9)	64.9(10)
Cu - Te[3] - Cu x 2	112.6(12)	111.1(12)	114.6(11)
U - Cu - Te[2]	167(2)	165(2)	170.7(19)
U - Cu - Te[3]	119.9(16)	117.9(15)	121.2(16)
U - Cu - Te[3] x 2	61.2(9)	59.4(10)	62.3(10)
U - Cu - Cu x 2	91.0(14)	88.5(13)	92.6(15)
Te[2] - Cu - Te[3]	73.0(13)	70.6(15)	74.6(15)
Te[2] - Cu - Te[3] x 2	114.1(11)	111.4(13)	117.9(12)
Te[2] - Cu - Cu x 2	96.5(15)	95.7(17)	97.9(15)
Te[3] - Cu - Te[3] x 6	118.4(12)	114.7(11)	120.9(12)
Te[3] - Cu - Cu x 4	59.5(13)	58.6(12)	60.1(14)
Te[3] - Cu - Cu x 2	148(2)	142(2)	152(2)
Cu - Cu - Cu x 2	110(2)	106(2)	113(3)

Table 7.13. Crystal data and structure refinement for Cu_{0.40(1)}UTe₃ at 100 K.

Empirical formula	Cu _{0.40(1)} UTe ₃
Formula weight	646.2
Temperature	100.0(3) K
Wavelength	0.70926 Å
Crystal system	triclinic
Space group	P-1($\alpha\beta\gamma$)0
Unit cell dimensions	$a = 6.0856(6)$ Å, $\alpha = 90^\circ$
	$b = 4.2005(4)$ Å, $\beta = 99.037^\circ$
	$c = 10.3326(11)$ Å, $\gamma = 90^\circ$
q-vector(1)	$0.2225(8)a^* + 0.2711(5)b^* + 0.513(1)c^*$
Volume	$260.85(5)$ Å ³
Z	2
Density (calculated)	8.2252 g/cm ³
Absorption coefficient	18.616 mm ⁻¹
F(000)	519
Crystal size	$0.16 \times 0.14 \times 0.08$ mm ³
Theta range for data collection	1.89 to 29.14°
Index ranges	$-8 \leq h \leq 8$, $-6 \leq k \leq 6$, $-14 \leq l \leq 13$, $-1 \leq m \leq 1$
Reflections collected	7444 (2469 main + 4975 satellites)
Independent reflections	3856 (1277 main + 2579 satellites) [$R_{\text{int}} = 0.0398$]
Completeness to $\theta = 21.52^\circ$	95%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3856 / 0 / 140
Goodness-of-fit on F^2	1.22
Final R indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0479$, $wR_{\text{obs}} = 0.0953$
R indices (all data)	$R_{\text{all}} = 0.0764$, $wR_{\text{all}} = 0.1026$
Final R main indices [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.0331$, $wR_{\text{obs}} = 0.0796$
R main indices (all data)	$R_{\text{all}} = 0.0341$, $wR_{\text{all}} = 0.0798$
Final R 1 st order satellites [$I > 2\sigma(I)$]	$R_{\text{obs}} = 0.1267$, $wR_{\text{obs}} = 0.2127$
R 1 st order satellites (all data)	$R_{\text{all}} = 0.2303$, $wR_{\text{all}} = 0.2508$
Extinction coefficient	0.000259
T _{min} and T _{max} coefficients	0.0212 and 0.0573
Largest diff. peak and hole	3.76 and -4.12 e.Å ⁻³
$R = \sum F_o - F_c / \sum F_o $, $wR = \{ \sum [w(F_o ^2 - F_c ^2)^2] / \sum [w(F_o ^4)] \}^{1/2}$ and $w = 1/(\sigma^2(I) + 0.0016I^2)$	

Table 7.14. Atomic coordinates ($\times 10^4$), Fourier components of the displacive modulation ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$) for $\text{Cu}_{0.40(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	x	y	z	Occupancy	U_{eq}
U	0	7923(1)	2500(1)	1629(1)	1	11(1)
	sin, 1	24(1)	0(1)	20(1)		
	cos, 1	1(1)	-13(1)	-15(1)		
Te[1]	0	2660(1)	2501(1)	593(1)	1	11(1)
	sin, 1	17(1)	-5(2)	17(1)		
	cos, 1	-5(1)	-49(3)	-9(1)		
Te[2]	0	4013(1)	2494(1)	6632(1)	1	14(1)
	sin, 1	-126(2)	-45(3)	-51(1)		
	cos, 1	-19(2)	6(3)	24(1)		
Te[3]	0	9054(1)	2502(1)	6692(1)	1	14(1)
	sin, 1	76(2)	-84(3)	1(1)		
	cos, 1	165(2)	10(3)	-41(1)		
Cu	0	963(11)	2473(19)	4663(6)	0.399(6)	6(2)
	sin, 1	-32(9)	-21(17)	3(6)		
	cos, 1	-43(17)	-45(30)	0(10)		

Table 7.15. Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.40(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
U	0	13(1)	7(1)	14(1)	0(1)	3(1)	0(1)
	sin, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	0(1)	0(1)	0(1)	0(1)
Te[1]	0	14(1)	7(1)	13(1)	1(1)	3(1)	1(1)
	sin, 1	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)
Te[2]	0	18(1)	8(1)	16(1)	0(1)	6(1)	0(1)
	sin, 1	-1(1)	1(1)	-1(1)	1(1)	-1(1)	0(1)
	cos, 1	-1(1)	1(1)	0(1)	0(1)	0(1)	0(1)
Te[3]	0	19(1)	9(1)	15(1)	1(1)	0(1)	0(1)
	sin, 1	-2(1)	0(1)	-1(1)	1(1)	1(1)	0(1)
	cos, 1	0(1)	0(1)	1(1)	0(1)	0(1)	0(1)

Table 7.15. (Cont'd) Fourier components of the atomic thermal parameters modulation ($\times 10^3$) for $\text{Cu}_{0.40(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Cu	0	9(4)	4(4)	5(4)	3(3)	1(2)	-4(3)
	sin, 1	-12(3)	-3(4)	-6(3)	1(2)	-2(2)	-3(2)
	cos, 1	-21(6)	-6(7)	-14(6)	5(4)	-5(4)	-9(4)

Table 7.16. Fourier components of the occupational modulation for $\text{Cu}_{0.40(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Wave	Occupational component
Cu	sin, 1	-0.187(11)
	cos, 1	-0.404(11)

Table 7.17. Bond lengths distributions [$\text{\AA}$] for $\text{Cu}_{0.40(1)}\text{UTe}_3$ at 100 K with e.s.d.'s in parentheses.

Atom	Average Distance	Minimum Distance	Maximum Distance
U - Te[1]	3.2139(10)	3.1947(10)	3.2330(10)
U - Te[1]	3.2288(12)	3.2217(12)	3.2360(12)
U - Te[1] x 2	3.0910(12)	3.0855(12)	3.0967(12)
U - Te[2]	3.1129(14)	3.0935(14)	3.1306(14)
U - Te[2]	3.1161(14)	3.1038(14)	3.1270(14)
U - Te[3] x 2	3.1333(13)	3.0952(13)	3.1714(13)
U - Cu	3.378(10)	3.365(11)	3.395(11)
Te[2] - Te[3]	3.0295(16)	2.8435(16)	3.2135(16)
Te[2] - Te[3]	3.0579(16)	2.9294(16)	3.1879(16)
Te[2] - Cu	2.540(10)	2.467(9)	2.594(10)
Te[3] - Cu	2.571(11)	2.438(13)	2.668(13)
Te[3] - Cu x 2	2.526(12)	2.461(14)	2.575(14)
Cu - Cu x 2	2.548(17)	2.473(19)	2.608(19)

Table 7.18. Bond angles distributions [°] for Cu_{0.40(1)}UTe₃ at 100 K with e.s.d.'s in parentheses.

Atom	Average Angle	Minimum Angle	Maximum Angle
Te[1] - U - Te[1] x 2	141.67(3)	141.31(3)	142.04(3)
Te[1] - U - Te[1] x 8	76.13(3)	75.38(3)	76.90(3)
Te[1] - U - Te[2] x 2	75.17(3)	73.33(3)	77.04(3)
Te[1] - U - Te[3] x 2	130.73(4)	129.05(4)	132.37(4)
Te[1] - U - Cu x 3	133.02(16)	132.14(16)	133.68(16)
Te[1] - U - Te[2] x 2	129.08(4)	127.76(4)	130.35(4)
Te[1] - U - Te[3] x 2	72.93(3)	71.01(3)	74.90(3)
Te[1] - U - Cu	85.37(16)	85.00(16)	85.87(16)
Te[1] - U - Te[1] x 2	85.61(3)	84.85(3)	86.38(3)
Te[1] - U - Te[2] x 2	87.76(3)	86.70(3)	88.83(3)
Te[1] - U - Te[2] x 2	151.33(3)	149.28(3)	153.39(3)
Te[1] - U - Te[3] x 2	86.82(3)	85.87(3)	87.78(3)
Te[1] - U - Te[3] x 2	148.91(4)	147.03(4)	150.83(4)
Te[2] - U - Te[2] x 2	84.84(4)	84.53(4)	85.18(4)
Te[2] - U - Te[3] x 2	58.05(3)	54.60(3)	61.39(3)
Te[2] - U - Te[3] x 2	112.04(3)	108.76(3)	115.28(3)
Te[2] - U - Cu x 2	70.84(17)	67.94(17)	73.02(17)
Te[3] - U - Te[3] x 2	84.27(3)	83.55(3)	84.97(3)
Te[3] - U - Cu x 2	45.41(18)	44.26(18)	46.27(18)
U - Te[1] - U x 2	141.67(4)	141.56(4)	141.78(4)
U - Te[1] - U x 8	103.99(3)	103.81(3)	104.19(3)
U - Te[1] - U x 2	85.62(3)	85.35(3)	85.88(3)
U - Te[2] - U x 2	84.81(3)	84.41(3)	85.27(3)
U - Te[2] - Te[3] x 2	61.30(3)	59.89(3)	62.80(4)
U - Te[2] - Te[3] x 2	117.27(4)	114.56(4)	119.97(4)
U - Te[2] - Cu x 2	99.2(2)	97.6(2)	101.3(2)
Te[3] - Te[2] - Te[3] x 2	177.45(5)	174.67(5)	179.82(6)
Te[3] - Te[2] - Cu	53.7(2)	53.2(2)	54.3(2)
Te[3] - Te[2] - Cu	128.4(2)	126.2(2)	131.0(2)
U - Te[3] - U x 2	84.21(3)	83.39(3)	85.04(3)
U - Te[3] - Te[2] x 2	120.68(5)	117.64(5)	123.67(5)
U - Te[3] - Te[2] x 2	60.65(3)	58.62(3)	62.79(4)
U - Te[3] - Cu x 2	97.9(2)	95.0(2)	102.1(2)

Table 7.18. (Cont'd) Bond angles distributions [°] for Cu_{0.40(1)}UTe₃ at 100 K with e.s.d.'s in parentheses.

U - Te[3] - Cu x 2	72.3(2)	70.85(19)	74.3(2)
U - Te[3] - Cu x 2	144.5(2)	140.5(2)	148.9(2)
Te[2] - Te[3] - Te[2] x 2	177.42(5)	175.00(5)	179.78(6)
Te[2] - Te[3] - Cu	124.78(19)	122.88(19)	126.35(19)
Te[2] - Te[3] - Cu x 2	94.2(2)	93.3(2)	94.7(2)
Te[2] - Te[3] - Cu	52.83(18)	50.98(18)	55.38(19)
Te[2] - Te[3] - Cu x 2	84.3(2)	82.7(2)	86.4(2)
Cu - Te[3] - Cu x 4	60.0(4)	59.4(4)	60.7(4)
Cu - Te[3] - Cu x 2	112.1(3)	110.6(3)	114.7(3)
U - Cu - Te[2]	166.3(4)	165.1(4)	167.4(4)
U - Cu - Te[3]	120.1(3)	117.9(4)	123.0(4)
U - Cu - Te[3] x 2	62.3(2)	61.4(2)	62.9(2)
U - Cu - Cu x 2	92.6(4)	91.6(4)	93.9(4)
Te[2] - Cu - Te[3]	73.5(3)	70.7(3)	75.4(3)
Te[2] - Cu - Te[3] x 2	112.7(4)	111.6(5)	114.2(5)
Te[2] - Cu - Cu x 2	95.5(4)	94.7(5)	96.1(5)
Te[3] - Cu - Te[3] x 4	120.0(5)	117.9(4)	122.0(4)
Te[3] - Cu - Cu x 4	59.1(3)	58.3(4)	60.3(4)
Te[3] - Cu - Te[3] x 2	112.6(4)	112.1(5)	113.2(5)
Te[3] - Cu - Cu x 2	150.9(5)	149.6(4)	152.2(4)
Cu - Cu - Cu x 2	110.3(5)	109.3(6)	111.9(6)

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Chapter 8

Conclusions and Outlook

The new information reported in this Dissertation regarding the CDW distortions in polytellurides opens fresh perspectives on how to think about these systems. An overview of the most important results will be presented in this Chapter. Size effect (section 8.1) and temperature (section 8.2), and dimensionality (section 8.3) on CDW modulations will be discussed. Furthermore, an outlook for CDW materials design (section 8.5) and thermoelectric application (8.6) will be reported.

8.1. Size effect on Charge Density Wave modulations (Chemical pressure)

In Chapter 2 a systematic study on the effect of the RE size (RE = Rare earth) in the CDW distortions in RETe_3 at 300 K was presented.¹ From the bigger in size La to the smaller Dy atom the length of the incommensurate component of the q-vector increases from 0.2751(4) (LaTe_3) to 0.2984(3) (DyTe_3), Table 8.1. The lanthanide contraction decreases the Te-Te distances and thickness of the RETe_3 slabs while the separation of the slabs that is defined by the van der Waals gap remains practically constant at a distance of ~ 3.6 Å. The average Te-Te distance in the distorted Te nets decreases from 3.095(5) Å in LaTe_3 to 3.025(3) Å in DyTe_3 . This so-called chemical pressure influences the CDW distortions. The CDW transition temperature (T_{CDW}) decreases with increasing pressure. For CeTe_3 the T_{CDW} is well above 450 K and for TmTe_3 is at ~ 240 K.² The T_{CDW} goes below room temperature for ErTe_3 , HoTe_3 and TmTe_3 that exhibit an ideal square net at 300 K judging from the vanishing of the modulation vector.

The effect of chemical pressure is more apparent in the RETe_2 family. The synthesis of the RETe_{2-x} (RE = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Yb) family was first reported in 1960 using a direct combination of the pure elements at high

temperature.^{3,4,5,6,7} Several attempts³ to prepare HoTe_{2-x} and ErTe_{2-x} resulted in a mixture of the mono- and tritellurides making the authors to predict that RETe_{2-x} phases with Te-Te distances of less than 3.015 Å do not form. A few years latter a high pressure (~ 50 Kbars) high temperature (~ 1300 °C) synthesis for YTe_{2-x} , HoTe_{2-x} , ErTe_{2-x} , TmTe_{2-x} , LuTe_{2-x} , and LuTe_3 was reported.⁸ The average electron count of the planar Te nets in the RETe_{2-x} family is $-(1-x)$ and it is much lower than the average oxidation state of -0.5 found in the RETe_3 family. Since the Te atoms are more reduced in the RETe_{2-x} members they have a tendency to be further apart and separated with longer distances from the ones present in the RETe_3 family. The extreme case would be a planar net of isolated Te^{2-} atoms with distances of more than 4 Å. Although the CDW distortion in most of the RETe_{2-x} members is unknown up to date (LaTe_2 ⁹ and SmTe_{2-x} ¹⁰ are the only two compounds with resolved distortions), and little is known about the role of vacancies, some general comments can be made. It seems that vacancies act as a pressure relief medium to the chemical pressure effect as the lanthanide atom gets small. Interestingly, only the larger La^{3+} atom¹¹ (minimum chemical pressure) can form a stoichiometric compound with no vacancies (LaTe_2) although an off-stoichiometric phase (LaTe_{2-x}) has been reported.¹²

In contrast to RETe_{2-x} and RETe_3 phases, the RE_2Te_5 family is structurally almost unexplored. The RE_2Te_5 is an intergrowth compound composed of layers found in RETe_2 and RETe_3 substructures. This result in the coexistence of two individual Te nets with different average oxidation states of 0.5- and 1- and two modulation vectors (Chapter 5). Most of the characterization work has been done for $\text{Sm}_2\text{Te}_{5-x}$ ¹³ and the synthesis of most of the RE_2Te_5 compounds has been reported. The analogues with the larger lanthanide

atom, La_2Te_5 ^{12a} and Ce_2Te_5 ,¹⁴ are reported to be high temperature phases. In the RE_2Te_5 family hypostoichiometry is also present in the Te^{1-} net that again it may be due to the higher applied pressure.

A detailed structural study of RETe_{2-x} and $\text{RE}_2\text{Te}_{5-x}$ with temperature and RE is necessary in order to elucidate and compare their CDW distortions and understand the exact role of vacancies.

8.2. Temperature effect on Charge Density Wave modulations

In Chapter 3 the role of temperature on the CDW modulations in RETe_3 was presented.¹⁵ The temperature depended (100 – 500 K) single crystal X-ray diffraction experiment gave unique information for the behavior of the CDW periodicity, Table 8.2. The CDW modulation dependence as a function of decreasing RE radius and decreasing temperature follows opposite trends, even though both factors cause a unit cell contraction. It seems that the band dispersion is effected differently with temperature and RE size and that influences the overall topology of the Fermi surface. Thus, the nesting properties change. Interestingly, the band structure calculations (DFT) capture the trend of temperature and RE size. Theoretical calculations were performed by Zsolt Rak and Prof. Subhendra D. Mahanti at the Physics Department at Michigan State University. The subcells (i.e. undistorted structures) of LaTe_3 , YTe_3 and LuTe_3 were used in the calculation and the temperature parameter was modeled by simple changing the volume of each cell. Qualitatively, the results are in agreement with the experimental observations that showed quantitatively a much large change of the nesting vector (q -

vector). Detailed analysis of the theoretical results is in progress in order to understand the physics behind this anomalous behavior.

8.3. Dimensionality effect on Charge Density Wave distortions

In Chapter 4 the study of an intergrowth AMRETe_4 ($A = \text{Na, K; M} = \text{Cu, Ag; RE} = \text{La, Ce}$) phase was reported.¹⁶ The structure can be seen as a combination of neutral RETe_3 and AMTe layers in a 1:1 ratio. The average oxidation state on the planar distorted Te net (RETe_3 substructure) remains 0.5- since there is no apparent electron transfer between the layers. Surprisingly, despite the fact that the distorted Te nets in AMRETe_4 and RETe_3 are isoelectronic the length of the modulation q-vector changes significantly from $\sim 2/7$ in RETe_3 to $\sim 1/3$, Table 8.3. The report of the effect of the cross-plane interactions on the CDW modulations gave new information and a different perspective on how we should think about CDW distortions.

In Chapter 6, the CDW modulations found in Cu_xEuTe_2 and AM_2EuTe_4 family (Chapter 6) give additional information to the dimensionality issue. The different size of the alkali metal cation that is located in between the distorted Te nets in the quasi-two-dimensional AM_2EuTe_4 gave a series of isoelectronic compound with different layer-layer separation. A decrease in the length of the q-vector was observed with the increase of the alkali metal size, Table 8.4. When the alkali metal was substituted with Eu^{2+} atoms to give the isostructural Cu_xEuTe_2 compound which however now lack a van der Waals gap the presence of two modulations along the same direction was observed. This is a unique behavior that has not been seen before in any of the reported CDW distorted layered polytelluride systems. A plausible explanation suggests that there is a competition

between the modulations coming from cross-plane interactions and the distortions that rise from in-plane interactions (chemical pressure). The distortion stress that is generated from the two competing effects is relieved on the van der Waals gap that gives one overall average modulation vector in AM_2EuTe_4 . In the extended three-dimensional Cu_xEuTe_2 structure there is no van der Waals gap and the two different effects seem to be expressed with two different modulation vectors.

The existence of two CDW modulations along the same direction cannot be explained with the information we have so far from the behavior of the CDW distortions found in RETe_{2-x} , RETe_3 , $\text{RE}_2\text{Te}_{5-x}$, and AMRETe_4 . The interpretation we gave above gives a reasonable answer but it may not be the only one. A systematic study of the ARE_3Te_8 ¹⁷ family as a function of A and RE size, and temperature may give more information.

8.4. Indexing and proper characterization of modulated structures

During our study of the RETe_3 series several publications from different groups mainly on physical characterization (transport properties, ARPES, STM) were reported. A question/issue that was addressed was about the indexing of these incommensurate modulated structures. STM data suggested¹⁸ that the fundamental q-vector is $\sim 5/7$ (1-q) and not $\sim 2/7$ (q). In this section we address the problems and artifacts that may come from indexing modulated structures using intensity information from reflections obtained from electron diffraction and STM experiments.

Electron diffraction has proven to be a powerful tool for detecting weak long range supercell modulations. The high energy of electrons typically used in a TEM ($\geq$

200 KeV) produces electron diffraction images that are very sensitive to small distortions in respect with an X-ray diffraction pattern obtained from an in house X-ray single crystal diffractometer. The integrated intensity calculated from an electron diffraction pattern though has to be corrected for possible dynamic scattering effects that may come from correlation between crystallographic planes perpendicular to the beam. A good example would be the selected area electron diffraction pattern that was collected on CeTe_3 at room temperature (Figure 2.3), Figure 8.1. Assuming that this was the only information we had from this system regarding the fundamental q-vector we could conclude that the q-vector is actually $\sim 5/7$ since the peaks at this position are more intense than the ones found at $\sim 2/7$. Furthermore there is a set of satellite reflections around every main reflection.

STM on the other hand is one of the fundamental techniques used for the direct observation of CDW distortions in layered compounds. Through a tunneling mechanism, electrons are ejected or added on the surface of the material through a conducting fine tip (nm size). It is important to understand that the STM tip does not “see” the atoms directly but instead it interacts with the density of states around the atoms. In that sense, depending on the bias of the tip (positive bias removes electrons and negative bias adds electrons on the surface) atoms in the STM images may appear brighter or darker. Therefore, the intensity of the periodicity peaks in the Fourier transform of the “real space” image obtained from STM will depend on the bias as well.¹⁹ Therefore, the assignment of a fundamental vector from FFT STM data will never be unequivocal since for almost every tip bias there is a corresponding FFT pattern with different relative intensities.

The data we reported and used for the refinements described in this Dissertation come from single crystal X-ray diffraction experiments. In this case, we can easily reconstruct the reciprocal space and study the position and intensity of each reflection. The data we have collected on all RETe_3 members suggest a q -vector of $\sim 2/7$ along c^* . Precession photographs from the data collected on CeTe_3 at 100 K along the long b -axis ($k=0, 1, 2$) verify the presence of satellite reflections at $q \sim 2/7$ around the main reflections, Figure 8.2. Furthermore, all the observed reflections obey the extinction condition of a C-centered system ($h + k = 2n$). Crystallographically there is no difference in indexing either with a q -vector component of $2/7$ or $5/7$ ($1-q$) especially when the lattice centering is C type. In more detail, all the observed reflections can be indexed in three-dimensional space as $h, k, l + m \cdot q_c$ where m is the index along the fourth dimension and q_c the component of the q vector (0.28 along c^*). Each reflection can be indexed with the new vector $q_c' = 1 - q_c$ as $h', k', l' + m' \cdot (1 - q_c)$. Since a given reflection represents a unique point in the reciprocal lattice we have $h' = h, k' = k, l' + m' = l$ and $m' = -m$ which means that the C-centering condition will not be effected from the transformation. This is not true for any other type of centering (A or B).

A proper characterization protocol for this type of incommensurate modulated structures should involve single crystal diffraction studies (in house X-rays / synchrotron or neutrons) accompanied with thermodynamic measurements (mainly heat capacity) from a wide temperature range for the investigation of (additional) weak structural transitions. Transport properties on single crystals and not pellets made from polycrystalline powders would also be useful for this reason. Additionally, total

scattering techniques, like PDF, could give more information hidden underneath the Bragg peaks (diffuse scattering) regarding the short range ordering of the CDW.²⁰

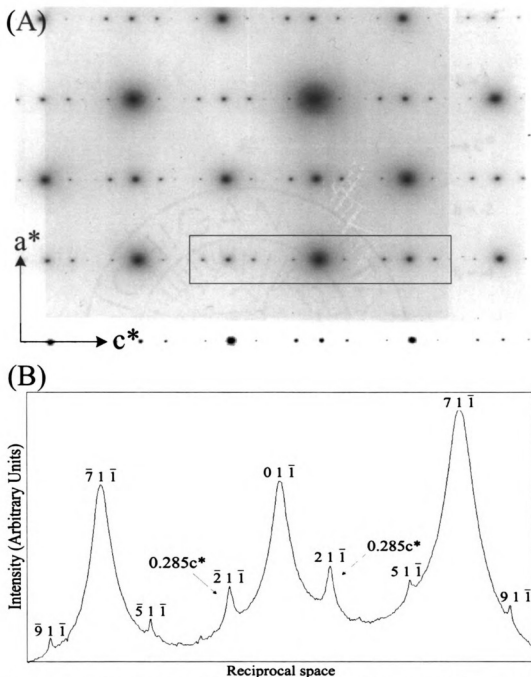


Figure 8.1. (A) Selected area electron diffraction (SAED) pattern for CeTe_3 at the $[010]_l$ orientation showing the 7-fold superlattice. (B) Intensity scan along the c^* axis of the SAED pattern (shown in rectangular box) and approximate indexing based on supercell. The q -vector is also indicated.¹

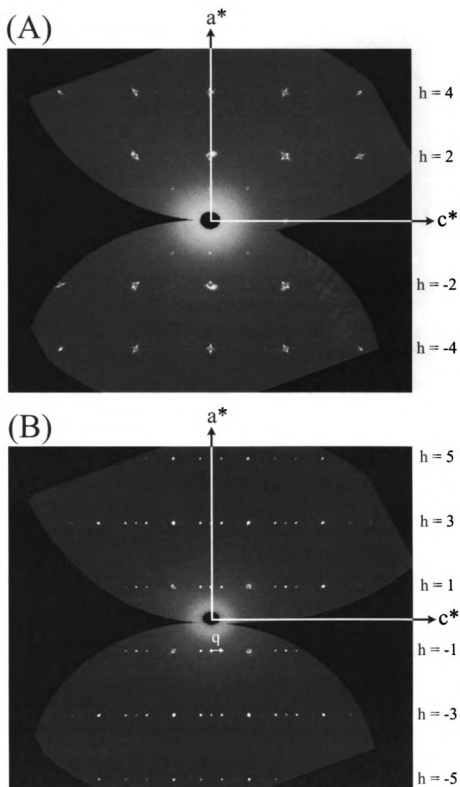


Figure 8.2. Precession photograph of CeTe_3 at 100K of (A) The $h0l$ layer. (B) The $h1l$ layer. (C) The $h2l$ layer. Rows of reflections with $h = 2n$ are absent since the structure is C-centered.

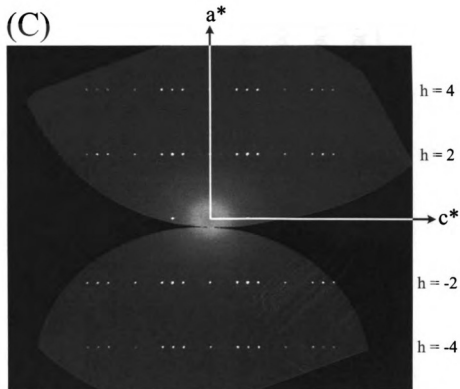


Figure 8.2. (Cont'd) Precession photograph of CeTe_3 at 100K of (A) The $h0l$ layer. (B) The $h1l$ layer. (C) The $h2l$ layer. Rows of reflections with $h = 2n$ are absent since the structure is C-centered.

8.5. Design on new Charge Density Wave materials

The number of CDW compounds is limited with respect to the known superconducting phases. Polychalcogenide and halide fluxes are useful synthetic tools for the discovery and crystal growth of new CDW phases. The existence and structure of intergrowth compounds like RE_2Te_5 , AMRETe_4 , and $\text{K}_2\text{Ag}_4\text{RE}_2\text{Te}_{10}$ could be used as a model for the design of new polytelluride CDW phases. It may be possible to combine layers of different compounds that have similar in plane cell parameters (i.e. NaCuTe and $\text{K}_2\text{Ag}_4\text{Te}_4$) with the $[\text{RETe}_3]$ or $[\text{RE}_2\text{Te}_5]$ layer and create homologous series of compounds. For example, phases like AMRE_2Te_6 that combine a $[\text{AMTe}]$ and $[\text{RE}_2\text{Te}_5]$ layer could exist.

Table 8.1. Summary of supercell parameters of RETe₃ (RE = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Y) at 300 K.

Compound	Cell parameters	q-vector	Average Distance (Å)	Minimum Distance (Å)	Maximum Distance (Å)
LaTe ₃	a = 4.3944(8) Å, b = 26.227(4) Å, c = 4.4076(7) Å	0.2751(4)c*	3.095(5)	2.934(5)	3.261(5)
CeTe ₃	a = 4.3732(5) Å, b = 25.973(4) Å, c = 4.3849(5) Å	0.2801(3)c*	3.095(2)	2.9564(16)	3.2350(17)
PrTe ₃	a = 4.3569(9) Å, b = 25.896(5) Å, c = 4.3666(9) Å	0.2818(4)c*	3.068(3)	2.943(2)	3.197(2)
NdTe ₃	a = 4.3433(6) Å, b = 25.809(4) Å, c = 4.3538(5) Å	0.2827(3)c*	3.0598(18)	2.9420(16)	3.1786(17)
SmTe ₃	a = 4.3218(6) Å, b = 25.609(5) Å, c = 4.3342(8) Å	0.2874(4)c*	3.050(3)	2.955(2)	3.144(3)
GdTe ₃	a = 4.3083(4) Å, b = 25.528(2) Å, c = 4.3154(5) Å	0.2916(3)c*	3.030(3)	2.946(2)	3.113(3)
TbTe ₃	a = 4.2995(8) Å, b = 25.420(6) Å, c = 4.3078(9) Å	0.2957(5)c*	3.039(4)	2.987(4)	3.090(4)
DyTe ₃	a = 4.2994(6) Å, b = 25.353(5) Å, c = 4.2930(6) Å	0.2984(3)c*	3.025(3)	2.991(2)	3.059(3)
YTe ₃	a = 4.2947(7) Å, b = 25.404(4) Å, c = 4.2968(9) Å	0.2969(5)c*	3.0283(12)	2.9733(11)	3.0842(11)

Table 8.2. Summary of supercell parameters of RETe₃ (RE = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Y) at 100 K.

Compound	Cell parameters	q-vector	Average Distance (Å)	Minimum Distance (Å)	Maximum Distance (Å)
LaTe ₃	a = 4.3779(10) Å, b = 26.149(5) Å, c = 4.3968(8) Å	0.2757(4)c*	3.090(7)	2.929(6)	3.256(7)
CeTe ₃	a = 4.3566(6) Å, b = 25.920(3) Å, c = 4.3722(5) Å	0.2790(3)c*	3.078(3)	2.925(2)	3.235(3)
PrTe ₃	a = 4.3475(9) Å, b = 25.800(5) Å, c = 4.3548(9) Å	0.2825(5)c*	3.0694(18)	2.9306(16)	3.2131(18)
NdTe ₃	a = 4.3316(7) Å, b = 25.705(5) Å, c = 4.3419(7) Å	0.2824(4)c*	3.0617(17)	2.9321(15)	3.1947(16)
SmTe ₃	a = 4.3055(6) Å, b = 25.553(5) Å, c = 4.3247(6) Å	0.2865(3)c*	3.033(2)	2.9189(18)	3.1483(19)
GdTe ₃	a = 4.2954(4) Å, b = 25.443(2) Å, c = 4.3097(5) Å	0.2884(3)c*	3.020(3)	2.909(2)	3.134(3)
YTe ₃	a = 4.2840(7) Å, b = 25.312(4) Å, c = 4.2932(9) Å	0.2907(5)c*	3.030(2)	2.9349(15)	3.1282(15)
TbTe ₃	a = 4.2801(7) Å, b = 25.307(5) Å, c = 4.3052(9) Å	0.2912(5)c*	3.0317(18)	2.9387(16)	3.1251(17)
DyTe ₃	a = 4.2831(6) Å, b = 25.250(5) Å, c = 4.2887(6) Å	0.2926(3)c*	3.0260(18)	2.9379(16)	3.1139(17)
HoTe ₃	a = 4.2723(8) Å, b = 25.203(4) Å, c = 4.2855(6) Å	0.2935(3)c*	3.023(2)	2.9453(19)	3.101(2)
ErTe ₃	a = 4.2641(8) Å, b = 25.164(6) Å, c = 4.2791(8) Å	0.2992(4)c*	3.019(3)	2.9522(18)	3.0865(19)
TmTe ₃	a = 4.2617(6) Å, b = 25.092(4) Å, c = 4.2714(8) Å	0.3026(4)c*	3.007(4)	2.944(4)	3.069(4)

Table 8.3. Summary of supercell parameters of AMRETe₄ (A = Na, K; M = Cu, Ag; RE = La, Ce).

Compound	Cell parameters	q-vector	Average Distance (Å)	Minimum Distance (Å)	Maximum Distance (Å)
KAgCeTe ₄ at 100 K	a = 4.4445(9) Å, b = 4.4800(8) Å, c = 21.398(4) Å	0.3358(10)b* + 1/2c*	3.145(9)	2.896(9)	3.402(9)
KAgCeTe ₄ at 300 K	a = 4.4657(9) Å, b = 4.4927(8) Å, c = 21.525(4) Å	0.3381(8)b* + 1/2c*	3.160(8)	2.907(8)	3.422(8)
K _{0.71} Ag _{1.29} LaTe ₄ at 100 K	a = 4.4838(5) Å, b = 4.5057(6) Å, c = 20.877(3) Å	0.3466(7)b* + 1/2c*	3.183(4)	2.929(4)	3.437(4)
KCuCeTe ₄ at 100 K	a = 4.4065(6) Å, b = 4.4220(6) Å, c = 21.086(3) Å	0.3550(8)b* + 1/2c*	3.121(2)	2.972(2)	3.275(2)
KCuCeTe ₄ at 300 K	a = 4.4229(3) Å, b = 4.4371(3) Å, c = 21.1976(17) Å	0.3538(4)b* + 1/2c*	3.133(2)	2.958(2)	3.318(2)
KCuLaTe ₄ at 100 K	a = 4.4421(4) Å, b = 4.4517(4) Å, c = 19.7507(18) Å	0.3861(5)b* + 1/2c*	3.147(4)	2.910(5)	3.392(4)
Na _{0.78} Ag _{1.22} CeTe ₄ at 100 K	a = 4.4139(7) Å, b = 4.4185(8) Å, c = 20.245(3) Å	0.3681(8)b*	3.122(2)	2.985(3)	3.264(3)
Na _{0.70} Ag _{1.30} LaTe ₄ at 100 K	a = 4.4415(6) Å, b = 4.4467(7) Å, c = 20.239(3) Å	0.3660(8)b* + 1/2c*	3.142(4)	3.016(3)	3.273(3)
Na _{0.78} Cu _{1.22} CeTe ₄ at 100 K	a = 4.3850(6) Å, b = 4.3973(6) Å, c = 19.810(3) Å	0.3621(7)b*	3.105(2)	2.977(3)	3.239(2)
Na _{0.6} Cu _{1.4} LaTe ₄ at 100 K	a = 4.4178(6) Å, b = 4.4257(7) Å, c = 19.760(3) Å	0.3632(8)b* + 1/2c*	3.127(4)	2.999(4)	3.260(4)

Table 8.4. Summary of supercell parameters of AM₂EuTe₄ (A = Na, K, Rb, Cs; M = Cu, Ag).

Compound	Cell parameters	q-vector	Average Distance (Å)	Minimum Distance (Å)	Maximum Distance (Å)
Na _{0.80(1)} Cu ₂ Eu _{1.20(1)} Te ₄ at 100 K	a = 4.3692(7) Å, b = 4.3790(6) Å, c = 10.5877(18) Å	0.3122(7)b* + 1/2c*	3.094(4)	2.961(3)	3.234(4)
Na _{0.81(1)} Ag ₂ Eu _{1.19(1)} Te ₄ at 100 K	a = 4.4185(6) Å, b = 4.4435(7) Å, c = 11.0767(17) Å	0.3134(6)b* + 1/2c*	3.133(5)	2.984(5)	3.284(5)
Na _{0.81(1)} Ag ₂ Eu _{1.19(1)} Te ₄ at 300 K	a = 4.4376(5) Å, b = 4.4599(7) Å, c = 11.1258(14) Å	0.3118(5)b* + 1/2c*	3.150(3)	2.973(3)	3.329(4)
KCu ₂ EuTe ₄ at 100 K	a = 4.3862(5) Å, b = 4.4074(7) Å, c = 11.2228(16) Å	0.2822(6)b* + 1/2c*	3.105(4)	2.934(4)	3.284(4)
K _{0.97(1)} Ag ₂ Eu _{1.03(1)} Te ₄ at 100 K	a = 4.4641(5) Å, b = 4.4964(8) Å, c = 11.3501(17) Å	0.2853(5)b* + 1/2c*	3.163(6)	2.940(5)	3.398(6)
RbCu ₂ EuTe ₄ at 100 K	a = 4.3984(7) Å, b = 4.4281(7) Å, c = 11.5510(17) Å	0.2656(8)b* + 1/2c*	3.122(6)	2.932(5)	3.320(5)
RbAg ₂ EuTe ₄ at 100 K	a = 4.4814(7) Å, b = 4.4928(8) Å, c = 11.9199(19) Å	0.2625(7)b* + 1/2c*	3.174(3)	3.167(3)	3.181(3)
CsAg ₂ EuTe ₄ at 100 K	a = 4.4911(6) Å, b = 4.5068(7) Å, c = 12.3484(18) Å	0.2631(6)b* + 1/2c*	3.187(3)	2.937(2)	3.442(3)
CsAg ₂ EuTe ₄ at 300 K	a = 4.5094(4) Å, b = 4.5226(4) Å, c = 12.3962(13) Å	0.2650(4)b* + 1/2c*	3.195(2)	2.951(2)	3.453(2)
Cu _{0.63(1)} EuTe ₂ at 100 K	a = 4.4536(2) Å, b = 4.4723(2) Å, c = 20.2982(6) Å	q ₁ = 0.2910(2)b*, q ₂ = 0.3557(3)b*	3.159(5)	2.935(5)	3.280(5)

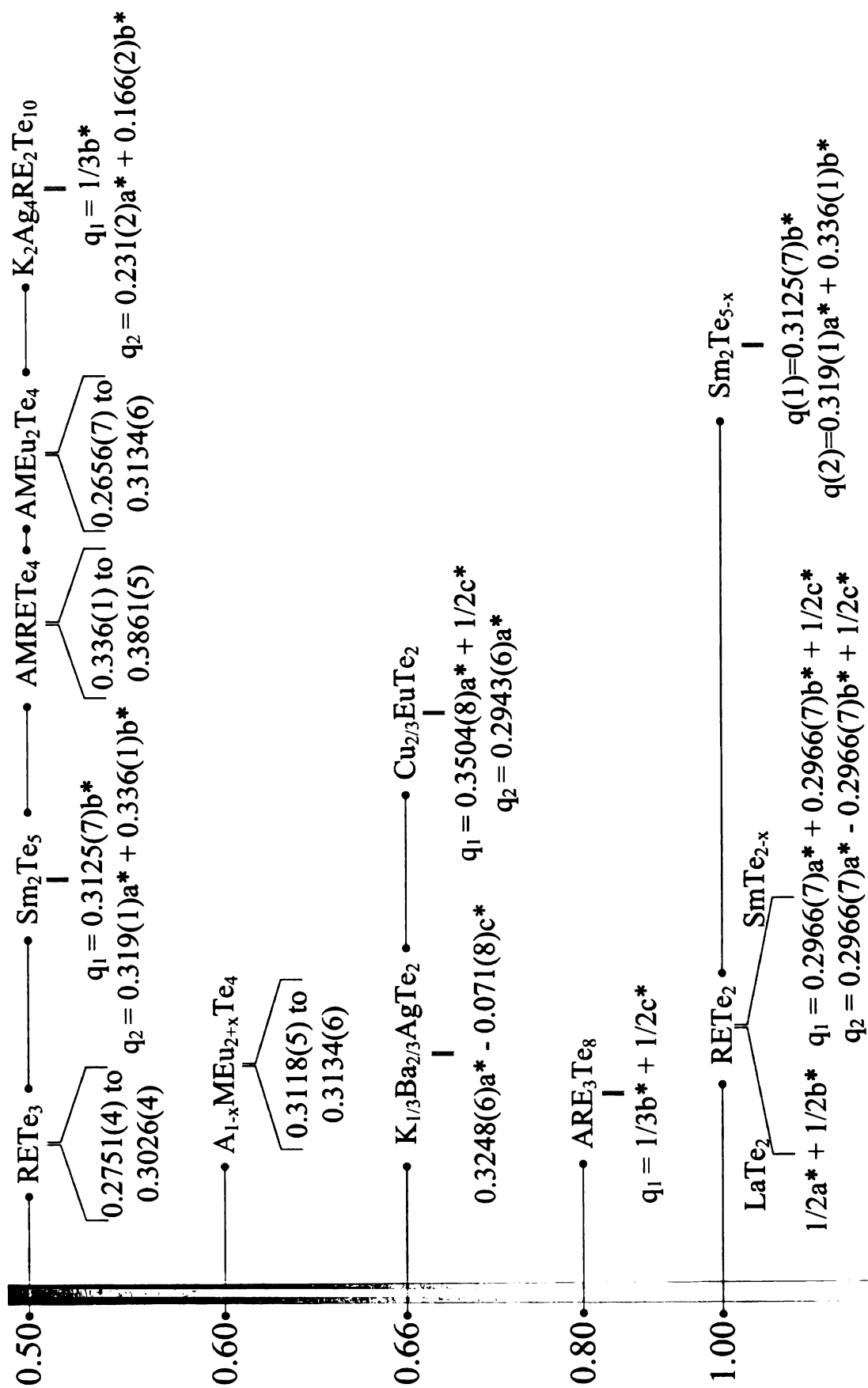


Figure 8.3. Overview of the modulation vectors of most of the known CDW distorted polytelluride phases.

8.6. Charge Density Waves Distortions and Thermoelectrics

Semimetals or narrow bandgap semiconductors with heavy metals seems to be the more promising materials for thermoelectric applications.²¹ A complex electronic structure close to the Fermi level will enhance the thermopower (see expression 1.4). On the other hand, a CDW distortion opens up a gap in the Fermi surface which may create a narrow semiconductor with a complex band structure.

Nevertheless, in all the compounds reported here, the CDW distortion does not create a fully gapped Fermi surface but instead a gap opens in a specific direction in the Fermi surface. This results in a poor metallic behavior (semimetal) in which the electrical conductivity is relative high (compared to semiconductors) and still metallic in character but the thermopower remains low ($< 100 \mu\text{V/K}$ characteristic for metals). Proper understanding of CDW distortions in materials could provide a unique method for creating narrow band gap semiconductors. In that sense, manipulation of CDW modulations could be an excellent synthetic tool for designing material suitable for thermoelectric applications.

8.7. Closing remarks

This is just the beginning of microscopic understanding of the CDW behavior in quasi-two-dimensional systems. In this work most of the know CDW distorted polytelluride systems were systematically studied, Figure 8.3. The distorted Te nets found in these materials are not effected only by the average electron count as it was originally assumed (numbers at the left side of Figure 8.3 represent the average oxidation state of the Te atoms in the CDW distorted nets) but temperature, size of atoms and

dimensionality play a very important role on defining the CDW modulations. Interactions along all three directions must be taken into account and the “quasi” description has to be used with caution.

The CDW study reported here was focused on polytelluride compounds with distorted Te nets. Recently, two more classes of compounds with CDW instabilities that contain Sb and Ga planar nets respectively were reported. Single crystal synchrotron data along a single zone revealed CDW superstructure reflections in LaAgSb_2 that are temperature dependent.²² Furthermore, a complete crystallographic solution of CDW distorted Ga nets in $\text{GdCo}_{1-x}\text{Ga}_3\text{Ge}$ was found.²³ The study of distorted compounds with different atoms in planar arrangements than Te can give more information for the behavior of CDW states.

It will be very exciting to see a well developed theory that can explain and predict the experimental results we presented in this thesis. Furthermore, these new information contributed here can be used in conjunction with the developing unified theory for the description of CDW and superconductivity. Theoretical calculations (DFT) on the undistorted crystal systems were very useful on describing the Fermi surface and correlating the crystallographically observed modulation q-vector to the nesting vectors. Advancement on the development of computational electronic structure codes that can treat incommensurate superstructures will help significantly our understanding of CDW formation, stability, and dynamics.

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