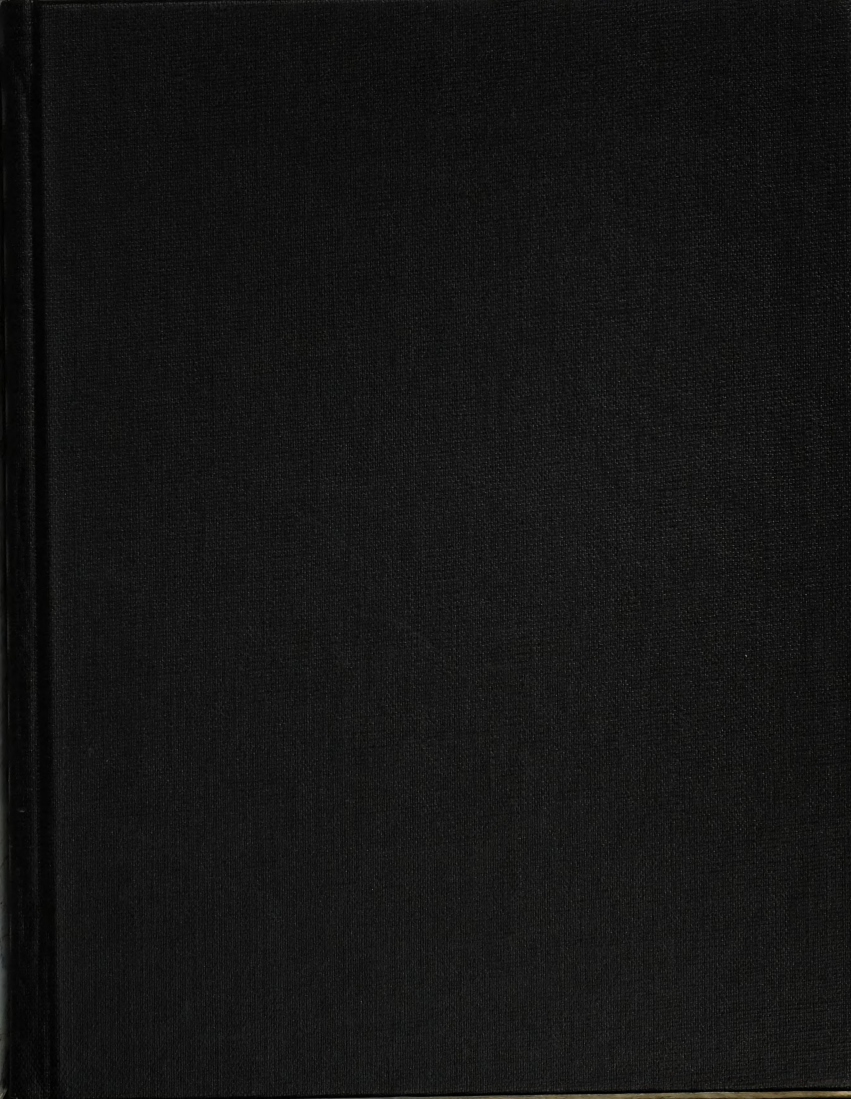






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AN ANALYSIS OF THE ν_2 FUNDAMENTAL INFRARED

ABSORPTION BANDS OF H_2S AND H_2Se

presented by

William Charles Lane

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Ph. D. degree in PHYSICS

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AN ANALYSIS OF THE ν_2 FUNDAMENTAL INFRARED

ABSORPTION BANDS OF H_2S AND H_2Se

By

William Charles Lane

A DISSERTATION

Submitted to

Michigan State University

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ABSTRACT

AN ANALYSIS OF THE ν_2 FUNDAMENTAL INFRARED
ABSORPTION BANDS OF H_2S AND H_2Se

By

William Charles Lane

The ν_2 fundamental infrared absorption bands of H_2S and H_2Se were run on the 50 cm Fourier transform infrared spectrometer system at the University of Denver with a resolution limit of 0.04 cm^{-1} for ν_2 of H_2S and 0.025 cm^{-1} for ν_2 of H_2Se . The two sets of spectra were analyzed at the Molecular Spectroscopy Laboratory at Michigan State University.

We initially analyzed the H_2^{32}S ν_2 spectrum using Typke's Hamiltonian, limited to terms through order P^6 . We determined ground state constants for H_2^{32}S by fitting our infrared ground state combination differences (GSCD's) and the available microwave transitions of Helminger, Cook, and De Lucia. Keeping the ground state constants fixed to the values obtained in our ground state fit, we determined (010) upper state constants for H_2^{32}S by a fit of the ν_2 spectral lines. We then used an isotopic mass adjustment analysis to simultaneously fit the small number of observed H_2^{33}S and H_2^{34}S ν_2 lines together with the many H_2^{32}S ν_2 lines.

Following the report of improved ground state constants for H_2S by Flaud, Camy-Peyret, and Johns, we reanalyzed the ν_2 band of H_2S with Watson's A-reduced Hamiltonian, including terms through order P^8 . Using their H_2^{32}S , H_2^{33}S , and H_2^{34}S ground state constants we determined (010) upper state constants for each of the three isotopic species of H_2S by

separately fitting the H_2^{32}S , H_2^{33}S and H_2^{34}S ν_2 spectral lines.

We similarly analyzed the ν_2 spectra of the five most abundant isotopic species of H_2Se as individual spectra, using Watson's A-reduced Hamiltonian. To analyze the small number of assigned H_2^{74}Se ν_2 lines, we used the method of isotopic mass adjustment to analyze the ground states and the (010) upper states of the six stable isotopic species of H_2Se .

TO MY PARENTS

FRANKLIN CHARLES LANE AND MARY LANE POWELL

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INTRODUCTION

The molecules hydrogen sulfide, H_2S , and hydrogen selenide, H_2Se , are two examples of the bent triatomic molecules of the same symmetry group (C_{2v}), as the water vapor molecule, H_2O . H_2S in particular is an important constituent of planetary atmospheres. On earth H_2S is a pollutant, produced both naturally and by the burning of sulfur-containing fossil fuels, and is a contributing factor in the formation of acid rain. On the larger planets of our solar system, notably Jupiter, H_2S is a major atmospheric component (1). A more complete knowledge of its infrared absorption spectrum will contribute to the understanding of the chemistry of planetary atmospheres.

The analysis in this dissertation completes a study of the three fundamental vibration-rotation infrared bands of these two molecules at Michigan State University. Over the years, the Molecular Spectroscopy Laboratory at Michigan State University has developed methods of analysis and computer programs suitable for analyzing high-resolution infrared spectra. Before this particular research was begun, the conclusions that had been drawn about the best methods of analysis for spectra of asymmetric top molecules were based on data gathered from the MSU grating infrared spectrometer. However, with the availability of higher resolution spectra from other laboratories, we have modified some of our conclusions and methods of analysis.

This work was done in cooperation with the Upper Atmosphere Research Group at the University of Denver. We provided the samples,

they ran the spectra on the Denver University Fourier Transform Interferometer, which operates in regions inaccessible to our spectrometer, and the analysis was carried out here at MSU.

In this dissertation the vibration-rotation infrared spectrum of the ν_2 fundamental band of H_2S in the $8.5\ \mu\text{m}$ region and the ν_2 fundamental band of H_2Se in the $9.7\ \mu\text{m}$ region are analyzed. The H_2S analysis includes the first reported ν_2 spectra for the molecular species H_2^{33}S and H_2^{34}S , and the H_2Se analysis includes the first reporting of H_2^{74}Se spectra anywhere.

Chapter I provides a brief overview of the general theory involved in the development of a vibration-rotation Hamiltonian suitable for analyzing asymmetric top molecules. Chapters II and III give the details of our analysis of the ν_2 bands of H_2S and H_2Se , respectively. A reprint of our 1982 paper on ν_2 of H_2S , tables of data for H_2S and H_2Se , and a new subroutine for our fitting programs are contained in the Appendices.

CHAPTER I

VIBRATION-ROTATION HAMILTONIANS FOR ASYMMETRIC TOP MOLECULES

Overview

This chapter traces the development of a Hamiltonian suitable for calculating the vibration-rotation energies of asymmetric top molecules. The analysis of spectroscopic data is regularly performed with an "effective Hamiltonian," i.e. one which effectively fits the spectral lines but is not explicitly expressed in terms of fundamental molecular parameters, such as the equilibrium values of the principal moments of inertia and the force constants of the molecular potential energy. The "effective constants" associated with such a Hamiltonian may be used successfully to predict the positions and intensities of the spectral lines of the specific vibration-rotation band from which they were determined, but are not directly related to the structure of the molecule. Furthermore, the specific values of the constants depend on which of several available effective Hamiltonians is used and on how a Cartesian coordinate system is chosen to be aligned with the "body-fixed" rotational axes of the molecule. It is nevertheless possible to transform these effective constants in a way which allows spectroscopists to compare the results of different fits of the spectrum using different Hamiltonians. The transformed constants are called the "determinable coefficients" of the molecule.

The General Form of the Hamiltonian

Darling and Dennison (2) constructed the first general Hermitian expression for the vibration-rotation Hamiltonian. This Hamiltonian is given by

$$H = \frac{1}{2} \sum_{\alpha \beta} \mu^{1/4} (p_{\alpha} - p_{\alpha}) \mu_{\alpha \beta} \mu^{-1/2} (p_{\beta} - p_{\beta}) \mu^{1/4} \\ + \frac{1}{2} \sum_k \mu^{1/4} p_k \mu^{-1/2} p_k \mu^{1/4} + V, \quad (I-1)$$

where α and β may be x, y or z, and the summation over k is a summation over the normal modes of the molecule. V is the vibrational potential energy which may be expanded as a Taylor series in the normal coordinate displacements from equilibrium. The operators p_{α} are the components of the angular momentum along body-fixed axes. These operators obey the commutation relations

$$[p_{\alpha}, p_{\beta}] = -i \epsilon_{\alpha \beta \gamma} p_{\gamma}, \quad (I-2)$$

where $\epsilon_{\alpha \beta \gamma}$ is the Levi-Civita tensor. The operators p_k are the components of the linear momenta conjugate to the normal coordinate displacements, given by

$$p_k = -i \hbar \frac{\partial}{\partial q_k}. \quad (I-3)$$

The operators p_{α} are the components of the "internal angular momentum." A familiar example of internal angular momentum is the linear combination of the two components of the degenerate bending mode of vibration of CO_2 . In general, the components of the internal angular momentum are defined as

$$p_{\alpha} = \sum_k \sum_{k'} \zeta_{kk'}^{\alpha} q_k p_{k'}, \quad (I-4)$$

where the constants $\zeta_{kk'}^{\alpha}$ are the "Coriolis coupling coefficients." For H_2S and H_2Se , only the asymmetric-stretch vibrational mode, v_3 , has any

internal angular momentum associated with it. The parameters $\mu_{\alpha\beta}$ are the cofactors of the determinant μ of the inertia tensor. The inertia tensor is composed of the instantaneous moments and products of inertia, which are functions of the normal coordinates:

$$I_{\alpha\alpha} = I_{\alpha\alpha}^e + \sum_k a_k^{\alpha\alpha} q_k + \sum_k \sum_{k'} A_{kk'}^{\alpha\alpha} q_k q_{k'}$$

and

(I-5)

$$I_{\alpha\beta} = \sum_k a_k^{\alpha\beta} q_k + \sum_k \sum_{k'} A_{kk'}^{\alpha\beta} q_k q_{k'},$$

where $I_{\alpha\alpha}^e$ are the equilibrium moments of inertia. Because the moments of inertia are functions of the normal coordinates, they will have different values for each vibrational state.

The Perturbation Expansion

Unfortunately, Schrodinger's equation cannot be solved exactly for the Darling-Dennison Hamiltonian, so a general perturbation approach must be used. The Darling-Dennison Hamiltonian may be expanded in a standard perturbation expression:

$$H = H_0 + \lambda H_1 + \lambda^2 H_2 + \dots, \quad (\text{I-6})$$

where the zeroth order term, H_0 , corresponds to the Hamiltonian for a "rigid" harmonic oscillator:

$$H_0 = \frac{1}{2} \sum_{\alpha} \frac{p_{\alpha}^2}{I_{\alpha}} + \frac{1}{2} \sum_k \hbar \lambda_k^{1/2} [(p_k/\hbar)^2 + q_k^2], \quad (\text{I-7})$$

where I_{α} are the equilibrium moments of inertia ($I_{\alpha\alpha}^e$ above) and $\lambda_k^{1/2}$ are the frequencies of the normal modes of vibration. This approach was taken by Wilson and Howard (3), who showed that the Hamiltonian can be made diagonal with respect to the vibrational quantum numbers to any

order λ by a sufficient number of "contact transformations." The result is a Hamiltonian of the form

$$H = h_v + \frac{1}{2} \sum_{\alpha} \sum_{\beta} \sigma_{\alpha\beta} P_{\alpha} P_{\beta} + \frac{1}{4} \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \sum_{\delta} T_{\alpha\beta\gamma\delta} P_{\alpha} P_{\beta} P_{\gamma} P_{\delta} + \dots, \quad (I-8)$$

where h_v is a collection of purely vibrational terms whose expectation values for a given vibrational state are constant, in the absence of any perturbing resonances. Only even powers of angular momentum operators appear in this expansion. Watson (4) has shown that this is a consequence of the requirement that the Hamiltonian be Hermitian and invariant under time reversal. The vibrational contact transformation introduces a dependence on the vibrational state into the coefficients of the angular momentum terms in Eq. (I-8), so these coefficients are now referred to as "effective" constants, i.e. they are constants only for a given vibrational state. The P_{α} terms of quartic and higher order are called the "centrifugal distortion" terms of the Hamiltonian. These terms are the result of changes in the average geometry of the molecule as its angular momentum increases and as the molecule vibrates.

The Vibrational Contact Transformation

Two successive contact transformations of the form e^{iS} are necessary to diagonalize the vibrational matrix elements of the Darling-Dennison Hamiltonian through order λ^4 , which includes angular momentum terms through sixth power in Eq. (I-8). These transformations have been carried out in excruciating detail in a series of papers by Goldsmith, Amat and Nielsen (5,6) and Amat and Nielsen (7,8,9). Using this as a groundwork, Chung and Parker (10,11,12) carried out an extensive theoretical derivation of the rotational and centrifugal

distortion constants in an effort to express them as functions of more fundamental parameters, such as the equilibrium moments of inertia and the equilibrium bond angle. They also made effective use of symmetry considerations to reduce the number of centrifugal distortion terms in Eq. (I-8).

Reduction of the Rotational Hamiltonian

There are six terms quadratic in P_α in Eq. (I-8), but by using the principal axes of inertia, only three constants need be determined. Since each index in Eq. (I-8) has three possible labels, and owing to the noncommutative nature of the angular momentum operators, in general there are 81 quartic terms and 729 sextic terms. Chung and Parker (11) showed that for orthorhombic molecules, a class which includes the symmetry group C_{2v} to which both H_2S and H_2Se belong, there are 15 independent quartic terms and 105 independent sextic terms.

Kneizys, Freedman and Clough (13) used the commutation relations of Eq. (I-2) to manipulate the rotational Hamiltonian to the following Cartesian form:

$$H = H^{(2)} + H^{(4)} + H^{(6)} + \dots \quad (I-9)$$

where

$$\begin{aligned} H^{(2)} &= X P_x^2 + Y P_y^2 + Z P_z^2, \\ H^{(4)} &= T_{xx} P_x^4 + T_{yy} P_y^4 + T_{zz} P_z^4 + T_{xy} (P_x^2 P_y^2 + P_y^2 P_x^2) \\ &\quad + T_{xz} (P_x^2 P_z^2 + P_z^2 P_x^2) + T_{yz} (P_y^2 P_z^2 + P_z^2 P_y^2), \\ H^{(6)} &= \phi_{xxx} P_x^6 + \phi_{yyy} P_y^6 + \phi_{zzz} P_z^6 \\ &\quad + \phi_{xxy} (P_x^4 P_y^2 + P_y^2 P_x^4) + \phi_{yyx} (P_y^4 P_x^2 + P_x^2 P_y^4) \end{aligned}$$

$$\begin{aligned}
& + \phi_{xxz} (p_x^4 p_z^2 + p_z^2 p_x^4) + \phi_{zzx} (p_z^4 p_x^2 + p_x^2 p_z^4) \\
& + \phi_{yyz} (p_y^4 p_z^2 + p_z^2 p_y^4) + \phi_{zzy} (p_z^4 p_y^2 + p_y^2 p_z^4) \\
& + \phi_{xyz} (p_x^2 p_y^2 p_z^2 + p_z^2 p_y^2 p_x^2)
\end{aligned}$$

The notation used above for the coefficients of the Cartesian Hamiltonian differs slightly from that used by Kneizys et al. in that in this version the Cartesian nature of the coefficients is explicitly shown. Thus there are 3 quadratic terms, 6 quartic terms and 10 sextic terms. Similarly, Rao (14) has shown that there are 15 octic terms in the Cartesian Hamiltonian. The use of the commutation relations to manipulate the angular momentum operators results in higher order centrifugal distortion constants contributing to lower order terms in the rotational Hamiltonian. Kneizys et al. also expressed this Hamiltonian in terms of the spherical operators p_x^2 , p_z^2 and $(p_x^2 - p_y^2)$ instead of p_x^2 , p_y^2 and p_z^2 to take advantage of the diagonal nature of p_x^2 and p_z^2 in the symmetric top basis.

The Rotational Contact Transformation

Even with this tremendous decrease in the number of centrifugal distortion terms, it is not possible to determine experimentally all the centrifugal distortion constants for any given order by fitting observed spectra. Watson (4) has suggested that this is because the eigenvalues of the rotational Hamiltonian depend on certain linear combinations of the Hamiltonian constants and that only these linear combinations may be experimentally determined. He proposed that the rotational Hamiltonian be subjected to a set of successive unitary transformations of the form $\exp(iS_n)$, where S_n is a Hermitian matrix given by

$$S_n = \sum_{p,q,r} \sum_{p,q,r} s_{pqr} (p_x^p p_y^q p_z^r + p_z^r p_y^q p_x^p), \quad (I-13)$$

where n , p , q and r are integers, and $n = p + q + r$. By applying appropriate symmetry restrictions, Watson found that only odd values of n , p , q and r are possible. The transformed Hamiltonian, denoted by $\tilde{H}$, is related to the untransformed Hamiltonian, H , by

$$\tilde{H} = \dots e^{-iS_5} e^{-iS_3} e^{-iS_1} H e^{iS_1} e^{iS_3} e^{iS_5} \dots \quad (I-14)$$

The coefficients s_{pqr} may be chosen to eliminate specific terms in the transformed or "reduced" Hamiltonian. The matrix S_1 transforms the body-fixed rotational axes to the principal axes of inertia. Furthermore, there is only one non-zero coefficient for S_3 (s_{111}), three for S_5 (s_{113} , s_{131} and s_{311}) and six for S_7 (s_{115} , s_{151} , s_{511} , s_{133} , s_{331} and s_{313}). Carrying out the transformation to lowest order will allow the elimination of one quartic term in the transformed Hamiltonian by a judicious choice of the s_{111} parameter. Similarly, by transforming the Hamiltonian to successively higher orders, the three S_5 parameters allow the elimination of three of the sextic terms and the six S_7 parameters reduce the octic terms from 15 to 9. Unfortunately, the reduction is not unique because the transformation parameters are arbitrary.

Choice of Reductions

Several different reductions of the rotational Hamiltonian have been used to fit experimental data. Using a spherical form of the rotational Hamiltonian similar to the one constructed by Kneizys et al., Watson chose a reduction that contained terms that had only diagonal and second off-diagonal matrix elements in the symmetric top basis set.

This reduction is called the Watson "A-reduced" Hamiltonian. A particular formulation of this Hamiltonian by Yallabandi and Parker (15) is given by

$$H^{(A)} = H^{(2)} + H^{(4)} + H^{(6)} + H^{(8)} + \dots, \quad (I-15)$$

where

$$H^{(2)} = X^2 P_x^2 + Y^2 P_y^2 + Z^2 P_z^2,$$

$$H^{(4)} = -\Delta_J P^4 - \Delta_{JK} P^2 P_z^2 - \Delta_K P_z^4 - 2\delta_J P^2 P_{xy}^2 \\ - \delta_K [P_z^2 P_{xy}^2 + P_{xy}^2 P_z^2],$$

$$H^{(6)} = H_J P^6 + H_{JK} P^4 P_z^2 + H_{KJ} P^2 P_z^4 + H_K P_z^6 + 2h_J P^4 P_{xy}^2 \\ + h_{JK} P^2 [P_z^2 P_{xy}^2 + P_{xy}^2 P_z^2] + h_K [P_z^4 P_{xy}^2 + P_{xy}^2 P_z^4],$$

$$H^{(8)} = L_J P^8 + L_{JK} P^6 P_z^2 + L_{JK} P^4 P_z^4 + L_{KKJ} P^2 P_z^6 + L_K P_z^8 \\ + 2\ell_J P^6 P_{xy}^2 + \ell_{JK} P^4 [P_z^2 P_{xy}^2 + P_{xy}^2 P_z^2] \\ + \ell_{KJ} P^2 [P_z^4 P_{xy}^2 + P_{xy}^2 P_z^4] + \ell_K [P_z^6 P_{xy}^2 + P_{xy}^2 P_z^6],$$

and

$$P_{xy}^2 = (P_x^2 - P_y^2).$$

The designation "A-reduced" refers to the fact that it was specifically designed for asymmetric top molecules far from either the oblate or prolate symmetry limits.

Watson proposed another reduction that would be useful for molecules near the oblate or prolate symmetry limits, the "S-reduced" Hamiltonian. Typke (16) introduced a related form of this reduction in response to the problems experienced by Carpenter (17) when he attempted to use the A-reduced Hamiltonian to calculate energy levels for several oblate molecules. This Hamiltonian has the form

$$H = H^{(2)} + H^{(4)} + H^{(6)} + H^{(8)} + \dots \quad (I-16)$$

where

$$\begin{aligned} H^{(2)} &= B_x^- P_x^2 + B_y^- P_y^2 + B_z^- P_z^2, \\ H^{(4)} &= -D_J^- P^4 - D_{JK}^- P^2 P_z^2 - D_K^- P_z^4 - 2\delta_J^- P^2(P_x^2 - P_y^2) - 2R_6^- O, \\ H^{(6)} &= H_J^- P^6 + H_{JK}^- P^4 P_z^2 + H_{KJ}^- P^2 P_z^4 + H_K^- P_z^6 + H_5^- P^4(P_x^2 - P_y^2) \\ &\quad + \frac{1}{2}H_6^- P^2 O + H_{10}^- (P_x^2 - P_y^2)^3, \end{aligned}$$

and

$$O = P_x^4 + P_y^4 - 3(P_x^2 P_y^2 + P_y^2 P_x^2). \quad (I-17)$$

Typke did not carry out the transformation to order S_7 , so the actual form of the octic terms for this reduction is not known. If we assume that they would be appropriate octic combinations of the operators present in the lower order terms and if we use Watson's S-reduced Hamiltonian as a guide, a possible expression for the Typke Hamiltonian octic terms is

$$\begin{aligned} H^{(8)} &= L_J^- P^8 + L_{JK}^- P^6 P_z^2 + L_{JK}^- P^4 P_z^4 + L_{KKJ}^- P^2 P_z^6 + L_K^- P_z^8 \quad (I-18) \\ &\quad + \ell_6 P^6(P_x^2 - P_y^2) + \ell_7 P^4 O + \ell_8 P^2(P_x^2 - P_y^2)^3 + \ell_9 O^2. \end{aligned}$$

Watson's A-reduced Hamiltonian has generally been the most widely used reduction, although, as previously stated, for certain cases it does not work well in fitting observed spectra.

Choice of Rotational Representations

There are six possible ways of associating the body-fixed rotational axes a, b, and c of the molecule with a set of Cartesian axes. These associations are called the "rotational representations"

(see Table 1).

Table 1. Rotational Representations

Body-Fixed Axes		Cartesian Axes				
a	z	x	y	z	x	y
b	x	z	z	y	y	x
c	y	y	x	x	z	z
Representation	I ^r	I ^l	II ^r	II ^l	III ^r	III ^l

Historically, "oblate" asymmetric tops such as H₂S and H₂Se have been analyzed with a rotational Hamiltonian in the III^r representation and "prolate" asymmetric tops have been analyzed with a Hamiltonian in the I^r rotational representation. These choices have a certain theoretical justification and tend to reduce the size of the off-diagonal matrix elements of the rotational Hamiltonian, an important consideration for the numerical diagonalization of the Hamiltonian before the availability of large, high-speed, digital computers. These choices for rotational representation cause no difficulty with Typke's Hamiltonian. However, it was soon observed that the spectra of asymmetric top molecules even moderately close to the oblate symmetric-top limit were hard to fit using Watson's A-reduced Hamiltonian in the III^r rotational representation. Van Eijck (18) explained this as a result of the large size of the s₁₁₁ parameter in the A-reduction for the III^r representation. For this reduction, the s₁₁₁ parameter is

$$s_{111} = \frac{1}{4} \frac{(T_{xx} + T_{yy} - 2T_{xy})}{(X - Y)} . \quad (\text{I-19})$$

In the III^r representation, X = A, Y = B and Z = C, where A, B and C are

the coefficients of the quadratic terms in the rotational Hamiltonian, and are inversely proportional to the moments of inertia about the rotational axes a, b and c. As a molecule approaches the oblate symmetry limit, A and B become closer in value and the magnitude of s_{111} increases dramatically. This parameter is one factor which determines how much of the lower order terms of the rotational Hamiltonian is transformed into the higher order terms by the rotational contact transformation. For example, the quartic constants of the transformed Cartesian Hamiltonian, denoted by tildes, are related to the constants of the untransformed Hamiltonian, by the following set of equations derived by Watson (19):

$$\begin{aligned}\tilde{T}_{xx} &= T_{xx}, \quad \tilde{T}_{yy} = T_{yy}, \quad \tilde{T}_{zz} = T_{zz}, \\ \tilde{T}_{xy} &= T_{xy} + 2(Y - X)s_{111}, \\ \tilde{T}_{xz} &= T_{xz} + 2(X - Z)s_{111}, \\ \tilde{T}_{yz} &= T_{yz} + 2(Z - Y)s_{111}.\end{aligned}\tag{I-20}$$

Thus for the last two transformed quartic terms to have the same order of magnitude effect as the untransformed quartic terms for the same angular momentum state, s_{111} should be approximately the ratio of a typical quartic constant to a typical quadratic constant. A similar argument is applicable to the sextic and octic coefficients. In general, the s-parameters should obey the order of magnitude relation derived by Watson (4), given by

$$s_{pqr} \sim \kappa^{2(p+q+r-1)},\tag{I-21}$$

where κ is a small parameter on the order of the ratio of the nuclear displacements from equilibrium in a molecule for a low vibrational state

to the equilibrium bond length. Strow (20) has calculated the value of the s_{111} parameter for two reductions and two representations in his analysis of the ground vibrational state and the ν_2 upper state of H_2S . He discovered that the value of s_{111} for the A-reduction in the III^r representation is 12 times larger in the ground state and 25 times larger in the (010) upper state than for the A-reduction in the I^r representation, or the S-reduction in either representation. Since H_2Se is closer to the oblate symmetric-top limit than H_2S , the effect should be even more pronounced for H_2Se . Thus if the A-reduced Hamiltonian is used to calculate rotational energies for an oblate molecule such as H_2S or H_2Se , the rotational representations III^r or III^l should not be used. Since our fitting programs are designed to use only I^r and III^r representations, we now use the I^r rotational representation with the A-reduced Hamiltonian.

Watson's Determinable Coefficients

Watson (18) pointed out that because the s-parameters in the rotational contact transformation are arbitrarily chosen, the eigenvalues of the Hamiltonian cannot depend on them. Thus he constructed a set of linear combinations of the reduced Hamiltonian coefficients that does not contain any of the s-parameters. Such a set of "determinable coefficients" should be independent of the reduction and of the rotational representation used. Using the Cartesian Hamiltonian, the transformed rotational constants are related to the untransformed rotational constants by

$$\tilde{X} = X + 4(Z - Y)s_{111} , \quad (\text{I-22})$$



$$\tilde{Y} = Y + 4(X - Z)s_{111} ,$$

$$\tilde{Z} = Z + 4(Y - X)s_{111} ,$$

where contributions of the order of quartic centrifugal distortion constants have been included in the transformed rotational constants. Thus using Eq. (I-20), determinable rotational coefficients A, B and C may be defined as

$$A = \tilde{X} - 2\tilde{T}_{yz} = X - 2T_{yz} \quad (I-23)$$

$$B = \tilde{Y} - 2\tilde{T}_{xz} = Y - 2T_{xz}$$

$$C = \tilde{Z} - 2\tilde{T}_{xy} = Z - 2T_{xy}$$

where the III^T rotational representation has been assumed. Watson noted that T_{xx} , T_{yy} , T_{zz} , ϕ_{xxx} , ϕ_{yyy} , ϕ_{zzz} , and all higher order centrifugal distortion constants that are "diagonal" in the Cartesian subscripts are independent of the contact transformation if certain small contributions to the transformed constants are ignored, and are thus determinable.

Additionally, he chose as the remaining quartic terms

$$T_1 = T_{xy} + T_{xz} + T_{yz} , \quad (I-24)$$

$$T_2 = ZT_{xy} + YT_{xz} + XT_{yz} ,$$

and as the remaining sextic terms

$$\phi_1 = 3 \sum_{\alpha} \sum_{\beta} \phi_{\alpha\alpha\beta} + \phi_{xyz} , \quad (I-25)$$

$$\phi_2 = (X - Z)\phi_{xxy} + (X - Y)\phi_{xxz} - 2(T_{xx} - T_{xy})(T_{xx} - T_{xz}) ,$$

$$\phi_3 = (Y - X)\phi_{yyz} + (Y - Z)\phi_{yyx} - 2(T_{yy} - T_{yz})(T_{yy} - T_{yx}) ,$$

$$\phi_4 = (Z - Y)\phi_{zzx} + (Z - X)\phi_{zzy} - 2(T_{zz} - T_{zx})(T_{zz} - T_{zy}) .$$

Rao (14) has constructed a set of octic determinable coefficients but we

have not yet incorporated them into our fitting programs.

To calculate the determinable coefficients, a subroutine in our fitting programs first determines the Cartesian coefficients from the constants of the reduced Hamiltonian used to fit the observed spectra, using the relations tabulated by Murphy (21) (see Appendix F). If the "wrong" rotational representation was used (e.g. I^r for an "oblate" molecule), the Cartesian coefficients are suitably relabeled to account for the permutation of the rotational axes. The determinable coefficients are then calculated with the aid of Eqs. (I-23), (I-24) and (I-25). Trial calculations using the ground state and (010) upper state of H_2S and H_2Se (with the rotational Hamiltonians truncated to sextic terms because Typke's Hamiltonian did not contain octic terms), have shown that our quadratic and quartic determinable coefficients were essentially invariant to reduction and representation, but the sextic coefficients were not. This may be because without octic terms present in the Hamiltonian, the sextic terms are trying to fit transitions between higher angular momentum states than they are intended to fit, and are thus poorly determined. Another possible explanation is that the small contributions to the transformed centrifugal distortion constants that Watson ignored in his formulation of the determinable coefficients are not negligible.



CHAPTER II

ANALYSIS OF ν_2 OF H_2S

Introduction

When we first began to analyze the ν_2 fundamental band of H_2S , we were confronted with two major difficulties:

- (1) We found that fits of our spectral data did not converge to a stable set of Hamiltonian constants using Watson's A-reduced Hamiltonian in the III^r rotational representation. At that time, we had tried Watson's A-reduced Hamiltonian only in the III^r representation. Thus we initially chose to use Typke's Hamiltonian, for which only terms through order P^6 are available. This restriction limited our ability to accurately fit and predict transitions with high values of J and K_a .
- (2) Because we did not have enough ground state transitions (infrared and microwave) for the molecular species H_2^{33}S and H_2^{34}S , we could not determine separate ground state rotational constants and centrifugal distortion constants for these isotopic species, or "isotopomers." Therefore, at that stage we initially limited our analysis of the H_2^{33}S and H_2^{34}S ground states to a simultaneous fit of infrared ground state combination differences (GSCD's) and microwave transitions for all three isotopomers, using linear isotopic mass adjustment constants for A, B, and C. Similarly our initial analysis of the (010) upper states of H_2^{33}S and H_2^{34}S consisted of a simultaneous fit of ν_2 lines for all three isotopomers using isotopic mass adjustment constants for ν_0 , A, B,

and C.

We published our analysis of the ν_2 band of H_2S with the limitations listed above (22). Appendix A contains a reprint of this paper, which is an essential part of our analysis of ν_2 of H_2S . Interested parties should read this paper as carefully as the remaining material in this chapter.

Recently Flaud, Camy-Peyret, and Johns more precisely determined the ground state constants of each of the three isotopomers from their analysis of the far-infrared and microwave pure rotational spectra of H_2S (23). Using their ground state constants through P^8 terms, we have reanalyzed our ν_2 data and obtained the first individual (010) upper state constants (also through P^8 terms) for H_2^{33}S and H_2^{34}S . Since our 1982 publication, we have followed the examples of Carpenter (17) and Strow (19) and have used the I^r rotational representation of Watson's A-Reduced Hamiltonian, as did Flaud et al. This modification of our analysis allowed us to use P^8 terms in the calculation of rotational energy levels, which particularly improved the fit of the high J, high K_a lines in our data set.

Results

For comparison with the results of Flaud et al., we determined a set of Watson A-reduced ground state constants for H_2^{32}S by fitting our H_2^{32}S GSCD's combined with the microwave transitions of Helminger, Cook and De Lucia (24). Both sets of constants are listed in Table 2, and the standard deviations of our fit of the infrared and microwave data are shown in Table 3.

Table 2. Comparison of H_2^{32}S Ground State Constants

	GSCD Fit		Flaud et al. ^b	
	Constant (cm^{-1})	(95 % SCI ^a)	Constant (cm^{-1})	(Error ^c)
A	10.36016 ₅₅	0.000021	10.3601594 ₀	0.0000021
B	9.01814 ₁₉	0.000021	9.0181358 ₂	0.0000020
C	4.73078 ₉₁	0.000010	4.7307832 ₁	0.0000010
$\Delta_J (\times 10^3)$	0.6529 ₇₂	0.00086	0.652598 ₅	0.000040
Δ_{JK} "	-2.280 ₄₆	0.0020	-2.28026 ₈	0.00010
Δ_K "	3.703 ₅₈	0.0028	3.70326 ₆	0.00011
δ_J "	0.2956 ₁₈	0.00035	0.295517 ₁	0.000019
δ_K "	-0.132 ₇₄	0.0011	-0.132618 ₈	0.000053
$H_J (\times 10^6)$	0.27 ₉₁	0.019	0.27098 ₃	0.00043
H_{JK} "	-1.55 ₆₈	0.059	-1.5329 ₃	0.0015
H_{KJ} "	1.31 ₄₉	0.098	1.2592 ₁	0.0044
H_K "	1.3 ₅₁	0.12	1.3811 ₆	0.0040
h_J "	0.138 ₅₃	0.0086	0.13541 ₃	0.00021
h_{JK} "	-0.48 ₁₉	0.033	-0.48509 ₅	0.00092
h_K "	1.20 ₂₆	0.060	1.2290 ₀	0.0029
$L_J (\times 10^9)$	-0.1 ₈₃	0.14	-0.1395 ₁	0.0014
L_{JK} "	1.3 ₈₈	0.40	1.1843 ₈	0.0059
L_{JK} "	-2.79	2.8	-3.319 ₆	0.038
L_{KKJ} "	2.60	1.4	5.480 ₁	0.088
L_K "	-2.20	1.5	-4.478 ₁	0.064
l_J "	-0.09 ₁₉	0.067	-0.07044 ₀	0.00072
l_{JK} "	0.5 ₆₄	0.29	0.4051 ₃	0.0038
l_{KJ} "	-1.1 ₇₈	0.95	-0.302 ₄	0.020
l_K "	(Constrained to 0)		-1.757 ₉	0.041

^a95% simultaneous confidence intervals, here about 6 times the standard error of each constant.

^bOnly terms through order P^8 are listed for comparison.

^cQuoted errors are "one standard deviation."

Table 3. Ground State Fit of H_2^{32}S

Ground State Data	Standard Deviation	Number of Data	Average Weight
Infrared GSCD's	0.0019 cm^{-1}	414	3.194
Microwave Data	0.10 MHz	39	100 000

The agreement between our constants and the constants of Flaud et al. is very good for A, B, and C and for the quartic centrifugal distortion constants, but is only fair for the sextic and octic centrifugal distortion constants. This is probably because our ground state data had a maximum J value of 15 and a maximum K_a value of 8, and we used only up through octic terms in the Hamiltonian, whereas Flaud et al. analyzed pure rotational lines with J as high as 22 and K_a as high as 15, and in addition they included several 10^{th} power terms in the Hamiltonian. The limited range of J and K_a values and the precision of our data does not warrant the inclusion of P^{10} terms. This assumption is supported by the fact that their ground state constants through P^8 terms predict our observed GSCD's with a standard deviation of 0.0019 cm^{-1} , which is the limit of the precision of our data. For consistency among the three isotopomers and also for greater accuracy, we have used their ground state constants (through P^8 terms) for our new fit of the (010) upper state of H_2^{32}S , as well as for the other two isotopomers.

Keeping the ground state constants fixed to the values determined by Flaud et al., we determined a set of (010) upper state constants for each isotopomer by individually fitting the three sets of ν_2 lines.



With the improved ground state and (010) state energies available from the new sets of constants, we discarded two of our previous line assignments for H_2^{33}S and seven for H_2^{34}S . We were also able to assign one additional H_2^{34}S line. Our set of ν_2 line assignments for H_2^{33}S and H_2^{34}S has a smaller range of J and K_a values than the H_2^{32}S ν_2 lines, owing to the low intensities of the lines of H_2^{33}S and H_2^{34}S (relative abundances 4.2 % and 0.7 % respectively), hence we could not determine as many centrifugal distortion constants for ν_2 of H_2^{33}S and H_2^{34}S as we determined for ν_2 of H_2^{32}S . Following a procedure similar to the one used by Flaud et al., we fixed the upper state H_{KJ} and the octic constants for H_2^{33}S and H_2^{34}S to the corresponding values for H_2^{32}S . Furthermore, for the analysis of ν_2 of H_2^{33}S we fixed the upper state δ_K and all sextic constants except H_{KJ} to the weighted average of the corresponding constants for H_2^{32}S and H_2^{34}S . The standard deviations of our (010) upper state fits, reported in Table 4, are from 60 % to 34 % smaller than the standard deviation of the fits of each isotopomer in our previous simultaneous analysis.

Table 4. Individual Upper State Fits of ν_2 of H_2S Isotopomers

Isotopomer	Standard Deviation (cm^{-1})	Number of Lines	Average Weight	Number of Parameters
32	0.0010	386	2.802	25
33	0.0012	15	0.923	8
34	0.0016	69	1.241	15



Table 5. Upper State Constants for ν_2 of H_2S Isotopomers

Constant (cm^{-1})	H_2^{32}S	H_2^{33}S	H_2^{34}S
ν_0	$1182.574_{20} \pm 0.0015$	$1182.01_{61} \pm 0.018$	$1181.498_{20} \pm 0.0068$
A	$10.7220_{06} \pm 0.00024$	$10.703_{71} \pm 0.0014$	$10.6856_{31} \pm 0.00096$
B	$9.2244_{32} \pm 0.00027$	$9.222_{62} \pm 0.0035$	$9.223_{88} \pm 0.0013$
C	$4.6688_{56} \pm 0.00013$	$4.665_{64} \pm 0.0016$	$4.6616_{36} \pm 0.00062$
$\Delta_J (\times 10^3)$	$0.756_{44} \pm 0.0050$	$0.74_{68} \pm 0.034$	$0.764_{54} \pm 0.0018$
Δ_{JK} "	$-2.74_{01} \pm 0.018$	$-2.7_{30} \pm 0.10$	$-2.73_{17} \pm 0.0097$
Δ_K "	$4.55_{80} \pm 0.014$	$4.5_{74} \pm 0.11$	$4.57_{88} \pm 0.0099$
δ_J "	$0.347_{54} \pm 0.0028$	$0.33_{76} \pm 0.020$	$0.34_{97} \pm 0.017$
δ_K "	$-0.018_{70} \pm 0.0054$	-0.01_{94}	$-0.03_{32} \pm 0.024$
$H_J (\times 10^6)$	$0.38_{77} \pm 0.066$	0.41_{15}	$0.41_{24} \pm 0.013$
H_{JK} "	$-1.9_{36} \pm 0.23$	-1.9_4	$-2.0_1 \pm 1.1$
H_{KJ} "	$0.9_{93} \pm 0.11$		
H_K "	$2.6_{12} \pm 0.20$	2.6_{23}	$2.8_{22} \pm 0.84$
h_J "	$0.19_{34} \pm 0.034$	0.1_{94}	$0.1_{99} \pm 0.17$
h_{JK} "	$-0.61_{60} \pm 0.064$	-0.6_{20}	$-0.6_{58} \pm 0.20$
h_K "	$2.1_{29} \pm 0.12$	2.1_{24}	$2.0_{65} \pm 0.41$
$L_J (\times 10^9)$	$-0.2_{91} \pm 0.27$		
L_{JJK} "	$1.9_{27} \pm 0.93$		
L_{JK} "	$-5.9_{79} \pm 3.0$		
L_{KKJ} "	$11.5_6 \pm 3.3$		
L_K "	$-9.0_{38} \pm 0.88$		
ℓ_J "	$-0.1_{46} \pm 0.14$		
ℓ_{JK} "	$0.5_{23} \pm 0.26$		
ℓ_{KJ} "	$-0.8_{52} \pm 0.73$		
ℓ_K "	$-3.5_{26} \pm 0.94$		



Our (010) upper state constants for the three isotopomers are listed in Table 5. A blank entry means that we fixed the constant to the corresponding value for H_2^{32}S . Those H_2^{33}S constants without a listed uncertainty were fixed to the weighted average of the corresponding constants for H_2^{32}S and H_2^{34}S . Quoted errors are 95% simultaneous confidence intervals, approximately 6 standard errors of each constant for H_2^{32}S and approximately 5 standard errors of each constant for H_2^{33}S and H_2^{34}S . Our (010) constants are in good agreement with those of Strow (19) for H_2^{32}S . However, we determined values for the upper state octic constants, and the standard errors of our lower order terms are somewhat smaller than his.

We have calculated Watson's determinable coefficients (4) for H_2^{32}S , from the ground state constants of Flaud et al. and from our (010) upper state constants. These determinable coefficients are listed in Table 6. A complete set of our final line assignments for all ν_2 lines of H_2S are contained in Appendix B, and Appendix C contains our weighted averaged GSCD's for H_2^{32}S , combined from the infrared bands (010), (020), (100), (001), (110), (011), (210), and (111).



Table 6. Determinable Coefficients of H_2^{32}S

Constant [‡]	Ground State [*]	(010) Upper State
X	10.36146 ₄₆	10.7235 ₁₉
Y	9.01683 ₁₆	9.2225 ₄₈
Z	4.73013 ₃₉	4.6682 ₈₆
$T_{xx} (\times 10^3)$	-2.075 ₆₀	-2.57 ₄₄
T_{yy} "	-1.243 ₆₃	-1.45 ₁₆
T_{zz} "	-0.0615 ₆₄	-0.061 ₄₆
T_1 "	0.322 ₄₇	0.470 ₄₈
T_2 "	0.640 ₄₆	1.91 ₀₁
$\phi_{xxx} (\times 10^6)$	1.3 ₇₈	2.0 ₅₇
ϕ_{yyy} "	0.54 ₁₈	0.77 ₄₄
ϕ_{zzz} "	0.0001 ₅₇	0.0009 ₄₃
ϕ_1 "	-3.4 ₂₂	-4.7 ₅₅
ϕ_2 "	-12.78	-18.82
ϕ_3 "	-5.0 ₄₃	-6.3 ₈₁
ϕ_4 "	-0.05 ₉₆	-0.23 ₇₀

[‡]All constants have units of cm^{-1} , except for T_2 , ϕ_2 , ϕ_3 , and ϕ_4 , which have units of cm^{-2} .

^{*}These determinable coefficients are calculated from the ground state constants of Flaud et al.

The number of significant digits reported for these constants is an estimate on our part.



CHAPTER III

ANALYSIS OF ν_2 OF H_2Se

Introduction

The ν_2 fundamental band of H_2Se was first studied at low resolution by Cameron, Sears, and Nielsen (25) in 1939, and at moderate resolution by Palik (26) in 1959. Helminger and De Lucia (27) investigated the microwave spectrum of H_2Se and assigned 109 ground state transitions for the five most abundant H_2Se isotopomers. Using these transitions and the available infrared ground state combination differences formed by Hill and Edwards (28), who made a preliminary analysis of the $2\nu_2$, ν_1 and ν_3 bands of H_2Se , Helminger and De Lucia calculated ground state constants for the five most abundant isotopomers.

In 1981, Gillis and Edwards (29) finished the analysis of these three bands at a resolution limit of 0.04 cm^{-1} with a standard deviation of 0.0084 cm^{-1} for the simultaneous fit of the Coriolis interacting bands ν_1 and ν_3 , and 0.0038 cm^{-1} for the fit of $2\nu_2$. In this work the ν_2 band has been run at a resolution limit of 0.025 cm^{-1} , and we have assigned about 1600 spectral lines, including some for H_2^{74}Se . As a result we have revised the existing ground state constants and obtained (010) upper state constants through octic terms in angular momentum operators.

Experimental Details

Our sample of H_2Se was purchased from the Matheson Company, Inc. The sample was used without further purification, and no impurities were observed in the spectrum.

Several runs of the spectrum of ν_2 of H_2Se were recorded using the University of Denver 50 cm FTIR spectrometer system, as described in our paper on ν_2 of H_2S (see Appendix A). The experimental conditions for each run are summarized in Table 7. All spectra were recorded at room temperature ($\sim 22^\circ\text{C}$). Several scans for each run were recorded and co-added to improve the signal-to-noise ratio. Calibration was performed using the $(10^00 - 00^00)$ $^{14}\text{N}_2^{16}\text{O}$ line positions reported by Olson, Maki, and Lafferty (30). Although the instrument resolution is nominally 0.020 cm^{-1} , the actual observed full widths at half height of weak to moderate intensity well-resolved lines are pressure-broadened to values ranging from 0.025 cm^{-1} to 0.060 cm^{-1} , depending on the sample pressure. Unfortunately, only short sample cells were available, making relatively high sample pressure necessary for adequate absorption.

Table 7. Experimental Conditions for ν_2 of H_2Se

Run number	1	2	3	4
Region (cm^{-1})	905 - 1320	885 - 1300	890 - 1310	1147 - 1347
Sample pressure (torr)	29.5	105	175	51
Path length (cm)	22	22	22	45
Linewidth (cm^{-1})	0.045	0.045	0.060	0.025
Number of scans co-added	6	7	8	6
Calibration method	N_2O^a	b	b	b

^aThe spectrum of 29 torr of N_2O in a 5 cm cell was recorded simultaneously with the H_2Se spectrum. See ref. (30) for the N_2O line positions.

^bCalibrated against well-resolved H_2Se lines from run 1.



Analysis of Individual Isotopomers

The basic procedure that we used to analyze the ν_2 band of H_2S (22) was also used to analyze ν_2 of H_2Se (see Appendix A). However, the natural abundances of the selenium isotopes, as listed at the bottom of Table 8, are such that the isotopomers of H_2Se produce five overlapping spectra of "comparable intensity," resulting in many blended lines. Our approach to this problem was first to assign as many lines as possible for the most abundant isotopomer, H_2^{80}Se . Using the intensity signature characteristic of H_2Se isotopic multiplets, we easily assigned many lines of the other isotopomers. After assigning and fitting a sufficient number of lines for each of five isotopomers, we predicted a spectrum of the most intense type B transitions for each isotopomer, and the analysis of each spectrum proceeded iteratively as usual.

Table 8. Range of Rotational Quantum Numbers for H_2Se Data Sets

GSCD's	H_2^{74}Se	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
J_{max}	7	14	14	17	18	12
$K_{\text{a,max}}$	2	7	8	9	12	7
$K_{\text{c,max}}$	7	14	14	17	18	12
ν_2 lines	H_2^{74}Se	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
J_{max}	15	17	17	18	19	16
$K_{\text{a,max}}$	11	13	13	14	14	13
$K_{\text{c,max}}$	17	15	15	17	19	15
# lines $\Delta K_{\text{a}} = 3$	1	16	11	32	40	13
# lines $\Delta K_{\text{c}} = 3$	0	0	0	0	3	0
Natural Abundances (%)	1	9	8	24	50	9



Table 9. H_2^{76}Se Molecular ConstantsWatson's A-Reduced Hamiltonian, I^r Representation

	Ground State		(010) State	
	Constant (cm^{-1})	(95 % SCI [*])	Constant (cm^{-1})	(95 % SCI [*])
ν_0	-	-	1034.514 ₄₀	0.0046
A	8.18043 ₀₉	0.000031	8.4299 ₂₀	0.00072
B	7.72688 ₅₀	0.000033	7.9071 ₇₉	0.00068
C	3.90400 ₀₂	0.000018	3.8579 ₇₀	0.00028
Δ_J ($\times 10^3$)	0.527 ₂₄	0.0022	0.616 ₇₇	0.0077
Δ_{JK} "	-1.848 ₆₈	0.0055	-2.20 ₈₂	0.032
Δ_K "	2.640 ₉₁	0.0042	3.18 ₆₀	0.029
δ_J "	0.242 ₉₃	0.0012	0.286 ₈₄	0.0042
δ_K "	-0.182 ₉₆	0.0022	-0.128 ₆₀	0.0056
H_J ($\times 10^6$)	0.21 ₄₈	0.025	0.33 ₆₇	0.049
H_{JK} "	-1.3 ₇₆	0.12	-1.7 ₂₄	0.26
H_{KJ} "	1.6 ₂₂	0.13	1.5 ₃₇	0.63
H_K "	0.24 ₅₆	0.072	0.8 ₆₂	0.29
h_J "	0.11 ₁₇	0.012	0.16 ₇₇	0.025
h_{JK} "	-0.40 ₅₆	0.084	-0.51 ₃₁	0.067
h_K "	0.7 ₈₁	0.14	1.21 ₀₅	0.070
L_J ($\times 10^9$)	-0.11 ₄₀ [‡]		-0.27 ₁₈	0.084
L_{JJK} "	1.6 ₄	1.4	1.8 ₉₈	0.66
L_{JK} "	-4.40	1.5	-4.1 ₆	1.2
L_{KKJ} "	4.71	1.6	4.4 ₆₀ [‡]	
L_K "	-2.3 ₆₇	0.71	-2.6 ₅	1.4
l_J "	-0.05 ₉₈ [‡]		-0.1 ₃₂ [‡]	
l_{JK} "	0.4 ₆₈ [‡]		0.5 ₀₁ [‡]	
l_{KJ} "	-0.95	1.1	-0.7 ₅₉ [‡]	
l_K "	(Constrained to 0)		-0.8 ₅₂ [‡]	

* 95 % simultaneous confidence intervals, here about 6 times the standard error of each constant.

‡ These constants were fixed to the corresponding values for H_2^{80}Se .



Table 10. H_2^{77}Se Molecular ConstantsWatson's A-Reduced Hamiltonian, I^r Representation

	<u>Ground State</u>		<u>(010) State</u>	
	Constant (cm^{-1})	(95 % SCI [*])	Constant (cm^{-1})	(95 % SCI [*])
ν_0	-	-	1034.425 ₅₀	0.0071
A	8.17769 ₂₃	0.000021	8.4270 ₉₁	0.00082
B	7.72689 ₂₂	0.000024	7.9069 ₈₈	0.00088
C	3.90337 ₄₅	0.000019	3.8571 ₉₉	0.00039
Δ_J ($\times 10^3$)	0.528 ₃₆	0.0023	0.611 ₆₃	0.0093
Δ_{JK} "	-1.846 ₀₂	0.0056	-2.18 ₀₅	0.038
Δ_K "	2.637 ₇₈	0.0016	3.15 ₉₀	0.035
δ_J "	0.2430 ₈₁	0.00047	0.284 ₉₈	0.0059
δ_K "	-0.1834 ₀₁	0.00062	-0.12 ₁₇	0.014
H_J ($\times 10^6$)	0.22 ₅₁	0.025	0.28 ₉₂	0.056
H_{JK} "	-1.35 ₀₈	0.063	-1.4 ₂₁	0.34
H_{KJ} "	1.67 ₄₅	0.053	1.3 ₄₁	0.68
H_K "	0.14 ₈₅	0.077	0.7 ₃₂	0.40
h_J "	0.11 ₅₆	0.010	0.14 ₂₄	0.044
h_{JK} "	-0.49 ₈₉	0.050	-0.4 ₃₈	0.13
h_K "	0.9 ₃₅	0.12	1.2 ₄₉	0.25
L_J ($\times 10^9$)	-0.11 ₄₀ [‡]		-0.2 ₅₅ [‡]	
L_{JK} "	0.8 ₆₁	0.51	2.3 ₉₂	0.96
L_{JK} "	-3.1 ₆₃	0.32	-9.7 ₁	5.6
L_{KKJ} "	4.3 ₆₂	0.60	1 _{4.7}	11
L_K "	-2.4 ₇₃	0.67	-7.6 ₅	6.1
l_J "	-0.05 ₉₈ [‡]		-0.10 ₁₉	0.074
l_{JK} "	0.4 ₆₈ [‡]		0.5 ₀₁ [‡]	
l_{KJ} "	-1.3 ₂₈	0.87	-1.6 ₃	1.8
l_K "	(Constrained to 0)		-0.8 ₅₂ [‡]	

* 95 % simultaneous confidence intervals, here about 7 times the standard error of each constant.

‡ These constants were fixed to the corresponding values for H_2^{80}Se .

Table 11. H_2^{78}Se Molecular ConstantsWatson's A-Reduced Hamiltonian, I^R Representation

	Ground State		(010) State	
	Constant (cm^{-1})	(95 % SCI [*])	Constant (cm^{-1})	(95 % SCI [*])
ν_0	-	-	1034.335 ₉₀	0.0023
A	8.17500 ₈₇	0.000029	8.4242 ₈₅	0.00037
B	7.72687 ₈₈	0.000028	7.9069 ₅₂	0.00030
C	3.90276 ₅₅	0.000020	3.8566 ₇₈	0.00016
Δ_J ($\times 10^3$)	0.528 ₂₀	0.0020	0.614 ₃₉	0.0037
Δ_{JK} "	-1.849 ₄₃	0.0055	-2.20 ₈₉	0.016
Δ_K "	2.638 ₂₇	0.0044	3.18 ₅₅	0.016
δ_J "	0.2424 ₀₀	0.00080	0.285 ₇₆	0.0020
δ_K "	-0.182 ₇₁	0.0026	-0.129 ₆₉	0.0053
H_J ($\times 10^6$)	0.21 ₀₂	0.021	0.31 ₉₀	0.023
H_{JK} "	-1.20 ₂₈	0.051	-1.7 ₀₁	0.12
H_{KJ} "	1.1 ₆₈	0.22	1.4 ₁₃	0.23
H_K "	0.5 ₁₈	0.24	0.9 ₆₅	0.23
h_J "	0.103 ₉₉	0.0093	0.16 ₁₂	0.013
h_{JK} "	-0.38 ₈₀	0.055	-0.55 ₉₂	0.052
h_K "	0.7 ₆₂	0.12	1.2 ₆₃	0.10
L_J ($\times 10^9$)	-0.12 ₁₇	0.045	-0.2 ₅₅ [‡]	
L_{JJK} "	1.3 ₀₈	0.70	1.7 ₈₅ [‡]	
L_{JK} "	-4.3 ₃₇	1.4	-4.0 ₃₅	0.71
L_{KKJ} "	6.8 ₂	1.3	5.7 ₇	2.0
L_K "	-4.1 ₁₄	1.3	-3.9 ₉	1.6
ℓ_J "	-0.05 ₉₈ [‡]		-0.13 ₃₄	0.015
ℓ_{JK} "	0.4 ₆₈ [‡]		0.5 ₇₂	0.13
ℓ_{KJ} "	-1.0 ₇₄	0.68	-0.7 ₅₉ [‡]	
ℓ_K "	(Constrained to 0)		-1.1 ₁₉	0.68

* 95% simultaneous confidence intervals, here about 7 times the standard error of each constant.

‡ These constants were fixed to the corresponding values for H_2^{80}Se .

Table 12. H_2^{80}Se Molecular ConstantsWatson's A-Reduced Hamiltonian, I^r Representation

	<u>Ground State</u>		<u>(010) State</u>	
	Constant (cm^{-1})	(95 % SCI [*])	Constant (cm^{-1})	(95 % SCI [*])
ν_0	-	-	1034.165 ₂₀	0.0019
A	8.16985 ₅₅	0.000021	8.4190 ₁₉	0.00032
B	7.72686 ₇₂	0.000023	7.9068 ₈₇	0.00034
C	3.90157 ₉₁	0.000014	3.8554 ₇₂	0.00012
Δ_J ($\times 10^3$)	0.527 ₈₂	0.0013	0.614 ₁₇	0.0056
Δ_{JK} "	-1.849 ₈₁	0.0012	-2.20 ₇₀	0.022
Δ_K "	2.637 ₁₂	0.0028	3.18 ₁₄	0.017
δ_J "	0.2423 ₉₉	0.00062	0.285 ₉₂	0.0030
δ_K "	-0.1834 ₅₄	0.00078	-0.128 ₅₃	0.0049
H_J ($\times 10^6$)	0.21 ₁₄	0.018	0.31 ₈₈	0.061
H_{JK} "	-1.28 ₂₆	0.021	-1.7 ₀₀	0.26
H_{KJ} "	1.37 ₈₂	0.063	1.4 ₇₁	0.14
H_K "	0.38 ₄₈	0.027	0.8 ₉₄	0.11
h_J "	0.10 ₆₂	0.010	0.16 ₁₃	0.032
h_{JK} "	-0.40 ₇₄	0.040	-0.52 ₅₃	0.052
h_K "	0.76 ₃₄	0.057	1.22 ₉₅	0.064
L_J ($\times 10^9$)	-0.11 ₄₀	0.097	-0.2 ₅₅	0.20
L_{JK} "	1.2 ₄₉	0.67	1.7 ₈₅	0.77
L_{JK} "	-2.5 ₄	1.7	-3.7 ₆	2.6
L_{KKJ} "	1.7 ₁	1.2	4.4 ₆₀	0.66
L_K "	-0.7 ₃₂	0.25	-2.8 ₇	1.3
l_J "	-0.05 ₉₈	0.051	-0.1 ₃₂	0.10
l_{JK} "	0.4 ₆₈	0.39	0.5 ₀₁	0.13
l_{KJ} "	-0.7 ₄₀	0.45	-0.7 ₅₉	0.29
l_K "	(Constrained to 0)		-0.8 ₅₂	0.44

* 95% simultaneous confidence intervals, here about 7 times the standard error of each constant.



Table 13. H_2^{82}Se Molecular ConstantsWatson's A-Reduced Hamiltonian, I^R Representation

	Ground State		(010) State	
	Constant (cm^{-1})	(95 % SCI [*])	Constant (cm^{-1})	(95 % SCI [*])
ν_0	-	-	1034.005 ₂₀	0.0046
A	8.16494 ₇₈	0.000030	8.4138 ₄₉	0.00069
B	7.72686 ₀₂	0.000033	7.9069 ₂₀	0.00056
C	3.90045 ₄₂	0.000028	3.8544 ₁₇	0.00030
$\Delta_J (\times 10^3)$	0.528 ₄₆	0.0040	0.619 ₈₉	0.0062
Δ_{JK}	-1.856 ₅₁	0.0024	-2.23 ₀₁	0.028
Δ_K	2.640 ₇₉	0.0017	3.19 ₄₁	0.032
δ_J	0.2416 ₆₇	0.00051	0.287 ₈₀	0.0023
δ_K	-0.1808 ₉₁	0.00097	-0.125 ₄₀	0.0067
$H_J (\times 10^6)$	0.23 ₉₈	0.057	0.42 ₃₁	0.050
H_{JK}	-1.60 ₇₆	0.059	-2.1 ₉₈	0.36
H_{KJ}	1.83 ₀₇	0.062	1.8 ₁₄	0.62
H_K	0.19 ₉₉	0.044	0.9 ₁₇	0.53
h_J	0.09 ₁₁	0.011	0.1 ₉₅	0.12
h_{JK}	-0.35 ₂₄	0.048	-0.48 ₅₄	0.082
h_K	0.85 ₉₄	0.064	1.37 ₉₄	0.081
$L_J (\times 10^9)$	-0.3 ₈₀	0.22	-0.7 ₈₅	0.25
L_{JK}	3.1 ₇₇	0.45	4.1 ₁₈	1.3
L_{JK}	-4.2 ₀₄	0.66	-5.1 ₁₂	2.2
L_{KKJ}	1.7 ₇₁ [‡]		4.4 ₆₀ [‡]	
L_K	-0.7 ₃₂ [‡]		-3.4 ₀	2.2
ℓ_J	-0.05 ₉₈ [‡]		-0.32 ₆₇	0.093
ℓ_{JK}	0.4 ₆₈ [‡]		0.5 ₀₁ [‡]	
ℓ_{KJ}	-2.5 ₆₈	0.84	-2.3 ₁	1.3
ℓ_K	(Constrained to 0)		-0.8 ₅₂ [‡]	

* 95 % simultaneous confidence intervals, here about 7 times the standard error of each constant.

‡ These constants were fixed to the corresponding values for H_2^{80}Se .



Because the relative intensity of lines within an isotopic multiplet depends on the natural abundance of the selenium isotopes, the number and selection of spectral lines was greatest for H_2^{80}Se (~50% abundance). As a result, we were able to assign spectral lines and form GSCD's with the widest range of rotational quantum numbers for this isotopomer. This was also the only isotopomer for which we observed any of the weak $\Delta K_c = 3$ lines. The range of quantum numbers exhibited by the six sets of GSCD's and ν_2 spectral lines and the natural abundances of the six isotopomers were given in Table 8. The molecular constants and the 95% simultaneous confidence intervals for the separate ground state and upper state fits of the five most abundant isotopomers were listed in Tables 9 through 13.

We obtained ground state constants for each isotopomer by fitting infrared GSCD's together with the microwave transitions observed by Helminger and De Lucia (27). The results of the individual ground state fits are summarized in Table 14, and the five sets of ground state constants are listed in Table 15 for comparison.

Table 14. Individual Ground State Fits of H_2Se Isotopomers

Isotopomer	Std Dev of IR GSCD Fit (cm^{-1})	No. of GSCD's	Av Wt	Std Dev of MW Fit (MHz)	No. of MW Transitions
76	0.0035	160	0.531	0.35	21
77	0.0037	143	0.228	0.31	21
78	0.0028	355	1.386	0.080	21
80	0.0021	510	1.756	0.089	25
82	0.0035	153	0.548	0.098	21
Weighted Average	0.0025	1321	1.203	0.22	109



Table 15. H_2Se Ground State Constants for Individual IsotopomersWatson's A-Reduced Hamiltonian, I^r Representation

Constant [#]	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
A	8.18043 ₀₉	8.17769 ₂₃	8.17500 ₈₇	8.16985 ₅₅	8.16494 ₇₈
B	7.72688 ₅₀	7.72689 ₂₂	7.72687 ₈₈	7.72686 ₇₂	7.72686 ₀₂
C	3.90400 ₀₂	3.90337 ₄₅	3.90276 ₅₅	3.90157 ₉₁	3.90045 ₄₂
$\Delta_J (\times 10^3)$	0.527 ₂₄	0.528 ₃₆	0.528 ₂₀	0.527 ₈₂	0.528 ₄₆
Δ_{JK}	-1.848 ₆₈	-1.846 ₀₂	-1.849 ₄₃	-1.849 ₈₁	-1.856 ₅₁
Δ_K	2.640 ₉₁	2.637 ₇₈	2.638 ₂₇	2.637 ₁₂	2.640 ₇₉
δ_J	0.242 ₉₃	0.2430 ₈₁	0.2424 ₀₀	0.2423 ₉₉	0.2416 ₆₇
δ_K	-0.182 ₉₆	-0.1834 ₀₁	-0.182 ₇₁	-0.1834 ₅₄	-0.1808 ₉₁
$H_J (\times 10^6)$	0.21 ₄₈	0.22 ₅₁	0.21 ₀₂	0.21 ₁₄	0.23 ₉₈
H_{JK}	-1.3 ₇₆	-1.35 ₀₈	-1.20 ₂₈	-1.28 ₂₆	-1.60 ₇₆
H_{KJ}	1.6 ₂₂	1.67 ₄₅	1.1 ₆₈	1.37 ₈₂	1.83 ₀₇
H_K	0.24 ₅₆	0.14 ₈₅	0.5 ₁₈	0.38 ₄₈	0.19 ₉₉
h_J	0.11 ₁₇	0.11 ₅₆	0.103 ₉₉	0.10 ₆₂	0.09 ₁₁
h_{JK}	-0.40 ₅₆	-0.49 ₈₉	-0.38 ₈₀	-0.40 ₇₄	-0.35 ₂₄
h_K	0.7 ₈₁	0.9 ₃₅	0.7 ₆₂	0.76 ₃₄	0.85 ₉₄
$L_J (\times 10^9)$			-0.12 ₁₇	-0.11 ₄₀	-0.3 ₈₀
L_{JK}	1.64	0.8 ₆₁	1.3 ₀₈	1.2 ₄₉	3.1 ₇₇
L_{JK}	-4.40	-3.1 ₆₃	-4.37	-2.54	-4.2 ₀₄
L_{KKJ}	4.71	4.3 ₆₂	6.82	1.71	
L_K	-2.3 ₆₇	-2.4 ₇₃	-4.14	-0.7 ₃₂	
l_J				-0.05 ₉₈	
l_{JK}				0.4 ₆₈	
l_{KJ}	-0.95	-1.3 ₂₈	-1.0 ₇₄	-0.7 ₄₀	-2.5 ₆₈
l_K	* * *	* * *	* * *	* * *	* * *

[#]All constants are in units of cm^{-1} . A blank entry means that the constant was fixed to the corresponding value for H_2^{80}Se .

The infrared GSCD's, listed in Appendix E, are weighted averages of all GSCD's formed from the (010) spectral lines of this analysis and the (020), (100), and (001) spectral lines from the analysis of Gillis and Edwards (29). The relative fit of each isotopomer's GSCD's is consistent with our previous comparison of the data sets and the number and average weights of the GSCD's. The weighted average of the microwave fit is 0.22 MHz, which is comparable to the experimental accuracy of the microwave techniques used by Helminger and De Lucia. We gave the microwave transitions a uniform weight of 100 000, compared to an average weight of 1.203 for the infrared GSCD's. This weighting scheme is consistent with the relative accuracies of the microwave frequencies and the ν_2 spectral line positions, and is approximately the square of the ratio of the standard deviations of the infrared and microwave fits. The centrifugal distortion constants are free of any regular mass dependencies. Therefore, when an octic centrifugal distortion constant proved not to be statistically significant, we fixed its value to the corresponding value for H_2^{80}Se . Only ℓ_K was not significant for all five isotopomers, so we fixed its value to zero for all ground state fits.

We determined the ν_2 upper state constants for each isotopomer by fitting the ν_2 spectral lines for each isotopomer (see Appendix D), keeping the ground state constants (determined from our ground state fits) fixed. The five sets of upper state constants are listed in Table 16 for comparison, and the results of the five individual fits are summarized in Table 17. The weighted average standard deviation of the fits for all five isotopomers is 0.0017 cm^{-1} , which is comparable to the standard deviation of the calibration run, 0.0020 cm^{-1} .

Table 16. ν_2 Constants for Individual Isotopomers of H_2Se Watson's A-Reduced Hamiltonian, I^r Representation

Constant [#]	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
ν_0	1034.514 ₄₀	1034.425 ₅₀	1034.335 ₉₀	1034.165 ₂₀	1034.005 ₂₀
A	8.4299 ₂₀	8.4270 ₉₁	8.4244 ₈₅	8.4190 ₁₉	8.4138 ₄₉
B	7.9071 ₇₉	7.9069 ₈₈	7.9069 ₅₂	7.9068 ₈₇	7.9069 ₂₀
C	3.8579 ₇₀	3.8571 ₉₉	3.8566 ₇₈	3.8554 ₇₂	3.8544 ₁₇
$\Delta_J (\times 10^3)$	0.616 ₇₇	0.611 ₆₃	0.614 ₃₉	0.614 ₁₇	0.619 ₈₉
Δ_{JK}	-2.20 ₈₂	-2.18 ₀₅	-2.20 ₈₉	-2.20 ₇₀	-2.23 ₀₁
Δ_K	3.18 ₆₀	3.15 ₉₀	3.18 ₅₅	3.18 ₁₄	3.19 ₄₁
δ_J	0.286 ₈₄	0.284 ₉₈	0.285 ₇₆	0.285 ₉₂	0.287 ₈₀
δ_K	-0.128 ₆₀	-0.12 ₁₇	-0.129 ₆₉	-0.128 ₅₃	-0.125 ₄₀
$H_J (\times 10^6)$	0.33 ₆₇	0.28 ₉₂	0.31 ₉₀	0.31 ₈₈	0.42 ₃₁
H_{JK}	-1.7 ₂₄	-1.4 ₂₁	-1.7 ₀₁	-1.7 ₀₀	-2.1 ₉₈
H_{KJ}	1.5 ₃₇	1.3 ₄₁	1.4 ₁₃	1.4 ₇₁	1.8 ₁₄
H_K	0.8 ₆₂	0.7 ₃₂	0.9 ₆₅	0.8 ₉₄	0.9 ₁₇
h_J	0.16 ₇₇	0.14 ₂₄	0.16 ₁₂	0.16 ₁₃	0.1 ₉₅
h_{JK}	-0.51 ₃₁	-0.4 ₃₈	-0.55 ₉₂	-0.52 ₅₃	-0.48 ₅₄
h_K	1.21 ₀₅	1.2 ₄₉	1.2 ₆₃	1.22 ₉₅	1.37 ₉₄
$L_J (\times 10^9)$	-0.27 ₁₈			-0.2 ₅₅	-0.7 ₈₅
L_{JK}	1.8 ₉₈	2.3 ₉₂		1.7 ₈₅	4.1 ₈
L_{JK}	-4.1 ₆	-9.7 ₁	-4.0 ₃₅	-3.7 ₆	-5.1 ₂
L_{KKJ}		1.4 ₇	5.7 ₇	4.4 ₆₀	
L_K	-2.6 ₅	-7.6 ₅	-3.9 ₉	-2.8 ₇	-3.4 ₀
l_J		-0.10 ₁₉	-0.13 ₃₄	-0.1 ₃₂	-0.32 ₆₇
l_{JK}			0.5 ₇₂	0.5 ₀₁	
l_{KJ}		-1.6 ₃		-0.7 ₅₉	-2.3 ₁
l_K			-1.1 ₁₉	-0.8 ₅₂	

[#]All constants are in units of cm^{-1} . A blank entry means that the constant was fixed to the corresponding value for H_2^{80}Se .

Table 17. Individual Upper State Fits of ν_2 of H_2Se

Isotopomer	Standard Deviation of Infrared Lines (cm^{-1})	Number of Weighted Lines	Average Weight
76	0.0021	233	1.162
77	0.0021	206	0.714
78	0.0016	386	1.874
80	0.0014	502	2.028
82	0.0019	243	1.149
Weighted			
	0.0017	1570	1.553
Average			

Again, the relative magnitudes of the five standard deviations are consistent with the range of quantum numbers exhibited by the five sets of ν_2 lines, as reported in Table 8, and in the number of weighted lines and average line weight for each isotopomer reported in Table 17. In contrast with the ground state case, the octic centrifugal distortion constant ℓ_K was determined to be statistically significant in the upper states of both H_2^{80}Se and H_2^{78}Se .

Simultaneous Analysis of All Isotopomers

The number and variety of spectral lines observed for H_2^{74}Se were inadequate to permit an independent analysis of this isotopomer, so an alternate simultaneous analysis of all six isotopomers was done using isotopic mass adjustment terms in the energy expressions, as done by Willson et al (31), by Moncur et al (32,33), by Gillis and Edwards (29,34,35), and by Lane et al (22) (see Appendix A). We calculated frequencies using the formula

$$F = \nu_0 + \xi^m \Delta M + \xi^{mm} \Delta M^2 + \sum_i (x_a^i + \xi_a^i \Delta M + \xi_a^{ii} \Delta M^2) \langle X_a^i \rangle \quad (\text{III-1})$$

$$- \sum_i (x_b^i + \xi_b^i \Delta M + \xi_b^{ii} \Delta M^2) \langle X_b^i \rangle ,$$

where the subscripts a and b refer to the upper and ground states, respectively, $\Delta M = 80 - M$, where M is the mass of the selenium isotope in the isotopomer, and x_b^i and $\langle X_b^i \rangle$ are, respectively, the Hamiltonian parameters and the expectation values of the associated angular momentum operators. The number of isotopomers (six), the number of lines observed (1593), and the reasonably large range of mass differences present make the H_2Se spectrum an excellent test of the validity of this procedure.

Table 18. Simultaneous Ground State Fit of All H_2Se Isotopomers

Isotopomer	Std Dev of IR GSCD Fit (cm^{-1})	No. of GSCD's	Av Wt	Std Dev of MW Fit (MHz)	No. of MW Transitions
74	0.0083	4	0.040	-	None
76	0.0051	160	0.531	11	21
77	0.0048	143	0.228	5.7	21
78	0.0033	356	1.386	4.3	21
80	0.0027	507	1.762	6.5	25
82	0.0042	156	0.548	9.0	21
Weighted Average	0.0032	1326	1.199	7.6	109

Inspection of the ground state rotational constants listed in Table 15 shows a monotonic dependence on the selenium mass for A and C, and no discernible mass dependence for B. This is not surprising since the b rotational axis passes through the selenium atom. As a result, we anticipated no isotopic mass correction term for B, and indeed, none was ultimately needed. The results of the simultaneous fit of all ground state data using isotopic mass correction terms are summarized in Table

18. Because the number of H_2^{74}Se lines assigned was small, we were only able to form four infrared GSCD's of non-zero weight for H_2^{74}Se . Furthermore, no microwave transitions were available for H_2^{74}Se . For these reasons, the relative fit for the H_2^{74}Se ground state data was poor compared to the fits observed for the other isotopomers. The weighted average standard deviation of the fit of the infrared GSCD's for all six isotopomers is larger than the corresponding value for the separate isotopomeric fits, but is of roughly comparable magnitude. On the other hand, the standard deviations of the microwave fits are from one to two orders of magnitude larger for the simultaneous fit than the corresponding standard deviations of the separate fits. Possibly more mass adjustment terms are needed to fit the microwave transitions simultaneously. However, for fitting the infrared GSCD's and microwave transitions together, only a linear mass adjustment term for C and a linear and quadratic term for A were statistically significant.

Table 19. Simultaneous Upper State Fit of ν_2 of All H_2Se Isotopomers

Isotopomer	Standard Deviation of Infrared Lines (cm^{-1})	Number of Weighted Lines	Average Weight
74	0.0049	25	0.048
76	0.0036	233	1.162
77	0.0028	206	0.714
78	0.0022	384	1.884
80	0.0020	502	2.028
82	0.0033	243	1.149
Weighted	0.0025	1593	1.531
Average			

Table 20. H₂Se Molecular and Isotopic Mass Adjustment ConstantsWatson's A - Reduced Hamiltonian, I^r Representation

	Ground State		(010) State	
	Constant (cm ⁻¹)	(95 % SCI [*])	Constant (cm ⁻¹)	(95 % SCI [#])
ν_0	-	-	1034.164 ₈₀	0.0022
A	8.16991 ₁₀	0.000076	8.4190 ₈₆	0.00032
B	7.72685 ₅₁	0.000069	7.9068 ₉₁	0.00030
C	3.90164 ₃₄	0.000052	3.8555 ₄₃	0.00012
Δ_J ($\times 10^3$)	0.528 ₂₃	0.0039	0.614 ₀₅	0.0033
Δ_{JK} "	-1.84 ₉₂	0.012	-2.20 ₄₅	0.013
Δ_K "	2.638 ₇₃	0.0079	3.18 ₀₉	0.015
δ_J "	0.242 ₄₃	0.0016	0.285 ₆₂	0.0018
δ_K "	-0.184 ₁₀	0.0043	-0.128 ₄₄	0.0057
H_J ($\times 10^6$)	0.21 ₇₃	0.036	0.31 ₅₂	0.018
H_{JK} "	-1.2 ₂₇	0.15	-1.6 ₅₁	0.18
H_{KJ} "	1.1 ₈₄	0.10	1.3 ₉₉	0.44
H_K "	0.5 ₅₃	0.68	0.9 ₂₉	0.28
h_J "	0.10 ₉₀	0.016	0.159 ₁₅	0.0099
h_{JK} "	-0.4 ₁₆	0.12	-0.54 ₁₁	0.094
h_K "	0.7 ₉₇	0.19	1.26 ₉₂	0.093
L_J ($\times 10^9$)			-0.2 ₂₉	0.13
L_{JJK} "	1.2 ₄₁	0.44	1.7 ₃₅	0.95
L_{JK} "			-3.9 ₂	3.2
L_{KKJ} "			4.6 ₂	3.7
L_K "			-2.7 ₈	1.7
l_J "			-0.118 ₆₇	0.0084
l_{JK} "	0.5 ₅₅	0.40	0.5 ₇₇	0.48
l_{KJ} "			-0.6 ₈₅	0.90
l_K "	(Constrained to 0)		-1.0 ₄₉	0.71

Table 20 (cont'd.)

	<u>Ground State</u>		<u>(010) State</u>	
	Constant (cm ⁻¹)	(95 % SCI ^a)	Constant (cm ⁻¹)	(95 % SCI ^b)
$\xi^m (\times 10^2)$	-	-	8.33 ₂₅	0.068
$\xi^{mm} (\times 10^3)$	-	-	1.2 ₂₅	0.21
$\xi^a (\times 10^3)$	2.470 ₀₀	0.0038	2.53 ₂₆	0.019
$\xi^{aa} (\times 10^5)$	3.3 ₄₀	0.14	3.0 ₇₀	0.66
$\xi^c (\times 10^4)$	5.6 ₄₀	0.10	5.59 ₀₆	0.065

* 95 % simultaneous confidence intervals, here about 6 times the standard errors of each constant.

† 95 % simultaneous confidence intervals, here about 8 times the standard errors of each constant.

A blank entry means the constant was fixed to the corresponding value for H₂⁸⁰Se.

The simultaneous fit of the ν_2 upper states was apparently more successful in approaching the goodness of fit of the separate fits of the isotopomers. The results of this fit are summarized in Table 19. The weighted standard deviation is 0.0025 cm^{-1} , which is close to the standard deviation of the calibration fit. The upper state constants in Table 16 show a mass dependence similar to the one observed for the ground state constants, with the obvious addition of the band centers, ν_0 . The molecular constants and isotopic mass adjustment constants that we obtained from the simultaneous ground state fit and from the simultaneous upper state fit (keeping our constants determined in the simultaneous ground state fit fixed) are listed in Table 20.

Determinable Coefficients of H_2Se

In addition to the molecular constants corresponding to Watson's A-reduced Hamiltonian, evaluated in the I^r representation, we are reporting Watson's determinable coefficients for the ground state and the ν_2 upper state for the five most abundant isotopomers of H_2Se . The ground state determinable coefficients for the five most abundant isotopomers are listed in Table 21 and the ν_2 upper state determinable coefficients are listed in Table 22. The variation in the sign and magnitude of the values obtained for the constants ϕ_{zzz} and ϕ_4 in both the ground and upper states suggest that either they are not well determined, or that the small terms ignored by Watson in his formulation of the determinable coefficients are not negligible.

Table 21. Ground State Determinable Coefficients of H_2Se

Constant [‡]	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
X	8.18148 ₅₄	8.17874 ₉₀	8.17606 ₅₁	8.17091 ₁₁	8.16600 ₄₇
Y	7.72597 ₀₉	7.72598 ₃₅	7.72596 ₆₄	7.72595 ₅₂	7.72593 ₉₁
Z	3.90332 ₅₉	3.90270 ₄₆	3.90209 ₁₈	3.90090 ₂₈	3.89977 ₆₂
$T_{xx} (\times 10^3)$	-1.319 ₄₇	-1.320 ₁₂	-1.317 ₀₄	-1.315 ₁₄	-1.312 ₇₄
T_{yy} "	-1.013 ₁₀	-1.014 ₅₂	-1.013 ₀₀	-1.012 ₆₂	-1.011 ₇₉
T_{zz} "	-0.041 ₃₈	-0.042 ₂₀	-0.043 ₄₀	-0.043 ₀₂	-0.045 ₁₃
T_1 "	0.266 ₉₆	0.260 ₉₄	0.264 ₈₃	0.266 ₃₄	0.271 ₁₃
T_2 "	0.534 ₈₃	0.497 ₃₁	0.521 ₅₅	0.530 ₆₈	0.566 ₂₅
$\phi_{xxx} (\times 10^6)$	0.70 ₆₄	0.69 ₇₃	0.69 ₃₄	0.69 ₁₈	0.66 ₂₈
ϕ_{yyy} "	0.43 ₈₂	0.45 ₆₃	0.41 ₈₂	0.42 ₃₈	0.42 ₂₀
ϕ_{zzz} "	-0.00 ₈₆	-0.00 ₆₁	-0.00 ₂₂	-0.00 ₁₀	0.05 ₇₆
ϕ_1 "	-2.45 ₀₀	-1.73 ₁₅	-2.21 ₈₀	-2.34 ₉₄	-3.38 ₉₉
ϕ_2 "	-5.17 ₂₃	-4.59 ₅₅	-5.47 ₀₂	-5.39 ₁₀	-5.13 ₃₄
ϕ_3 "	-3.60 ₃₈	-3.83 ₁₄	-3.27 ₉₂	-3.48 ₃₃	-3.85 ₃₈
ϕ_4 "	0.28 ₆₀	-0.19 ₈₅	-0.01 ₂₆	0.07 ₇₉	0.39 ₁₄

[‡]All constants have units of cm^{-1} , except for T_2 , ϕ_2 , ϕ_3 , and ϕ_4 , which have units of cm^{-2} .



Table 22. (010) Upper State Determinable Coefficients of H_2Se

Constant [#]	H_2^{76}Se	H_2^{77}Se	H_2^{78}Se	H_2^{80}Se	H_2^{82}Se
X	8.4311 ₅₃	8.4283 ₁₅	8.4255 ₁₄	8.4202 ₄₈	8.4150 ₈₉
Y	7.9058 ₈₈	7.9057 ₀₄	7.9056 ₆₀	7.9055 ₉₃	7.9056 ₀₅
Z	3.8573 ₁₁	3.8565 ₆₈	3.8560 ₁₀	3.8548 ₀₈	3.8537 ₅₂
$T_{xx} (\times 10^3)$	-1.594 ₅₅	-1.590 ₁₁	-1.591 ₀₀	-1.588 ₅₈	-1.583 ₈₄
T_{yy} "	-1.190 ₄₅	-1.181 ₅₉	-1.185 ₉₂	-1.186 ₀₂	-1.195 ₄₉
T_{zz} "	-0.043 ₀₉	-0.041 ₆₇	-0.042 ₈₇	-0.042 ₃₂	-0.044 ₂₉
T_1 "	0.357 ₉₂	0.345 ₆₅	0.365 ₆₉	0.364 ₄₉	0.370 ₄₆
T_2 "	1.175 ₁₄	1.137 ₇₅	1.220 ₉₉	1.222 ₆₁	1.266 ₃₈
$\phi_{xxx} (\times 10^6)$	1.01 ₂₃	0.94 ₁₀	0.99 ₆₅	0.98 ₃₉	0.95 ₆₅
ϕ_{yyy} "	0.67 ₂₀	0.57 ₃₉	0.64 ₁₅	0.64 ₁₄	0.81 ₄₀
ϕ_{zzz} "	0.00 ₁₃	0.00 ₄₅	-0.00 ₃₄	-0.00 ₃₈	0.03 ₂₃
ϕ_1 "	-2.52 ₅₆	-1.50 ₉₇	-3.19 ₇₁	-3.02 ₀₇	-3.83 ₈₆
ϕ_2 "	-7.40 ₉₀	-6.25 ₄₅	-7.73 ₀₅	-7.54 ₆₇	-7.49 ₉₇
ϕ_3 "	-4.25 ₉₈	-3.74 ₅₄	-4.53 ₃₂	-4.39 ₀₅	-4.44 ₃₉
ϕ_4 "	-0.02 ₆₉	-0.05 ₁₁	-0.11 ₄₅	0.02 ₆₄	0.30 ₂₅

[#]All constants have units of cm^{-1} , except for T_2 , ϕ_2 , ϕ_3 , and ϕ_4 , which have units of cm^{-2} .

SUMMARY AND CONCLUSIONS

We have reviewed the development of an effective Hamiltonian suitable for calculating the vibration-rotation energy levels of an asymmetric top molecule, from the Darling-Dennison Hamiltonian to the reduced Hamiltonians proposed by Watson. Because the contact transformations necessary to properly reduce the Hamiltonian through terms of order P^8 have only been carried out rigorously for Watson's A-reduced Hamiltonian, we used this Hamiltonian for our final calculations. However, we found it necessary to use the I^r rotational representation, formerly reserved for "prolate" asymmetric top molecules, to obtain stable fits of spectral data for "oblate" asymmetric top molecules with Watson's A-reduced Hamiltonian. Several investigators have identified the reason for this anomaly to be the large size of the s_{111} parameter in this reduction for oblate asymmetric top molecules in the III^r rotational representation. Therefore, we report the effective constants obtained by fitting the data to Watson's A-reduced Hamiltonian in the I^r rotational representation for the ν_2 bands of H_2S and H_2Se . In addition, in order to simplify the comparison of our results with the results of other investigators who may use different reduced Hamiltonians or different rotational representations, we have calculated and reported Watson's determinable coefficients for $H_2^{32}S$ and five of the isotopomers of H_2Se .

Because Watson's A-reduced Hamiltonian in the III^r rotational representation apparently failed to produce a stable fit of spectral data, we used Typke's Hamiltonian, limited to terms through order P^6 ,

for our initial analysis of ν_2 of H_2S . With our new understanding about the appropriate rotational representation for Watson's A-reduced Hamiltonian, we have reanalyzed our ν_2 data for H_2S using Watson's A-reduced Hamiltonian including terms through order P^8 . Using the ground state constants for all three isotopomers of H_2S determined by Flaud et al., we have obtained separate ν_2 upper state constants for H_2^{33}S and H_2^{34}S , as well as H_2^{32}S ground state and ν_2 upper state constants that are in good agreement with the results of other investigators.

We have individually analyzed the ground state and ν_2 upper state of the five most abundant isotopomers of H_2Se . We have also performed a simultaneous analysis of all six naturally occurring isotopomers, including H_2^{74}Se , using isotopic mass adjustments on some of the molecular constants. Using this procedure, we have fit about 1600 H_2Se spectral lines from all six stable isotopomers using only 56 constants in place of the 240 constants that are required to fit five isotopomers individually.



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APPENDICES



APPENDIX A

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Analysis of ν_2 of H_2S

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The infrared absorption spectrum of ν_2 of H_2S in the region from 1000 to 1500 cm^{-1} was obtained with a resolution limit of $<0.05 \text{ cm}^{-1}$ on the University of Denver 50-cm FTIR spectrometer system. We have assigned 387 lines due to H_2^{32}S , 75 lines due to H_2^{34}S , and 15 lines due to H_2^{33}S , and have analyzed them using Typke's reduction of Watson's Hamiltonian. Slightly revised ground-state constants for the 32 isotope were obtained from a simultaneous fit of the microwave transitions observed by Helminger, Cook, and De Lucia, combined with weighted averaged ground-state combination differences formed from the infrared bands (010), (020), (100), (001), (110), (011), (210), and (111). The standard deviation for the fit was 0.0018 cm^{-1} for the infrared data and 0.000032 cm^{-1} for the microwave lines. Upper-state constants for the 32 isotope were obtained from a least-squares fit of the spectral lines of ν_2 , keeping the ground-state constants fixed to the values determined by the combination difference fit. The standard deviation of the (010) line fit was 0.0017 cm^{-1} for the 32 isotope. Ground-state and upper-state isotopic mass adjustment constants were determined in a simultaneous fit of lines of H_2^{33}S and H_2^{34}S , keeping the ground-state and upper-state constants for the 32 isotope fixed.

I. INTRODUCTION

Low-resolution studies of the ν_2 bending fundamental band of H_2S date back at least as far as 1905 when Coblenz (1) located several H_2S infrared absorption bands with a low dispersion prism spectrometer. Among these bands was one centered at 8.46 microns, or 1182 cm^{-1} , a value remarkably close to the currently accepted value of the ν_2 band center. Later investigators such as Rollefson (2), Mischke (3), Mecke (4), Bailey *et al.* (5), and Sprague and Nielsen (6) reported different values for the band center, ranging from 1180 to 1250 cm^{-1} .

In 1951, Allen and Cross (7) reanalyzed the data of the previous investigators and concluded that the band center of ν_2 was near 1183 cm^{-1} . Reasonable estimates of A , B , and C were also produced. In 1956, Allen and Plyler (8) obtained a new spectrum at a resolution limit of 0.3 cm^{-1} . They identified about 55 transitions for $J \leq 6$, fit the spectrum with an average deviation of 0.08 cm^{-1} , and produced better values for A , B , and C .

Recently Gillis and Edwards (9) analyzed the other two fundamentals ν_1 and ν_3 , as well as $2\nu_2$, at a resolution limit of 0.05 cm^{-1} and with a standard deviation of 0.0052 cm^{-1} for the simultaneous fit of ν_1 and ν_3 , and 0.0040 cm^{-1} for the fit of $2\nu_2$.

TABLE I
Experimental Conditions

Run	1	2	3	4	5
Region (cm^{-1})	1010-1350	1010-1350	950-1350	1150-1500	1150-1500
Sample Pressure (torr)	88	88	210	41	161
Path Length (cm)	22	22	22	45	45
Linewidth (cm^{-1})	0.06	0.06	0.10	0.04	0.08
Number of scans co-added	5	7	8	3	4
Calibration	N_2O^*	†	†	†	†

* Spectrum of 28 torr N_2O in a 5 cm cell was recorded simultaneously with H_2S spectrum. See ref. (10) for N_2O line positions.

† Calibrated against well resolved H_2S lines from run 1.

In this work we have run the ν_2 band under higher resolution, assigned 477 transitions, including some for H_2^{34}S and H_2^{33}S , revised the existing vibration-rotation constants, and obtained values for the upper-state constants through sextic terms in angular momentum.

II. EXPERIMENTAL DETAILS

A sample of electronic grade H_2S (99.99% purity, less than 50 ppm CO_2) donated by Scientific Gas Products, Incorporated, was used without further purification. Several runs of the spectrum of ν_2 of H_2S were recorded using the University of Denver 50-cm FTIR spectrometer system. All spectra were recorded at room temperature ($\sim 22^\circ\text{C}$). Several scans for each run were recorded and coadded to improve the signal-to-noise ratio. Experimental conditions are given in Table I. Although the instrument resolution is nominally 0.02 cm^{-1} , the actual observed full widths at half-height of weak to moderate intensity well-resolved lines are pressure broadened from 0.04 to 0.10 cm^{-1} depending on sample pressure. Only short sample cells were available, making necessary relatively high pressure for adequate absorption.

In run 1 the spectra of H_2S and N_2O were recorded simultaneously. The precisely measured ($10^\circ 0' - 00^\circ 0'$) $^{14}\text{N}_2^{16}\text{O}$ line positions of Olson *et al.* (10) were used for calibration. The calibration fit of run 1 indicated that the line positions of well-resolved lines are accurate to $\pm 0.002\text{ cm}^{-1}$. Calibrations of the remaining spectra were performed using well-resolved H_2S lines from run 1 as secondary calibration standards. It was observed that strongly absorbing, heavily pressure-broadened lines in the high-pressure spectra are shifted systematically about 0.007 cm^{-1} toward lower frequency relative to the line positions of run 1 or 2. As line intensity and linewidth decrease, the shift in line position decreases smoothly to zero. This effect is caused by small errors in the phase correction of the interferograms before transformation. These phase errors cause the lineshapes in the transformed spectra to be slightly asymmetric, and line centers are shifted more for broad lines than for narrow lines. In order to minimize line position errors, the line positions used for fitting the

TABLE II
Ground-State Constants of H_2^{32}S

	Constant (cm^{-1})	[†] 95% SCI (cm^{-1})
A'	10.3616 ₁₇	0.00011
B'	9.0161 ₅₈	0.00010
C'	4.73125 ₆₃	0.000050
D' _J	1.103 ₀₁ $\times 10^{-3}$	0.0025 $\times 10^{-3}$
D' _{JK}	-1.968 ₄₂ $\times 10^{-3}$	0.0038 $\times 10^{-3}$
D' _K	0.927 ₈₀ $\times 10^{-3}$	0.0026 $\times 10^{-3}$
δ'_J	0.208 ₆₅ $\times 10^{-3}$	0.0015 $\times 10^{-3}$
R' ₆	-0.2779 ₃₄ $\times 10^{-3}$	0.00052 $\times 10^{-3}$
H' _J	0.44 ₉₅ $\times 10^{-6}$	0.025 $\times 10^{-6}$
H' _{JK}	-1.57 ₀₅ $\times 10^{-6}$	0.072 $\times 10^{-6}$
H' _{KJ}	1.86 ₆₉ $\times 10^{-6}$	0.095 $\times 10^{-6}$
H' _K	-0.74 ₅₃ $\times 10^{-6}$	0.045 $\times 10^{-6}$
H' ₅	0.33 ₄₅ $\times 10^{-6}$	0.045 $\times 10^{-6}$
H' ₆	0.89 ₄₁ $\times 10^{-6}$	0.050 $\times 10^{-6}$
H' ₁₀	0.24 ₂₈ $\times 10^{-6}$	0.020 $\times 10^{-6}$

Standard deviation of 414 weighted averaged infrared GSCD's = 0.0018 cm^{-1} .

Standard deviation of 39 microwave transitions* = 0.000032 cm^{-1} (0.96 MHz).

[†]95% SCI (simultaneous confidence intervals), here ± 6 standard errors of the associated rotational constants.

*See reference (19).

spectra were taken from the lowest-pressure run which gave adequate absorption to observe the line.

Because the spectrometer system has about a 1-m optical path open to the atmosphere, some atmospheric water lines appear in the high-frequency end of the spectrum. The spacings between these lines are wide enough so that very few H_2S lines are obscured.

III. THEORY

We analyzed the spectra using Typke's reduction of Watson's Hamiltonian (11) for the rotational part of the vibration-rotation Hamiltonian, viz.,

$$\begin{aligned}
 H = & A'P_x^2 + B'P_y^2 + C'P_z^2 - D'_JP^4 - D'_{JK}P^2P_z^2 - D'_KP_z^4 - 2\delta'_JP^2(P_x^2 - P_y^2) \\
 & + 2R'_6\mathcal{O} + H'_JP^6 + H'_{JK}P^4P_z^2 + H'_{KJ}P^2P_z^4 + H'_KP_z^6 + H'_5P^4(P_x^2 - P_y^2) \\
 & + (1/2)H'_6P^2\mathcal{O} + H'_{10}(P_x^2 - P_y^2)^3, \quad (1)
 \end{aligned}$$

TABLE III
Upper-State Constants for ν_2 of H_2^{32}S

	*Line Fit		USCD Fit	
	Constants (cm^{-1})	$\dagger 95\%$ SCI (cm^{-1})	Constants (cm^{-1})	$\dagger 95\%$ SCI (cm^{-1})
A'	10.7235 ₄₅	0.00020	10.7239 ₀₉	0.00033
B'	9.2218 ₆₈	0.00022	9.2217 ₁₄	0.00028
C'	4.6694 ₉₄	0.00010	4.6695 ₅₈	0.00017
D _J ¹	1.349 ₆₃ $\times 10^{-3}$	0.0022 $\times 10^{-3}$	1.352 ₅₅ $\times 10^{-3}$	0.0047 $\times 10^{-3}$
D _{JK} ¹	-2.559 ₈₉ $\times 10^{-3}$	0.0053 $\times 10^{-3}$	-2.563 ₇₅ $\times 10^{-3}$	0.0086 $\times 10^{-3}$
D _K ¹	1.272 ₅₄ $\times 10^{-3}$	0.0035 $\times 10^{-3}$	1.274 ₃₉ $\times 10^{-3}$	0.0048 $\times 10^{-3}$
δ_J^1	0.278 ₀₂ $\times 10^{-3}$	0.0020 $\times 10^{-3}$	0.282 ₆₅ $\times 10^{-3}$	0.0044 $\times 10^{-3}$
R ₆ ¹	-0.3271 ₃₄ $\times 10^{-3}$	0.00072 $\times 10^{-3}$	-0.328 ₁₇ $\times 10^{-3}$	0.0015 $\times 10^{-3}$
H _J ¹	0.64 ₁₉ $\times 10^{-6}$	0.012 $\times 10^{-6}$	0.66 ₃₇ $\times 10^{-6}$	0.034 $\times 10^{-6}$
H _{JK} ¹	-2.38 ₆₂ $\times 10^{-6}$	0.047 $\times 10^{-6}$	-2.43 ₅₀ $\times 10^{-6}$	0.089 $\times 10^{-6}$
H _{KJ} ¹	2.98 ₁₂ $\times 10^{-6}$	0.061 $\times 10^{-6}$	3.03 ₁₁ $\times 10^{-6}$	0.095 $\times 10^{-6}$
H _K ¹	-1.23 ₆₇ $\times 10^{-6}$	0.027 $\times 10^{-6}$	-1.25 ₈₄ $\times 10^{-6}$	0.038 $\times 10^{-6}$
H ₅ ¹	0.45 ₂₉ $\times 10^{-6}$	0.022 $\times 10^{-6}$	0.52 ₄₉ $\times 10^{-6}$	0.084 $\times 10^{-6}$
H ₆ ¹	1.14 ₃₈ $\times 10^{-6}$	0.024 $\times 10^{-6}$	1.20 ₂₉ $\times 10^{-6}$	0.092 $\times 10^{-6}$
H ₁₀ ¹	0.31 ₀₂ $\times 10^{-6}$	0.014 $\times 10^{-6}$	0.33 ₇₃ $\times 10^{-6}$	0.030 $\times 10^{-6}$
ν_0	1182.575 ₃₀	0.0018		

Standard deviation of 387 H_2^{32}S lines = 0.0017 cm^{-1} .

Standard deviation of 328 H_2^{32}S ν_2 upper state combination differences = 0.0019 cm^{-1} .

$\dagger 95\%$ SCI (simultaneous confidence intervals), here ≈ 6 standard errors of the associated constant.

*Recommended set of constants.

where

$$\mathcal{O} = P_x^4 + P_y^4 - 3(P_x^2 P_y^2 + P_y^2 P_x^2).$$

Because H_2S is an oblate asymmetric rotor molecule, rotational Hamiltonians were evaluated in the III' representation ($a = x$, $b = y$, $c = z$) with the molecule in the xy plane. The analysis was performed treating the ν_2 band as unperturbed.

The number and selection of transitions observed for H_2^{34}S and H_2^{33}S was inadequate to permit good separate analyses for those isotopic species; hence the H_2^{33}S and H_2^{34}S isotopic species were fit simultaneously using isotopic mass adjustment terms in the energy expressions, as done by Willson *et al.* (12), by Moncur *et al.* (13, 14), and by Gillis and Edwards (9, 15, 16). Frequencies were calculated via the

TABLE IV
Isotopic Constants from ν_2 of H_2S

	Constant (cm^{-1})	$\dagger 95\%$ SCI (cm^{-1})
ξ_b^A	$18.3_{31} \times 10^{-3}$	0.68×10^{-3}
ξ_b^B	$0.1_{32} \times 10^{-3}$	0.33×10^{-3}
ξ_b^C	$3.8_{13} \times 10^{-3}$	0.18×10^{-3}
ξ_a^A	$18.6_{29} \times 10^{-3}$	0.52×10^{-3}
ξ_a^B	$0.3_{97} \times 10^{-3}$	0.31×10^{-3}
ξ_a^C	$3.7_{52} \times 10^{-3}$	0.16×10^{-3}
ξ^m	0.580_{39}	0.0081
ξ^{mm}	0.021_{89}	0.0039

Isotope	Standard Deviation of Fit (cm^{-1})	Number of Weighted Lines	Average Weight
H_2^{32}S	0.0017	387	2.882
H_2^{33}S	0.0035	15	0.923
H_2^{34}S	0.0027	75	1.579
All	0.0018	477	2.615

$\dagger 95\%$ SCI (simultaneous confidence intervals), here ≈ 4 standard errors of the associated constant.

formula:

$$F = \nu_0 + \xi^m \Delta M + \xi^{mm} (\Delta M)^2 + \sum_i (x_a^i + \xi_a^i \Delta M) \langle X^i \rangle_a - \sum_i (x_b^i + \xi_b^i \Delta M) \langle X^i \rangle_b, \quad (2)$$

where a and b refer to the upper and ground states, respectively, $\Delta M = 32 - M$, where M is the mass of the sulfur isotope involved in the particular transition and x^i and $\langle X^i \rangle$ are, respectively, the Hamiltonian parameters and the expectation values of the associated momentum operators in the Hamiltonian space of the 32 isotope.

IV. ANALYSIS

The analysis of ν_2 of H_2S was straightforward and presented few difficulties for the following reasons:

- (1) The spectrum was well enough resolved that most observed lines were



TABLE V
Assigned Transitions of ν_2 of H_2S

UPPER J K- K+			LOWER J K- K+			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
7	3	4	8	6	3	1003.456	0.003	0.05	32
13	6	8	14	5	9	1025.427	-0.016	0.05	32
13	0	13	14	1	14	1039.307	0.009	1.25	32
7	7	0	8	8	1	1040.125	0.009	0.05	32
7	6	1	8	7	2	1043.280	0.002	0.25	32
12	1	12	13	0	13	1049.843	0.004	0.25	32
6	5	2	7	6	1	1054.392	0.005	0.05	32
6	6	1	7	7	0	1055.193	0.007	0.05	32
11	0	11	12	1	12	1060.284	0.000	1.25	32
10	2	9	11	1	10	1067.382	-0.011	0.00	32
10	1	10	11	0	11	1070.631	0.000	1.25	32
9	2	7	10	3	8	1072.205	0.004	0.05	32
11	0	11	11	1	10	1076.184	-0.002	0.05	32
9	1	8	10	2	9	1076.930	0.006	1.25	32
9	0	9	10	1	10	1080.878	0.001	1.25	32
8	2	7	9	1	8	1086.360	0.001	5.00	32
10	1	10	10	2	9	1086.804	-0.003	0.05	32
7	2	5	8	3	6	1089.556	0.002	0.05	32
8	1	8	9	0	9	1091.021	0.001	5.00	32
7	1	6	8	2	7	1095.698	0.004	1.25	32
9	0	9	9	1	8	1097.332	-0.004	0.05	32
6	3	4	7	2	5	1098.271	0.005	0.25	32
7	0	7	8	1	8	1101.059	0.001	5.00	32
6	2	5	7	1	6	1104.930	-0.002	1.25	32
5	2	3	6	3	4	1105.720	0.002	0.25	32
8	1	8	8	2	7	1107.759	-0.013	0.00	32
6	1	6	7	0	7	1110.988	-0.001	5.00	32
5	1	4	6	2	5	1114.010	-0.002	1.25	32
12	4	9	12	5	8	1117.482	-0.007	0.25	32
3	2	1	4	3	2	1118.589	0.006	0.05	32
5	0	5	6	1	6	1120.811	0.002	5.00	32
4	1	3	5	2	4	1122.853	0.001	0.00	32
4	2	3	5	1	4	1123.231	-0.004	1.25	32
4	1	4	5	0	5	1130.519	-0.003	5.00	32
3	1	2	4	2	3	1131.019	-0.001	1.25	32
3	2	2	4	1	3	1132.845	0.001	0.05	32
2	1	1	3	2	2	1138.443	-0.001	0.05	32
3	0	3	4	1	4	1140.084	0.000	0.00	32
2	2	1	3	1	2	1144.264	-0.001	1.25	32
1	1	0	2	2	1	1147.354	-0.002	1.25	32
2	0	2	3	1	3	1149.403	0.002	1.25	32
2	1	2	3	0	3	1149.768	-0.002	5.00	32
1	0	1	2	1	2	1158.167	-0.001	5.00	32
3	0	3	3	1	2	1159.209	0.004	0.05	32
4	2	3	4	3	2	1159.484	-0.001	0.25	32
1	1	1	2	0	2	1159.947	-0.002	1.25	32
6	4	3	6	5	2	1162.426	0.006	0.05	32
7	3	4	7	4	3	1162.681	0.003	0.05	32
4	1	3	4	2	2	1162.782	0.001	0.05	32
6	5	2	6	6	1	1164.464	0.000	0.05	32

individual transitions. In addition there were few molecular contaminants. We observed only a few atmospheric water vapor lines in the high-frequency end of the spectrum.

(2) All the strong lines were attributable to H_2^{32}S because of the high natural abundance of ^{32}S (95%), compared to ^{33}S (0.8%) and ^{34}S (4.2%).

(3) No perturbations with other bands were expected or observed.

(4) The ground-state constants were already well known.

(5) The known values for the ground-state constants and the $2\nu_2$ upper-state constants permitted good initial estimates of the ν_2 upper-state constants by averaging corresponding ground-state constants and $2\nu_2$ upper-state constants, e.g.,



TABLE V—Continued

UPPER J K ⁻ K ⁺			LOWER J K ⁻ K ⁺			OBSERVED (CM ⁻¹)	OBS-CALC (CM ⁻¹)	WEIGHT	ISO
4	3	2	4	4	1	1165.170	-0.001	1.25	32
2	1	2	2	2	1	1166.032	0.000	1.25	32
5	2	3	5	3	2	1167.128	0.002	1.25	32
0	0	0	1	1	1	1167.481	-0.004	0.25	32
5	4	1	5	5	0	1170.509	0.000	0.25	32
6	3	3	6	4	2	1171.486	0.006	0.00	32
3	1	2	3	2	1	1172.070	-0.001	1.25	32
4	2	2	4	3	1	1174.012	0.001	0.25	32
7	4	3	7	5	2	1175.056	0.001	0.05	32
5	3	2	5	4	1	1175.084	-0.002	0.25	32
3	2	1	3	3	0	1175.157	-0.001	5.00	32
2	1	1	2	2	0	1176.466	-0.001	1.25	32
1	0	1	1	1	0	1177.089	-0.001	5.00	32
9	6	3	9	7	2	1178.082	-0.002	0.05	32
1	1	0	1	0	1	1188.771	-0.001	5.00	32
2	2	0	2	1	1	1191.543	0.000	1.25	32
3	3	0	3	2	1	1196.171	0.001	5.00	32
2	1	1	2	0	2	1196.819	-0.001	1.25	32
3	2	1	3	1	2	1197.494	0.000	5.00	32
1	1	1	0	0	0	1197.964	-0.001	5.00	32
4	3	1	4	2	2	1199.527	0.000	5.00	32
2	2	1	2	1	2	1201.024	0.001	5.00	32
4	4	0	4	3	1	1202.822	0.001	5.00	32
5	4	1	5	3	2	1203.448	0.001	5.00	32
3	3	1	3	2	2	1205.040	0.001	5.00	32
2	0	2	1	1	1	1205.776	0.000	5.00	32
2	1	2	1	0	1	1207.447	-0.001	5.00	32
3	1	2	3	0	3	1208.014	0.000	5.00	32
4	2	2	4	1	3	1208.518	-0.001	5.00	32
5	3	2	5	2	3	1209.080	0.000	5.00	32
3	2	2	3	1	3	1209.522	0.002	5.00	32
6	5	1	6	4	2	1209.597	0.000	5.00	32
4	4	1	4	3	2	1210.360	0.002	5.00	32
6	4	2	6	3	3	1210.426	0.000	1.25	32
5	5	0	5	4	1	1211.188	0.001	5.00	32
4	3	2	4	2	3	1212.414	0.000	5.00	32
7	5	2	7	4	3	1213.385	0.000	5.00	32
3	0	3	2	1	2	1215.963	-0.001	5.00	32
3	1	3	2	0	2	1216.294	-0.001	5.00	32
5	4	2	5	3	3	1216.436	0.003	5.00	32
5	5	1	5	4	2	1216.858	0.001	5.00	32
7	6	1	7	5	2	1217.986	0.000	5.00	32
8	6	2	8	5	3	1218.601	0.000	1.25	32
4	1	3	4	0	4	1218.944	-0.001	5.00	32
4	2	3	4	1	4	1219.275	0.000	5.00	32
2	2	1	1	1	0	1219.946	0.001	5.00	32
6	6	0	6	5	1	1220.590	0.002	0.25	32
5	2	3	5	1	4	1220.647	0.000	5.00	32
6	5	2	6	4	3	1221.675	0.001	5.00	32
5	3	3	5	2	4	1221.861	0.000	5.00	32

$$A'(010) \cong (1/2)[A'(000) + A'(020)]. \quad (3)$$

Inserting the estimated constants into our program INTCAL1, we predicted a spectrum which matched the observed spectrum well enough to enable us to assign transitions and weights to many lines. Also available for assigning transitions was our program LINESRT, which searches the spectrum for lines separated by frequency intervals equal to ground-state combination differences (GSCDs). The ground-state quantum numbers of the line pairs are determined by the matching GSCD, and the upper-state assignments are specified by quantum numbers consistent with the selection rules and constraints on J , K_- , K_+ for the band type being analyzed. This procedure requires a good set of GSCDs and improved as our set of combined GSCDs was refined.

TABLE V—Continued

UPPER			LOWER			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
J	K-	K+	J	K-	K+				
6	3	3	6	2	4	1221.992	-0.001	5.00	32
7	4	3	7	3	4	1222.931	0.000	5.00	32
8	5	3	8	4	4	1223.949	-0.001	1.25	32
3	1	2	2	2	1	1224.278	0.001	1.25	32
6	6	1	6	5	2	1224.331	-0.001	1.25	32
6	4	3	6	3	4	1225.159	0.001	5.00	32
4	0	4	3	1	3	1225.394	0.000	0.25	32
4	1	4	3	0	3	1225.442	0.001	1.25	32
9	6	3	9	5	4	1225.981	0.003	5.00	32
9	7	2	9	6	3	1226.395	-0.001	5.00	32
2	2	0	1	1	1	1227.593	0.000	5.00	32
7	6	2	7	5	3	1228.131	-0.003	5.00	32
5	1	4	5	0	5	1229.272	0.001	5.00	32
5	2	4	5	1	5	1229.336	0.006	1.25	32
3	2	2	2	1	1	1229.845	0.000	5.00	32
7	7	0	7	6	1	1230.330	-0.001	5.00	32
6	2	4	6	1	5	1231.862	-0.001	5.00	32
6	3	4	6	2	5	1232.143	0.001	5.00	32
7	7	1	7	6	2	1232.523	-0.001	1.25	32
7	3	4	7	2	5	1234.434	-0.001	5.00	32
5	0	5	4	1	4	1234.578	0.001	0.25	32
7	4	4	7	3	5	1235.375	0.001	5.00	32
8	7	2	8	6	3	1235.704	-0.001	5.00	32
8	4	4	8	3	5	1236.651	0.000	1.25	32
4	1	3	3	2	2	1236.724	0.000	5.00	32
4	4	0	4	1	3	1237.324	-0.005	0.05	32
9	5	4	9	4	5	1238.236	0.000	5.00	32
4	2	3	3	1	2	1238.396	0.000	5.00	32
8	5	4	8	4	5	1239.130	0.001	5.00	32
9	8	1	9	7	2	1239.173	-0.002	0.25	32
6	2	5	6	1	6	1239.335	-0.003	0.25	32
8	8	0	8	7	1	1239.995	-0.001	0.25	32
9	7	3	9	6	4	1241.029	-0.005	1.25	32
8	8	1	8	7	2	1241.165	-0.002	5.00	32
4	2	2	3	3	1	1241.321	0.002	1.25	32
7	2	5	7	1	6	1242.500	0.000	5.00	32
7	3	5	7	2	6	1242.556	-0.001	0.25	32
3	3	1	2	2	0	1243.064	0.001	5.00	32
6	1	6	5	0	5	1243.614	-0.001	5.00	32
9	8	2	9	7	3	1244.187	0.003	0.05	32
5	5	0	5	2	3	1245.181	0.000	0.25	32
8	3	5	8	2	6	1245.844	0.000	5.00	32
8	4	5	8	3	6	1246.075	-0.001	5.00	32
5	1	4	4	2	3	1247.196	0.000	5.00	32
5	2	4	4	1	3	1247.535	0.001	5.00	32
3	3	0	2	2	1	1248.378	0.001	5.00	32
10	8	3	10	7	4	1248.608	-0.001	1.25	32
10	7	4	10	6	5	1248.905	0.002	1.25	32
9	4	5	9	3	6	1249.156	-0.001	1.25	32
7	1	6	7	0	7	1249.221	0.002	5.00	32

Keeping the ground-state constants fixed, a least-squares fit of the assigned lines produced revised upper-state constants using our program ISPCFIT, a single band fitting program. These revised upper-state constants were used to predict the spectrum again, allowing more assignments, a new fit, etc. This cycle was repeated several times and we employed two internal checks on the assignments obtained:

(1) Both GSCDs and USCDs (upper-state combination differences) were formed from the assigned lines using our program CDFORM. Repeated formations of the same combination difference via different levels were grouped together for the purpose of averaging. This procedure helped to detect bad assignments by associating together lines involving the same upper-state energy levels or the same

TABLE V—Continued

UPPER J K- K+			LOWER J K- K+			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
9	9	0	9	8	1	1249.434	-0.002	0.25	32
9	5	5	9	4	6	1249.898	-0.001	1.25	32
10	5	5	10	4	6	1252.128	0.004	0.05	32
7	0	7	6	1	6	1252.520	-0.001	5.00	32
8	3	6	8	2	7	1252.872	-0.002	5.00	32
10	9	2	10	8	3	1253.320	0.004	0.25	32
4	3	2	3	2	1	1253.465	0.001	5.00	32
10	6	5	10	5	6	1254.094	0.002	5.00	32
3	2	1	2	1	2	1254.253	0.000	5.00	32
9	3	6	9	2	7	1256.730	0.000	1.25	32
5	3	2	4	4	1	1256.763	0.001	0.05	32
5	2	3	4	3	2	1256.897	0.000	5.00	32
6	1	5	5	2	4	1257.009	0.001	1.25	32
6	2	5	5	1	4	1257.066	0.000	5.00	32
8	2	7	8	1	8	1258.967	0.001	5.00	32
10	4	6	10	3	7	1260.706	-0.001	1.25	32
10	5	6	10	4	7	1260.907	0.002	5.00	32
8	1	8	7	0	7	1261.296	-0.001	5.00	32
5	3	3	4	2	2	1261.791	0.001	5.00	32
9	2	7	9	1	8	1263.042	0.000	5.00	32
3	3	1	2	0	2	1263.414	-0.001	1.25	32
11	5	6	11	4	7	1264.615	0.001	1.25	32
11	6	6	11	5	7	1265.231	0.004	0.05	32
7	1	6	6	2	5	1266.589	0.003	5.00	32
4	4	1	3	3	0	1266.934	0.001	5.00	32
10	4	7	10	3	8	1267.347	-0.003	5.00	32
9	1	8	9	0	9	1268.576	0.001	5.00	32
6	2	4	5	3	3	1269.065	0.000	5.00	32
9	0	9	8	1	8	1269.943	0.000	5.00	32
4	4	0	3	3	1	1270.130	0.001	5.00	32
6	3	4	5	2	3	1270.402	0.001	5.00	32
6	4	2	5	5	1	1270.834	-0.003	0.05	32
11	4	7	11	3	8	1271.777	0.001	1.25	32
11	5	7	11	4	8	1271.830	0.003	0.25	32
10	3	8	10	2	9	1273.059	0.000	5.00	32
4	3	1	3	2	2	1273.470	0.000	5.00	32
6	3	3	5	4	2	1275.803	-0.002	5.00	32
8	2	7	7	1	6	1276.022	0.000	5.00	32
12	6	7	12	5	8	1276.435	0.006	1.25	32
11	3	8	11	2	9	1277.740	0.000	5.00	32
10	2	9	10	1	10	1278.051	0.002	5.00	32
5	4	2	4	3	1	1278.178	0.000	5.00	32
10	1	10	9	0	9	1278.457	-0.001	5.00	32
7	2	5	6	3	4	1279.705	0.000	5.00	32
7	3	5	6	2	4	1279.993	0.001	5.00	32
12	5	8	12	4	9	1282.567	-0.002	1.25	32
11	2	9	11	1	10	1282.921	-0.002	5.00	32
7	5	2	6	6	1	1284.048	0.004	0.05	32
7	5	2	7	2	5	1285.131	-0.011	0.25	32
4	2	2	3	1	3	1285.193	-0.001	1.25	32

ground-state energy levels, thus allowing anomalies to be easily recognized. The GSCDs formed from the (010) band were also compared with the corresponding weighted averaged GSCDs already available from the (020), (100), and (001) line assignments of Gillis and Edwards (9), the (110) and (011) line assignments of Snyder and Edwards (17), and the (210) and (111) line assignments of Edwards, Moncur, and Snyder (18). Such comparisons, using our program CDCOMPARE, also aided in identifying any bad GSCDs formed from incorrectly assigned lines.

(2) Our program USEN grouped together lines involving transitions to the same upper-state energy level. Using the ground-state constants from previous analyses to determine ground-state energy levels, upper-state energy levels were calculated by adding the appropriate observed transition frequency to each ground-state

TABLE V—Continued

UPPER J K- K+			LOWER J K- K+			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
9	1	8	8	2	7	1285.327	0.000	5.00	32
6	4	3	5	3	2	1286.566	0.000	5.00	32
11	0	11	10	1	10	1286.840	-0.002	5.00	32
11	1	10	11	0	11	1287.390	0.002	5.00	32
12	4	9	12	3	10	1287.961	-0.002	1.25	32
4	4	1	3	1	2	1289.271	0.002	5.00	32
4	3	2	3	0	3	1289.408	0.000	5.00	32
8	2	6	7	3	5	1289.835	-0.001	1.25	32
8	3	6	7	2	5	1289.892	0.000	5.00	32
7	3	4	6	4	3	1290.545	-0.001	5.00	32
5	5	1	4	4	0	1291.162	0.001	5.00	32
12	3	10	12	2	11	1292.636	-0.001	5.00	32
5	5	0	4	4	1	1292.864	0.001	5.00	32
7	4	3	6	5	2	1292.922	-0.004	0.05	32
5	4	1	4	3	2	1293.219	0.000	5.00	32
7	4	4	6	3	3	1294.381	0.000	5.00	32
10	2	9	9	1	8	1294.509	0.001	5.00	32
12	1	12	11	0	11	1295.091	-0.002	5.00	32
12	2	11	12	1	12	1296.599	0.004	5.00	32
13	3	10	13	2	11	1298.014	0.001	1.25	32
9	2	7	8	3	6	1299.760	0.002	5.00	32
8	3	5	7	4	4	1302.463	-0.001	5.00	32
13	0	13	12	1	12	1303.210	-0.002	5.00	32
8	4	5	7	3	4	1303.494	0.000	5.00	32
11	1	10	10	2	9	1303.565	0.001	5.00	32
6	5	2	5	4	1	1303.702	0.000	5.00	32
5	3	2	4	2	3	1304.005	0.000	5.00	32
13	1	12	13	0	13	1305.676	0.005	1.25	32
14	4	11	14	3	12	1307.902	0.005	0.25	32
8	5	3	7	6	2	1308.172	0.001	1.25	32
10	3	8	9	2	7	1309.542	-0.001	5.00	32
8	4	4	7	5	3	1310.979	0.000	5.00	32
14	1	14	13	0	13	1311.196	-0.001	5.00	32
14	3	12	14	2	13	1311.627	-0.001	1.25	32
12	2	11	11	1	10	1312.498	0.001	5.00	32
7	5	3	6	4	2	1312.590	0.000	5.00	32
5	4	2	4	1	3	1312.686	0.001	5.00	32
9	3	6	8	4	5	1313.261	-0.001	5.00	32
9	4	6	8	3	5	1313.501	-0.001	5.00	32
6	5	1	5	4	2	1313.921	0.000	5.00	32
14	2	13	14	1	14	1314.623	0.005	0.25	32
6	6	1	5	5	0	1315.538	-0.001	5.00	32
6	6	0	5	5	1	1316.370	-0.001	5.00	32
5	2	3	4	1	4	1316.687	0.000	5.00	32
5	5	1	4	2	2	1317.626	-0.002	5.00	32
5	3	3	4	0	4	1317.954	0.001	1.25	32
15	0	15	14	1	14	1319.049	0.000	1.25	32
11	2	9	10	3	8	1319.197	-0.001	5.00	32
8	5	4	7	4	3	1319.777	0.001	5.00	32
15	2	13	15	1	14	1320.912	0.003	0.05	32

energy level. Upper states were then checked for inconsistencies, which would indicate a poorly measured or misassigned line.

After bad assignments had been eliminated and the lines were properly weighted to reflect the precision of the frequency measurements relative to the previous infrared band measurements (9, 15, 16), new GSCDs and USCDs were formed from the (010) observed frequencies. These GSCDs were combined with the previous set of combined GSCDs to produce our final set of weighted averaged GSCDs including data from the infrared bands (010), (020), (100), (001), (110), (011), (210), and (111).

Slightly revised ground-state constants were obtained by using our program ICDFIT to fit the combined GSCDs simultaneously with the 39 H₂³²S microwave

TABLE V—Continued

UPPER			LOWER			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
J	K-	K+	J	K-	K+				
13	1	12	12	2	11	1321.308	0.001	5.00	32
9	6	3	8	7	2	1321.893	0.002	0.25	32
6	4	2	5	3	3	1322.549	0.000	5.00	32
10	3	7	9	4	6	1323.661	-0.001	0.25	32
10	4	7	9	3	6	1323.713	-0.002	5.00	32
9	4	5	8	5	4	1324.920	-0.002	5.00	32
16	1	16	15	0	15	1326.767	0.000	1.25	32
9	5	5	8	4	4	1327.864	0.000	5.00	32
12	3	10	11	2	9	1328.728	-0.003	5.00	32
7	6	2	6	5	1	1329.616	0.001	5.00	32
14	2	13	13	1	12	1329.997	0.003	5.00	32
11	3	8	10	4	7	1333.872	0.000	5.00	32
17	0	17	16	1	16	1334.355	0.005	0.25	32
7	6	1	6	5	2	1335.857	0.000	5.00	32
6	3	3	5	2	4	1336.649	0.003	0.25	32
10	4	6	9	5	5	1336.691	-0.007	0.05	32
10	5	6	9	4	5	1337.511	0.000	5.00	32
6	5	2	5	2	3	1337.698	0.001	5.00	32
13	2	11	12	3	10	1338.139	-0.003	5.00	32
15	1	14	14	2	13	1338.555	-0.006	0.05	32
8	6	3	7	5	2	1339.579	0.000	5.00	32
7	7	1	6	6	0	1340.020	-0.002	5.00	32
6	4	3	5	1	4	1340.088	0.001	5.00	32
7	7	0	6	6	1	1340.406	-0.002	5.00	32
7	5	2	6	4	3	1341.254	0.001	5.00	32
12	4	9	11	3	8	1343.943	-0.003	5.00	32
10	5	5	9	6	4	1346.485	-0.004	0.05	32
9	6	4	8	5	3	1346.636	0.002	5.00	32
16	2	15	15	1	14	1347.014	0.006	0.05	32
6	2	4	5	1	5	1347.115	0.002	0.25	32
6	3	4	5	0	5	1347.403	-0.002	0.25	32
11	4	7	10	5	6	1347.637	-0.001	5.00	32
11	5	7	10	4	6	1347.846	0.001	1.25	32
6	6	1	5	3	2	1348.479	0.001	5.00	32
10	6	5	9	5	4	1353.505	0.003	5.00	32
13	4	10	12	3	9	1353.885	-0.002	0.25	32
8	7	2	7	6	1	1355.509	-0.002	5.00	32
7	4	3	6	3	4	1355.664	-0.001	5.00	32
15	2	13	14	3	12	1356.603	-0.004	0.25	32
12	4	8	11	5	7	1358.250	0.001	0.05	32
12	5	8	11	4	7	1358.299	-0.001	1.25	32
8	7	1	7	6	2	1358.974	-0.001	5.00	32
11	5	6	10	6	5	1359.841	0.001	5.00	32
11	7	4	10	8	3	1360.357	0.000	0.05	32
8	6	2	7	5	3	1360.641	0.001	5.00	32
11	6	6	10	5	5	1362.158	0.005	1.25	32
7	5	3	6	2	4	1363.104	0.001	1.25	32
14	4	11	13	3	10	1363.701	-0.003	1.25	32
8	8	1	7	7	0	1364.600	-0.001	5.00	32
8	8	0	7	7	1	1364.775	0.000	5.00	32

lines of Helminger, Cook, and De Lucia (19). The microwave transitions were given a uniform weight of 1000 compared to an average weight of 5.136 for the infrared data. The results of the ground-state fit are reported in Table II.

Keeping our revised ground-state constants fixed, a fit of 387 H_2^{32}S lines was made. The upper-state constants determined in this fit are reported in Table III.

A set of upper-state constants (with the exception of ν_0) was also determined from our (010) USCDs using ICDFIT, for comparison with the results of the line fit. Such a USCD fit does not depend on the ground-state constants and of course uses only (010) data. The results of this fit are included in Table III.

The two sets of constants are in good agreement. Only the values for A' and δ'_j determined in the line fit fall outside the 95% simultaneous confidence interval of

TABLE V—Continued

UPPER			LOWER			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
J	K-	K+	J	K-	K+				
7	6	2	6	3	3	1364.986	-0.002	1.25	32
16	3	14	15	2	13	1365.647	-0.017	0.05	32
11	6	5	10	7	4	1366.384	-0.004	1.25	32
9	7	3	8	6	2	1367.106	-0.001	5.00	32
6	6	0	5	3	3	1368.077	-0.006	0.05	32
7	3	4	6	2	5	1368.309	-0.001	5.00	32
13	4	9	12	5	8	1368.681	0.002	0.25	32
7	4	4	6	1	5	1369.300	-0.002	5.00	32
12	5	7	11	6	6	1371.543	0.002	0.25	32
12	6	7	11	5	6	1372.220	0.005	1.25	32
15	3	12	14	4	11	1373.393	-0.006	0.25	32
8	5	3	7	4	4	1373.845	-0.001	0.25	32
17	2	15	16	3	14	1374.591	-0.016	0.05	32
10	7	4	9	6	3	1374.722	0.002	5.00	32
7	2	5	6	1	6	1376.908	0.002	1.25	32
7	3	5	6	0	6	1376.964	-0.001	0.25	32
14	5	10	13	4	9	1378.973	0.005	1.25	32
11	7	5	10	6	4	1380.707	0.005	0.25	32
9	7	2	8	6	3	1381.221	0.000	0.25	32
12	6	6	11	7	5	1382.175	-0.004	0.05	32
13	5	8	12	6	7	1382.590	0.004	1.25	32
9	8	1	8	7	2	1382.981	-0.001	5.00	32
8	6	3	7	3	4	1387.459	0.003	0.05	32
12	7	6	11	6	5	1387.847	0.010	0.25	32
8	4	4	7	3	5	1388.826	0.000	1.25	32
15	4	11	14	5	10	1389.127	0.009	0.05	32
9	9	1	8	8	0	1389.248	0.003	1.25	32
9	9	0	8	8	1	1389.326	0.003	5.00	32
8	5	4	7	2	5	1391.535	0.001	5.00	32
9	6	3	8	5	4	1391.632	0.001	5.00	32
17	3	14	16	4	13	1392.449	0.019	0.01	32
10	8	3	9	7	2	1394.650	-0.002	1.25	32
8	7	2	7	4	3	1394.928	-0.001	5.00	32
13	6	7	12	7	6	1395.119	0.003	0.05	32
7	7	0	6	4	3	1397.620	0.003	0.05	32
7	6	1	6	3	4	1398.595	-0.001	0.05	32
8	3	5	7	2	6	1398.779	-0.001	1.25	32
8	4	5	7	1	6	1399.023	0.001	1.25	32
10	8	2	9	7	3	1403.254	-0.001	5.00	32
11	8	4	10	7	3	1403.603	0.004	1.25	32
8	3	6	7	0	7	1406.397	-0.003	1.25	32
10	9	2	9	8	1	1406.673	0.001	5.00	32
10	9	1	9	8	2	1407.549	0.000	5.00	32
9	5	4	8	4	5	1408.215	0.000	5.00	32
12	8	5	11	7	4	1409.432	0.008	0.25	32
10	7	3	9	6	4	1409.646	0.001	1.25	32
9	7	3	8	4	4	1413.737	0.001	1.25	32
10	10	1	9	9	0	1413.912	0.008	0.00	32
10	10	0	9	9	1	1413.943	0.005	0.00	32
9	6	4	8	3	5	1414.346	0.001	1.25	32

the corresponding constant from the USCD fit. Each set of constants exhibits the usual correlations between terms involving similar angular momentum operators. No unusually high correlations were observed, and both sets of constants had comparable correlation matrices. We prefer the upper-state constants determined by the line fit because of the narrower simultaneous confidence intervals on the constants and the slightly superior fit they yield. An alternative choice would be to use weighted averages of each constant.

Since there were not enough H_2^{33}S and H_2^{34}S lines to form sufficient GSCDs to fit the ground-state isotopic constants independently, the H_2^{33}S and H_2^{34}S lines were



TABLE V—Continued

UPPER J K- K+			LOWER J K- K+			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
9	4	5	8	3	6	1420.348	0.000	5.00	32
9	5	5	8	2	6	1421.141	0.001	5.00	32
11	9	3	10	8	2	1421.783	-0.001	5.00	32
8	7	1	7	4	4	1424.646	-0.005	0.05	32
10	6	4	9	5	5	1426.299	0.000	1.25	32
11	9	2	10	8	3	1426.599	-0.002	5.00	32
9	8	2	8	5	3	1427.473	-0.001	0.05	32
11	8	3	10	7	4	1428.581	-0.005	1.25	32
9	3	6	8	2	7	1428.648	-0.001	1.25	32
9	4	6	8	1	7	1428.705	0.000	0.25	32
11	10	2	10	9	1	1432.001	0.004	1.25	32
11	10	1	10	9	2	1432.419	0.005	5.00	32
12	9	4	11	8	3	1432.685	0.004	1.25	32
9	2	7	8	1	8	1435.649	0.000	5.00	32
10	7	4	9	4	5	1438.145	0.001	5.00	32
10	5	5	9	4	6	1441.224	-0.002	1.25	32
10	8	3	9	5	4	1442.545	-0.001	1.25	32
11	7	4	10	6	5	1443.367	0.001	0.00	32
10	6	5	9	3	6	1443.390	0.001	0.25	32
12	10	3	11	9	2	1448.347	-0.003	1.25	32
12	9	3	11	8	4	1449.015	-0.011	0.05	32
10	4	6	9	3	7	1450.748	-0.002	1.25	32
12	10	2	11	9	3	1450.871	-0.005	1.25	32
10	5	6	9	2	7	1450.959	0.000	5.00	32
9	8	1	8	5	4	1452.721	-0.001	0.25	32
12	11	2	11	10	1	1457.208	0.006	0.05	32
12	11	1	11	10	2	1457.406	0.009	0.05	32
10	4	7	9	1	8	1458.191	0.001	0.05	32
9	7	2	8	4	5	1459.799	0.001	0.05	32
11	6	5	10	5	6	1460.911	-0.004	5.00	32
10	9	2	9	6	3	1462.142	-0.001	0.05	32
10	3	8	9	0	9	1464.711	0.000	0.05	32
11	7	5	10	4	6	1465.973	0.002	0.25	32
11	5	6	10	4	7	1472.474	-0.001	1.25	32
11	6	6	10	3	7	1473.136	0.002	0.05	32
11	4	7	10	3	8	1480.571	0.001	1.25	32
12	8	5	11	5	6	1489.252	0.001	0.25	32
12	9	4	11	6	5	1491.152	-0.002	0.05	32
12	6	6	11	5	7	1493.484	0.000	0.05	32
11	2	9	10	1	10	1493.574	-0.005	0.25	32
12	7	6	11	4	7	1495.282	0.004	0.25	32
11	11	0	10	10	1	1438.539	0.005	1.25	32
12	12	1	11	11	0	1463.029	-0.006	1.25	32
13	10	3	12	9	4	1471.103	-0.026*	-0.25	32
13	11	2	12	10	3	1475.670	-0.016	0.25	32
13	12	1	12	11	2	1482.379	0.000	0.25	32
14	11	3	13	10	4	1494.640	0.032*	-0.05	32
7	5	2	7	4	3	1212.791	0.007	0.05	33
3	1	3	2	0	2	1215.705	0.000	0.05	33
4	1	4	3	0	3	1224.850	0.003	0.25	33

fit simultaneously using ISPCFIT. For these isotopes, only isotopic constants were varied, using linear mass adjustment terms for A' , B' , and C' in the ground and upper states, and both linear and quadratic mass adjustment terms for the band center ν_0 , as shown in Eq. (2). During this fit the ground-state and upper-state constants for H_2^{32}S were not varied. The results of this fit are reported in Table IV.

A separate fit of the H_2^{34}S lines was also attempted. However, while the constants obtained were in reasonable agreement with the results of the simultaneous isotopic fit, several were not statistically significant. We attribute this to the relatively low number of assigned lines and the large number of constants to be determined. Therefore we report only the results of the simultaneous fit of H_2^{33}S and H_2^{34}S .

TABLE V—Continued

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K-	K+	J	K-	K+	(CM-1)	(CM-1)		
5	0	5	4	1	4	1233.987	0.011	0.05	33
4	2	3	3	1	2	1237.772	0.000	5.00	33
5	1	4	4	2	3	1246.599	0.009	0.05	33
7	0	7	6	1	6	1251.908	0.002	0.05	33
6	2	5	5	1	4	1256.454	0.009	0.25	33
4	4	1	3	3	0	1266.226	-0.001	0.05	33
9	0	9	8	1	8	1269.318	0.003	0.05	33
6	3	4	5	2	3	1269.750	0.005	1.25	33
5	5	0	4	4	1	1292.151	-0.001	5.00	33
6	6	1	5	5	0	1314.752	-0.007	1.25	33
6	5	2	5	4	1	1302.911	-0.008	0.25	33
9	8	1	8	7	2	1382.173	0.006	0.25	33
5	0	5	6	1	6	1119.834	-0.003	0.05	34
4	1	4	5	0	5	1129.530	-0.004	0.25	34
2	1	2	3	0	3	1148.733	-0.009	0.05	34
1	1	0	1	0	1	1187.667	-0.001	1.25	34
3	3	0	3	2	1	1194.917	0.001	0.25	34
3	2	1	3	1	2	1196.418	0.000	1.25	34
2	2	1	2	1	2	1199.856	-0.004	1.25	34
5	4	1	5	3	2	1202.205	0.002	5.00	34
2	1	2	1	0	1	1206.310	-0.004	0.05	34
3	1	2	3	0	3	1206.942	0.005	1.25	34
3	0	3	2	1	2	1214.843	-0.001	1.25	34
5	4	2	5	3	3	1215.201	0.005	0.05	34
4	1	3	4	0	4	1217.826	-0.003	0.25	34
4	2	3	4	1	4	1218.139	0.000	1.25	34
2	2	1	1	1	0	1218.752	0.000	5.00	34
5	2	3	5	1	4	1219.565	-0.005	1.25	34
3	2	2	2	1	1	1228.640	0.005	0.05	34
6	3	4	6	2	5	1230.994	-0.002	0.25	34
5	0	5	4	1	4	1233.419	0.000	5.00	34
7	4	4	7	3	5	1234.228	0.004	0.05	34
4	2	3	3	1	2	1237.190	-0.001	5.00	34
8	5	4	8	4	5	1237.961	0.000	0.05	34
6	2	5	6	1	6	1238.173	-0.001	0.05	34
3	3	1	2	2	0	1241.783	0.003	0.05	34
6	1	6	5	0	5	1242.446	0.003	0.05	34
5	2	4	4	1	3	1246.341	0.000	0.25	34
7	1	6	7	0	7	1248.047	0.009	1.25	34
7	0	7	6	1	6	1251.339	0.004	5.00	34
8	3	6	8	2	7	1251.692	-0.004	5.00	34
4	3	2	3	2	1	1252.157	0.000	0.25	34
6	1	5	5	2	4	1255.815	0.000	0.25	34
6	2	5	5	1	4	1255.869	0.001	1.25	34
8	2	7	8	1	8	1257.774	0.007	0.05	34
8	1	8	7	0	7	1260.097	0.000	5.00	34
5	3	3	4	2	2	1260.485	0.003	0.05	34
7	1	6	6	2	5	1265.376	0.000	1.25	34
4	4	1	3	3	0	1265.564	0.000	5.00	34
6	2	4	5	3	3	1267.885	-0.002	0.25	34

Table V lists the observed frequencies, assignments, and deviations grouped by isotope.

V. CONCLUSION

Our analysis of the spectrum of ν_2 of H_2^{32}S has led to a set of well-determined molecular constants, and very good agreement between observed and calculated frequencies. We have also assigned some lines due to H_2^{33}S and H_2^{34}S , but the number and quality of these lines is insufficient for an analysis of quality comparable to that for H_2^{32}S .



ν_2 OF H_2S

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TABLE V—Continued

UPPER			LOWER			OBSERVED (CM-1)	OBS-CALC (CM-1)	WEIGHT	ISO
J	K-	K+	J	K-	K+				
9	0	9	8	1	8	1268.730	0.000	1.25	34
4	4	0	3	3	1	1268.844	0.004	5.00	34
6	3	4	5	2	3	1269.131	-0.002	0.25	34
4	3	1	3	2	2	1272.346	0.007	0.05	34
8	2	7	7	1	6	1274.795	-0.001	5.00	34
10	2	9	10	1	10	1276.823	0.008	0.25	34
10	1	10	9	0	9	1277.229	-0.002	5.00	34
9	1	8	8	2	7	1284.085	-0.001	0.25	34
6	4	3	5	3	2	1285.131	0.003	0.25	34
11	0	11	10	1	10	1285.596	-0.005	0.25	34
11	1	10	11	0	11	1286.147	0.009	0.25	34
8	3	6	7	2	5	1288.632	-0.005	0.25	34
5	5	1	4	4	0	1289.715	-0.001	1.25	34
5	5	0	4	4	1	1291.483	-0.001	5.00	34
5	4	1	4	3	2	1292.056	0.001	5.00	34
12	1	12	11	0	11	1293.844	0.004	1.25	34
9	2	7	8	3	6	1298.490	-0.001	5.00	34
6	5	2	5	4	1	1302.179	-0.001	0.05	34
11	1	10	10	2	9	1302.292	-0.001	0.05	34
9	3	6	8	4	5	1311.975	-0.003	0.05	34
6	6	1	5	5	0	1314.020	-0.003	5.00	34
6	6	0	5	5	1	1314.896	-0.004	5.00	34
11	2	9	10	3	8	1317.893	-0.005	0.05	34
8	5	4	7	4	3	1318.229	0.005	0.05	34
10	3	7	9	4	6	1322.346	-0.007	0.05	34
10	4	7	9	3	6	1322.393	-0.008	0.05	34
7	6	2	6	5	1	1328.008	0.000	0.25	34
7	6	1	6	5	2	1334.510	0.000	5.00	34
8	6	3	7	5	2	1337.866	0.005	0.05	34
7	7	1	6	6	0	1338.434	0.000	0.25	34
7	7	0	6	6	1	1338.846	-0.001	5.00	34
7	5	2	6	4	3	1340.189	0.000	0.25	34
8	7	2	7	6	1	1353.846	0.002	0.05	34
7	4	3	6	3	4	1354.578	-0.007	0.05	34
8	8	1	7	7	0	1362.942	0.004	5.00	34
9	7	2	8	6	3	1379.984	0.003	0.25	34
9	8	1	8	7	2	1381.400	0.005	1.25	34

*Not included in the fit.

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APPENDIX B

ASSIGNED TRANSITIONS OF ν_2 OF H_2S

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	3	4	8	6	3	1003.456	0.004	0.05	32
13	0	13	14	1	14	1039.307	0.003	1.25	32
7	7	0	8	8	1	1040.125	0.006	0.05	32
7	6	1	8	7	2	1043.280	0.003	0.25	32
12	1	12	13	0	13	1049.843	0.000	0.25	32
6	5	2	7	6	1	1054.392	0.005	0.05	32
6	6	1	7	7	0	1055.193	0.007	0.05	32
11	0	11	12	1	12	1060.284	-0.002	1.25	32
10	2	9	11	1	10	1067.382	-0.014	0.00	32
10	1	10	11	0	11	1070.631	-0.001	1.25	32
9	2	7	10	3	8	1072.205	0.003	0.05	32
11	0	11	11	1	10	1076.184	-0.002	0.05	32
9	1	8	10	2	9	1076.930	0.004	1.25	32
9	0	9	10	1	10	1080.878	0.001	1.25	32
8	2	7	9	1	8	1086.360	-0.001	5.00	32
10	1	10	10	2	9	1086.804	-0.003	0.05	32
7	2	5	8	3	6	1089.556	0.002	0.05	32
8	1	8	9	0	9	1091.021	0.001	5.00	32
7	1	6	8	2	7	1095.698	0.003	1.25	32
9	0	9	9	1	8	1097.332	-0.004	0.05	32
6	3	4	7	2	5	1098.271	0.004	0.25	32
7	0	7	8	1	8	1101.059	0.001	5.00	32
6	2	5	7	1	6	1104.930	-0.002	1.25	32
5	2	3	6	3	4	1105.720	0.002	0.25	32
8	1	8	8	2	7	1107.759	-0.013	0.00	32
6	1	6	7	0	7	1110.988	-0.001	5.00	32
5	1	4	6	2	5	1114.010	-0.003	1.25	32
12	4	9	12	5	8	1117.482	-0.002	0.25	32
3	2	1	4	3	2	1118.589	0.006	0.05	32
5	0	5	6	1	6	1120.811	0.002	5.00	32
4	1	3	5	2	4	1122.853	0.001	0.00	32
4	2	3	5	1	4	1123.231	-0.005	1.25	32
4	1	4	5	0	5	1130.519	-0.003	5.00	32
3	1	2	4	2	3	1131.019	-0.001	1.25	32
3	2	2	4	1	3	1132.845	0.001	0.05	32
2	1	1	3	2	2	1138.443	0.000	0.05	32
3	0	3	4	1	4	1140.084	0.001	0.00	32
2	2	1	3	1	2	1144.264	-0.001	1.25	32
1	1	0	2	2	1	1147.354	-0.002	1.25	32
2	0	2	3	1	3	1149.403	0.003	1.25	32
2	1	2	3	0	3	1149.768	-0.001	5.00	32
1	0	1	2	1	2	1158.167	0.000	5.00	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	0	3	3	1	2	1159.209	0.004	0.05	32
4	2	3	4	3	2	1159.484	-0.002	0.25	32
1	1	1	2	0	2	1159.947	-0.001	1.25	32
6	4	3	6	5	2	1162.426	0.006	0.05	32
7	3	4	7	4	3	1162.681	0.004	0.05	32
4	1	3	4	2	2	1162.782	0.001	0.05	32
6	5	2	6	6	1	1164.464	-0.001	0.05	32
4	3	2	4	4	1	1165.170	-0.002	1.25	32
2	1	2	2	2	1	1166.032	0.000	1.25	32
5	2	3	5	3	2	1167.128	0.003	1.25	32
0	0	0	1	1	1	1167.481	-0.003	0.25	32
5	4	1	5	5	0	1170.509	0.000	0.25	32
6	3	3	6	4	2	1171.486	0.007	0.00	32
3	1	2	3	2	1	1172.070	0.000	1.25	32
4	2	2	4	3	1	1174.012	0.002	0.25	32
7	4	3	7	5	2	1175.056	0.002	0.05	32
5	3	2	5	4	1	1175.084	-0.002	0.25	32
3	2	1	3	3	0	1175.157	-0.001	5.00	32
2	1	1	2	2	0	1176.466	0.000	1.25	32
1	0	1	1	1	0	1177.089	0.000	5.00	32
9	6	3	9	7	2	1178.082	-0.004	0.05	32
1	1	0	1	0	1	1188.771	0.000	5.00	32
2	2	0	2	1	1	1191.543	0.000	1.25	32
3	3	0	3	2	1	1196.171	0.000	5.00	32
2	1	1	2	0	2	1196.819	0.000	1.25	32
3	2	1	3	1	2	1197.494	0.000	5.00	32
1	1	1	0	0	0	1197.964	0.000	5.00	32
4	3	1	4	2	2	1199.527	0.000	5.00	32
2	2	1	2	1	2	1201.024	0.000	5.00	32
4	4	0	4	3	1	1202.822	0.000	5.00	32
5	4	1	5	3	2	1203.448	0.000	5.00	32
3	3	1	3	2	2	1205.040	0.000	5.00	32
2	0	2	1	1	1	1205.776	0.001	5.00	32
2	1	2	1	0	1	1207.447	0.000	5.00	32
3	1	2	3	0	3	1208.014	0.000	5.00	32
4	2	2	4	1	3	1208.518	0.000	5.00	32
5	3	2	5	2	3	1209.080	0.000	5.00	32
3	2	2	3	1	3	1209.522	0.002	5.00	32
6	5	1	6	4	2	1209.597	0.000	5.00	32
4	4	1	4	3	2	1210.360	0.001	5.00	32
6	4	2	6	3	3	1210.426	0.000	1.25	32
5	5	0	5	4	1	1211.188	0.001	5.00	32
4	3	2	4	2	3	1212.414	-0.001	5.00	32
7	5	2	7	4	3	1213.385	0.000	5.00	32
3	0	3	2	1	2	1215.963	0.000	5.00	32
3	1	3	2	0	2	1216.294	0.000	5.00	32
5	4	2	5	3	3	1216.436	0.002	5.00	32
5	5	1	5	4	2	1216.858	0.000	5.00	32
7	6	1	7	5	2	1217.986	0.001	5.00	32



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	6	2	8	5	3	1218.601	0.000	1.25	32
4	1	3	4	0	4	1218.944	-0.001	5.00	32
4	2	3	4	1	4	1219.275	0.000	5.00	32
2	2	1	1	1	0	1219.946	0.000	5.00	32
6	6	0	6	5	1	1220.590	0.003	0.25	32
5	2	3	5	1	4	1220.647	0.000	5.00	32
6	5	2	6	4	3	1221.675	0.001	5.00	32
5	3	3	5	2	4	1221.861	0.000	5.00	32
6	3	3	6	2	4	1221.992	0.000	5.00	32
7	4	3	7	3	4	1222.931	0.000	5.00	32
8	5	3	8	4	4	1223.949	-0.001	1.25	32
3	1	2	2	2	1	1224.278	0.001	1.25	32
6	6	1	6	5	2	1224.331	0.000	1.25	32
6	4	3	6	3	4	1225.159	0.000	5.00	32
4	0	4	3	1	3	1225.394	0.001	0.25	32
4	1	4	3	0	3	1225.442	0.001	1.25	32
9	6	3	9	5	4	1225.981	0.001	5.00	32
9	7	2	9	6	3	1226.395	-0.001	5.00	32
2	2	0	1	1	1	1227.593	0.000	5.00	32
7	6	2	7	5	3	1228.131	-0.002	5.00	32
5	1	4	5	0	5	1229.272	0.000	5.00	32
5	2	4	5	1	5	1229.336	0.005	1.25	32
3	2	2	2	1	1	1229.845	0.000	5.00	32
7	7	0	7	6	1	1230.330	0.001	5.00	32
6	2	4	6	1	5	1231.862	-0.001	5.00	32
6	3	4	6	2	5	1232.143	0.001	5.00	32
7	7	1	7	6	2	1232.523	0.001	1.25	32
7	3	4	7	2	5	1234.434	-0.001	5.00	32
5	0	5	4	1	4	1234.578	0.002	0.25	32
7	4	4	7	3	5	1235.375	0.000	5.00	32
8	7	2	8	6	3	1235.704	0.001	5.00	32
8	4	4	8	3	5	1236.651	0.001	1.25	32
4	1	3	3	2	2	1236.724	0.000	5.00	32
4	4	0	4	1	3	1237.324	-0.006	0.05	32
9	5	4	9	4	5	1238.236	0.000	5.00	32
4	2	3	3	1	2	1238.396	-0.001	5.00	32
8	5	4	8	4	5	1239.130	0.000	5.00	32
9	8	1	9	7	2	1239.173	-0.001	0.25	32
6	2	5	6	1	6	1239.335	-0.004	0.25	32
8	8	0	8	7	1	1239.995	0.001	0.25	32
9	7	3	9	6	4	1241.029	-0.004	1.25	32
8	8	1	8	7	2	1241.165	0.000	5.00	32
4	2	2	3	3	1	1241.321	0.003	1.25	32
7	2	5	7	1	6	1242.500	0.000	5.00	32
7	3	5	7	2	6	1242.556	-0.001	0.25	32
3	3	1	2	2	0	1243.064	0.000	5.00	32
6	1	6	5	0	5	1243.614	-0.001	5.00	32
9	8	2	9	7	3	1244.187	0.004	0.05	32
5	5	0	5	2	3	1245.181	-0.001	0.25	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	3	5	8	2	6	1245.844	0.000	5.00	32
8	4	5	8	3	6	1246.075	-0.001	5.00	32
5	1	4	4	2	3	1247.196	-0.001	5.00	32
5	2	4	4	1	3	1247.535	0.001	5.00	32
3	3	0	2	2	1	1248.378	0.000	5.00	32
10	8	3	10	7	4	1248.608	0.000	1.25	32
10	7	4	10	6	5	1248.905	0.001	1.25	32
9	4	5	9	3	6	1249.156	0.000	1.25	32
7	1	6	7	0	7	1249.221	0.001	5.00	32
9	9	0	9	8	1	1249.434	0.000	0.25	32
9	5	5	9	4	6	1249.898	-0.002	1.25	32
10	5	5	10	4	6	1252.128	0.005	0.05	32
7	0	7	6	1	6	1252.520	0.000	5.00	32
8	3	6	8	2	7	1252.872	-0.003	5.00	32
10	9	2	10	8	3	1253.320	0.004	0.25	32
4	3	2	3	2	1	1253.465	0.000	5.00	32
10	6	5	10	5	6	1254.094	0.000	5.00	32
3	2	1	2	1	2	1254.253	0.001	5.00	32
9	3	6	9	2	7	1256.730	0.000	1.25	32
5	3	2	4	4	1	1256.763	0.001	0.05	32
5	2	3	4	3	2	1256.897	0.000	5.00	32
6	1	5	5	2	4	1257.009	0.000	1.25	32
6	2	5	5	1	4	1257.066	-0.001	5.00	32
8	2	7	8	1	8	1258.967	0.000	5.00	32
10	4	6	10	3	7	1260.706	-0.001	1.25	32
10	5	6	10	4	7	1260.907	0.001	5.00	32
8	1	8	7	0	7	1261.296	-0.001	5.00	32
5	3	3	4	2	2	1261.791	0.001	5.00	32
9	2	7	9	1	8	1263.042	0.001	5.00	32
3	3	1	2	0	2	1263.414	-0.002	1.25	32
11	5	6	11	4	7	1264.615	0.001	1.25	32
11	6	6	11	5	7	1265.231	0.001	0.05	32
7	1	6	6	2	5	1266.589	0.002	5.00	32
4	4	1	3	3	0	1266.934	-0.001	5.00	32
10	4	7	10	3	8	1267.347	-0.002	5.00	32
9	1	8	9	0	9	1268.576	0.000	5.00	32
6	2	4	5	3	3	1269.065	0.000	5.00	32
9	0	9	8	1	8	1269.943	0.001	5.00	32
4	4	0	3	3	1	1270.130	0.000	5.00	32
6	3	4	5	2	3	1270.402	0.001	5.00	32
6	4	2	5	5	1	1270.834	-0.003	0.05	32
11	4	7	11	3	8	1271.777	0.000	1.25	32
11	5	7	11	4	8	1271.830	0.002	0.25	32
10	3	8	10	2	9	1273.059	0.000	5.00	32
4	3	1	3	2	2	1273.470	0.000	5.00	32
6	3	3	5	4	2	1275.803	-0.001	5.00	32
8	2	7	7	1	6	1276.022	-0.001	5.00	32
12	6	7	12	5	8	1276.435	0.000	1.25	32
11	3	8	11	2	9	1277.740	0.000	5.00	32



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	2	9	10	1	10	1278.051	0.001	5.00	32
5	4	2	4	3	1	1278.178	0.000	5.00	32
10	1	10	9	0	9	1278.457	0.000	5.00	32
7	2	5	6	3	4	1279.705	0.000	5.00	32
7	3	5	6	2	4	1279.993	0.001	5.00	32
12	5	8	12	4	9	1282.567	-0.005	1.25	32
11	2	9	11	1	10	1282.921	-0.001	5.00	32
7	5	2	6	6	1	1284.048	0.004	0.05	32
7	5	2	7	2	5	1285.131	-0.011	0.25	32
4	2	2	3	1	3	1285.193	0.000	1.25	32
9	1	8	8	2	7	1285.327	-0.001	5.00	32
6	4	3	5	3	2	1286.566	0.000	5.00	32
11	0	11	10	1	10	1286.840	0.000	5.00	32
11	1	10	11	0	11	1287.390	0.000	5.00	32
12	4	9	12	3	10	1287.961	-0.002	1.25	32
4	4	1	3	1	2	1289.271	0.001	5.00	32
4	3	2	3	0	3	1289.408	-0.001	5.00	32
8	2	6	7	3	5	1289.835	-0.001	1.25	32
8	3	6	7	2	5	1289.892	0.000	5.00	32
7	3	4	6	4	3	1290.545	-0.001	5.00	32
5	5	1	4	4	0	1291.162	0.000	5.00	32
12	3	10	12	2	11	1292.636	0.000	5.00	32
5	5	0	4	4	1	1292.864	0.000	5.00	32
7	4	3	6	5	2	1292.922	-0.004	0.05	32
5	4	1	4	3	2	1293.219	0.000	5.00	32
7	4	4	6	3	3	1294.381	-0.001	5.00	32
10	2	9	9	1	8	1294.509	0.000	5.00	32
12	1	12	11	0	11	1295.091	0.000	5.00	32
12	2	11	12	1	12	1296.599	0.001	5.00	32
13	3	10	13	2	11	1298.014	-0.001	1.25	32
9	2	7	8	3	6	1299.760	0.002	5.00	32
8	3	5	7	4	4	1302.463	-0.001	5.00	32
13	0	13	12	1	12	1303.210	0.000	5.00	32
8	4	5	7	3	4	1303.494	0.000	5.00	32
11	1	10	10	2	9	1303.565	0.000	5.00	32
6	5	2	5	4	1	1303.702	-0.001	5.00	32
5	3	2	4	2	3	1304.005	0.000	5.00	32
13	1	12	13	0	13	1305.676	0.000	1.25	32
14	4	11	14	3	12	1307.902	0.001	0.25	32
8	5	3	7	6	2	1308.172	0.001	1.25	32
10	3	8	9	2	7	1309.542	-0.001	5.00	32
8	4	4	7	5	3	1310.979	0.001	5.00	32
14	1	14	13	0	13	1311.196	0.000	5.00	32
14	3	12	14	2	13	1311.627	-0.001	1.25	32
12	2	11	11	1	10	1312.498	0.000	5.00	32
7	5	3	6	4	2	1312.590	0.000	5.00	32
5	4	2	4	1	3	1312.686	0.000	5.00	32
9	3	6	8	4	5	1313.261	0.000	5.00	32
9	4	6	8	3	5	1313.501	0.000	5.00	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	5	1	5	4	2	1313.921	-0.001	5.00	32
14	2	13	14	1	14	1314.623	-0.001	0.25	32
6	6	1	5	5	0	1315.538	0.000	5.00	32
6	6	0	5	5	1	1316.370	-0.001	5.00	32
5	2	3	4	1	4	1316.687	0.000	5.00	32
5	5	1	4	2	2	1317.626	-0.002	5.00	32
5	3	3	4	0	4	1317.954	0.000	1.25	32
15	0	15	14	1	14	1319.049	0.000	1.25	32
11	2	9	10	3	8	1319.197	0.001	5.00	32
8	5	4	7	4	3	1319.777	0.000	5.00	32
15	2	13	15	1	14	1320.912	0.002	0.05	32
13	1	12	12	2	11	1321.308	0.000	5.00	32
9	6	3	8	7	2	1321.893	0.000	0.25	32
6	4	2	5	3	3	1322.549	0.000	5.00	32
10	3	7	9	4	6	1323.661	0.001	0.25	32
10	4	7	9	3	6	1323.713	-0.001	5.00	32
9	4	5	8	5	4	1324.920	-0.001	5.00	32
16	1	16	15	0	15	1326.767	-0.001	1.25	32
9	5	5	8	4	4	1327.864	0.000	5.00	32
12	3	10	11	2	9	1328.728	-0.001	5.00	32
7	6	2	6	5	1	1329.616	0.002	5.00	32
14	2	13	13	1	12	1329.997	0.000	5.00	32
11	3	8	10	4	7	1333.872	0.002	5.00	32
17	0	17	16	1	16	1334.355	0.002	0.25	32
7	6	1	6	5	2	1335.857	0.000	5.00	32
6	3	3	5	2	4	1336.649	0.003	0.25	32
10	4	6	9	5	5	1336.691	-0.005	0.05	32
10	5	6	9	4	5	1337.511	0.000	5.00	32
6	5	2	5	2	3	1337.698	0.001	5.00	32
13	2	11	12	3	10	1338.139	0.000	5.00	32
15	1	14	14	2	13	1338.555	-0.009	0.05	32
8	6	3	7	5	2	1339.579	0.000	5.00	32
7	7	1	6	6	0	1340.020	-0.001	5.00	32
6	4	3	5	1	4	1340.088	0.000	5.00	32
7	7	0	6	6	1	1340.406	-0.001	5.00	32
7	5	2	6	4	3	1341.254	0.000	5.00	32
12	4	9	11	3	8	1343.943	0.000	5.00	32
10	5	5	9	6	4	1346.485	-0.002	0.05	32
9	6	4	8	5	3	1346.636	0.001	5.00	32
16	2	15	15	1	14	1347.014	0.002	0.05	32
6	2	4	5	1	5	1347.115	0.002	0.25	32
6	3	4	5	0	5	1347.403	0.002	0.25	32
11	4	7	10	5	6	1347.637	0.000	5.00	32
11	5	7	10	4	6	1347.846	0.002	1.25	32
6	6	1	5	3	2	1348.479	0.002	5.00	32
10	6	5	9	5	4	1353.505	0.001	5.00	32
13	4	10	12	3	9	1353.885	0.002	0.25	32
8	7	2	7	6	1	1355.509	0.000	5.00	32
7	4	3	6	3	4	1355.664	0.000	5.00	32



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
15	2	13	14	3	12	1356.603	0.002	0.25	32
12	4	8	11	5	7	1358.250	0.002	0.05	32
12	5	8	11	4	7	1358.299	-0.001	1.25	32
8	7	1	7	6	2	1358.974	0.000	5.00	32
11	5	6	10	6	5	1359.841	0.002	5.00	32
11	7	4	10	8	3	1360.357	0.006	0.05	32
8	6	2	7	5	3	1360.641	0.000	5.00	32
11	6	6	10	5	5	1362.158	0.002	1.25	32
7	5	3	6	2	4	1363.104	0.001	1.25	32
14	4	11	13	3	10	1363.701	0.001	1.25	32
8	8	1	7	7	0	1364.600	0.000	5.00	32
8	8	0	7	7	1	1364.775	0.000	5.00	32
7	6	2	6	3	3	1364.986	-0.001	1.25	32
16	3	14	15	2	13	1365.647	-0.008	0.05	32
11	6	5	10	7	4	1366.384	0.000	1.25	32
9	7	3	8	6	2	1367.106	0.000	5.00	32
6	6	0	5	3	3	1368.077	-0.006	0.05	32
7	3	4	6	2	5	1368.309	-0.001	5.00	32
13	4	9	12	5	8	1368.681	0.002	0.25	32
7	4	4	6	1	5	1369.300	-0.002	5.00	32
12	5	7	11	6	6	1371.543	0.001	0.25	32
12	6	7	11	5	6	1372.220	0.000	1.25	32
15	3	12	14	4	11	1373.393	-0.001	0.25	32
8	5	3	7	4	4	1373.845	-0.002	0.25	32
17	2	15	16	3	14	1374.591	-0.001	0.05	32
10	7	4	9	6	3	1374.722	0.000	5.00	32
7	2	5	6	1	6	1376.908	0.002	1.25	32
7	3	5	6	0	6	1376.964	-0.001	0.25	32
14	5	10	13	4	9	1378.973	0.001	1.25	32
11	7	5	10	6	4	1380.707	-0.001	0.25	32
9	7	2	8	6	3	1381.221	0.000	0.25	32
12	6	6	11	7	5	1382.175	0.000	0.05	32
13	5	8	12	6	7	1382.590	-0.002	1.25	32
9	8	1	8	7	2	1382.981	0.000	5.00	32
8	6	3	7	3	4	1387.459	0.003	0.05	32
12	7	6	11	6	5	1387.847	0.000	0.25	32
8	4	4	7	3	5	1388.826	0.001	1.25	32
15	4	11	14	5	10	1389.127	0.003	0.05	32
9	9	1	8	8	0	1389.248	0.000	1.25	32
9	9	0	8	8	1	1389.326	0.001	5.00	32
8	5	4	7	2	5	1391.535	0.001	5.00	32
9	6	3	8	5	4	1391.632	-0.001	5.00	32
10	8	3	9	7	2	1394.650	-0.001	1.25	32
8	7	2	7	4	3	1394.928	0.000	5.00	32
13	6	7	12	7	6	1395.119	0.001	0.05	32
7	7	0	6	4	3	1397.620	0.004	0.05	32
7	6	1	6	3	4	1398.595	0.000	0.05	32
8	3	5	7	2	6	1398.779	-0.001	1.25	32
8	4	5	7	1	6	1399.023	0.001	1.25	32



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	8	2	9	7	3	1403.254	0.000	5.00	32
11	8	4	10	7	3	1403.603	0.000	1.25	32
8	3	6	7	0	7	1406.397	-0.003	1.25	32
10	9	2	9	8	1	1406.673	0.000	5.00	32
10	9	1	9	8	2	1407.549	0.000	5.00	32
9	5	4	8	4	5	1408.215	0.000	5.00	32
12	8	5	11	7	4	1409.432	-0.004	0.25	32
10	7	3	9	6	4	1409.646	0.001	1.25	32
9	7	3	8	4	4	1413.737	0.002	1.25	32
10	10	1	9	9	0	1413.912	0.002	0.00	32
10	10	0	9	9	1	1413.943	-0.002	0.00	32
9	6	4	8	3	5	1414.346	0.000	1.25	32
9	4	5	8	3	6	1420.348	0.000	5.00	32
9	5	5	8	2	6	1421.141	0.001	5.00	32
11	9	3	10	8	2	1421.783	0.000	5.00	32
8	7	1	7	4	4	1424.646	-0.004	0.05	32
10	6	4	9	5	5	1426.299	0.000	1.25	32
11	9	2	10	8	3	1426.599	0.001	5.00	32
9	8	2	8	5	3	1427.473	0.000	0.05	32
11	8	3	10	7	4	1428.581	0.000	1.25	32
9	3	6	8	2	7	1428.648	0.000	1.25	32
9	4	6	8	1	7	1428.705	0.001	0.25	32
11	10	2	10	9	1	1432.001	-0.001	1.25	32
11	10	1	10	9	2	1432.419	0.000	5.00	32
12	9	4	11	8	3	1432.685	0.000	1.25	32
9	2	7	8	1	8	1435.649	0.001	5.00	32
10	7	4	9	4	5	1438.145	-0.001	5.00	32
10	5	5	9	4	6	1441.224	-0.002	1.25	32
10	8	3	9	5	4	1442.545	0.000	1.25	32
11	7	4	10	6	5	1443.367	0.007	0.00	32
10	6	5	9	3	6	1443.390	-0.002	0.25	32
12	10	3	11	9	2	1448.347	-0.001	1.25	32
12	9	3	11	8	4	1449.015	0.004	0.05	32
10	4	6	9	3	7	1450.748	-0.001	1.25	32
12	10	2	11	9	3	1450.871	0.001	1.25	32
10	5	6	9	2	7	1450.959	0.000	5.00	32
9	8	1	8	5	4	1452.721	0.000	0.25	32
12	11	2	11	10	1	1457.208	-0.001	0.00	32
12	11	1	11	10	2	1457.406	0.001	0.00	32
10	4	7	9	1	8	1458.191	0.003	0.05	32
9	7	2	8	4	5	1459.799	0.000	0.05	32
11	6	5	10	5	6	1460.911	-0.001	5.00	32
10	9	2	9	6	3	1462.142	-0.002	0.05	32
10	3	8	9	0	9	1464.711	0.002	0.05	32
11	7	5	10	4	6	1465.973	-0.003	0.25	32
11	5	6	10	4	7	1472.474	-0.002	1.25	32
11	6	6	10	3	7	1473.136	-0.002	0.05	32
11	4	7	10	3	8	1480.571	0.001	1.25	32
12	8	5	11	5	6	1489.252	-0.004	0.25	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	9	4	11	6	5	1491.152	-0.004	0.05	32
12	6	6	11	5	7	1493.484	0.003	0.05	32
11	2	9	10	1	10	1493.574	-0.002	0.25	32
12	7	6	11	4	7	1495.282	-0.003	0.25	32
11	11	0	10	10	1	1438.539	-0.002	1.25	32
12	12	1	11	11	0	1463.029	0.001	1.25	32
13	10	3	12	9	4	1471.103	0.004	0.25	32
13	11	2	12	10	3	1475.670	-0.003	0.25	32
13	12	1	12	11	2	1482.379	0.000	0.25	32
7	5	2	7	4	3	1212.791	-0.004	0.05	33
3	1	3	2	0	2	1215.705	-0.003	0.05	33
4	1	4	3	0	3	1224.850	-0.003	0.25	33
5	0	5	4	1	4	1233.987	0.003	0.05	33
4	2	3	3	1	2	1237.772	0.000	5.00	33
5	1	4	4	2	3	1246.599	0.006	0.05	33
7	0	7	6	1	6	1251.908	-0.008	0.05	33
6	2	5	5	1	4	1256.454	0.001	0.25	33
4	4	1	3	3	0	1266.226	-0.002	0.05	33
9	0	9	8	1	8	1269.318	0.000	0.05	33
6	3	4	5	2	3	1269.750	0.001	1.25	33
5	5	0	4	4	1	1292.151	0.000	5.00	33
6	5	2	5	4	1	1302.911	-0.006	0.25	33
6	6	1	5	5	0	1314.752	0.000	1.25	33
9	8	1	8	7	2	1382.173	0.001	0.25	33
5	0	5	6	1	6	1119.834	-0.006	0.05	34
4	1	4	5	0	5	1129.530	-0.005	0.05	34
2	1	2	3	0	3	1148.733	-0.007	0.05	34
1	1	0	1	0	1	1187.667	0.001	0.25	34
3	3	0	3	2	1	1194.917	0.000	0.05	34
3	2	1	3	1	2	1196.418	0.001	0.25	34
2	2	1	2	1	2	1199.856	-0.004	0.25	34
5	4	1	5	3	2	1202.205	0.002	1.25	34
2	1	2	1	0	1	1206.310	-0.002	0.05	34
3	1	2	3	0	3	1206.942	0.006	0.05	34
3	0	3	2	1	2	1214.843	0.000	0.25	34
5	4	2	5	3	3	1215.201	0.000	0.05	34
4	1	3	4	0	4	1217.826	-0.003	0.05	34
4	2	3	4	1	4	1218.139	-0.001	0.25	34
2	2	1	1	1	0	1218.752	0.000	5.00	34
5	2	3	5	1	4	1219.565	-0.004	1.25	34
3	2	2	2	1	1	1228.640	0.006	0.05	34
6	3	4	6	2	5	1230.994	-0.003	0.25	34
5	0	5	4	1	4	1233.419	-0.001	1.25	34
7	4	4	7	3	5	1234.228	0.000	0.05	34
4	2	3	3	1	2	1237.190	-0.001	5.00	34
8	5	4	8	4	5	1237.961	-0.008	0.05	34
6	2	5	6	1	6	1238.173	-0.001	0.05	34
3	3	1	2	2	0	1241.783	0.002	0.05	34
6	1	6	5	0	5	1242.446	0.002	0.05	34

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	2	4	4	1	3	1246.341	0.000	0.25	34
7	1	6	7	0	7	1248.047	0.012	0.05	34
7	0	7	6	1	6	1251.339	0.003	1.25	34
8	3	6	8	2	7	1251.692	-0.002	1.25	34
4	3	2	3	2	1	1252.157	-0.001	0.25	34
6	1	5	5	2	4	1255.815	0.000	1.25	34
6	2	5	5	1	4	1255.869	0.001	1.25	34
8	1	8	7	0	7	1260.097	-0.001	5.00	34
5	3	3	4	2	2	1260.485	0.005	0.05	34
7	1	6	6	2	5	1265.376	0.000	5.00	34
4	4	1	3	3	0	1265.564	-0.001	5.00	34
6	2	4	5	3	3	1267.885	0.001	0.25	34
9	0	9	8	1	8	1268.730	0.001	1.25	34
4	4	0	3	3	1	1268.844	0.002	5.00	34
6	3	4	5	2	3	1269.131	0.000	0.25	34
4	3	1	3	2	2	1272.346	0.007	0.05	34
8	2	7	7	1	6	1274.795	0.000	1.25	34
10	1	10	9	0	9	1277.229	-0.001	1.25	34
9	1	8	8	2	7	1284.085	0.001	0.05	34
6	4	3	5	3	2	1285.131	0.009	0.25	34
11	0	11	10	1	10	1285.596	-0.004	0.25	34
8	3	6	7	2	5	1288.632	-0.001	0.05	34
5	5	1	4	4	0	1289.715	0.001	1.25	34
5	5	0	4	4	1	1291.483	-0.001	5.00	34
5	4	1	4	3	2	1292.056	0.000	5.00	34
12	1	12	11	0	11	1293.844	0.003	0.25	34
9	2	7	8	3	6	1298.490	0.003	0.25	34
6	5	2	5	4	1	1302.179	0.005	0.05	34
9	3	6	8	4	5	1311.975	0.005	0.05	34
6	6	1	5	5	0	1314.020	0.001	5.00	34
6	6	0	5	5	1	1314.896	-0.002	5.00	34
10	3	7	9	4	6	1322.346	-0.001	0.05	34
10	4	7	9	3	6	1322.393	-0.001	0.05	34
7	6	2	6	5	1	1328.008	0.011	0.05	34
7	6	1	6	5	2	1334.510	-0.001	5.00	34
7	7	1	6	6	0	1338.434	0.003	0.25	34
7	7	0	6	6	1	1338.846	0.001	5.00	34
7	5	2	6	4	3	1340.189	0.004	0.25	34
8	7	2	7	6	1	1353.846	0.015	0.05	34
7	4	3	6	3	4	1354.578	0.006	0.05	34
8	7	1	7	6	2	1357.501	-0.005	0.05	34
8	8	1	7	7	0	1362.942	0.000	5.00	34
9	7	2	8	6	3	1379.984	0.000	0.25	34
9	8	1	8	7	2	1381.400	0.000	1.25	34

APPENDIX C

WEIGHTED AVERAGED GSCD'S OF H_2^{32}S

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
2	2	0	0	0	0	58.361	-0.008	1.56	32
2	2	0	2	0	2	20.352	-0.001	5.25	32
2	1	1	1	1	1	36.051	0.001	5.16	32
2	2	1	1	0	1	41.415	0.000	9.81	32
2	0	2	0	0	0	38.017	0.001	2.26	32
2	1	2	1	1	0	18.922	0.000	13.24	32
3	3	0	1	1	0	98.019	0.003	4.58	32
3	3	0	2	1	2	79.095	0.001	7.50	32
3	3	0	3	1	2	22.339	0.003	22.13	32
3	2	1	1	0	1	93.621	-0.001	4.90	32
3	3	1	1	1	1	100.248	-0.002	0.85	32
3	2	1	2	2	1	52.206	-0.001	16.25	32
3	3	1	2	1	1	64.200	0.000	3.75	32
3	2	1	3	0	3	35.945	0.001	13.86	32
3	3	1	3	1	3	43.873	-0.002	1.39	32
3	1	2	1	1	0	75.682	0.001	3.98	32
3	2	2	2	2	0	38.025	0.001	11.08	32
3	1	2	2	1	2	56.759	0.000	17.29	32
3	2	2	2	0	2	58.375	-0.001	2.90	32
3	0	3	1	0	1	57.677	-0.001	11.29	32
3	1	3	1	1	1	56.373	-0.002	7.78	32
3	0	3	2	2	1	16.261	-0.002	12.89	32
3	1	3	2	1	1	20.322	-0.003	12.05	32
4	4	0	2	2	0	138.433	0.000	0.40	32
4	4	0	2	0	2	158.778	-0.008	0.19	32
4	4	0	3	2	2	100.413	0.003	1.09	32
4	4	0	4	2	2	26.466	0.000	9.93	32
4	4	0	4	0	4	82.602	-0.028	0.00	32
4	3	1	2	1	1	131.509	0.001	0.44	32
4	4	1	2	2	1	140.495	-0.005	2.84	32
4	3	1	3	3	1	67.307	-0.001	9.87	32
4	4	1	3	2	1	88.294	0.001	5.61	32
4	3	1	3	1	3	111.183	0.000	0.62	32
4	4	1	3	0	3	124.237	0.000	2.78	32
4	3	1	4	1	3	34.508	0.000	7.58	32
4	4	1	4	2	3	47.242	-0.001	6.61	32
4	2	2	2	2	0	111.955	-0.012	0.55	32
4	2	2	2	0	2	132.322	0.002	0.06	32
4	3	2	2	1	2	135.668	-0.002	1.57	32
4	3	2	3	3	0	56.575	0.000	12.56	32
4	2	2	3	2	2	73.943	0.000	10.05	32
4	3	2	3	1	2	78.912	0.001	14.31	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
4	2	2	4	0	4	56.162	-0.002	2.40	32
4	3	2	4	1	4	59.790	0.000	6.78	32
4	1	3	2	1	1	97.001	0.001	1.67	32
4	2	3	2	2	1	93.257	0.000	9.70	32
4	1	3	3	3	1	32.802	0.002	4.34	32
4	2	3	3	2	1	41.049	-0.001	16.83	32
4	1	3	3	1	3	76.675	0.000	2.68	32
4	2	3	3	0	3	76.993	-0.001	15.75	32
4	0	4	2	0	2	76.157	0.001	0.04	32
4	1	4	2	1	2	75.875	-0.005	3.17	32
4	0	4	3	2	2	17.780	0.000	5.00	32
4	1	4	3	1	2	19.120	-0.001	8.61	32
5	5	0	3	3	0	179.285	-0.001	5.93	32
5	5	0	3	1	2	201.617	-0.004	0.44	32
5	5	0	4	3	2	122.714	0.004	2.50	32
5	5	0	5	3	2	32.940	0.001	8.31	32
5	4	1	3	2	1	169.967	-0.002	1.18	32
5	5	1	3	3	1	180.764	0.000	0.85	32
5	4	1	3	0	3	205.913	0.000	0.89	32
5	4	1	4	4	1	81.677	0.001	12.05	32
5	5	1	4	3	1	113.454	-0.002	1.46	32
5	4	1	4	2	3	128.918	-0.001	7.68	32
5	5	1	4	1	3	147.961	-0.003	0.05	32
5	4	1	5	2	3	33.994	0.000	12.05	32
5	5	1	5	3	3	51.710	-0.002	0.43	32
5	3	2	3	3	0	146.348	0.001	2.25	32
5	3	2	3	1	2	168.688	0.005	2.40	32
5	4	2	3	2	2	174.710	-0.004	0.33	32
5	4	2	4	4	0	74.304	0.000	7.86	32
5	3	2	4	3	2	89.771	-0.001	19.25	32
5	4	2	4	2	2	100.769	-0.001	6.06	32
5	3	2	4	1	4	149.560	-0.001	2.85	32
5	4	2	4	0	4	156.936	0.002	0.04	32
5	3	2	5	1	4	53.521	-0.001	10.68	32
5	4	2	5	2	4	60.846	0.005	1.78	32
5	3	2	6	1	6	35.807	0.013	0.02	32
5	2	3	3	2	1	135.975	0.000	2.90	32
5	3	3	3	3	1	129.051	-0.001	0.25	32
5	2	3	3	0	3	171.919	0.000	1.50	32
5	3	3	3	1	3	172.932	0.005	0.17	32
5	2	3	4	4	1	47.684	0.002	4.78	32
5	3	3	4	3	1	61.743	-0.001	10.06	32
5	2	3	4	2	3	94.926	0.001	16.86	32
5	3	3	4	1	3	96.252	0.000	12.07	32
5	2	3	5	0	5	77.001	0.001	2.45	32
5	3	3	5	1	5	78.050	0.002	0.60	32
5	1	4	3	1	2	115.162	0.001	8.56	32
5	2	4	3	2	2	113.871	-0.001	3.28	32
5	1	4	4	3	2	36.250	0.000	15.45	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	2	4	4	2	2	39.929	0.000	8.20	32
5	1	4	4	1	4	96.040	0.000	9.87	32
5	2	4	4	0	4	96.094	0.001	2.29	32
5	0	5	3	0	3	94.919	0.000	3.65	32
5	0	5	4	2	3	17.924	-0.001	9.25	32
5	1	5	4	1	3	18.199	-0.005	2.04	32
6	6	0	4	4	0	220.048	0.004	0.46	32
6	6	0	5	4	2	145.742	0.002	0.46	32
6	6	0	6	4	2	41.421	0.006	0.02	32
6	5	1	4	3	1	209.224	-0.015	0.12	32
6	6	1	4	4	1	220.917	0.003	0.41	32
6	5	1	4	1	3	243.736	-0.011	0.06	32
6	6	1	4	2	3	268.164	0.007	0.02	32
6	5	1	5	5	1	95.785	0.002	1.14	32
6	6	1	5	4	1	139.239	0.001	3.23	32
6	5	1	5	3	3	147.490	-0.005	1.78	32
6	6	1	5	2	3	173.234	0.002	0.10	32
6	5	1	6	3	3	35.370	-0.003	4.56	32
6	6	1	6	4	3	57.210	0.000	1.57	32
6	6	1	7	2	5	1.083	-0.015	0.08	32
6	4	2	4	4	0	178.629	0.000	2.09	32
6	4	2	4	2	2	205.096	0.001	0.16	32
6	5	2	4	3	2	213.920	0.002	1.95	32
6	5	2	4	1	4	273.708	0.001	0.02	32
6	5	2	5	5	0	91.209	0.002	8.75	32
6	4	2	5	4	2	104.324	-0.001	9.36	32
6	5	2	5	3	2	124.147	0.001	4.58	32
6	4	2	5	2	4	165.170	0.004	0.17	32
6	5	2	5	1	4	177.669	0.001	0.35	32
6	4	2	6	2	4	50.514	0.001	2.90	32
6	5	2	6	3	4	62.737	-0.001	3.56	32
6	3	3	4	3	1	173.862	-0.005	0.27	32
6	4	3	4	4	1	163.708	0.003	1.74	32
6	3	3	4	1	3	208.373	-0.002	0.06	32
6	4	3	4	2	3	210.949	0.001	4.62	32
6	3	3	5	5	1	60.415	0.004	0.36	32
6	4	3	5	4	1	82.030	0.001	12.24	32
6	3	3	5	3	3	112.122	-0.001	5.30	32
6	4	3	5	2	3	116.024	0.001	16.19	32
6	4	3	5	0	5	193.025	0.002	0.36	32
6	3	3	6	1	5	74.919	-0.002	5.13	32
6	4	3	6	2	5	77.764	0.000	6.28	32
6	2	4	4	2	2	154.583	0.001	0.96	32
6	3	4	4	3	2	151.183	0.004	2.82	32
6	2	4	4	0	4	210.743	-0.003	0.12	32
6	3	4	4	1	4	210.968	-0.001	1.10	32
6	2	4	5	4	2	53.811	-0.001	5.59	32
6	3	4	5	3	2	61.407	0.000	10.43	32
6	2	4	5	2	4	114.657	0.004	0.87	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	3	4	5	1	4	114.928	-0.001	8.32	32
6	2	4	6	0	6	96.971	-0.002	0.48	32
6	3	4	6	1	6	97.203	0.002	2.37	32
6	1	5	4	1	3	133.459	0.005	0.17	32
6	2	5	4	2	3	133.185	0.001	3.37	32
6	1	5	5	3	3	37.203	0.001	5.61	32
6	2	5	5	2	3	38.260	0.001	8.56	32
6	1	5	5	1	5	115.253	0.003	0.60	32
6	2	5	5	0	5	115.259	0.000	4.93	32
6	1	6	4	1	4	113.765	-0.002	3.06	32
6	1	6	5	1	4	17.727	-0.001	1.38	32
7	7	0	5	5	0	260.344	-0.008	0.27	32
7	7	0	5	3	2	293.287	-0.004	0.16	32
7	7	0	6	5	2	169.131	-0.014	0.27	32
7	7	0	7	5	2	51.264	-0.010	0.53	32
7	6	1	5	4	1	249.318	0.002	0.28	32
7	7	1	5	5	1	260.799	-0.003	0.08	32
7	6	1	5	2	3	283.306	-0.004	0.10	32
7	7	1	5	3	3	312.538	0.024	0.00	32
7	6	1	6	6	1	110.077	-0.001	6.34	32
7	6	1	6	4	3	167.292	0.005	2.62	32
7	6	1	7	4	3	39.421	0.003	7.80	32
7	7	1	7	3	5	141.397	0.012	0.05	32
7	5	2	5	5	0	209.083	0.004	4.72	32
7	5	2	5	3	2	242.017	-0.001	0.89	32
7	6	2	5	4	2	253.238	-0.001	0.10	32
7	6	2	6	6	0	107.497	-0.001	2.12	32
7	5	2	6	5	2	117.872	0.000	6.84	32
7	6	2	6	4	2	148.915	0.001	0.67	32
7	5	2	6	3	4	180.613	0.003	4.58	32
7	6	2	6	2	4	199.420	-0.007	0.02	32
7	5	2	7	3	4	47.878	0.001	5.15	32
7	6	2	7	4	4	65.673	-0.003	0.67	32
7	4	3	5	4	1	209.900	0.002	1.68	32
7	5	3	5	5	1	197.272	0.008	0.10	32
7	4	3	5	2	3	243.892	0.000	1.85	32
7	5	3	5	3	3	248.984	0.008	0.34	32
7	4	3	5	0	5	320.899	0.007	0.03	32
7	4	3	6	6	1	70.655	-0.005	0.76	32
7	5	3	6	5	1	101.484	0.003	6.52	32
7	4	3	6	4	3	127.869	0.000	9.07	32
7	5	3	6	3	3	136.854	0.001	3.14	32
7	4	3	6	2	5	205.630	-0.003	0.62	32
7	5	3	6	1	5	211.777	0.003	0.04	32
7	4	3	7	2	5	71.757	-0.001	7.37	32
7	5	3	7	3	5	77.847	0.001	2.00	32
7	3	4	5	3	2	194.139	-0.002	4.62	32
7	4	4	5	4	2	187.552	-0.011	0.33	32
7	3	4	5	1	4	247.657	-0.005	0.71	32



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	4	4	5	2	4	248.407	0.003	0.16	32
7	3	4	6	5	2	69.996	0.001	3.68	32
7	4	4	6	4	2	83.239	0.001	1.21	32
7	3	4	6	3	4	132.733	0.000	11.73	32
7	4	4	6	2	4	133.752	0.001	1.75	32
7	3	4	6	1	6	229.930	-0.005	0.10	32
7	4	4	6	0	6	230.738	0.014	0.01	32
7	3	4	7	1	6	95.529	0.001	3.90	32
7	4	4	7	2	6	96.316	0.000	2.12	32
7	4	4	8	0	8	79.215	-0.046	0.00	32
7	2	5	5	2	3	172.137	0.003	4.16	32
7	3	5	5	3	3	171.133	0.003	2.07	32
7	2	5	5	0	5	249.135	0.001	0.69	32
7	3	5	5	1	5	249.183	0.005	0.12	32
7	2	5	6	4	3	56.111	0.000	8.31	32
7	3	5	6	3	3	59.007	0.000	6.71	32
7	2	5	6	2	5	133.876	0.001	10.04	32
7	3	5	6	1	5	133.926	-0.002	5.78	32
7	2	5	7	0	7	116.508	0.000	3.73	32
7	3	5	7	1	7	116.512	-0.040	0.00	32
7	1	6	5	3	2	98.593	-0.020	0.02	32
7	1	6	5	1	4	152.133	-0.001	4.87	32
7	1	6	6	3	4	37.206	0.001	7.75	32
7	2	6	6	2	4	37.437	0.002	0.51	32
7	1	6	6	1	6	134.406	-0.001	4.12	32
7	2	6	6	0	6	134.408	0.000	0.25	32
7	0	7	5	0	5	132.625	-0.001	8.27	32
7	0	7	6	2	5	17.370	0.003	8.41	32
8	8	0	7	6	2	192.589	0.013	0.41	32
8	8	0	8	6	2	61.736	0.010	0.02	32
8	7	1	6	5	1	289.787	-0.012	0.06	32
8	8	1	6	6	1	300.286	-0.004	0.27	32
8	8	1	6	4	3	357.495	-0.004	0.05	32
8	7	1	7	7	1	124.780	0.000	0.58	32
8	8	1	7	6	1	190.206	-0.006	0.24	32
8	6	2	6	4	2	279.762	-0.002	0.06	32
8	7	2	6	5	2	292.579	-0.001	0.89	32
8	6	2	6	2	4	330.291	0.014	0.02	32
8	7	2	6	3	4	355.315	-0.004	0.08	32
8	7	2	7	7	0	123.435	0.000	5.25	32
8	6	2	7	6	2	130.849	-0.001	0.16	32
8	7	2	7	5	2	174.705	-0.003	0.96	32
8	6	2	7	4	4	196.524	-0.002	0.16	32
8	7	2	7	3	4	222.588	0.003	0.25	32
8	6	2	8	4	4	46.631	0.002	2.15	32
8	7	2	8	5	4	69.739	-0.002	1.03	32
8	5	3	6	5	1	243.531	0.010	0.10	32
8	6	3	6	6	1	229.882	-0.002	0.71	32
8	6	3	6	4	3	287.091	-0.002	1.63	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	6	3	6	2	5	364.853	-0.004	0.10	32
8	6	3	7	6	1	119.803	-0.003	6.37	32
8	5	3	7	5	3	142.040	0.000	2.65	32
8	6	3	7	4	3	159.224	0.000	6.63	32
8	5	3	7	3	5	219.885	-0.001	0.03	32
8	6	3	7	2	5	230.981	-0.001	1.07	32
8	5	3	8	3	5	67.710	-0.002	2.03	32
8	6	3	8	4	5	78.574	-0.004	0.82	32
8	4	4	6	4	2	233.130	-0.005	0.17	32
8	5	4	6	5	2	222.844	0.005	0.51	32
8	4	4	6	2	4	283.659	0.011	0.01	32
8	5	4	6	3	4	285.579	0.001	0.46	32
8	4	4	7	6	2	84.223	0.002	1.39	32
8	5	4	7	5	2	104.963	-0.005	0.47	32
8	4	4	7	4	4	149.887	-0.010	2.23	32
8	5	4	7	3	4	152.847	0.002	3.04	32
8	4	4	7	2	6	246.210	-0.003	0.03	32
8	5	4	7	1	6	248.373	0.000	0.28	32
8	4	4	8	2	6	93.277	0.001	5.09	32
8	5	4	8	3	6	95.428	0.001	5.83	32
8	3	5	6	3	3	211.177	-0.005	0.41	32
8	4	5	6	4	3	208.511	-0.005	1.54	32
8	3	5	6	1	5	286.105	0.003	0.08	32
8	4	5	6	2	5	286.277	-0.003	0.53	32
8	3	5	7	5	3	74.328	0.000	2.12	32
8	4	5	7	4	3	80.646	-0.001	8.18	32
8	3	5	7	3	5	152.174	-0.001	1.35	32
8	4	5	7	2	5	152.403	-0.002	7.34	32
8	3	5	8	1	7	115.204	0.002	0.48	32
8	4	5	8	2	7	115.387	0.000	2.85	32
8	2	6	6	2	4	190.370	-0.001	0.04	32
8	3	6	6	3	4	190.148	-0.003	1.42	32
8	2	6	6	0	6	287.357	0.013	0.01	32
8	3	6	6	1	6	287.352	0.000	0.27	32
8	2	6	7	4	4	56.619	-0.001	5.15	32
8	3	6	7	3	4	57.418	0.000	6.72	32
8	2	6	7	2	6	152.935	-0.001	2.06	32
8	3	6	7	1	6	152.947	0.001	3.92	32
8	2	6	8	0	8	135.834	-0.048	0.00	32
8	3	6	8	1	8	135.889	-0.001	5.30	32
8	2	7	6	2	5	170.895	0.003	9.89	32
8	2	7	7	2	5	37.019	0.002	7.37	32
8	2	7	7	0	7	153.523	-0.002	6.93	32
8	1	8	6	1	6	151.460	-0.002	6.90	32
8	1	8	7	1	6	17.056	0.000	9.52	32
9	8	1	7	6	1	330.097	-0.006	0.10	32
9	8	1	8	8	1	139.892	0.001	0.48	32
9	8	1	9	6	3	55.469	-0.002	0.15	32
9	7	2	7	3	4	366.395	0.003	0.41	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	7	2	8	7	2	143.808	0.001	0.57	32
9	7	2	8	5	4	213.549	0.001	0.34	32
9	7	2	9	5	4	47.895	0.000	1.35	32
9	6	3	7	6	1	274.627	-0.005	0.10	32
9	7	3	7	7	1	261.795	0.003	0.03	32
9	7	3	8	7	1	137.014	0.002	0.06	32
9	6	3	8	6	3	154.826	0.000	0.48	32
9	7	3	8	5	3	183.286	-0.004	0.05	32
9	6	3	8	4	5	233.404	0.001	0.10	32
9	6	3	9	4	5	63.423	-0.001	5.00	32
9	6	4	7	6	2	256.932	0.009	0.05	32
9	6	4	7	4	4	322.600	0.001	0.10	32
9	5	4	8	7	2	95.912	0.000	0.48	32
9	6	4	8	6	2	126.077	0.004	2.10	32
9	5	4	8	5	4	165.651	-0.002	5.00	32
9	6	4	8	4	4	172.707	0.004	1.34	32
9	5	4	9	3	6	89.885	-0.003	0.48	32
9	6	4	9	4	6	94.737	-0.001	0.12	32
9	4	5	7	4	3	250.625	-0.001	3.92	32
9	5	5	7	5	3	245.095	-0.004	0.10	32
9	4	5	7	2	5	322.383	-0.001	0.67	32
9	5	5	7	3	5	322.943	-0.003	0.03	32
9	4	5	8	6	3	91.402	0.000	1.75	32
9	5	5	8	5	3	103.059	0.000	0.06	32
9	4	5	8	4	5	169.979	0.000	5.24	32
9	5	5	8	3	5	170.771	0.000	0.10	32
9	4	5	9	2	7	113.448	0.001	5.12	32
9	5	5	9	3	7	114.057	0.005	0.10	32
9	3	6	7	3	4	228.609	0.000	1.92	32
9	4	6	7	4	4	227.862	0.001	0.23	32
9	3	6	7	1	6	324.137	-0.001	0.41	32
9	4	6	7	2	6	324.176	-0.001	0.04	32
9	3	6	8	5	4	75.763	-0.002	3.12	32
9	4	6	8	4	4	77.967	0.003	2.23	32
9	3	6	8	3	6	171.193	0.001	2.67	32
9	4	6	8	2	6	171.243	0.002	2.07	32
9	3	6	9	1	8	134.471	-0.004	0.24	32
9	2	7	7	2	5	208.943	0.007	0.85	32
9	2	7	7	0	7	325.440	-0.004	0.38	32
9	2	7	8	4	5	56.530	-0.002	4.47	32
9	3	7	8	3	5	56.739	0.021	0.00	32
9	2	7	8	2	7	171.919	0.000	4.46	32
9	3	7	8	1	7	171.920	-0.001	0.13	32
9	2	7	9	0	9	155.166	-0.001	0.32	32
9	1	8	7	1	6	189.661	-0.002	11.25	32
9	1	8	8	3	6	36.720	0.003	7.94	32
9	1	8	8	1	8	172.607	0.000	12.17	32
9	2	8	8	0	8	172.603	-0.004	0.08	32
9	0	9	7	0	7	170.272	-0.005	9.38	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	0	9	8	2	7	16.751	-0.001	6.56	32
10	8	3	9	8	1	153.353	-0.002	0.48	32
10	8	3	9	6	3	208.822	-0.004	0.08	32
10	7	4	9	7	2	146.042	0.001	1.25	32
10	7	4	9	5	4	193.937	0.001	1.25	32
10	6	4	10	4	6	85.266	-0.002	0.25	32
10	7	4	10	5	6	94.527	0.000	2.00	32
10	6	5	9	6	3	125.817	0.001	2.00	32
10	6	5	9	4	5	189.240	-0.001	2.00	32
10	5	5	10	3	7	110.978	-0.002	0.10	32
10	6	5	10	4	7	112.633	-0.002	2.00	32
10	4	6	9	6	4	94.357	-0.007	0.05	32
10	5	6	9	5	4	99.411	0.002	5.08	32
10	4	6	9	4	6	189.096	-0.006	0.10	32
10	5	6	9	3	6	189.297	0.000	0.71	32
10	5	6	10	3	8	132.934	0.002	2.00	32
10	4	7	8	4	5	246.590	0.005	2.40	32
10	4	7	8	2	7	361.967	-0.005	0.01	32
10	3	7	9	5	5	75.985	-0.005	0.10	32
10	4	7	9	4	5	76.605	-0.001	5.62	32
10	3	7	9	3	7	190.044	0.001	1.67	32
10	4	7	9	2	7	190.052	-0.001	5.66	32
10	3	8	8	3	6	227.560	0.003	1.70	32
10	3	8	8	1	8	363.444	-0.003	0.10	32
10	3	8	9	3	6	56.365	0.000	5.46	32
10	3	8	9	1	8	190.838	-0.002	1.53	32
10	3	8	10	1	10	174.378	-0.003	0.57	32
10	2	9	8	2	7	208.404	0.001	6.90	32
10	1	9	9	3	7	36.483	0.001	0.01	32
10	2	9	9	2	7	36.484	0.000	7.74	32
10	2	9	9	0	9	191.649	-0.002	3.48	32
10	0	10	8	0	8	189.057	-0.008	0.02	32
10	1	10	8	1	8	189.065	0.000	8.75	32
10	0	10	9	2	8	16.466	0.007	0.01	32
10	1	10	9	1	8	16.458	-0.001	6.06	32
11	8	3	11	6	5	58.467	-0.007	0.10	32
11	7	4	11	5	6	79.820	-0.001	0.25	32
11	6	5	11	4	7	107.435	0.001	0.25	32
11	7	5	11	5	7	111.309	0.006	0.05	32
11	4	7	9	4	5	284.467	0.001	0.08	32
11	4	7	10	6	5	95.226	0.001	2.00	32
11	5	7	10	5	5	96.927	0.000	0.10	32
11	4	7	10	4	7	207.859	-0.001	1.32	32
11	5	7	10	3	7	207.905	-0.002	0.05	32
11	3	8	9	3	6	265.152	-0.007	0.03	32
11	3	8	10	5	6	75.860	-0.002	2.00	32
11	4	8	10	4	6	76.016	-0.002	0.41	32
11	3	8	10	3	8	208.794	0.000	1.34	32
11	2	9	9	2	7	246.182	-0.003	0.38	32

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
11	2	9	10	4	7	56.132	0.000	5.40	32
11	2	9	10	2	9	209.696	-0.005	0.69	32
11	2	9	11	0	11	193.526	0.000	0.04	32
11	1	10	9	1	8	227.117	0.003	4.75	32
11	1	10	10	3	8	36.276	0.002	5.91	32
11	1	10	10	1	10	210.656	0.001	1.81	32
11	0	11	9	0	9	207.827	0.001	4.43	32
11	0	11	10	2	9	16.175	0.000	6.02	32
12	5	8	11	5	6	95.785	-0.002	1.25	32
12	5	8	11	3	8	226.461	0.006	0.48	32
12	5	8	12	3	10	170.479	0.006	0.41	32
12	4	9	10	4	7	283.594	0.002	0.21	32
12	4	9	11	4	7	75.732	0.000	1.25	32
12	4	9	11	2	9	227.461	0.001	0.13	32
12	3	10	10	3	8	264.768	-0.008	0.44	32
12	3	10	11	3	8	55.982	0.000	2.09	32
12	3	10	11	1	10	228.491	-0.011	0.31	32
12	2	11	10	2	9	245.793	0.001	2.59	32
12	2	11	11	2	9	36.092	0.001	5.19	32
12	2	11	11	0	11	229.614	-0.003	0.69	32
12	1	12	10	1	10	226.559	0.004	3.87	32
12	1	12	11	1	10	15.899	-0.001	5.28	32
13	3	10	11	3	8	302.022	-0.003	0.10	32
13	3	10	12	3	10	246.049	0.006	0.06	32
13	2	11	11	2	9	283.329	-0.002	0.13	32
13	1	12	11	1	10	264.437	0.002	0.71	32
13	1	12	12	1	12	248.531	-0.004	0.10	32
13	0	13	11	0	11	245.249	-0.001	1.18	32
13	0	13	12	2	11	15.632	-0.001	2.00	32
14	3	12	13	3	10	55.799	-0.004	0.41	32
14	2	13	12	2	11	283.030	-0.007	0.13	32
14	1	14	12	1	12	263.903	-0.005	2.40	32
14	1	14	13	1	12	15.374	0.001	0.48	32
15	1	14	14	3	12	35.691	0.008	0.08	32
15	0	15	13	0	13	282.533	0.008	0.60	32

APPENDIX D

ASSIGNED TRANSITIONS OF ν_2 OF H_2Se

UPPER			LOWER			OBSERVED (cm^{-1})	OBS-CALC (cm^{-1})	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c				
10	1	10	11	0	11	942.592	-0.016	0.01	74
9	0	9	10	1	10	950.999	-0.002	0.00	74
7	1	6	8	2	7	962.885	-0.008	0.01	74
5	2	3	6	3	4	971.716	-0.012	0.05	74
6	1	6	7	0	7	975.696	-0.010	0.05	74
5	1	4	6	2	5	978.052	-0.004	0.25	74
4	1	4	5	0	5	991.760	-0.008	0.01	74
3	0	3	4	1	4	999.662	-0.006	0.05	74
2	1	2	3	0	3	1007.508	-0.010	0.01	74
3	3	0	3	2	1	1042.886	0.000	0.05	74
5	5	0	5	4	1	1049.603	-0.002	0.01	74
5	4	1	5	3	2	1050.586	-0.012	0.00	74
2	1	2	1	0	1	1054.853	-0.001	0.01	74
3	0	3	2	1	2	1062.365	-0.003	0.05	74
6	1	6	5	0	5	1085.179	-0.001	0.25	74
3	3	0	2	2	1	1088.514	-0.004	0.01	74
4	3	2	3	2	1	1090.766	-0.009	0.01	74
7	0	7	6	1	6	1092.584	0.000	0.01	74
6	2	5	5	1	4	1096.044	0.006	0.01	74
9	0	9	8	1	8	1107.105	0.004	0.05	74
10	2	9	9	1	8	1127.088	-0.004	0.01	74
9	3	6	8	4	5	1142.170	0.009	0.01	74
15	0	15	14	1	14	1148.291	-0.004	0.01	74
10	4	7	9	3	6	1150.696	0.008	0.01	74
9	9	0	8	8	1	1197.966	0.000	0.25	74
8	5	4	7	2	5	1207.214	-0.004	0.01	74
11	11	0	10	10	1	1236.665	0.003	0.01	74
13	0	13	14	1	14	916.809	-0.010	0.25	76
12	3	10	13	2	11	920.947	0.002	0.25	76
12	1	12	13	0	13	925.427	-0.002	0.25	76
11	2	9	12	3	10	928.404	0.002	0.05	76
6	6	1	7	7	0	930.892	0.002	0.25	76
11	0	11	12	1	12	933.972	0.004	1.25	76
10	3	8	11	2	9	935.787	-0.005	0.05	76
9	3	6	10	4	7	938.442	0.000	0.25	76
10	2	9	11	1	10	939.404	0.001	1.25	76
10	1	10	11	0	11	942.436	0.002	1.25	76
9	2	7	10	3	8	943.117	0.003	0.25	76
5	5	1	6	6	0	943.641	0.003	0.05	76
8	4	5	9	3	6	945.188	0.005	0.05	76
5	5	0	6	6	1	946.432	-0.004	0.05	76
9	1	8	10	2	9	947.252	0.003	1.25	76

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	0	9	10	1	10	950.827	0.002	1.25	76
7	3	4	8	4	5	951.777	-0.003	0.05	76
8	2	7	9	1	8	955.021	-0.001	1.25	76
4	4	1	5	5	0	956.795	-0.003	0.05	76
7	2	5	8	3	6	957.533	-0.004	0.25	76
6	4	3	7	3	4	958.595	0.003	0.05	76
8	1	8	9	0	9	959.139	0.000	5.00	76
4	4	0	5	5	1	960.701	-0.010	0.05	76
7	1	6	8	2	7	962.721	0.000	1.25	76
5	3	2	6	4	3	963.718	-0.004	0.05	76
6	3	4	7	2	5	964.636	-0.007	0.05	76
7	0	7	8	1	8	967.372	-0.002	1.25	76
6	2	5	7	1	6	970.340	-0.002	0.05	76
5	2	3	6	3	4	971.553	-0.005	0.25	76
6	1	6	7	0	7	975.528	0.001	1.25	76
5	1	4	6	2	5	977.881	0.001	1.25	76
4	3	2	5	2	3	979.009	0.000	0.25	76
5	0	5	6	1	6	983.597	-0.001	0.25	76
2	2	1	3	3	0	984.450	0.000	0.25	76
4	2	3	5	1	4	985.354	-0.003	0.05	76
3	3	1	4	2	2	987.620	0.000	0.05	76
2	2	0	3	3	1	990.860	0.000	0.25	76
4	1	4	5	0	5	991.585	-0.001	1.25	76
7	1	6	7	2	5	993.062	-0.003	0.25	76
5	0	5	5	1	4	998.181	0.003	1.25	76
3	0	3	4	1	4	999.484	0.000	1.25	76
2	2	1	3	1	2	1000.998	0.001	0.25	76
7	2	5	7	3	4	1004.045	-0.001	0.05	76
1	1	0	2	2	1	1006.515	0.001	0.25	76
2	1	2	3	0	3	1007.330	-0.001	0.25	76
5	1	4	5	2	3	1008.725	-0.002	0.25	76
9	4	5	9	5	4	1011.579	0.001	0.25	76
1	0	1	2	1	2	1014.756	-0.001	0.25	76
1	1	1	2	0	2	1015.321	-0.008	0.25	76
4	2	3	4	3	2	1016.085	0.000	1.25	76
8	5	4	8	6	3	1017.280	0.000	0.05	76
5	3	3	5	4	2	1017.977	0.003	0.05	76
5	2	3	5	3	2	1019.361	0.000	1.25	76
6	4	3	6	5	2	1020.093	0.002	0.25	76
2	1	2	2	2	1	1021.942	-0.003	0.25	76
4	3	2	4	4	1	1023.435	0.001	0.25	76
3	1	2	3	2	1	1024.998	0.000	1.25	76
7	4	3	7	5	2	1026.162	-0.001	0.25	76
4	2	2	4	3	1	1027.065	-0.004	0.25	76
5	3	2	5	4	1	1029.282	0.000	1.25	76
3	2	1	3	3	0	1031.064	0.003	1.25	76
6	4	2	6	5	1	1031.483	0.005	0.25	76
5	4	1	5	5	0	1031.896	-0.004	0.05	76
7	5	2	7	6	1	1033.537	0.002	0.25	76

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
1	1	0	1	0	1	1039.220	-0.001	1.25	76
2	2	0	2	1	1	1040.568	-0.003	1.25	76
3	3	0	3	2	1	1042.668	-0.002	5.00	76
4	4	0	4	3	1	1045.578	-0.006	1.25	76
2	1	1	2	0	2	1046.934	-0.002	0.05	76
3	2	1	3	1	2	1047.606	-0.003	1.25	76
2	2	1	2	1	2	1048.461	0.002	0.25	76
5	5	0	5	4	1	1049.348	0.001	5.00	76
5	4	1	5	3	2	1050.406	-0.004	0.25	76
4	4	1	4	3	2	1053.171	-0.001	0.25	76
2	1	2	1	0	1	1054.651	-0.001	1.25	76
3	2	2	3	1	3	1056.313	0.006	0.05	76
5	5	1	5	4	2	1056.453	0.003	0.05	76
4	2	2	4	1	3	1057.284	-0.004	1.25	76
4	3	2	4	2	3	1058.096	0.000	1.25	76
5	3	2	5	2	3	1058.661	-0.004	0.25	76
7	7	0	7	6	1	1059.165	0.002	0.25	76
6	4	2	6	3	3	1060.149	0.000	1.25	76
6	6	1	6	5	2	1060.268	0.001	0.05	76
5	4	2	5	3	3	1060.407	-0.003	0.25	76
3	0	3	2	1	2	1062.166	-0.001	0.25	76
6	5	2	6	4	3	1063.280	-0.001	1.25	76
2	2	1	1	1	0	1064.076	0.003	5.00	76
9	8	1	9	7	2	1065.689	0.002	0.25	76
5	2	3	5	1	4	1066.502	0.005	0.05	76
5	3	3	5	2	4	1066.627	-0.007	1.25	76
7	6	2	7	5	3	1066.719	-0.008	0.05	76
6	4	3	6	3	4	1068.997	0.001	0.05	76
4	1	4	3	0	3	1069.881	-0.003	1.25	76
3	1	2	2	2	1	1070.644	0.006	0.05	76
7	4	3	7	3	4	1070.841	0.000	1.25	76
3	2	2	2	1	1	1072.283	-0.004	0.25	76
5	1	4	5	0	5	1072.997	0.002	0.25	76
6	3	4	6	2	5	1075.308	0.000	0.05	76
5	0	5	4	1	4	1077.480	0.004	1.25	76
7	3	4	7	2	5	1077.857	-0.013	0.05	76
4	2	3	3	1	2	1079.877	-0.001	1.25	76
6	2	5	6	1	6	1081.246	-0.004	1.25	76
3	3	1	2	2	0	1081.973	0.000	1.25	76
10	8	3	10	7	4	1082.757	0.003	0.25	76
7	2	5	7	1	6	1083.904	0.002	1.25	76
9	6	4	9	5	5	1084.132	-0.005	0.25	76
6	1	6	5	0	5	1084.972	-0.002	5.00	76
4	2	2	3	3	1	1087.008	0.004	0.25	76
5	1	4	4	2	3	1087.817	0.002	0.05	76
3	3	0	2	2	1	1088.310	0.000	1.25	76
7	1	6	7	0	7	1089.394	-0.005	1.25	76
4	3	2	3	2	1	1090.551	0.002	5.00	76
7	0	7	6	1	6	1092.377	0.002	5.00	76

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	2	5	5	1	4	1095.827	-0.002	5.00	76
5	2	3	4	3	2	1097.231	0.006	5.00	76
5	3	3	4	2	2	1098.046	-0.003	0.25	76
8	1	8	7	0	7	1099.680	0.000	5.00	76
9	2	7	9	1	8	1100.770	0.005	0.05	76
7	1	6	6	2	5	1103.731	0.001	5.00	76
10	4	7	10	3	8	1104.331	-0.006	0.25	76
6	3	4	5	2	3	1106.157	0.001	1.25	76
9	0	9	8	1	8	1106.887	0.000	5.00	76
11	4	7	11	3	8	1108.131	0.001	0.05	76
5	4	2	4	3	1	1109.419	0.005	0.05	76
8	2	7	7	1	6	1111.538	-0.001	5.00	76
10	2	9	10	1	10	1113.243	0.008	0.05	76
6	3	3	5	4	2	1114.868	0.002	0.05	76
9	1	8	8	2	7	1119.256	0.003	0.05	76
11	0	11	10	1	10	1121.007	-0.001	5.00	76
4	3	2	3	0	3	1121.572	-0.002	0.05	76
5	5	0	4	4	1	1123.157	0.001	5.00	76
10	2	9	9	1	8	1126.876	0.002	5.00	76
6	5	2	5	4	1	1128.840	-0.001	5.00	76
9	2	7	8	3	6	1130.917	0.001	5.00	76
7	4	3	6	5	2	1132.340	0.000	5.00	76
8	4	5	7	3	4	1133.364	-0.002	0.25	76
11	1	10	10	2	9	1134.399	-0.003	0.05	76
13	0	13	12	1	12	1134.737	0.000	1.25	76
7	5	3	6	4	2	1136.176	0.000	0.05	76
6	6	1	5	5	0	1138.464	0.000	5.00	76
10	3	8	9	2	7	1139.003	-0.001	5.00	76
12	2	11	11	1	10	1141.834	-0.003	1.25	76
9	3	6	8	4	5	1141.942	0.001	1.25	76
8	4	4	7	5	3	1142.931	-0.006	0.25	76
8	5	4	7	4	3	1143.910	0.002	5.00	76
6	5	1	5	4	2	1145.163	0.000	0.25	76
11	2	9	10	3	8	1146.999	0.000	5.00	76
15	0	15	14	1	14	1148.070	0.001	1.25	76
13	1	12	12	2	11	1149.182	0.001	5.00	76
8	5	3	7	6	2	1149.431	0.000	0.05	76
10	4	7	9	3	6	1150.464	-0.001	5.00	76
9	4	5	8	5	4	1152.304	-0.008	1.25	76
9	5	5	8	4	4	1152.517	0.005	0.05	76
16	1	16	15	0	15	1154.582	-0.003	0.25	76
12	3	10	11	2	9	1154.902	0.000	1.25	76
8	6	3	7	5	2	1156.189	0.004	0.05	76
14	2	13	13	1	12	1156.435	0.002	1.25	76
6	6	1	5	3	2	1156.983	0.008	0.05	76
7	7	1	6	6	0	1157.829	0.000	1.25	76
6	5	2	5	2	3	1158.224	0.000	0.25	76
11	3	8	10	4	7	1158.890	0.003	1.25	76
7	7	0	6	6	1	1159.738	-0.001	5.00	76



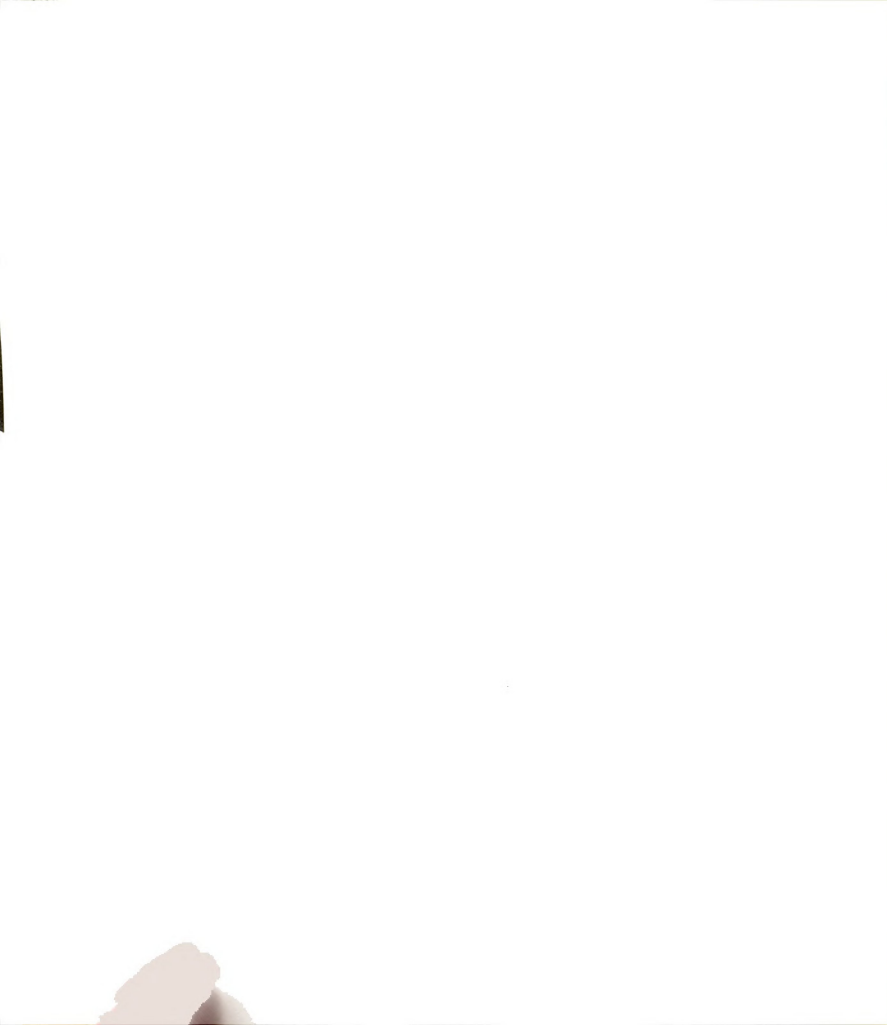
UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	4	6	9	5	5	1161.306	0.003	0.05	76
10	5	6	9	4	5	1161.346	0.004	0.25	76
7	6	1	6	5	2	1162.322	-0.004	0.25	76
13	2	11	12	3	10	1162.714	0.000	5.00	76
15	1	14	14	2	13	1163.596	0.002	0.05	76
6	4	3	5	1	4	1163.935	0.000	0.25	76
9	6	3	8	7	2	1165.947	0.005	0.05	76
12	4	9	11	3	8	1167.212	-0.003	5.00	76
8	7	2	7	6	1	1169.087	-0.001	5.00	76
11	4	7	10	5	6	1170.138	0.003	5.00	76
16	2	15	15	1	14	1170.665	0.002	0.25	76
10	6	5	9	5	4	1171.920	0.002	1.25	76
13	3	10	12	4	9	1175.450	0.002	1.25	76
8	8	1	7	7	0	1177.306	0.001	5.00	76
8	8	0	7	7	1	1178.583	0.000	1.25	76
12	5	8	11	4	7	1178.854	-0.003	0.25	76
8	7	1	7	6	2	1179.850	-0.001	0.25	76
11	5	6	10	6	5	1180.764	-0.003	1.25	76
7	4	3	6	3	4	1181.243	-0.002	1.25	76
7	5	3	6	2	4	1182.232	0.000	0.05	76
14	4	11	13	3	10	1183.587	-0.002	0.25	76
10	7	4	9	6	3	1183.621	0.002	0.05	76
16	3	14	15	2	13	1185.609	-0.002	0.25	76
13	4	9	12	5	8	1187.476	0.001	1.25	76
7	3	4	6	2	5	1188.533	-0.002	0.25	76
7	4	4	6	1	5	1188.614	0.006	0.05	76
12	6	7	11	5	6	1189.910	-0.001	0.25	76
11	6	5	10	7	4	1190.445	-0.001	0.25	76
11	7	5	10	6	4	1191.631	-0.004	0.05	76
17	2	15	16	3	14	1193.062	0.002	0.05	76
7	2	5	6	1	6	1194.815	0.005	0.05	76
9	9	0	8	8	1	1197.689	0.002	0.25	76
9	8	1	8	7	2	1197.823	0.000	5.00	76
10	8	3	9	7	2	1197.910	0.000	1.25	76
8	5	3	7	4	4	1198.795	-0.005	0.05	76
13	5	8	12	6	7	1198.869	0.002	0.25	76
8	8	1	7	5	2	1200.509	0.004	0.25	76
12	7	6	11	6	5	1200.568	0.003	0.25	76
8	6	3	7	3	4	1200.863	0.000	1.25	76
9	7	2	8	6	3	1204.847	-0.001	5.00	76
8	5	4	7	2	5	1206.978	0.004	0.05	76
10	9	2	9	8	1	1210.393	0.000	5.00	76
12	8	5	11	7	4	1211.756	-0.002	0.05	76
8	4	5	7	1	6	1213.221	-0.002	0.25	76
9	6	3	8	5	4	1216.052	0.002	0.05	76
10	10	0	9	9	1	1216.965	-0.002	1.25	76
8	3	6	7	0	7	1219.073	0.003	0.25	76
10	8	2	9	7	3	1221.623	-0.003	0.05	76
9	5	4	8	4	5	1224.970	0.001	1.25	76

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	9	4	11	8	3	1225.840	0.001	0.25	76
11	10	2	10	9	1	1231.101	0.000	0.05	76
9	4	5	8	3	6	1231.717	0.003	0.25	76
10	7	3	9	6	4	1232.912	-0.001	0.05	76
11	10	1	10	9	2	1235.187	0.000	1.25	76
11	11	1	10	10	0	1235.985	0.002	0.25	76
11	11	0	10	10	1	1236.351	0.000	5.00	76
9	3	6	8	2	7	1237.684	-0.001	0.25	76
10	8	3	9	5	4	1239.418	-0.002	0.25	76
12	10	3	11	9	2	1241.181	-0.004	0.25	76
10	7	4	9	4	5	1244.220	0.001	0.25	76
11	8	3	10	7	4	1249.395	-0.001	0.25	76
10	6	5	9	3	6	1250.378	0.000	0.05	76
12	11	2	11	10	1	1251.720	0.000	1.25	76
12	12	1	11	11	0	1255.531	-0.001	0.25	76
10	5	6	9	2	7	1256.388	-0.002	0.25	76
11	7	4	10	6	5	1260.743	0.000	0.05	76
10	4	7	9	1	8	1261.990	0.002	0.05	76
13	13	0	12	12	1	1275.209	0.001	0.25	76
11	5	6	10	4	7	1275.106	-0.001	0.05	76
11	4	7	10	3	8	1280.834	0.000	0.05	76
11	3	8	10	2	9	1286.130	0.005	0.05	76
13	0	13	14	1	14	916.742	-0.002	0.25	77
12	3	10	13	2	11	920.866	0.004	0.05	77
12	1	12	13	0	13	925.355	-0.002	0.05	77
11	2	9	12	3	10	928.314	-0.006	0.05	77
6	6	1	7	7	0	930.816	-0.008	0.05	77
11	1	10	12	2	11	931.413	0.004	0.05	77
9	3	6	10	4	7	938.355	-0.012	0.05	77
10	2	9	11	1	10	939.322	-0.001	0.25	77
10	1	10	11	0	11	942.361	0.001	0.05	77
9	2	7	10	3	8	943.036	0.001	0.05	77
8	4	5	9	3	6	945.100	-0.008	0.05	77
5	5	0	6	6	1	946.380	-0.001	0.05	77
9	1	8	10	2	9	947.166	-0.003	0.05	77
8	3	6	9	2	7	950.287	0.001	0.05	77
9	0	9	10	1	10	950.750	0.001	0.25	77
7	3	4	8	4	5	951.710	0.004	1.25	77
8	2	7	9	1	8	954.944	0.002	0.25	77
4	4	1	5	5	0	956.718	-0.003	0.05	77
7	2	5	8	3	6	957.454	-0.005	0.05	77
8	1	8	9	0	9	959.061	0.001	1.25	77
7	1	6	8	2	7	962.638	-0.003	0.05	77
7	0	7	8	1	8	967.295	0.002	1.25	77
5	2	3	6	3	4	971.475	-0.005	0.05	77
4	3	2	5	2	3	978.924	0.001	0.25	77
3	2	1	4	3	2	983.742	-0.001	0.05	77
2	2	1	3	3	0	984.366	-0.002	0.05	77
2	2	0	3	3	1	990.789	0.003	0.05	77

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
4	1	4	5	0	5	991.500	-0.002	0.25	77
7	1	6	7	2	5	992.983	0.002	0.05	77
8	3	6	8	4	5	996.563	0.000	0.05	77
5	0	5	5	1	4	998.092	-0.001	0.05	77
3	0	3	4	1	4	999.400	0.000	0.25	77
2	2	1	3	1	2	1000.900	-0.008	0.05	77
1	1	0	2	2	1	1006.421	-0.012	0.00	77
2	1	2	3	0	3	1007.252	0.007	0.25	77
5	1	4	5	2	3	1008.631	-0.009	0.05	77
1	0	1	2	1	2	1014.671	-0.001	0.25	77
1	1	1	2	0	2	1015.241	0.000	0.25	77
4	2	3	4	3	2	1016.002	0.003	0.25	77
8	5	4	8	6	3	1017.199	-0.001	0.05	77
5	3	3	5	4	2	1017.883	-0.007	0.05	77
5	2	3	5	3	2	1019.262	-0.003	0.25	77
6	4	3	6	5	2	1020.004	-0.006	0.05	77
2	1	2	2	2	1	1021.860	-0.002	0.05	77
0	0	0	1	1	1	1022.344	-0.001	0.05	77
4	3	2	4	4	1	1023.355	-0.004	0.05	77
3	1	2	3	2	1	1024.901	-0.004	0.05	77
7	4	3	7	5	2	1026.060	-0.001	0.05	77
4	2	2	4	3	1	1026.978	0.003	0.25	77
5	3	2	5	4	1	1029.191	0.001	1.25	77
3	2	1	3	3	0	1030.981	0.000	1.25	77
6	4	2	6	5	1	1031.400	0.007	0.25	77
1	1	0	1	0	1	1039.128	-0.001	0.25	77
2	2	0	2	1	1	1040.468	-0.008	0.05	77
3	3	0	3	2	1	1042.568	-0.001	1.25	77
4	4	0	4	3	1	1045.466	-0.008	0.05	77
3	2	1	3	1	2	1047.517	-0.005	0.25	77
5	5	0	5	4	1	1049.223	-0.001	5.00	77
5	4	1	5	3	2	1050.304	-0.016	0.00	77
4	4	1	4	3	2	1053.063	-0.002	1.25	77
2	1	2	1	0	1	1054.558	0.000	0.25	77
4	2	2	4	1	3	1057.195	-0.004	0.25	77
4	3	2	4	2	3	1057.995	-0.004	0.25	77
7	7	0	7	6	1	1059.012	0.002	0.25	77
6	5	2	6	4	3	1063.175	-0.002	0.25	77
2	2	1	1	1	0	1063.977	0.002	0.25	77
4	2	3	4	1	4	1064.540	-0.020	0.00	77
9	8	1	9	7	2	1065.550	0.001	0.25	77
6	4	3	6	3	4	1068.880	-0.019	0.00	77
4	1	4	3	0	3	1069.785	-0.003	0.25	77
7	4	3	7	3	4	1070.754	0.000	1.25	77
3	2	2	2	1	1	1072.185	-0.001	0.25	77
5	1	4	5	0	5	1072.901	0.003	0.25	77
5	0	5	4	1	4	1077.378	0.001	1.25	77
4	2	3	3	1	2	1079.777	-0.001	0.25	77
6	2	5	6	1	6	1081.152	0.001	0.25	77

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	3	1	2	2	0	1081.871	0.003	1.25	77
9	6	4	9	5	5	1084.035	-0.008	0.05	77
6	1	6	5	0	5	1084.874	0.000	1.25	77
8	4	5	8	3	6	1086.752	-0.007	0.05	77
5	1	4	4	2	3	1087.721	0.006	0.05	77
3	3	0	2	2	1	1088.210	-0.002	0.25	77
7	1	6	7	0	7	1089.304	0.005	0.25	77
4	3	2	3	2	1	1090.441	0.001	1.25	77
7	0	7	6	1	6	1092.278	0.003	1.25	77
10	6	5	10	5	6	1093.449	-0.007	0.05	77
6	2	5	5	1	4	1095.727	-0.001	1.25	77
5	2	3	4	3	2	1097.125	-0.003	0.05	77
8	2	7	8	1	8	1097.347	0.003	0.25	77
5	3	3	4	2	2	1097.950	0.007	0.05	77
8	1	8	7	0	7	1099.580	0.001	5.00	77
4	4	1	3	3	0	1100.308	0.005	0.25	77
9	2	7	9	1	8	1100.657	-0.005	0.25	77
5	3	2	4	4	1	1103.013	-0.003	0.05	77
7	1	6	6	2	5	1103.629	0.001	1.25	77
10	4	7	10	3	8	1104.239	0.006	0.05	77
4	4	0	3	3	1	1105.411	-0.008	0.25	77
6	3	4	5	2	3	1106.048	-0.004	0.25	77
9	0	9	8	1	8	1106.783	-0.003	5.00	77
11	4	7	11	3	8	1108.026	0.002	0.05	77
5	4	2	4	3	1	1109.299	0.004	0.25	77
8	2	7	7	1	6	1111.433	-0.003	1.25	77
10	2	9	10	1	10	1113.129	-0.006	0.05	77
10	1	10	9	0	9	1113.880	-0.016	0.25	77
7	2	5	6	3	4	1114.348	0.001	0.05	77
6	3	3	5	4	2	1114.768	-0.003	0.05	77
9	1	8	8	2	7	1119.151	0.001	0.05	77
11	0	11	10	1	10	1120.910	0.002	5.00	77
8	3	6	7	2	5	1122.634	0.002	0.25	77
5	5	0	4	4	1	1123.049	-0.001	1.25	77
7	3	4	6	4	3	1124.340	0.004	0.05	77
7	4	4	6	3	3	1124.725	0.006	0.05	77
12	3	10	12	2	11	1125.119	0.006	0.05	77
10	2	9	9	1	8	1126.772	0.002	1.25	77
12	1	12	11	0	11	1127.821	0.001	1.25	77
6	5	2	5	4	1	1128.712	0.000	5.00	77
9	2	7	8	3	6	1130.811	0.000	5.00	77
7	4	3	6	5	2	1132.253	0.001	1.25	77
8	4	5	7	3	4	1133.257	-0.003	0.25	77
13	0	13	12	1	12	1134.630	-0.001	1.25	77
6	6	1	5	5	0	1138.337	0.001	5.00	77
10	3	8	9	2	7	1138.897	-0.001	5.00	77
6	6	0	5	5	1	1141.125	-0.003	0.05	77
14	1	14	13	0	13	1141.341	0.004	0.05	77
8	4	4	7	5	3	1142.827	-0.008	0.05	77

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	5	4	7	4	3	1143.794	0.001	1.25	77
6	5	1	5	4	2	1145.076	0.004	0.05	77
11	2	9	10	3	8	1146.893	0.002	1.25	77
15	0	15	14	1	14	1147.964	0.031	0.00	77
7	6	2	6	5	1	1148.629	0.004	0.05	77
13	1	12	12	2	11	1149.072	-0.003	1.25	77
8	5	3	7	6	2	1149.354	-0.001	0.25	77
10	4	7	9	3	6	1150.360	0.002	5.00	77
9	4	5	8	5	4	1152.203	-0.002	5.00	77
6	4	2	5	3	3	1154.582	0.003	0.25	77
12	3	10	11	2	9	1154.793	0.001	5.00	77
8	6	3	7	5	2	1156.050	0.002	0.25	77
14	2	13	13	1	12	1156.323	-0.002	0.25	77
6	6	1	5	3	2	1156.817	-0.001	0.05	77
7	7	1	6	6	0	1157.697	0.002	1.25	77
6	5	2	5	2	3	1158.106	0.004	0.25	77
11	3	8	10	4	7	1158.774	-0.003	1.25	77
7	7	0	6	6	1	1159.619	-0.001	1.25	77
10	5	6	9	4	5	1161.236	0.003	0.05	77
9	5	4	8	6	3	1161.264	-0.003	0.05	77
7	6	1	6	5	2	1162.234	0.001	0.25	77
13	2	11	12	3	10	1162.602	0.001	1.25	77
6	3	3	5	2	4	1163.418	-0.001	0.25	77
9	6	3	8	7	2	1165.877	-0.004	0.05	77
12	4	9	11	3	8	1167.102	0.000	5.00	77
8	7	2	7	6	1	1168.938	-0.001	5.00	77
14	3	12	13	2	11	1170.318	-0.002	0.25	77
16	2	15	15	1	14	1170.549	0.005	0.05	77
7	5	2	6	4	3	1171.376	-0.002	0.25	77
10	6	5	9	5	4	1171.799	-0.004	0.25	77
13	3	10	12	4	9	1175.334	0.003	0.25	77
9	7	3	8	6	2	1176.640	0.001	0.25	77
8	8	1	7	7	0	1177.167	0.000	5.00	77
15	2	13	14	3	12	1177.950	0.000	0.05	77
8	8	0	7	7	1	1178.455	-0.002	0.05	77
12	5	8	11	4	7	1178.746	0.001	0.25	77
8	7	1	7	6	2	1179.755	0.001	0.25	77
7	4	3	6	3	4	1181.143	0.001	0.25	77
7	5	3	6	2	4	1182.120	0.004	0.05	77
10	7	4	9	6	3	1183.482	0.002	1.25	77
13	4	9	12	5	8	1187.356	-0.001	1.25	77
7	3	4	6	2	5	1188.422	0.001	0.05	77
9	8	2	8	7	1	1189.522	0.000	0.05	77
12	6	7	11	5	6	1189.802	0.003	0.05	77
11	6	5	10	7	4	1190.336	-0.003	0.25	77
17	2	15	16	3	14	1192.946	0.003	0.05	77
9	9	1	8	8	0	1196.706	0.005	0.05	77
9	9	0	8	8	1	1197.556	0.002	0.05	77
9	8	1	8	7	2	1197.721	0.004	0.05	77



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	5	3	7	4	4	1198.702	0.000	0.05	77
13	5	8	12	6	7	1198.749	-0.003	0.05	77
8	6	3	7	3	4	1200.744	0.003	1.25	77
11	8	4	10	7	3	1204.256	0.007	0.05	77
9	7	2	8	6	3	1204.770	-0.001	1.25	77
8	5	4	7	2	5	1206.854	-0.003	0.25	77
10	9	2	9	8	1	1210.232	0.000	5.00	77
12	8	5	11	7	4	1211.624	0.004	0.05	77
8	4	5	7	1	6	1213.095	-0.009	0.25	77
9	6	3	8	5	4	1215.961	0.001	1.25	77
10	10	1	9	9	0	1216.264	0.000	5.00	77
10	10	0	9	9	1	1216.826	-0.001	1.25	77
9	7	3	8	4	4	1219.765	0.002	0.05	77
10	8	2	9	7	3	1221.546	-0.002	0.05	77
9	5	4	8	4	5	1224.855	0.000	1.25	77
9	6	4	8	3	5	1225.384	-0.004	0.05	77
12	9	4	11	8	3	1225.666	0.003	0.25	77
11	10	2	10	9	1	1230.935	-0.003	0.05	77
9	4	5	8	3	6	1231.595	0.002	0.25	77
10	7	3	9	6	4	1232.830	0.000	0.05	77
11	10	1	10	9	2	1235.062	0.001	1.25	77
11	11	0	10	10	1	1236.206	0.001	1.25	77
9	3	6	8	2	7	1237.566	0.004	0.25	77
11	9	2	10	8	3	1238.554	-0.004	0.25	77
10	8	3	9	5	4	1239.277	-0.001	0.25	77
12	10	3	11	9	2	1240.991	-0.012	0.05	77
10	7	4	9	4	5	1244.096	-0.001	0.05	77
11	8	3	10	7	4	1249.322	0.007	0.05	77
10	6	5	9	3	6	1250.254	-0.002	0.25	77
12	11	2	11	10	1	1251.555	0.000	0.25	77
12	12	1	11	11	0	1255.378	0.001	0.25	77
10	5	6	9	2	7	1256.261	-0.003	0.25	77
11	7	4	10	6	5	1260.641	0.012	0.05	77
10	4	7	9	1	8	1261.863	0.003	0.05	77
13	13	0	12	12	1	1275.051	-0.003	0.05	77
11	5	6	10	4	7	1274.978	0.002	0.05	77
11	4	7	10	3	8	1280.707	0.006	0.05	77
16	1	16	17	0	17	890.401	-0.014	0.05	78
9	9	0	10	10	1	895.711	0.006	0.05	78
15	0	15	16	1	16	899.233	-0.001	0.25	78
14	4	11	15	3	12	903.573	0.007	0.05	78
8	8	1	9	9	0	906.562	-0.003	0.05	78
14	1	14	15	0	15	907.988	0.001	1.25	78
13	1	12	14	2	13	915.312	0.000	0.25	78
13	0	13	14	1	14	916.670	-0.001	1.25	78
7	7	0	8	8	1	919.736	-0.001	1.25	78
11	4	7	12	5	8	920.409	-0.008	0.05	78
12	3	10	13	2	11	920.796	-0.004	0.25	78
10	6	5	11	5	6	921.637	0.006	0.05	78



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	2	11	13	1	12	923.360	0.001	1.25	78
7	6	1	8	7	2	924.727	0.003	0.25	78
12	1	12	13	0	13	925.283	-0.001	5.00	78
9	5	4	10	6	5	927.004	0.005	0.25	78
11	2	9	12	3	10	928.257	0.002	1.25	78
6	6	1	7	7	0	930.756	0.002	1.25	78
10	4	7	11	3	8	931.487	-0.001	0.05	78
6	6	0	7	7	1	932.705	0.007	0.25	78
9	4	5	10	5	6	933.076	0.007	0.25	78
11	0	11	12	1	12	933.824	0.001	5.00	78
7	5	2	8	6	3	935.105	0.001	0.25	78
10	3	8	11	2	9	935.643	-0.002	1.25	78
9	3	6	10	4	7	938.294	-0.001	1.25	78
10	2	9	11	1	10	939.257	0.002	1.25	78
10	1	10	11	0	11	942.289	0.001	5.00	78
9	2	7	10	3	8	942.965	0.000	5.00	78
5	5	1	6	6	0	943.489	-0.002	0.25	78
7	4	3	8	5	4	944.796	0.001	0.05	78
8	4	5	9	3	6	945.029	-0.004	1.25	78
5	5	0	6	6	1	946.325	0.003	5.00	78
9	1	8	10	2	9	947.100	0.002	5.00	78
4	3	2	5	4	1	949.438	-0.004	0.25	78
8	3	6	9	2	7	950.212	-0.001	5.00	78
9	0	9	10	1	10	950.677	0.000	5.00	78
7	3	4	8	4	5	951.628	-0.002	0.25	78
8	2	7	9	1	8	954.868	-0.001	1.25	78
4	4	1	5	5	0	956.642	0.000	5.00	78
7	2	5	8	3	6	957.386	0.003	1.25	78
6	3	3	7	4	4	957.983	0.001	0.25	78
6	4	3	7	3	4	958.437	0.003	5.00	78
8	1	8	9	0	9	958.986	-0.001	5.00	78
4	4	0	5	5	1	960.591	0.005	0.25	78
7	1	6	8	2	7	962.565	0.000	5.00	78
5	3	2	6	4	3	963.585	0.001	1.25	78
6	3	4	7	2	5	964.478	-0.008	0.25	78
5	4	2	6	3	3	965.715	-0.001	0.25	78
7	0	7	8	1	8	967.215	-0.003	5.00	78
4	3	1	5	4	2	968.508	-0.001	0.25	78
6	2	5	7	1	6	970.183	-0.001	0.25	78
8	1	8	8	2	7	972.845	0.003	0.05	78
6	1	6	7	0	7	975.369	0.001	1.25	78
3	3	0	4	4	1	975.422	0.003	0.05	78
2	1	2	3	2	1	976.124	-0.007	0.05	78
9	1	8	9	2	7	977.054	-0.011	0.05	78
5	1	4	6	2	5	977.721	0.002	0.25	78
4	3	2	5	2	3	978.839	-0.001	5.00	78
7	0	7	7	1	6	981.306	0.002	0.25	78
10	3	8	10	4	7	981.617	-0.010	0.05	78
5	0	5	6	1	6	983.435	-0.001	5.00	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	2	1	4	3	2	983.668	-0.001	0.05	78
2	2	1	3	3	0	984.283	-0.001	5.00	78
4	2	3	5	1	4	985.189	-0.004	0.05	78
11	3	8	11	4	7	986.490	-0.004	0.05	78
3	3	1	4	2	2	987.432	0.004	0.25	78
9	2	7	9	3	6	989.074	-0.003	0.05	78
6	1	6	6	2	5	989.692	-0.001	1.25	78
2	2	0	3	3	1	990.709	-0.002	1.25	78
4	1	4	5	0	5	991.420	-0.001	5.00	78
3	1	2	4	2	3	992.381	-0.001	5.00	78
7	1	6	7	2	5	992.885	-0.013	0.25	78
10	4	7	10	5	6	993.470	-0.002	0.05	78
8	3	6	8	4	5	996.479	0.000	0.25	78
5	0	5	5	1	4	998.010	0.001	5.00	78
3	0	3	4	1	4	999.318	0.002	1.25	78
6	2	5	6	3	4	1000.719	-0.001	0.05	78
2	2	1	3	1	2	1000.819	0.002	1.25	78
7	2	5	7	3	4	1003.877	0.003	0.25	78
10	5	6	10	6	5	1004.658	-0.004	0.05	78
1	1	0	2	2	1	1006.353	0.001	1.25	78
2	1	2	3	0	3	1007.161	0.001	0.25	78
5	1	4	5	2	3	1008.552	-0.001	5.00	78
6	3	4	6	4	3	1011.043	0.003	1.25	78
6	2	4	6	3	3	1011.330	0.002	0.05	78
9	4	5	9	5	4	1011.400	0.002	0.05	78
7	4	4	7	5	3	1013.954	0.007	0.05	78
1	0	1	2	1	2	1014.592	0.005	0.25	78
1	1	1	2	0	2	1015.154	0.001	5.00	78
4	2	3	4	3	2	1015.916	0.001	5.00	78
4	1	3	4	2	2	1016.552	0.001	1.25	78
8	5	4	8	6	3	1017.114	0.003	1.25	78
5	3	3	5	4	2	1017.804	-0.003	0.25	78
8	4	4	8	5	3	1018.449	-0.003	0.05	78
5	2	3	5	3	2	1019.172	0.002	5.00	78
6	4	3	6	5	2	1019.930	0.000	5.00	78
2	1	2	2	2	1	1021.779	0.001	5.00	78
6	3	3	6	4	2	1022.346	-0.001	0.25	78
3	2	2	3	3	1	1022.425	0.008	0.05	78
4	3	2	4	4	1	1023.284	-0.001	5.00	78
10	7	4	10	8	3	1023.953	-0.002	0.25	78
5	4	2	5	5	1	1024.414	0.009	0.05	78
3	1	2	3	2	1	1024.813	0.002	1.25	78
7	4	3	7	5	2	1025.953	-0.003	1.25	78
4	2	2	4	3	1	1026.879	-0.001	5.00	78
7	6	2	7	7	1	1027.547	-0.002	0.05	78
5	3	2	5	4	1	1029.098	0.001	5.00	78
8	7	2	8	8	1	1029.674	-0.004	0.25	78
1	0	1	1	1	0	1030.197	0.000	5.00	78
2	1	1	2	2	0	1030.506	0.002	0.25	78



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	2	1	3	3	0	1030.902	0.000	5.00	78
5	4	1	5	5	0	1031.777	-0.001	5.00	78
6	5	1	6	6	0	1032.261	0.006	0.25	78
7	6	1	7	7	0	1032.881	0.001	0.25	78
7	5	2	7	6	1	1033.384	0.005	0.25	78
9	6	3	9	7	2	1033.609	-0.002	0.25	78
9	7	2	9	8	1	1036.857	0.000	0.25	78
1	1	0	1	0	1	1039.039	0.002	5.00	78
2	2	0	2	1	1	1040.382	0.002	5.00	78
3	3	0	3	2	1	1042.468	0.000	5.00	78
4	4	0	4	3	1	1045.363	-0.001	5.00	78
2	1	1	2	0	2	1046.762	0.002	0.25	78
3	2	1	3	1	2	1047.433	-0.002	5.00	78
2	2	1	2	1	2	1048.266	-0.001	1.25	78
4	3	1	4	2	2	1048.541	-0.001	1.25	78
5	5	0	5	4	1	1049.101	-0.001	5.00	78
5	4	1	5	3	2	1050.232	0.000	5.00	78
6	5	1	6	4	2	1052.659	0.004	1.25	78
4	4	1	4	3	2	1052.957	-0.001	5.00	78
6	6	0	6	5	1	1053.632	-0.012	0.25	78
2	0	2	1	1	1	1053.953	-0.003	1.25	78
2	1	2	1	0	1	1054.463	-0.001	5.00	78
3	1	2	3	0	3	1055.841	0.001	1.25	78
3	2	2	3	1	3	1056.125	0.006	0.05	78
5	5	1	5	4	2	1056.217	-0.003	0.25	78
4	2	2	4	1	3	1057.108	-0.001	5.00	78
4	3	2	4	2	3	1057.903	-0.002	5.00	78
5	3	2	5	2	3	1058.495	0.000	1.25	78
7	7	0	7	6	1	1058.856	-0.002	5.00	78
8	7	1	8	6	2	1060.184	0.006	0.05	78
5	4	2	5	3	3	1060.215	0.001	0.05	78
3	0	3	2	1	2	1061.982	0.002	0.25	78
3	1	3	2	0	2	1062.034	0.003	0.05	78
6	5	2	6	4	3	1063.076	-0.001	5.00	78
2	2	1	1	1	0	1063.875	-0.001	5.00	78
4	2	3	4	1	4	1064.462	-0.004	0.05	78
9	8	1	9	7	2	1065.413	0.000	1.25	78
5	2	3	5	1	4	1066.308	-0.002	0.05	78
5	3	3	5	2	4	1066.449	0.005	0.05	78
6	4	3	6	3	4	1068.805	0.000	0.05	78
4	1	4	3	0	3	1069.691	-0.002	1.25	78
3	1	2	2	2	1	1070.459	0.000	0.05	78
2	2	0	1	1	1	1071.275	0.005	0.25	78
7	5	3	7	4	4	1071.562	-0.004	0.05	78
3	2	2	2	1	1	1072.086	-0.001	1.25	78
5	1	4	5	0	5	1072.796	-0.008	1.25	78
11	9	2	11	8	3	1074.272	0.001	0.05	78
8	6	3	8	5	4	1074.753	-0.001	1.25	78
6	3	4	6	2	5	1075.109	-0.008	0.05	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	6	3	9	5	4	1075.175	0.002	0.05	78
5	0	5	4	1	4	1077.282	0.000	5.00	78
7	3	4	7	2	5	1077.679	-0.001	0.05	78
7	4	4	7	3	5	1077.757	0.007	0.25	78
10	10	1	10	9	2	1078.698	0.006	0.05	78
4	2	3	3	1	2	1079.681	0.000	1.25	78
8	5	4	8	4	5	1080.693	0.000	1.25	78
6	2	5	6	1	6	1081.057	0.000	5.00	78
3	3	1	2	2	0	1081.763	0.001	5.00	78
10	8	3	10	7	4	1082.533	-0.002	1.25	78
7	2	5	7	1	6	1083.711	0.002	1.25	78
6	1	6	5	0	5	1084.777	-0.001	5.00	78
8	4	5	8	3	6	1086.666	0.002	1.25	78
5	1	4	4	2	3	1087.620	0.002	0.25	78
3	3	0	2	2	1	1088.117	0.002	1.25	78
7	1	6	7	0	7	1089.209	0.005	5.00	78
9	4	5	9	3	6	1089.852	0.005	0.05	78
4	3	2	3	2	1	1090.334	0.000	5.00	78
11	8	4	11	7	5	1091.438	0.007	0.25	78
7	0	7	6	1	6	1092.181	0.003	5.00	78
10	6	5	10	5	6	1093.356	-0.003	0.05	78
3	2	1	2	1	2	1094.886	0.002	0.25	78
6	2	5	5	1	4	1095.629	-0.001	5.00	78
5	2	3	4	3	2	1097.038	0.006	1.25	78
5	3	3	4	2	2	1097.835	-0.005	1.25	78
10	5	6	10	4	7	1098.980	0.003	0.25	78
8	1	8	7	0	7	1099.481	0.000	5.00	78
4	4	1	3	3	0	1100.193	0.002	5.00	78
9	2	7	9	1	8	1100.566	-0.001	1.25	78
5	3	2	4	4	1	1102.941	0.001	1.25	78
7	1	6	6	2	5	1103.529	0.000	5.00	78
10	4	7	10	3	8	1104.137	-0.001	1.25	78
9	1	8	9	0	9	1105.194	0.000	0.05	78
4	4	0	3	3	1	1105.318	-0.001	1.25	78
6	3	4	5	2	3	1105.951	0.000	1.25	78
9	0	9	8	1	8	1106.686	0.000	5.00	78
11	4	7	11	3	8	1107.929	0.000	0.25	78
10	3	8	10	2	9	1108.828	0.002	0.25	78
5	4	2	4	3	1	1109.184	0.002	1.25	78
8	2	7	7	1	6	1111.335	-0.001	5.00	78
12	6	7	12	5	8	1111.913	-0.001	0.05	78
11	3	8	11	2	9	1112.683	-0.004	0.25	78
10	2	9	10	1	10	1113.036	-0.002	1.25	78
10	1	10	9	0	9	1113.796	0.001	5.00	78
7	2	5	6	3	4	1114.248	0.003	0.25	78
6	3	3	5	4	2	1114.676	-0.001	5.00	78
6	4	3	5	3	2	1116.573	-0.002	5.00	78
11	2	9	11	1	10	1116.973	-0.002	0.25	78
9	1	8	8	2	7	1119.048	0.000	0.25	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
11	0	11	10	1	10	1120.802	-0.003	5.00	78
4	3	2	3	0	3	1121.366	0.003	0.05	78
8	3	6	7	2	5	1122.533	0.004	1.25	78
5	5	0	4	4	1	1122.945	0.000	5.00	78
7	3	4	6	4	3	1124.231	-0.003	5.00	78
7	4	4	6	3	3	1124.618	0.004	1.25	78
12	3	10	12	2	11	1125.014	-0.001	0.25	78
13	4	9	13	3	10	1125.420	0.000	0.05	78
10	2	9	9	1	8	1126.668	0.000	5.00	78
12	1	12	11	0	11	1127.717	0.001	5.00	78
5	4	1	4	3	2	1128.096	0.003	1.25	78
6	5	2	5	4	1	1128.589	-0.001	5.00	78
9	2	7	8	3	6	1130.706	-0.001	5.00	78
7	4	3	6	5	2	1132.163	0.000	5.00	78
8	4	5	7	3	4	1133.155	0.000	0.25	78
11	1	10	10	2	9	1134.192	-0.001	1.25	78
13	0	13	12	1	12	1134.528	0.000	1.25	78
7	5	3	6	4	2	1135.934	0.003	1.25	78
13	1	12	13	0	13	1135.979	0.004	0.05	78
5	5	1	4	2	2	1136.251	-0.002	0.05	78
5	3	2	4	2	3	1137.561	0.001	1.25	78
6	6	1	5	5	0	1138.209	-0.001	5.00	78
10	3	8	9	2	7	1138.792	-0.001	5.00	78
5	4	2	4	1	3	1139.410	-0.001	0.25	78
14	1	14	13	0	13	1141.238	-0.003	1.25	78
12	2	11	11	1	10	1141.626	0.000	1.25	78
9	3	6	8	4	5	1141.730	0.003	1.25	78
8	4	4	7	5	3	1142.731	0.000	1.25	78
8	5	4	7	4	3	1143.681	0.000	5.00	78
6	5	1	5	4	2	1144.984	0.000	5.00	78
11	2	9	10	3	8	1146.784	-0.001	5.00	78
15	0	15	14	1	14	1147.855	-0.001	5.00	78
7	6	2	6	5	1	1148.494	0.000	5.00	78
13	1	12	12	2	11	1148.968	0.002	5.00	78
8	5	3	7	6	2	1149.275	-0.001	1.25	78
10	4	7	9	3	6	1150.249	-0.001	5.00	78
9	4	5	8	5	4	1152.090	-0.006	1.25	78
16	1	16	15	0	15	1154.373	0.001	5.00	78
12	3	10	11	2	9	1154.684	-0.001	5.00	78
8	6	3	7	5	2	1155.916	0.001	5.00	78
14	2	13	13	1	12	1156.215	0.000	1.25	78
6	6	1	5	3	2	1156.663	-0.001	5.00	78
7	7	1	6	6	0	1157.562	-0.001	1.25	78
6	5	2	5	2	3	1157.988	0.000	5.00	78
11	3	8	10	4	7	1158.669	0.000	5.00	78
7	7	0	6	6	1	1159.503	0.000	5.00	78
17	0	17	16	1	16	1160.789	-0.001	1.25	78
10	4	6	9	5	5	1161.085	0.001	0.05	78
10	5	6	9	4	5	1161.122	0.000	1.25	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	5	4	8	6	3	1161.164	0.000	1.25	78
7	6	1	6	5	2	1162.145	0.000	5.00	78
13	2	11	12	3	10	1162.494	0.000	5.00	78
9	6	4	8	5	3	1163.227	-0.003	1.25	78
6	3	3	5	2	4	1163.313	-0.001	0.25	78
15	1	14	14	2	13	1163.375	0.003	1.25	78
6	4	3	5	1	4	1163.714	-0.001	1.25	78
9	6	3	8	7	2	1165.818	-0.001	5.00	78
12	4	9	11	3	8	1166.993	0.000	5.00	78
8	7	2	7	6	1	1168.799	0.000	5.00	78
11	4	7	10	5	6	1169.914	0.001	5.00	78
14	3	12	13	2	11	1170.213	0.002	0.25	78
16	2	15	15	1	14	1170.437	-0.001	5.00	78
10	5	5	9	6	4	1171.185	0.004	1.25	78
7	5	2	6	4	3	1171.290	0.000	1.25	78
10	6	5	9	5	4	1171.688	0.000	5.00	78
13	3	10	12	4	9	1175.223	0.000	5.00	78
8	8	1	7	7	0	1177.030	0.000	5.00	78
15	2	13	14	3	12	1177.841	0.002	0.05	78
8	8	0	7	7	1	1178.334	0.001	5.00	78
12	5	8	11	4	7	1178.631	-0.001	1.25	78
8	7	1	7	6	2	1179.663	0.000	1.25	78
11	5	6	10	6	5	1180.542	0.001	5.00	78
11	6	6	10	5	5	1180.654	-0.001	1.25	78
7	4	3	6	3	4	1181.036	-0.002	5.00	78
7	5	3	6	2	4	1182.007	0.002	1.25	78
10	7	4	9	6	3	1183.349	0.002	5.00	78
18	2	17	17	1	16	1184.309	0.005	0.05	78
16	3	14	15	2	13	1185.381	0.003	0.25	78
13	4	9	12	5	8	1187.245	-0.001	1.25	78
8	6	2	7	5	3	1188.002	0.000	1.25	78
7	3	4	6	2	5	1188.310	-0.001	1.25	78
7	4	4	6	1	5	1188.383	0.000	0.25	78
9	8	2	8	7	1	1189.375	0.001	1.25	78
12	6	7	11	5	6	1189.678	-0.004	1.25	78
11	6	5	10	7	4	1190.228	0.002	5.00	78
11	7	5	10	6	4	1191.396	0.005	0.05	78
17	2	15	16	3	14	1192.833	0.004	0.25	78
7	2	5	6	1	6	1194.580	-0.002	0.25	78
14	5	10	13	4	9	1195.761	0.000	0.25	78
9	9	1	8	8	0	1196.562	0.002	5.00	78
8	7	2	7	4	3	1197.093	-0.001	5.00	78
10	8	3	9	7	2	1197.585	0.001	0.05	78
9	8	1	8	7	2	1197.619	-0.001	1.25	78
8	5	3	7	4	4	1198.609	0.005	0.05	78
13	5	8	12	6	7	1198.637	0.002	1.25	78
16	4	13	15	3	12	1199.353	-0.001	0.25	78
12	6	6	11	7	5	1200.034	0.003	0.05	78
12	7	6	11	6	5	1200.330	0.001	5.00	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	6	3	7	3	4	1200.626	0.000	5.00	78
11	8	4	10	7	3	1204.099	-0.001	0.25	78
15	4	11	14	5	10	1204.176	-0.002	0.25	78
9	7	2	8	6	3	1204.693	0.000	5.00	78
8	5	4	7	2	5	1206.746	0.002	5.00	78
17	3	14	16	4	13	1207.214	0.000	0.25	78
14	6	9	13	5	8	1207.500	-0.002	0.25	78
12	7	5	11	8	4	1209.065	0.000	0.25	78
13	6	7	12	7	6	1209.429	0.000	1.25	78
10	9	2	9	8	1	1210.076	-0.001	5.00	78
12	8	5	11	7	4	1211.488	-0.004	1.25	78
16	5	12	15	4	11	1212.497	0.000	0.25	78
8	4	5	7	1	6	1212.987	-0.003	1.25	78
10	9	1	9	8	2	1216.052	-0.004	0.25	78
10	10	1	9	9	0	1216.120	0.000	5.00	78
10	10	0	9	9	1	1216.690	0.000	5.00	78
9	8	2	8	5	3	1217.856	0.000	0.25	78
8	3	6	7	0	7	1218.836	0.001	1.25	78
11	9	3	10	8	2	1219.073	-0.002	1.25	78
13	7	6	12	8	5	1219.462	0.003	0.25	78
9	7	3	8	4	4	1219.640	0.000	0.25	78
10	8	2	9	7	3	1221.471	0.001	1.25	78
9	5	4	8	4	5	1224.746	-0.001	5.00	78
16	6	11	15	5	10	1224.911	0.000	0.05	78
9	6	4	8	3	5	1225.272	0.000	0.25	78
12	9	4	11	8	3	1225.494	-0.002	1.25	78
15	6	9	14	7	8	1227.719	0.002	0.25	78
14	8	7	13	7	6	1229.362	-0.007	0.05	78
11	10	2	10	9	1	1230.780	0.001	5.00	78
9	4	5	8	3	6	1231.478	0.001	1.25	78
9	5	5	8	2	6	1231.519	0.000	0.05	78
10	7	3	9	6	4	1232.753	-0.001	0.25	78
17	5	12	16	6	11	1233.453	-0.004	0.05	78
11	10	1	10	9	2	1234.944	0.000	5.00	78
11	11	1	10	10	0	1235.683	0.000	1.25	78
11	11	0	10	10	1	1236.062	-0.001	5.00	78
9	3	6	8	2	7	1237.446	0.001	1.25	78
11	9	2	10	8	3	1238.473	0.001	1.25	78
10	8	3	9	5	4	1239.147	0.002	1.25	78
10	9	2	9	6	3	1239.580	0.002	0.25	78
12	10	3	11	9	2	1240.807	0.000	1.25	78
10	6	4	9	5	5	1242.809	0.001	0.05	78
9	2	7	8	1	8	1242.947	0.000	0.25	78
10	7	4	9	4	5	1243.976	0.000	1.25	78
11	8	3	10	7	4	1249.252	-0.001	1.25	78
10	5	5	9	4	6	1250.019	0.003	0.25	78
10	6	5	9	3	6	1250.136	-0.001	1.25	78
12	11	2	11	10	1	1251.396	0.000	1.25	78
12	11	1	11	10	2	1254.208	0.000	0.25	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	12	1	11	11	0	1255.225	0.001	0.25	78
12	12	0	11	11	1	1255.482	0.001	0.25	78
12	10	2	11	9	3	1255.846	-0.001	0.05	78
10	5	6	9	2	7	1256.142	-0.002	1.25	78
11	9	3	10	6	4	1259.269	-0.003	0.05	78
11	7	4	10	6	5	1260.542	-0.001	1.25	78
10	4	7	9	1	8	1261.739	-0.001	1.25	78
10	3	8	9	0	9	1266.924	0.003	0.25	78
11	6	5	10	5	6	1268.507	0.000	1.25	78
14	11	4	13	10	3	1269.889	-0.002	0.05	78
13	11	2	12	10	3	1273.708	0.004	0.25	78
13	12	1	12	11	2	1273.748	0.000	0.05	78
13	13	1	12	12	0	1274.720	-0.001	0.05	78
11	5	6	10	4	7	1274.858	0.002	0.05	78
13	13	0	12	12	1	1274.896	-0.003	0.05	78
12	8	4	11	7	5	1277.773	0.003	0.05	78
12	10	3	11	7	4	1280.174	-0.003	0.05	78
11	4	7	10	3	8	1280.579	0.000	1.25	78
12	9	4	11	6	5	1282.101	-0.002	0.25	78
11	3	8	10	2	9	1285.868	0.000	0.25	78
12	8	5	11	5	6	1287.548	-0.001	0.25	78
14	13	2	13	12	1	1292.257	-0.002	0.05	78
12	7	6	11	4	7	1293.627	0.001	0.25	78
14	14	1	13	13	0	1294.158	0.006	0.05	78
12	6	7	11	3	8	1299.424	-0.001	0.25	78
12	5	8	11	2	9	1304.826	0.002	0.05	78
12	4	9	11	1	10	1309.833	0.000	0.05	78
13	6	7	12	5	8	1318.214	0.000	0.05	78
13	5	8	12	4	9	1323.749	0.002	0.05	78
13	4	9	12	3	10	1328.883	0.006	0.05	78
13	3	10	12	2	11	1333.635	0.002	0.05	78
16	1	16	17	0	17	890.288	0.002	0.25	80
9	9	0	10	10	1	895.613	0.000	0.25	80
15	1	14	16	2	15	898.913	0.006	0.05	80
15	0	15	16	1	16	899.109	0.002	1.25	80
8	7	2	9	8	1	902.516	0.003	0.25	80
14	4	11	15	3	12	903.431	0.000	0.05	80
14	3	12	15	2	13	905.575	0.003	0.05	80
8	8	1	9	9	0	906.450	-0.001	0.25	80
14	2	13	15	1	14	907.068	-0.006	0.25	80
8	8	0	9	9	1	907.314	-0.010	0.05	80
14	1	14	15	0	15	907.859	0.000	5.00	80
13	3	10	14	4	11	910.512	0.005	0.05	80
13	2	11	14	3	12	913.151	0.003	0.25	80
13	1	12	14	2	13	915.182	0.001	1.25	80
11	5	6	12	6	7	915.548	-0.003	0.05	80
10	7	4	11	6	5	916.216	0.002	0.05	80
13	0	13	14	1	14	916.537	-0.003	5.00	80
12	4	9	13	3	10	917.525	0.005	0.25	80

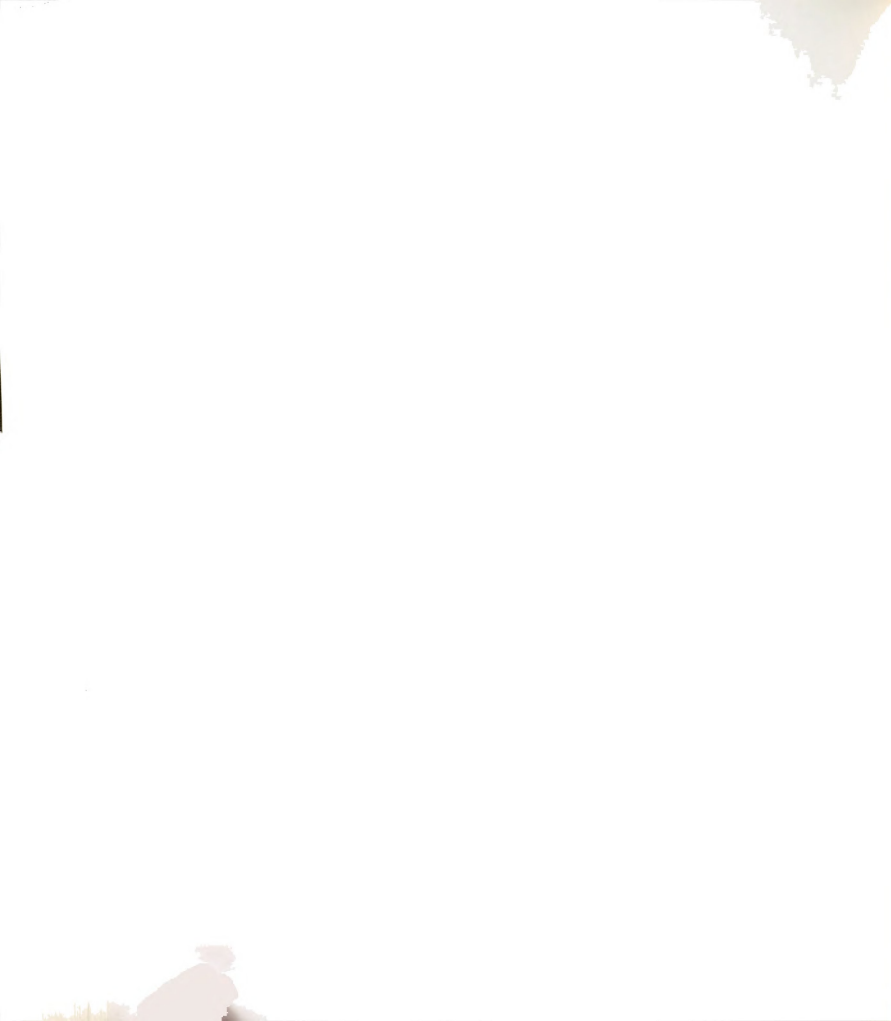


UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	7	1	8	8	0	918.319	0.002	1.25	80
7	7	0	8	8	1	919.639	0.000	1.25	80
11	4	7	12	5	8	920.281	-0.001	0.25	80
12	3	10	13	2	11	920.664	0.000	1.25	80
10	6	5	11	5	6	921.496	0.002	0.05	80
12	2	11	13	1	12	923.224	0.000	5.00	80
11	3	8	12	4	9	924.464	-0.004	1.25	80
7	6	1	8	7	2	924.643	0.002	0.05	80
6	5	2	7	6	1	924.988	0.005	0.05	80
12	1	12	13	0	13	925.150	0.001	5.00	80
5	3	2	6	6	1	926.266	0.001	0.05	80
10	5	6	11	4	7	926.661	-0.003	1.25	80
9	5	4	10	6	5	926.869	-0.001	0.05	80
11	2	9	12	3	10	928.118	0.002	5.00	80
6	6	1	7	7	0	930.623	0.001	5.00	80
11	1	10	12	2	11	931.201	-0.002	5.00	80
10	4	7	11	3	8	931.345	-0.002	0.05	80
8	7	2	9	6	3	931.960	0.004	0.25	80
6	6	0	7	7	1	932.600	0.005	1.25	80
9	4	5	10	5	6	932.930	0.001	0.25	80
11	0	11	12	1	12	933.685	0.001	5.00	80
8	6	3	9	5	4	933.895	0.000	0.25	80
7	5	2	8	6	3	935.011	0.000	0.25	80
10	3	8	11	2	9	935.503	0.000	5.00	80
5	4	2	6	5	1	936.855	0.003	0.05	80
4	2	3	5	3	2	937.896	0.003	0.05	80
9	3	6	10	4	7	938.151	-0.001	5.00	80
6	5	1	7	6	2	938.867	0.001	0.05	80
10	2	9	11	1	10	939.113	0.000	5.00	80
10	1	10	11	0	11	942.146	0.000	5.00	80
9	2	7	10	3	8	942.822	0.001	5.00	80
5	5	1	6	6	0	943.348	-0.002	1.25	80
7	4	3	8	5	4	944.666	0.002	1.25	80
8	4	5	9	3	6	944.885	-0.004	1.25	80
7	5	3	8	4	4	945.747	-0.001	0.25	80
5	5	0	6	6	1	946.215	0.002	5.00	80
9	1	8	10	2	9	946.955	0.001	5.00	80
6	4	2	7	5	3	949.213	0.005	0.05	80
4	3	2	5	4	1	949.269	0.002	0.05	80
8	3	6	9	2	7	950.067	0.000	5.00	80
9	0	9	10	1	10	950.532	0.001	5.00	80
7	3	4	8	4	5	951.484	-0.001	5.00	80
7	4	4	8	3	5	951.568	0.005	0.05	80
6	5	2	7	4	3	953.284	0.002	1.25	80
5	4	1	6	5	2	953.472	-0.004	0.05	80
8	2	7	9	1	8	954.722	0.000	5.00	80
4	4	1	5	5	0	956.494	0.001	5.00	80
7	2	5	8	3	6	957.235	0.001	5.00	80
6	3	3	7	4	4	957.837	-0.003	0.25	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	4	3	7	3	4	958.283	0.001	5.00	80
8	1	8	9	0	9	958.839	0.001	5.00	80
4	4	0	5	5	1	960.469	0.001	1.25	80
7	1	6	8	2	7	962.415	0.000	5.00	80
5	3	2	6	4	3	963.453	0.001	5.00	80
5	5	1	6	4	2	963.655	-0.006	0.25	80
6	3	4	7	2	5	964.328	-0.008	0.25	80
5	4	2	6	3	3	965.547	-0.003	1.25	80
7	0	7	8	1	8	967.065	-0.002	5.00	80
4	3	1	5	4	2	968.379	-0.004	1.25	80
10	2	9	10	3	8	968.916	0.004	0.25	80
6	2	5	7	1	6	970.031	-0.001	0.25	80
5	2	3	6	3	4	971.249	-0.001	5.00	80
5	3	3	6	2	4	971.399	0.000	0.05	80
8	1	8	8	2	7	972.692	0.003	0.25	80
4	4	1	5	3	2	974.892	-0.002	1.25	80
6	1	6	7	0	7	975.214	-0.001	1.25	80
3	3	0	4	4	1	975.285	-0.004	0.05	80
2	1	2	3	2	1	975.966	0.001	0.25	80
9	1	8	9	2	7	976.911	0.001	0.25	80
5	1	4	6	2	5	977.564	-0.001	5.00	80
4	2	2	5	3	3	977.766	-0.001	0.05	80
4	3	2	5	2	3	978.678	-0.001	5.00	80
7	0	7	7	1	6	981.150	0.001	1.25	80
10	3	8	10	4	7	981.468	-0.001	0.25	80
5	0	5	6	1	6	983.279	-0.001	5.00	80
3	2	1	4	3	2	983.523	-0.006	0.25	80
2	2	1	3	3	0	984.125	-0.001	5.00	80
8	2	7	8	3	6	984.851	-0.001	0.25	80
4	2	3	5	1	4	985.030	-0.007	0.05	80
11	3	8	11	4	7	986.334	-0.001	0.05	80
3	3	1	4	2	2	987.246	0.001	1.25	80
9	2	7	9	3	6	988.918	0.001	1.25	80
6	1	6	6	2	5	989.537	0.002	5.00	80
2	2	0	3	3	1	990.568	0.000	5.00	80
4	1	4	5	0	5	991.261	-0.001	5.00	80
3	1	2	4	2	3	992.226	-0.001	5.00	80
3	2	2	4	1	3	992.536	0.005	0.25	80
7	1	6	7	2	5	992.736	-0.002	0.25	80
10	4	7	10	5	6	993.308	-0.002	0.25	80
8	3	6	8	4	5	996.320	0.003	1.25	80
5	0	5	5	1	4	997.849	0.000	5.00	80
1	1	1	2	2	0	998.738	0.002	1.25	80
2	1	1	3	2	2	998.884	0.002	1.25	80
3	0	3	4	1	4	999.156	0.000	1.25	80
6	2	5	6	3	4	1000.565	0.007	0.05	80
2	2	1	3	1	2	1000.647	0.001	1.25	80
7	2	5	7	3	4	1003.708	0.000	0.25	80
10	5	6	10	6	5	1004.495	-0.001	0.25	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	4	6	10	5	5	1004.564	-0.007	0.05	80
4	1	4	4	2	3	1006.072	0.000	0.25	80
1	1	0	2	2	1	1006.201	0.003	1.25	80
2	0	2	3	1	3	1006.952	0.015	0.05	80
2	1	2	3	0	3	1006.997	0.000	1.25	80
5	2	4	5	3	3	1008.291	0.003	0.05	80
5	1	4	5	2	3	1008.389	0.002	5.00	80
11	5	6	11	6	5	1009.210	0.001	0.05	80
6	3	4	6	4	3	1010.876	0.001	5.00	80
6	2	4	6	3	3	1011.158	0.001	0.05	80
9	4	5	9	5	4	1011.216	-0.005	0.05	80
7	4	4	7	5	3	1013.784	0.001	1.25	80
3	1	3	3	2	2	1014.143	0.001	0.25	80
1	0	1	2	1	2	1014.428	0.003	1.25	80
1	1	1	2	0	2	1014.986	0.001	1.25	80
4	2	3	4	3	2	1015.754	0.001	5.00	80
4	1	3	4	2	2	1016.379	0.001	5.00	80
8	5	4	8	6	3	1016.949	0.001	1.25	80
5	3	3	5	4	2	1017.650	0.002	1.25	80
8	4	4	8	5	3	1018.264	0.003	0.25	80
5	2	3	5	3	2	1018.989	0.001	5.00	80
6	4	3	6	5	2	1019.776	0.001	5.00	80
9	6	4	9	7	3	1020.307	-0.001	0.05	80
11	6	5	11	7	4	1020.514	-0.004	0.05	80
2	1	2	2	2	1	1021.621	0.002	5.00	80
0	0	0	1	1	1	1022.097	0.003	0.25	80
6	3	3	6	4	2	1022.154	-0.002	0.05	80
3	2	2	3	3	1	1022.263	-0.003	0.25	80
9	5	4	9	6	3	1022.622	-0.001	0.25	80
2	0	2	2	1	1	1022.898	0.005	1.25	80
4	3	2	4	4	1	1023.144	0.000	5.00	80
10	7	4	10	8	3	1023.801	-0.001	0.25	80
5	4	2	5	5	1	1024.273	-0.002	1.25	80
8	6	3	8	7	2	1024.572	0.009	0.05	80
3	1	2	3	2	1	1024.635	0.001	1.25	80
6	5	2	6	6	1	1025.702	0.007	0.25	80
7	4	3	7	5	2	1025.758	0.001	1.25	80
4	2	2	4	3	1	1026.702	0.001	5.00	80
9	7	3	9	8	2	1027.180	0.002	0.05	80
7	6	2	7	7	1	1027.448	-0.001	0.25	80
5	3	2	5	4	1	1028.922	0.001	5.00	80
8	7	2	8	8	1	1029.594	0.000	0.25	80
1	0	1	1	1	0	1030.031	0.001	5.00	80
2	1	1	2	2	0	1030.346	0.003	0.25	80
3	2	1	3	3	0	1030.750	-0.001	5.00	80
6	4	2	6	5	1	1031.142	0.005	0.05	80
4	3	1	4	4	0	1031.199	-0.001	0.05	80
5	4	1	5	5	0	1031.661	0.000	5.00	80
6	5	1	6	6	0	1032.164	0.002	1.25	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	6	1	7	7	0	1032.812	0.001	0.25	80
7	5	2	7	6	1	1033.228	0.000	1.25	80
8	7	1	8	8	0	1033.795	0.010	0.05	80
8	6	2	8	7	1	1035.111	0.000	1.25	80
9	7	2	9	8	1	1036.753	-0.001	5.00	80
10	7	3	10	8	2	1037.022	0.003	0.25	80
10	9	1	10	10	0	1037.464	0.003	0.05	80
10	8	2	10	9	1	1038.196	0.002	0.25	80
1	1	0	1	0	1	1038.863	0.000	5.00	80
11	9	2	11	10	1	1039.559	-0.003	0.25	80
2	2	0	2	1	1	1040.201	0.002	5.00	80
3	3	0	3	2	1	1042.274	-0.001	5.00	80
4	4	0	4	3	1	1045.153	-0.001	5.00	80
1	1	1	0	0	0	1046.437	-0.002	5.00	80
2	1	1	2	0	2	1046.595	0.004	0.05	80
3	2	1	3	1	2	1047.268	-0.002	5.00	80
2	2	1	2	1	2	1048.083	0.000	5.00	80
4	3	1	4	2	2	1048.374	-0.003	1.25	80
5	5	0	5	4	1	1048.868	-0.001	5.00	80
5	4	1	5	3	2	1050.063	0.001	0.25	80
6	5	1	6	4	2	1052.473	0.001	5.00	80
4	4	1	4	3	2	1052.753	-0.001	1.25	80
6	6	0	6	5	1	1053.382	-0.001	1.25	80
2	0	2	1	1	1	1053.782	-0.001	5.00	80
2	1	2	1	0	1	1054.283	-0.001	5.00	80
3	1	2	3	0	3	1055.669	0.003	1.25	80
7	6	1	7	5	2	1055.735	-0.001	1.25	80
3	2	2	3	1	3	1055.937	-0.003	1.25	80
5	5	1	5	4	2	1056.000	-0.002	0.05	80
4	2	2	4	1	3	1056.938	-0.002	5.00	80
4	3	2	4	2	3	1057.722	-0.001	5.00	80
5	3	2	5	2	3	1058.331	-0.002	5.00	80
7	7	0	7	6	1	1058.565	-0.002	0.25	80
6	6	1	6	5	2	1059.784	0.002	1.25	80
6	4	2	6	3	3	1059.830	-0.005	0.05	80
5	4	2	5	3	3	1060.018	-0.009	0.05	80
7	5	2	7	4	3	1061.525	-0.001	1.25	80
3	0	3	2	1	2	1061.804	0.003	0.25	80
6	5	2	6	4	3	1062.880	-0.002	5.00	80
8	6	2	8	5	3	1063.576	0.002	0.05	80
2	2	1	1	1	0	1063.687	-0.002	5.00	80
4	2	3	4	1	4	1064.277	-0.009	0.05	80
9	8	1	9	7	2	1065.149	0.001	5.00	80
5	2	3	5	1	4	1066.131	-0.001	0.25	80
9	7	2	9	6	3	1066.197	0.000	0.05	80
6	3	3	6	2	4	1068.246	-0.001	1.25	80
6	4	3	6	3	4	1068.614	-0.009	0.05	80
4	1	4	3	0	3	1069.507	-0.004	1.25	80
9	9	0	9	8	1	1070.096	0.005	0.05	80



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	1	2	2	2	1	1070.290	0.002	1.25	80
7	4	3	7	3	4	1070.495	-0.004	0.05	80
2	2	0	1	1	1	1071.090	0.001	1.25	80
7	5	3	7	4	4	1071.377	-0.004	0.25	80
3	2	2	2	1	1	1071.898	0.002	5.00	80
5	1	4	5	0	5	1072.622	0.001	5.00	80
9	9	1	9	8	2	1073.420	-0.002	0.25	80
11	9	2	11	8	3	1074.048	-0.002	1.25	80
8	6	3	8	5	4	1074.564	-0.001	5.00	80
6	3	4	6	2	5	1074.928	-0.006	0.05	80
9	6	3	9	5	4	1075.030	0.001	0.25	80
5	0	5	4	1	4	1077.095	-0.003	5.00	80
7	4	4	7	3	5	1077.563	-0.004	0.25	80
9	7	3	9	6	4	1078.206	0.001	1.25	80
4	1	3	3	2	2	1079.235	0.002	1.25	80
4	2	3	3	1	2	1079.493	0.000	1.25	80
8	4	4	8	3	5	1080.318	0.002	1.25	80
8	5	4	8	4	5	1080.506	-0.004	1.25	80
6	2	5	6	1	6	1080.873	0.002	5.00	80
3	3	1	2	2	0	1081.561	0.000	5.00	80
10	8	3	10	7	4	1082.329	-0.002	1.25	80
9	5	4	9	4	5	1083.288	0.003	1.25	80
7	2	5	7	1	6	1083.525	0.002	1.25	80
6	1	6	5	0	5	1084.589	-0.002	5.00	80
8	4	5	8	3	6	1086.475	-0.003	1.25	80
5	1	4	4	2	3	1087.433	0.002	0.25	80
3	3	0	2	2	1	1087.930	0.000	1.25	80
7	1	6	7	0	7	1089.017	0.001	5.00	80
9	4	5	9	3	6	1089.665	0.003	0.05	80
4	3	2	3	2	1	1090.129	-0.001	5.00	80
11	8	4	11	7	5	1091.242	-0.001	0.00	80
7	0	7	6	1	6	1091.990	0.001	5.00	80
10	5	5	10	4	6	1093.061	-0.002	0.25	80
10	6	5	10	5	6	1093.172	-0.002	0.25	80
3	2	1	2	1	2	1094.710	0.002	1.25	80
6	2	5	5	1	4	1095.438	-0.002	1.25	80
11	6	5	11	5	6	1096.603	0.002	0.05	80
5	2	3	4	3	2	1096.848	0.000	5.00	80
5	3	3	4	2	2	1097.643	0.001	5.00	80
10	5	6	10	4	7	1098.786	-0.003	5.00	80
8	1	8	7	0	7	1099.289	0.000	5.00	80
4	4	1	3	3	0	1099.975	0.000	5.00	80
9	2	7	9	1	8	1100.383	0.007	0.05	80
11	5	6	11	4	7	1102.499	0.005	0.25	80
5	3	2	4	4	1	1102.799	0.001	1.25	80
7	1	6	6	2	5	1103.336	0.000	5.00	80
10	4	7	10	3	8	1103.946	-0.001	1.25	80
9	1	8	9	0	9	1105.002	0.002	0.25	80
4	4	0	3	3	1	1105.130	0.003	1.25	80



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	2	4	5	3	3	1105.636	0.002	0.25	80
6	3	4	5	2	3	1105.759	0.003	1.25	80
9	0	9	8	1	8	1106.492	-0.001	5.00	80
11	4	7	11	3	8	1107.737	0.000	1.25	80
10	3	8	10	2	9	1108.634	0.000	1.25	80
5	4	2	4	3	1	1108.962	0.001	1.25	80
13	7	6	13	6	7	1110.351	0.003	0.25	80
8	2	7	7	1	6	1111.140	-0.001	5.00	80
4	3	1	3	2	2	1111.229	-0.003	0.05	80
12	6	7	12	5	8	1111.719	-0.004	0.25	80
11	3	8	11	2	9	1112.496	0.003	1.25	80
10	2	9	10	1	10	1112.843	0.001	0.25	80
10	1	10	9	0	9	1113.601	0.002	5.00	80
7	2	5	6	3	4	1114.052	0.002	0.25	80
13	6	7	13	5	8	1115.853	0.003	1.25	80
6	4	3	5	3	2	1116.362	0.001	5.00	80
4	4	1	3	1	2	1116.502	0.008	0.05	80
11	2	9	11	1	10	1116.787	0.006	0.25	80
9	1	8	8	2	7	1118.851	0.000	0.05	80
11	0	11	10	1	10	1120.606	-0.002	5.00	80
4	3	2	3	0	3	1121.164	0.002	0.25	80
8	3	6	7	2	5	1122.330	-0.001	5.00	80
5	5	0	4	4	1	1122.743	-0.002	1.25	80
7	3	4	6	4	3	1124.038	0.000	5.00	80
7	4	4	6	3	3	1124.415	0.006	0.25	80
12	3	10	12	2	11	1124.820	0.001	0.25	80
13	4	9	13	3	10	1125.223	0.001	0.05	80
10	2	9	9	1	8	1126.468	0.000	5.00	80
12	1	12	11	0	11	1127.518	0.000	5.00	80
5	4	1	4	3	2	1127.922	0.000	1.25	80
6	5	2	5	4	1	1128.350	-0.001	5.00	80
13	3	10	13	2	11	1129.218	-0.002	0.25	80
9	2	7	8	3	6	1130.505	-0.001	5.00	80
7	4	3	6	5	2	1131.992	-0.001	5.00	80
8	4	5	7	3	4	1132.950	-0.002	0.25	80
11	1	10	10	2	9	1133.992	0.001	1.25	80
13	0	13	12	1	12	1134.326	-0.003	1.25	80
7	5	3	6	4	2	1135.698	0.001	1.25	80
13	1	12	13	0	13	1135.770	-0.004	0.05	80
5	3	2	4	2	3	1137.378	0.001	5.00	80
6	6	1	5	5	0	1137.965	-0.002	5.00	80
10	3	8	9	2	7	1138.588	-0.002	5.00	80
5	4	2	4	1	3	1139.205	0.005	1.25	80
6	6	0	5	5	1	1140.808	0.002	5.00	80
14	1	14	13	0	13	1141.030	-0.011	0.05	80
12	2	11	11	1	10	1141.425	0.003	1.25	80
9	3	6	8	4	5	1141.524	0.001	1.25	80
8	4	4	7	5	3	1142.535	0.000	1.25	80
8	5	4	7	4	3	1143.462	-0.002	5.00	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	5	1	5	4	2	1144.813	0.000	5.00	80
5	2	3	4	1	4	1145.381	-0.001	1.25	80
11	2	9	10	3	8	1146.579	0.000	5.00	80
15	0	15	14	1	14	1147.653	0.000	5.00	80
15	2	13	15	1	14	1148.292	-0.002	0.05	80
7	6	2	6	5	1	1148.236	0.000	5.00	80
13	1	12	12	2	11	1148.761	0.000	5.00	80
8	5	3	7	6	2	1149.126	0.001	1.25	80
10	4	7	9	3	6	1150.042	-0.001	5.00	80
15	1	14	15	0	15	1150.578	0.002	0.05	80
11	7	5	10	8	2	1150.912	0.001	0.05	80
9	4	5	8	5	4	1151.890	0.000	5.00	80
8	6	3	8	3	6	1153.930	0.004	0.05	80
16	1	16	15	0	15	1154.166	0.000	5.00	80
6	4	2	5	3	3	1154.312	0.001	0.05	80
12	3	10	11	2	9	1154.478	0.001	5.00	80
8	6	3	7	5	2	1155.658	0.000	5.00	80
14	2	13	13	1	12	1156.011	0.003	1.25	80
6	6	1	5	3	2	1156.369	0.001	1.25	80
7	7	1	6	6	0	1157.310	0.000	5.00	80
6	5	2	5	2	3	1157.763	0.000	1.25	80
11	3	8	10	4	7	1158.460	0.001	5.00	80
7	7	0	6	6	1	1159.278	0.000	5.00	80
17	0	17	16	1	16	1160.579	0.000	1.25	80
10	4	6	9	5	5	1160.876	0.002	0.05	80
10	5	6	9	4	5	1160.910	-0.001	1.25	80
9	5	4	8	6	3	1160.972	0.000	1.25	80
7	6	1	6	5	2	1161.972	0.001	5.00	80
13	2	11	12	3	10	1162.283	0.000	1.25	80
9	6	4	8	5	3	1162.990	-0.003	1.25	80
6	3	3	5	2	4	1163.116	0.004	0.05	80
15	1	14	14	2	13	1163.166	0.001	5.00	80
6	4	3	5	1	4	1163.504	-0.001	1.25	80
9	7	2	8	8	1	1163.835	0.000	0.25	80
9	6	3	8	7	2	1165.697	0.000	5.00	80
12	4	9	11	3	8	1166.780	-0.001	5.00	80
18	1	18	17	0	17	1166.894	0.002	0.25	80
8	7	2	7	6	1	1168.522	0.000	5.00	80
11	4	7	10	5	6	1169.702	0.002	5.00	80
14	3	12	13	2	11	1169.998	-0.001	1.25	80
16	2	15	15	1	14	1170.230	-0.001	0.25	80
10	5	5	9	6	4	1170.972	-0.001	5.00	80
7	5	2	6	4	3	1171.126	0.000	1.25	80
10	6	5	9	5	4	1171.465	0.000	5.00	80
19	0	19	18	1	18	1173.104	-0.001	0.25	80
13	3	10	12	4	9	1175.008	0.000	5.00	80
9	7	3	8	6	2	1176.209	0.001	1.25	80
8	8	1	7	7	0	1176.767	-0.001	5.00	80
7	6	2	6	3	3	1176.934	0.000	1.25	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
17	1	16	16	2	15	1177.206	-0.002	0.05	80
15	2	13	14	3	12	1177.624	-0.002	1.25	80
8	8	0	7	7	1	1178.095	0.000	5.00	80
12	5	8	11	4	7	1178.416	0.000	1.25	80
10	6	4	9	7	3	1179.151	0.001	1.25	80
8	7	1	7	6	2	1179.483	0.001	1.25	80
11	5	6	10	6	5	1180.326	0.000	5.00	80
11	6	6	10	5	5	1180.436	0.001	5.00	80
7	4	3	6	3	4	1180.841	0.001	1.25	80
7	5	3	6	2	4	1181.790	0.001	1.25	80
10	7	4	9	6	3	1183.086	0.002	5.00	80
14	4	11	13	3	10	1183.141	-0.001	1.25	80
18	2	17	17	1	16	1184.095	-0.001	0.25	80
16	3	14	15	2	13	1185.163	-0.002	1.25	80
13	4	9	12	5	8	1187.027	0.000	5.00	80
8	6	2	7	5	3	1187.849	0.001	1.25	80
7	3	4	6	2	5	1188.096	-0.001	1.25	80
7	4	4	6	1	5	1188.166	-0.001	1.25	80
9	8	2	8	7	1	1189.082	-0.001	5.00	80
12	6	7	11	5	6	1189.461	0.000	5.00	80
11	6	5	10	7	4	1190.018	-0.001	5.00	80
19	1	18	18	2	17	1190.894	-0.002	0.25	80
11	7	5	10	6	4	1191.151	0.000	0.05	80
15	3	12	14	4	11	1191.183	-0.001	0.05	80
17	2	15	16	3	14	1192.613	-0.003	0.05	80
7	2	5	6	1	6	1194.367	0.004	0.25	80
14	5	10	13	4	9	1195.540	0.000	1.25	80
9	9	1	8	8	0	1196.290	0.001	5.00	80
7	7	0	6	4	3	1196.470	0.005	0.05	80
8	7	2	7	4	3	1196.823	0.002	1.25	80
9	9	0	8	8	1	1197.171	-0.001	5.00	80
10	8	3	9	7	2	1197.274	0.000	1.25	80
9	8	1	8	7	2	1197.425	-0.002	1.25	80
13	5	8	12	6	7	1198.416	0.003	1.25	80
16	4	13	15	3	12	1199.134	0.000	1.25	80
8	8	1	7	5	2	1199.693	0.001	5.00	80
12	6	6	11	7	5	1199.813	0.002	1.25	80
18	3	16	17	2	15	1199.982	0.001	0.25	80
12	7	6	11	6	5	1200.097	-0.001	5.00	80
8	6	3	7	3	4	1200.400	0.000	5.00	80
11	8	4	10	7	3	1203.806	0.002	1.25	80
15	4	11	14	5	10	1203.956	0.001	1.25	80
9	7	2	8	6	3	1204.546	0.000	5.00	80
8	4	4	7	3	5	1206.318	-0.001	0.05	80
8	5	4	7	2	5	1206.524	0.000	5.00	80
17	3	14	16	4	13	1206.995	0.001	0.05	80
14	6	9	13	5	8	1207.272	-0.005	1.25	80
12	7	5	11	8	4	1208.863	-0.001	1.25	80
13	6	7	12	7	6	1209.204	0.000	5.00	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
13	7	7	12	6	6	1209.275	0.001	0.25	80
10	9	2	9	8	1	1209.775	0.000	5.00	80
12	8	5	11	7	4	1211.229	0.002	5.00	80
16	5	12	15	4	11	1212.272	0.000	1.25	80
8	4	5	7	1	6	1212.763	-0.004	5.00	80
12	8	4	11	9	3	1213.747	0.004	0.05	80
18	4	15	17	3	14	1214.769	0.006	0.05	80
9	6	3	8	5	4	1215.699	0.000	5.00	80
10	10	1	9	9	0	1215.842	0.001	5.00	80
10	10	0	9	9	1	1216.421	-0.005	1.25	80
9	8	2	8	5	3	1217.544	-0.001	1.25	80
14	7	8	13	6	7	1218.423	-0.004	0.25	80
8	3	6	7	0	7	1218.609	0.001	1.25	80
11	9	3	10	8	2	1218.742	0.001	1.25	80
13	7	6	12	8	5	1219.237	-0.001	1.25	80
9	7	3	8	4	4	1219.402	0.001	5.00	80
13	8	6	12	7	5	1219.919	-0.001	0.25	80
17	4	13	16	5	12	1220.493	0.002	0.25	80
10	8	2	9	7	3	1221.326	0.000	5.00	80
9	9	1	8	6	2	1222.452	0.000	0.25	80
9	5	4	8	4	5	1224.535	0.001	5.00	80
16	6	11	15	5	10	1224.685	0.004	0.25	80
9	6	4	8	3	5	1225.048	0.000	1.25	80
12	9	4	11	8	3	1225.163	-0.001	5.00	80
13	11	2	12	12	1	1225.329	0.004	0.05	80
13	8	5	12	9	4	1227.290	0.005	0.25	80
15	6	9	14	7	8	1227.482	-0.003	1.25	80
14	8	7	13	7	6	1229.127	0.000	0.25	80
13	9	4	12	10	3	1229.710	0.005	0.25	80
11	10	2	10	9	1	1230.472	0.000	5.00	80
9	4	5	8	3	6	1231.253	0.001	1.25	80
9	5	5	8	2	6	1231.292	-0.001	0.05	80
13	9	5	12	8	4	1231.818	0.002	0.25	80
10	7	3	9	6	4	1232.599	-0.002	1.25	80
17	5	12	16	6	11	1233.229	0.004	0.25	80
11	10	1	10	9	2	1234.715	-0.001	5.00	80
11	11	1	10	10	0	1235.397	0.000	5.00	80
11	11	0	10	10	1	1235.788	0.000	5.00	80
16	7	10	15	6	9	1236.439	-0.003	0.25	80
9	3	6	8	2	7	1237.214	0.000	5.00	80
11	9	2	10	8	3	1238.322	-0.001	1.25	80
10	8	3	9	5	4	1238.884	-0.001	5.00	80
10	9	2	9	6	3	1239.218	0.000	1.25	80
14	9	6	13	8	5	1239.961	-0.003	0.25	80
12	10	3	11	9	2	1240.453	0.000	5.00	80
10	6	4	9	5	5	1242.602	-0.001	1.25	80
9	2	7	8	1	8	1242.713	0.000	1.25	80
10	7	4	9	4	5	1243.748	0.002	5.00	80
13	10	4	12	9	3	1247.104	0.001	0.25	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
11	8	3	10	7	4	1249.120	-0.001	1.25	80
10	5	5	9	4	6	1249.790	0.001	1.25	80
10	6	5	9	3	6	1249.906	0.000	5.00	80
12	11	2	11	10	1	1251.086	0.001	5.00	80
12	11	1	11	10	2	1253.959	-0.002	1.25	80
12	12	1	11	11	0	1254.931	-0.001	5.00	80
12	12	0	11	11	1	1255.199	0.001	0.05	80
12	10	2	11	9	3	1255.682	-0.001	1.25	80
10	5	6	9	2	7	1255.909	-0.001	1.25	80
11	9	3	10	6	4	1258.983	0.002	0.25	80
11	7	4	10	6	5	1260.352	-0.002	1.25	80
10	4	7	9	1	8	1261.502	0.000	1.25	80
11	8	4	10	5	5	1262.655	0.000	0.05	80
10	3	8	9	0	9	1266.680	0.000	1.25	80
11	6	5	10	5	6	1268.282	0.001	1.25	80
11	7	5	10	4	6	1268.581	-0.001	0.25	80
14	11	4	13	10	3	1269.488	0.002	0.25	80
13	12	2	12	11	1	1271.578	0.001	0.25	80
13	12	1	12	11	2	1273.484	0.000	0.25	80
13	11	2	12	10	3	1273.516	0.000	0.05	80
13	13	1	12	12	0	1274.422	-0.002	0.05	80
13	13	0	12	12	1	1274.611	0.002	1.25	80
12	8	4	11	7	5	1277.600	-0.004	0.25	80
12	10	3	11	7	4	1279.841	-0.004	0.25	80
11	4	7	10	3	8	1280.338	0.001	5.00	80
13	10	3	12	9	4	1281.430	0.000	0.25	80
12	9	4	11	6	5	1281.847	-0.002	1.25	80
14	12	3	13	11	2	1283.835	0.002	0.25	80
11	3	8	10	2	9	1285.624	0.000	1.25	80
12	7	5	11	6	6	1286.617	0.003	0.25	80
12	8	5	11	5	6	1287.310	0.000	1.25	80
11	2	9	10	1	10	1290.511	0.002	0.05	80
14	13	2	13	12	1	1291.940	-0.001	0.25	80
12	6	6	11	5	7	1293.311	0.003	0.25	80
12	7	6	11	4	7	1293.385	0.001	1.25	80
14	14	1	13	13	0	1293.852	-0.003	0.25	80
12	6	7	11	3	8	1299.179	0.001	1.25	80
12	5	8	11	2	9	1304.576	0.002	0.25	80
12	4	9	11	1	10	1309.581	0.000	0.25	80
12	3	10	11	0	11	1314.201	0.001	0.25	80
13	6	7	12	5	8	1317.967	0.006	0.25	80
13	5	8	12	4	9	1323.494	0.004	0.25	80
13	4	9	12	3	10	1328.620	0.001	0.25	80
13	3	10	12	2	11	1333.376	0.001	0.25	80
12	2	11	13	1	12	923.089	-0.016	0.05	82
6	6	1	7	7	0	930.499	0.000	0.25	82
11	1	10	12	2	11	931.071	-0.002	0.25	82
11	0	11	12	1	12	933.556	-0.001	1.25	82
10	3	8	11	2	9	935.367	0.002	0.25	82

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	3	6	10	4	7	938.022	0.006	0.25	82
10	2	9	11	1	10	938.978	-0.001	0.25	82
10	1	10	11	0	11	942.013	0.004	1.25	82
9	2	7	10	3	8	942.683	-0.002	0.25	82
7	4	3	8	5	4	944.542	-0.001	0.25	82
5	5	0	6	6	1	946.115	0.005	0.25	82
9	1	8	10	2	9	946.822	0.004	1.25	82
8	3	6	9	2	7	949.932	0.002	0.25	82
9	0	9	10	1	10	950.388	-0.003	5.00	82
7	3	4	8	4	5	951.355	0.006	0.05	82
6	5	2	7	4	3	953.112	-0.003	0.05	82
8	2	7	9	1	8	954.583	-0.002	1.25	82
4	4	1	5	5	0	956.357	0.004	0.05	82
7	2	5	8	3	6	957.102	0.005	0.25	82
6	4	3	7	3	4	958.140	0.000	1.25	82
8	1	8	9	0	9	958.701	0.003	5.00	82
4	4	0	5	5	1	960.361	0.004	0.05	82
7	1	6	8	2	7	962.278	0.001	5.00	82
5	3	2	6	4	3	963.326	-0.002	1.25	82
6	3	4	7	2	5	964.183	-0.013	0.05	82
7	0	7	8	1	8	966.926	0.000	5.00	82
4	3	1	5	4	2	968.268	0.002	0.05	82
6	2	5	7	1	6	969.888	-0.003	0.05	82
5	2	3	6	3	4	971.111	0.001	0.25	82
4	4	1	5	3	2	974.697	-0.007	0.05	82
6	1	6	7	0	7	975.073	0.001	0.25	82
5	1	4	6	2	5	977.421	-0.001	1.25	82
4	3	2	5	2	3	978.527	-0.001	0.25	82
7	0	7	7	1	6	981.011	0.005	0.05	82
5	0	5	6	1	6	983.135	-0.001	1.25	82
2	2	1	3	3	0	983.976	-0.002	1.25	82
3	3	1	4	2	2	987.071	-0.002	0.05	82
6	1	6	6	2	5	989.391	0.002	0.25	82
2	2	0	3	3	1	990.433	-0.002	0.25	82
4	1	4	5	0	5	991.115	-0.001	5.00	82
3	1	2	4	2	3	992.085	0.004	1.25	82
8	3	6	8	4	5	996.173	0.007	0.05	82
5	0	5	5	1	4	997.692	-0.008	0.25	82
3	0	3	4	1	4	999.010	0.004	0.25	82
2	2	1	3	1	2	1000.487	0.003	0.05	82
7	3	5	7	4	4	1003.514	0.008	0.05	82
7	2	5	7	3	4	1003.551	-0.002	0.05	82
4	1	4	4	2	3	1005.925	0.004	0.05	82
2	1	2	3	0	3	1006.848	0.003	0.25	82
5	1	4	5	2	3	1008.239	0.007	0.00	82
6	3	4	6	4	3	1010.726	0.005	0.05	82
7	4	4	7	5	3	1013.629	0.001	0.05	82
1	0	1	2	1	2	1014.278	0.005	0.25	82
4	2	3	4	3	2	1015.604	0.003	1.25	82



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	5	4	8	6	3	1016.789	-0.007	0.05	82
4	1	3	4	2	2	1016.221	0.005	0.25	82
5	3	3	5	4	2	1017.497	-0.002	0.05	82
5	2	3	5	3	2	1018.819	0.001	1.25	82
6	4	3	6	5	2	1019.629	-0.001	0.25	82
2	1	2	2	2	1	1021.475	0.004	0.25	82
4	3	2	4	4	1	1023.020	0.009	0.05	82
3	1	2	3	2	1	1024.468	0.001	0.25	82
7	4	3	7	5	2	1025.575	0.006	0.05	82
4	2	2	4	3	1	1026.536	0.004	0.25	82
5	3	2	5	4	1	1028.757	0.002	1.25	82
1	0	1	1	1	0	1029.877	0.003	1.25	82
3	2	1	3	3	0	1030.606	-0.003	1.25	82
5	4	1	5	5	0	1031.555	0.003	0.25	82
7	5	2	7	6	1	1033.076	-0.008	0.25	82
8	6	2	8	7	1	1034.995	0.004	0.05	82
1	1	0	1	0	1	1038.699	0.000	1.25	82
2	2	0	2	1	1	1040.022	-0.007	0.25	82
3	3	0	3	2	1	1042.094	0.000	5.00	82
4	4	0	4	3	1	1044.956	0.000	1.25	82
1	1	1	0	0	0	1046.277	0.004	0.25	82
3	2	1	3	1	2	1047.114	-0.001	1.25	82
2	2	1	2	1	2	1047.910	-0.001	1.25	82
5	5	0	5	4	1	1048.643	-0.005	1.25	82
5	4	1	5	3	2	1049.905	0.003	0.05	82
6	5	1	6	4	2	1052.303	0.002	0.25	82
4	4	1	4	3	2	1052.560	-0.001	1.25	82
2	1	2	1	0	1	1054.117	0.001	1.25	82
3	1	2	3	0	3	1055.510	0.008	0.05	82
7	6	1	7	5	2	1055.547	0.001	0.05	82
4	2	2	4	1	3	1056.779	-0.001	0.25	82
4	3	2	4	2	3	1057.551	-0.001	1.25	82
5	3	2	5	2	3	1058.180	0.000	1.25	82
6	6	1	6	5	2	1059.560	0.002	1.25	82
7	5	2	7	4	3	1061.387	0.001	1.25	82
3	0	3	2	1	2	1061.641	0.008	0.05	82
6	5	2	6	4	3	1062.694	-0.004	1.25	82
2	2	1	1	1	0	1063.510	-0.002	1.25	82
5	2	3	5	1	4	1065.963	-0.002	0.25	82
6	3	3	6	2	4	1068.070	-0.013	0.05	82
4	1	4	3	0	3	1069.338	-0.004	1.25	82
2	2	0	1	1	1	1070.928	0.009	0.05	82
7	5	3	7	4	4	1071.205	-0.002	0.05	82
3	2	2	2	1	1	1071.721	0.003	0.25	82
5	1	4	5	0	5	1072.448	-0.003	1.25	82
8	6	3	8	5	4	1074.387	0.001	0.25	82
5	0	5	4	1	4	1076.925	-0.001	5.00	82
4	1	3	3	2	2	1079.058	-0.004	0.25	82
4	2	3	3	1	2	1079.317	-0.001	1.25	82



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	3	1	2	2	0	1081.373	0.001	1.25	82
9	5	4	9	4	5	1083.124	0.003	0.25	82
7	2	5	7	1	6	1083.346	-0.003	0.25	82
6	1	6	5	0	5	1084.417	-0.001	5.00	82
8	4	5	8	3	6	1086.298	-0.005	1.25	82
5	1	4	4	2	3	1087.259	0.003	0.05	82
7	1	6	7	0	7	1088.840	0.000	1.25	82
9	4	5	9	3	6	1089.489	0.002	0.05	82
4	3	2	3	2	1	1089.937	-0.001	0.25	82
7	0	7	6	1	6	1091.816	0.002	5.00	82
10	6	5	10	5	6	1092.998	0.003	0.05	82
3	2	1	2	1	2	1094.539	-0.003	0.05	82
9	3	6	9	2	7	1095.086	-0.008	0.25	82
6	2	5	5	1	4	1095.265	0.003	1.25	82
5	2	3	4	3	2	1096.675	0.000	1.25	82
5	3	3	4	2	2	1097.445	-0.010	0.05	82
10	5	6	10	4	7	1098.604	-0.003	0.05	82
8	1	8	7	0	7	1099.112	-0.001	5.00	82
4	4	1	3	3	0	1099.770	-0.002	1.25	82
5	3	2	4	4	1	1102.673	0.010	0.05	82
7	1	6	6	2	5	1103.156	-0.001	1.25	82
9	1	8	9	0	9	1104.822	0.006	0.05	82
6	3	4	5	2	3	1105.580	0.007	0.05	82
9	0	9	8	1	8	1106.314	0.000	5.00	82
11	4	7	11	3	8	1107.546	-0.002	0.25	82
10	3	8	10	2	9	1108.454	0.004	0.25	82
5	4	2	4	3	1	1108.755	0.002	0.05	82
8	2	7	7	1	6	1110.958	-0.001	5.00	82
11	3	8	11	2	9	1112.307	0.001	0.05	82
10	1	10	9	0	9	1113.419	0.001	5.00	82
6	4	3	5	3	2	1116.161	0.002	5.00	82
9	1	8	8	2	7	1118.668	0.001	0.05	82
11	0	11	10	1	10	1120.423	-0.001	5.00	82
8	3	6	7	2	5	1122.144	0.000	5.00	82
7	3	4	6	4	3	1123.853	0.000	5.00	82
10	2	9	9	1	8	1126.283	0.001	5.00	82
12	1	12	11	0	11	1127.331	0.001	5.00	82
9	2	7	8	3	6	1130.316	-0.001	5.00	82
7	4	3	6	5	2	1131.828	-0.003	1.25	82
8	4	5	7	3	4	1132.750	-0.009	0.25	82
11	1	10	10	2	9	1133.802	-0.002	1.25	82
7	5	3	6	4	2	1135.477	0.002	0.25	82
5	3	2	4	2	3	1137.206	0.002	0.25	82
6	6	1	5	5	0	1137.738	0.001	5.00	82
10	3	8	9	2	7	1138.402	0.004	0.25	82
6	6	0	5	5	1	1140.603	-0.002	0.25	82
8	4	4	7	5	3	1142.346	-0.003	0.05	82
8	5	4	7	4	3	1143.255	-0.002	1.25	82
6	5	1	5	4	2	1144.651	0.000	0.25	82



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
11	2	9	10	3	8	1146.384	-0.002	1.25	82
15	0	15	14	1	14	1147.464	0.000	1.25	82
7	6	2	6	5	1	1147.993	0.002	0.25	82
13	1	12	12	2	11	1148.568	0.000	5.00	82
10	4	7	9	3	6	1149.847	0.000	5.00	82
9	4	5	8	5	4	1151.694	-0.001	5.00	82
12	3	10	11	2	9	1154.282	0.000	0.05	82
8	6	3	7	5	2	1155.414	0.001	5.00	82
14	2	13	13	1	12	1155.814	0.001	5.00	82
6	6	1	5	3	2	1156.088	0.001	0.25	82
7	7	1	6	6	0	1157.070	0.000	5.00	82
11	3	8	10	4	7	1158.258	-0.003	0.25	82
7	7	0	6	6	1	1159.066	0.001	5.00	82
10	4	6	9	5	5	1160.673	-0.001	0.05	82
10	5	6	9	4	5	1160.711	0.001	1.25	82
7	6	1	6	5	2	1161.807	0.000	5.00	82
13	2	11	12	3	10	1162.083	-0.002	0.25	82
9	6	4	8	5	3	1162.766	-0.002	0.05	82
9	6	3	8	7	2	1165.581	-0.002	0.25	82
12	4	9	11	3	8	1166.580	-0.001	1.25	82
8	7	2	7	6	1	1168.259	-0.001	5.00	82
11	4	7	10	5	6	1169.501	0.003	5.00	82
14	3	12	13	2	11	1169.797	-0.001	1.25	82
10	5	5	9	6	4	1170.773	-0.002	0.05	82
10	6	5	9	5	4	1171.257	0.002	0.05	82
13	3	10	12	4	9	1174.804	-0.001	1.25	82
9	7	3	8	6	2	1175.940	0.001	0.25	82
8	8	1	7	7	0	1176.516	-0.002	5.00	82
7	6	2	6	3	3	1176.703	0.001	0.05	82
15	2	13	14	3	12	1177.420	0.000	1.25	82
8	8	0	7	7	1	1177.868	-0.001	0.05	82
12	5	8	11	4	7	1178.212	0.000	1.25	82
10	6	4	9	7	3	1178.981	0.000	0.05	82
8	7	1	7	6	2	1179.318	0.006	0.25	82
11	5	6	10	6	5	1180.121	-0.001	1.25	82
11	6	6	10	5	5	1180.226	-0.003	0.05	82
7	5	3	6	2	4	1181.577	-0.006	0.25	82
10	7	4	9	6	3	1182.837	-0.001	5.00	82
14	4	11	13	3	10	1182.937	0.003	0.25	82
16	3	14	15	2	13	1184.951	-0.002	0.05	82
13	4	9	12	5	8	1186.822	0.002	1.25	82
8	6	2	7	5	3	1187.704	0.003	0.05	82
9	8	2	8	7	1	1188.799	-0.007	0.05	82
12	6	7	11	5	6	1189.248	-0.007	0.05	82
11	6	5	10	7	4	1189.818	-0.004	0.05	82
7	2	5	6	1	6	1194.161	0.004	0.05	82
9	9	1	8	8	0	1196.033	0.001	5.00	82
9	9	0	8	8	1	1196.934	0.001	1.25	82
10	8	3	9	7	2	1196.981	-0.001	1.25	82



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
13	5	8	12	6	7	1198.204	0.002	0.05	82
8	5	3	7	4	4	1198.237	0.000	0.05	82
8	8	1	7	5	2	1199.317	0.001	0.05	82
12	7	6	11	6	5	1199.881	-0.005	1.25	82
8	6	3	7	3	4	1200.188	0.004	1.25	82
11	8	4	10	7	3	1203.525	-0.007	0.05	82
9	7	2	8	6	3	1204.407	0.000	5.00	82
14	6	9	13	5	8	1207.062	0.004	0.05	82
13	6	7	12	7	6	1208.988	-0.001	0.05	82
10	9	2	9	8	1	1209.490	0.000	5.00	82
12	8	5	11	7	4	1210.981	-0.009	0.05	82
8	4	5	7	1	6	1212.554	-0.001	0.25	82
9	6	3	8	5	4	1215.535	0.000	0.05	82
10	10	1	9	9	0	1215.575	-0.001	1.25	82
10	10	0	9	9	1	1216.172	-0.004	0.25	82
13	7	6	12	8	5	1219.031	0.012	0.05	82
9	7	3	8	4	4	1219.173	0.002	0.05	82
13	8	6	12	7	5	1219.693	-0.002	0.05	82
10	8	2	9	7	3	1221.188	0.001	0.05	82
9	5	4	8	4	5	1224.331	0.000	1.25	82
11	10	2	10	9	1	1230.177	-0.004	0.25	82
9	4	5	8	3	6	1231.039	0.003	0.25	82
9	5	5	8	2	6	1231.074	-0.002	0.05	82
10	7	3	9	6	4	1232.451	-0.003	0.05	82
11	10	1	10	9	2	1234.499	0.002	1.25	82
11	11	1	10	10	0	1235.122	-0.003	0.05	82
11	11	0	10	10	1	1235.527	0.000	5.00	82
9	3	6	8	2	7	1236.999	0.005	0.25	82
11	9	2	10	8	3	1238.178	0.006	0.25	82
10	8	3	9	5	4	1238.634	-0.001	1.25	82
12	10	3	11	9	2	1240.114	-0.010	0.05	82
10	6	4	9	5	5	1242.397	-0.009	0.05	82
9	2	7	8	1	8	1242.490	0.001	0.05	82
10	7	4	9	4	5	1243.527	0.003	0.25	82
10	6	5	9	3	6	1249.687	0.001	0.25	82
12	11	2	11	10	1	1250.790	-0.001	0.25	82
12	12	1	11	11	0	1254.651	-0.001	0.25	82
11	7	4	10	6	5	1260.171	0.008	0.05	82
10	4	7	9	1	8	1261.276	0.001	0.25	82
11	6	5	10	5	6	1268.068	0.009	0.05	82
13	13	0	12	12	1	1274.324	-0.001	0.05	82
11	4	7	10	3	8	1280.104	-0.002	0.05	82
12	9	4	11	6	5	1281.602	0.012	0.05	82

APPENDIX E

WEIGHTED AVERAGED GSCD'S OF H₂Se ISOTOPOMERS

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	2	1	2	2	1	45.628	-0.004	0.02	74
3	0	3	1	0	1	47.345	0.008	0.01	74
4	1	4	2	1	2	62.703	0.003	0.05	74
7	0	7	5	0	5	109.483	0.009	0.08	74
10	1	10	8	1	8	156.100	0.006	0.00	74
2	2	1	1	0	1	32.707	0.000	0.82	76
2	1	2	1	1	0	15.615	0.000	0.48	76
3	3	0	1	1	0	79.625	0.002	0.55	76
3	3	0	2	1	2	64.011	0.002	0.25	76
3	3	0	3	1	2	16.543	-0.004	1.57	76
3	2	1	2	2	1	45.642	0.002	2.09	76
3	3	1	2	1	1	49.708	-0.003	0.41	76
3	2	1	3	0	3	31.021	-0.005	0.10	76
3	3	1	3	1	3	33.721	-0.010	0.01	76
3	1	2	1	1	0	63.077	0.001	0.62	76
3	1	2	2	1	2	47.463	0.002	0.26	76
3	0	3	1	0	1	47.324	0.003	0.67	76
3	1	3	1	1	1	46.877	0.007	0.02	76
3	0	3	2	2	1	14.612	-0.002	0.25	76
3	1	3	2	1	1	15.970	-0.010	0.08	76
4	4	0	2	2	0	111.600	0.012	0.02	76
4	4	0	4	2	2	17.233	-0.002	0.10	76
4	4	1	2	2	1	112.753	-0.002	0.19	76
4	3	1	3	3	1	59.943	0.007	0.25	76
4	4	1	3	2	1	67.117	0.002	0.73	76
4	4	1	3	0	3	98.137	-0.004	0.08	76
4	3	1	4	1	3	30.219	0.000	0.41	76
4	4	1	4	2	3	34.661	-0.001	0.41	76
4	2	2	2	2	0	94.353	-0.001	0.10	76
4	3	2	3	3	0	47.244	-0.001	0.10	76
4	2	2	3	2	2	62.877	0.003	0.02	76
4	3	2	3	1	2	63.792	-0.001	1.25	76
4	1	3	2	1	1	79.433	0.006	0.05	76
4	1	3	3	3	1	29.724	0.007	0.41	76
4	2	3	3	2	1	32.455	0.002	2.07	76
4	2	3	3	0	3	63.476	-0.003	0.10	76
4	1	4	2	1	2	62.682	-0.002	0.41	76
4	1	4	3	1	2	15.225	0.003	0.02	76
5	5	0	4	3	2	96.376	0.002	0.08	76
5	5	0	5	3	2	18.513	0.002	0.23	76
5	4	1	3	2	1	140.922	-0.002	0.02	76
5	4	1	4	4	1	73.809	0.000	5.09	76



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	5	1	4	3	1	84.877	0.004	0.10	76
5	4	1	5	2	3	29.382	-0.001	0.98	76
5	3	2	4	3	2	77.870	0.006	2.00	76
5	4	2	4	2	2	80.069	-0.005	0.08	76
5	3	2	5	1	4	47.141	0.005	0.10	76
5	4	2	5	2	4	48.650	-0.010	0.10	76
5	2	3	3	2	1	111.542	0.002	0.48	76
5	2	3	3	0	3	142.563	-0.003	0.08	76
5	2	3	4	4	1	44.426	0.001	0.25	76
5	3	3	4	3	1	49.012	0.009	0.08	76
5	2	3	4	2	3	79.088	0.001	0.50	76
5	2	3	5	0	5	64.272	0.005	0.25	76
5	1	4	3	1	2	94.523	0.003	0.10	76
5	1	4	4	3	2	30.730	0.002	0.20	76
5	2	4	4	2	2	31.419	0.004	0.41	76
5	1	4	4	1	4	79.299	0.001	1.25	76
5	0	5	3	0	3	78.296	-0.003	1.25	76
5	0	5	4	2	3	14.820	0.000	0.08	76
6	6	0	4	4	0	175.655	0.003	0.02	76
6	6	0	5	4	2	112.812	0.000	0.05	76
6	6	1	4	4	1	176.724	0.005	0.12	76
6	6	1	5	4	1	102.916	0.005	0.10	76
6	5	1	6	3	3	28.666	-0.005	0.41	76
6	5	2	5	5	0	78.196	-0.002	0.20	76
6	5	2	5	3	2	96.715	0.007	0.05	76
6	5	2	5	1	4	143.842	-0.002	0.25	76
6	4	2	6	2	4	46.056	0.000	0.05	76
6	5	2	6	3	4	48.903	-0.002	2.09	76
6	3	3	4	3	1	143.521	-0.003	0.05	76
6	4	3	5	4	1	65.560	0.000	2.09	76
6	4	3	5	2	3	94.944	0.001	0.50	76
6	3	4	4	3	2	125.678	0.011	0.48	76
6	3	4	5	3	2	47.808	0.005	0.67	76
6	3	4	5	1	4	94.943	0.004	0.16	76
6	2	5	4	2	3	109.936	0.001	0.10	76
6	2	5	5	2	3	30.845	-0.003	0.53	76
6	2	5	5	0	5	95.116	0.001	0.41	76
6	1	6	4	1	4	93.885	0.008	1.67	76
6	1	6	5	1	4	14.582	0.003	2.42	76
7	7	0	5	5	0	207.572	-0.002	0.48	76
7	7	0	5	3	2	226.091	0.006	0.08	76
7	7	0	6	5	2	129.376	-0.001	0.08	76
7	7	0	7	5	2	23.203	0.003	0.48	76
7	6	1	5	2	3	232.875	0.004	0.02	76
7	6	1	6	6	1	100.573	-0.003	0.48	76
7	6	1	7	4	3	28.313	0.021	-0.02	76
7	5	2	6	5	2	106.178	0.001	0.48	76
7	5	2	6	3	4	155.081	-0.001	0.41	76
7	5	2	7	3	4	44.678	0.001	0.51	76



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	6	2	7	4	4	49.364	-0.004	0.05	76
7	4	3	7	2	5	63.066	0.000	0.51	76
7	3	4	5	1	4	205.340	-0.004	0.08	76
7	3	4	6	5	2	61.499	0.000	2.09	76
7	3	4	6	3	4	110.403	-0.001	1.38	76
7	3	4	6	1	6	190.770	0.006	0.05	76
7	3	4	7	1	6	79.858	0.002	0.35	76
7	2	5	5	2	3	141.518	0.005	0.16	76
7	3	5	6	3	3	46.889	0.003	0.01	76
7	2	5	6	2	5	110.670	0.005	0.60	76
7	2	5	7	0	7	96.332	-0.001	0.41	76
7	1	6	5	1	4	125.487	0.000	0.10	76
7	1	6	6	1	6	110.909	0.001	0.19	76
7	0	7	5	0	5	109.444	-0.003	2.01	76
7	0	7	6	2	5	14.337	0.005	2.00	76
8	7	2	8	5	4	50.105	-0.003	0.05	76
8	6	3	7	4	3	126.630	0.003	0.10	76
8	6	3	7	2	5	189.698	0.005	0.05	76
8	5	4	8	3	6	79.413	0.011	0.41	76
8	4	5	6	2	5	236.756	0.002	0.08	76
8	4	5	7	4	3	63.030	0.007	0.50	76
8	4	5	7	2	5	126.095	0.006	0.47	76
8	4	5	7	0	7	222.428	0.005	0.41	76
8	4	5	8	2	7	95.742	-0.003	0.41	76
8	3	6	6	3	4	156.916	0.003	0.05	76
8	3	6	6	1	6	237.282	0.009	0.08	76
8	3	6	7	3	4	46.512	0.003	0.08	76
8	3	6	7	1	6	126.371	0.005	0.42	76
8	2	7	6	2	5	141.010	0.000	2.25	76
8	2	7	7	2	5	30.341	-0.004	0.41	76
8	2	7	7	0	7	126.673	-0.005	1.25	76
8	1	8	6	1	6	125.005	0.003	2.07	76
9	7	2	8	7	2	132.134	-0.002	0.48	76
9	7	2	9	5	4	41.508	-0.002	0.41	76
9	6	3	9	4	5	60.599	-0.001	0.08	76
9	5	4	8	5	4	140.724	-0.009	0.51	76
9	5	4	8	3	6	220.138	0.003	0.25	76
9	5	4	9	3	6	78.458	-0.003	0.10	76
9	4	5	7	4	3	204.373	0.019	0.02	76
9	4	5	7	2	5	267.438	0.018	0.02	76
9	4	5	8	4	5	141.341	0.010	0.02	76
9	4	5	9	2	7	95.042	-0.006	0.25	76
9	3	6	7	3	4	188.176	-0.008	0.08	76
9	3	6	7	1	6	268.033	-0.007	0.08	76
9	3	6	8	3	6	141.678	0.003	0.02	76
9	3	6	9	1	8	111.526	0.003	0.10	76
9	2	7	7	0	7	268.708	0.003	0.41	76
9	2	7	8	4	5	46.280	-0.003	1.25	76
9	2	7	8	2	7	142.028	0.001	0.10	76



UPPER			LOWER			OBSERVED (cm ⁻¹)	OBS-CALC (cm ⁻¹)	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c				
9	1	8	7	1	6	156.517	0.000	2.00	76
9	1	8	8	3	6	30.147	-0.004	0.10	76
9	0	9	7	0	7	140.541	0.000	5.00	76
10	7	4	9	7	2	115.153	-0.003	0.41	76
10	7	4	9	5	4	156.661	-0.005	0.25	76
10	6	5	10	4	7	94.342	0.002	0.10	76
10	5	6	10	3	8	110.696	-0.003	0.10	76
10	4	7	8	4	5	203.500	0.002	0.41	76
10	4	7	8	2	7	299.242	-0.001	0.25	76
10	4	7	10	2	9	127.246	0.007	0.17	76
10	3	8	8	3	6	187.800	-0.002	0.48	76
10	3	8	9	3	6	46.133	0.005	0.48	76
10	3	8	9	1	8	157.655	0.004	0.25	76
10	2	9	8	2	7	172.004	-0.001	0.10	76
10	1	10	8	1	8	156.060	-0.002	2.00	76
10	1	10	9	1	8	13.633	-0.006	0.10	76
11	3	8	9	1	8	330.357	0.002	0.02	76
11	3	8	10	5	6	62.007	0.002	0.10	76
11	3	8	10	3	8	172.703	-0.001	0.05	76
11	2	9	9	2	7	203.216	0.004	0.10	76
11	1	10	9	1	8	187.472	0.001	2.00	76
11	1	10	10	1	10	173.839	0.007	0.10	76
12	3	10	10	3	8	218.595	-0.003	0.10	76
12	1	12	10	1	10	187.035	-0.005	2.01	76
13	2	11	11	2	9	233.955	-0.002	0.41	76
14	1	14	12	1	12	217.928	0.011	0.41	76
2	2	1	1	0	1	32.702	0.006	0.16	77
2	1	2	1	1	0	15.614	0.002	0.05	77
3	3	0	1	1	0	79.611	0.004	0.08	77
3	3	0	3	1	2	16.536	-0.004	0.55	77
3	2	1	2	2	1	45.642	-0.001	0.41	77
3	3	1	2	1	1	49.678	-0.012	0.06	77
3	1	2	1	1	0	63.072	0.005	0.17	77
3	1	2	2	1	2	47.470	0.015	0.02	77
3	0	3	1	0	1	47.308	-0.004	0.32	77
3	0	3	2	2	1	14.608	-0.008	0.08	77
4	4	0	3	2	2	80.070	-0.019	0.02	77
4	3	1	3	3	1	59.945	0.000	0.08	77
4	4	1	3	2	1	67.077	-0.004	0.43	77
4	4	1	3	0	3	98.111	0.003	0.02	77
4	3	1	4	1	3	30.217	-0.007	0.25	77
4	4	1	4	2	3	34.639	-0.001	0.28	77
4	3	2	3	3	0	47.244	0.005	0.60	77
4	3	2	3	1	2	63.776	-0.003	0.38	77
4	1	3	2	1	1	79.411	0.000	0.02	77
4	2	3	3	2	1	32.443	0.002	0.60	77
4	2	3	3	0	3	63.470	0.002	0.08	77
5	5	0	3	3	0	143.590	0.007	0.08	77
5	5	0	4	3	2	96.345	0.001	0.10	77

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	5	0	5	3	2	18.480	-0.002	0.10	77
5	4	1	4	4	1	73.826	0.000	2.15	77
5	4	1	5	2	3	29.391	0.001	0.69	77
5	3	2	4	3	2	77.863	0.001	0.08	77
5	4	2	4	2	2	80.066	0.013	0.06	77
5	4	2	5	2	4	48.650	0.002	0.08	77
5	2	3	3	2	1	111.517	0.000	0.50	77
5	2	3	4	4	1	44.431	-0.004	0.23	77
5	2	3	4	2	3	79.071	-0.005	0.25	77
5	2	3	5	0	5	64.272	0.014	0.08	77
5	1	4	4	3	2	30.725	0.001	0.02	77
5	1	4	4	1	4	79.286	0.001	0.10	77
5	0	5	3	0	3	78.285	-0.001	0.25	77
6	6	1	4	4	1	176.669	0.000	0.10	77
6	6	1	5	4	1	102.843	-0.001	0.10	77
6	5	1	5	3	3	123.182	-0.004	0.25	77
6	5	2	5	5	0	78.191	-0.003	1.25	77
6	5	2	5	3	2	96.674	-0.001	0.25	77
6	5	2	6	3	4	48.890	0.000	0.41	77
6	4	3	5	4	1	65.537	0.002	0.49	77
6	4	3	5	2	3	94.931	0.005	0.25	77
6	4	3	6	2	5	64.084	-0.001	0.06	77
6	3	4	4	3	2	125.650	0.002	0.05	77
6	3	4	5	3	2	47.787	0.001	0.08	77
6	2	5	5	2	3	30.840	-0.001	0.05	77
6	1	6	4	1	4	93.866	0.004	0.35	77
6	1	6	5	1	4	14.575	-0.002	0.42	77
7	7	0	5	5	0	207.521	0.009	0.10	77
7	7	0	5	3	2	226.001	0.007	0.05	77
7	6	1	5	4	1	203.455	0.001	0.41	77
7	6	1	5	2	3	232.839	-0.005	0.19	77
7	6	1	6	6	1	100.607	-0.003	0.41	77
7	6	1	7	4	3	28.308	0.016	0.10	77
7	5	2	6	5	2	106.193	0.002	0.10	77
7	5	2	6	3	4	155.083	0.003	0.08	77
7	5	2	7	3	4	44.694	0.001	0.51	77
7	6	2	7	4	4	49.348	0.001	0.08	77
7	4	3	7	2	5	63.060	-0.004	0.43	77
7	3	4	6	5	2	61.499	0.001	1.25	77
7	3	4	6	3	4	110.389	0.002	0.47	77
7	3	4	7	1	6	79.838	-0.006	0.25	77
7	2	5	6	4	3	46.560	-0.002	0.02	77
7	2	5	6	2	5	110.646	-0.001	0.10	77
7	2	5	7	0	7	96.321	0.003	0.08	77
7	1	6	6	1	6	110.900	0.010	0.02	77
7	0	7	5	0	5	109.430	0.002	0.05	77
7	0	7	6	2	5	14.325	-0.004	0.41	77
8	8	1	8	6	3	40.918	-0.001	0.10	77
8	6	2	8	4	4	43.125	0.001	0.08	77

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	7	2	8	5	4	50.084	0.005	0.10	77
8	6	3	7	4	3	126.595	0.002	0.19	77
8	6	3	7	2	5	189.655	-0.002	0.08	77
8	6	3	8	4	5	63.591	0.002	0.10	77
8	5	4	8	3	6	79.392	0.004	0.48	77
8	4	5	6	4	3	172.630	0.000	0.10	77
8	4	5	6	2	5	236.712	-0.003	0.10	77
8	4	5	7	2	5	126.071	0.003	0.08	77
8	3	6	6	3	4	156.889	0.001	0.10	77
8	3	6	6	3	5	156.894	-0.009	0.05	77
8	3	6	7	3	4	46.505	0.004	0.08	77
8	3	6	7	1	6	126.341	-0.004	0.12	77
8	2	7	6	2	5	140.994	0.007	0.19	77
8	2	7	7	2	5	30.345	0.004	0.05	77
8	2	7	7	0	7	126.666	0.008	0.08	77
8	1	8	6	1	6	124.983	0.002	1.25	77
8	1	8	7	1	6	14.086	-0.006	0.50	77
9	7	2	8	7	2	132.171	0.002	0.08	77
9	6	3	7	4	3	264.927	-0.002	0.26	77
9	6	3	7	2	5	327.990	-0.003	0.02	77
9	6	3	8	6	3	138.331	-0.005	0.02	77
9	6	3	9	4	5	60.614	-0.003	0.12	77
9	5	4	8	3	6	220.106	0.002	0.02	77
9	5	4	9	3	6	78.454	0.001	0.26	77
9	4	5	7	4	3	204.311	-0.001	0.43	77
9	4	5	7	2	5	267.377	0.001	0.01	77
9	4	5	8	6	3	77.716	-0.003	0.08	77
9	5	5	8	3	5	141.349	0.003	0.05	77
9	4	5	8	2	7	237.033	-0.003	0.02	77
9	4	5	9	2	7	95.025	-0.006	0.08	77
9	3	6	7	3	4	188.157	0.005	0.08	77
9	3	6	7	1	6	267.995	-0.001	0.08	77
9	3	6	8	3	6	141.658	0.007	0.15	77
9	3	6	9	1	8	111.503	0.001	0.10	77
9	2	7	7	2	5	172.347	0.002	0.08	77
9	2	7	8	4	5	46.276	-0.001	0.05	77
9	2	7	8	2	7	142.006	0.001	0.02	77
9	1	8	7	1	6	156.489	-0.005	0.41	77
9	1	8	8	3	6	30.154	0.005	0.48	77
9	1	8	8	1	8	142.405	0.003	0.31	77
9	0	9	7	0	7	140.519	0.000	2.00	77
9	0	9	8	2	7	13.865	0.004	0.10	77
10	6	5	10	4	7	94.325	0.005	0.08	77
10	5	6	8	3	6	298.463	0.012	0.02	77
10	5	6	9	5	4	78.350	0.003	0.08	77
10	5	6	9	3	6	156.805	0.005	0.08	77
10	5	6	10	3	8	110.679	0.004	0.02	77
10	4	7	8	2	7	299.211	0.016	0.08	77
10	4	7	10	2	9	127.217	0.003	0.08	77

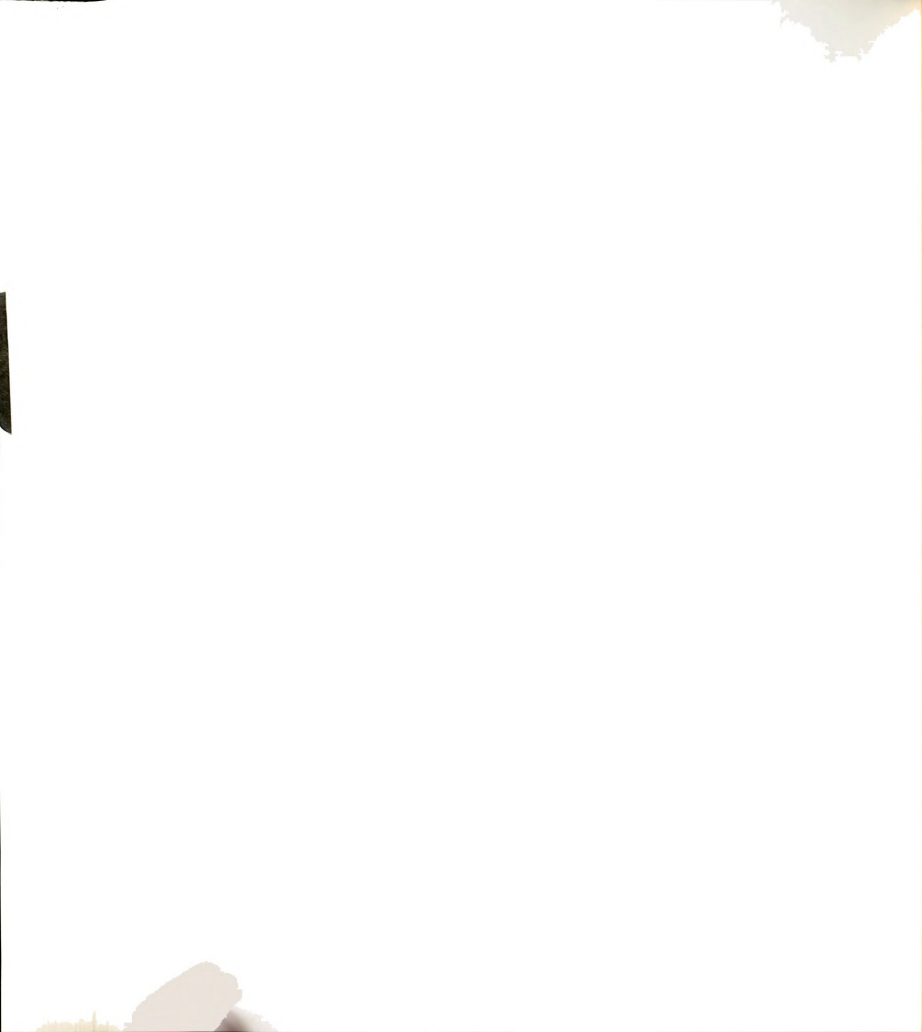


UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	3	8	8	3	6	187.775	-0.001	0.10	77
10	3	8	9	3	6	46.121	-0.004	0.10	77
10	3	8	9	1	8	157.622	-0.005	0.12	77
10	2	9	8	2	7	171.985	0.004	0.05	77
10	1	10	8	1	8	156.034	-0.004	0.55	77
10	1	10	9	1	8	13.634	-0.002	0.17	77
11	5	6	9	3	6	328.542	-0.009	0.19	77
11	4	7	10	4	7	172.202	0.003	0.02	77
11	3	8	10	3	8	172.681	0.004	0.05	77
11	1	10	9	1	8	187.450	0.003	0.41	77
11	1	10	10	1	10	173.807	-0.004	0.08	77
11	0	11	9	0	9	171.528	-0.009	0.15	77
12	5	8	10	5	6	249.536	-0.004	0.02	77
12	5	8	10	3	8	360.215	0.000	1.25	77
12	3	10	10	3	8	218.579	0.007	0.10	77
12	3	10	10	1	10	362.555	-0.008	0.06	77
12	2	11	11	2	9	29.670	-0.009	0.10	77
12	1	12	10	1	10	187.023	0.010	0.02	77
13	2	11	11	2	9	233.927	-0.003	0.10	77
13	2	11	12	2	11	204.257	0.007	0.05	77
13	0	13	11	0	11	202.466	0.002	0.10	77
14	1	14	12	1	12	217.888	0.001	0.41	77
2	2	0	0	0	0	47.726	0.007	0.02	78
2	2	0	2	0	2	16.256	0.000	0.36	78
2	1	1	1	1	1	30.893	0.003	0.48	78
2	2	1	1	0	1	32.685	0.000	7.09	78
2	0	2	0	0	0	31.467	0.004	0.06	78
2	1	2	1	1	0	15.609	-0.001	4.00	78
3	3	0	1	1	0	79.592	0.000	6.50	78
3	3	0	2	1	2	63.982	0.000	2.98	78
3	3	0	3	1	2	16.532	-0.001	8.75	78
3	2	1	1	0	1	78.338	0.005	0.12	78
3	3	1	1	1	1	80.566	0.007	0.41	78
3	2	1	2	2	1	45.649	0.002	2.60	78
3	3	1	2	1	1	49.672	0.002	2.18	78
3	2	1	3	0	3	31.029	0.000	1.54	78
3	3	1	3	1	3	33.700	-0.002	0.05	78
3	1	2	1	1	0	63.058	-0.001	3.32	78
3	2	2	2	2	0	31.464	-0.006	0.15	78
3	1	2	2	1	2	47.448	-0.001	2.09	78
3	2	2	2	0	2	47.719	-0.007	0.08	78
3	0	3	1	0	1	47.303	-0.001	1.00	78
3	1	3	1	1	1	46.859	0.001	0.02	78
3	0	3	2	2	1	14.618	0.000	0.58	78
3	1	3	2	1	1	15.961	-0.007	0.10	78
4	4	0	3	2	2	80.066	-0.003	0.12	78
4	4	0	4	2	2	17.209	0.004	1.50	78
4	4	1	2	2	1	112.695	-0.001	0.15	78
4	3	1	3	3	1	59.955	0.000	2.01	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
4	4	1	3	2	1	67.050	0.001	7.28	78
4	4	1	3	0	3	98.082	0.004	0.10	78
4	3	1	4	1	3	30.229	0.000	5.43	78
4	4	1	4	2	3	34.618	-0.001	7.75	78
4	2	2	2	2	0	94.331	-0.003	0.48	78
4	3	2	2	1	2	111.216	0.001	0.16	78
4	3	2	3	3	0	47.236	0.003	5.61	78
4	2	2	3	2	2	62.857	-0.008	0.12	78
4	3	2	3	1	2	63.766	0.000	2.75	78
4	3	2	4	1	4	48.549	-0.002	0.26	78
4	1	3	2	1	1	79.406	0.010	0.01	78
4	2	3	2	2	1	78.078	0.001	0.12	78
4	1	3	3	3	1	29.720	-0.006	0.08	78
4	2	3	3	2	1	32.430	0.001	9.10	78
4	2	3	3	0	3	63.460	0.002	2.20	78
4	1	4	2	1	2	62.664	0.000	0.42	78
4	1	4	3	1	2	15.221	0.007	0.69	78
5	5	0	3	3	0	143.551	0.002	5.66	78
5	5	0	4	3	2	96.316	0.000	7.00	78
5	5	0	5	3	2	18.455	0.001	11.70	78
5	4	1	3	2	1	140.896	0.004	0.48	78
5	5	1	3	3	1	144.728	-0.004	0.82	78
5	4	1	3	0	3	171.928	0.007	0.08	78
5	4	1	4	4	1	73.844	0.001	7.47	78
5	5	1	4	3	1	84.774	-0.003	0.76	78
5	4	1	4	2	3	108.463	0.000	2.56	78
5	5	1	4	1	3	115.002	-0.004	0.16	78
5	4	1	5	2	3	29.399	0.001	7.72	78
5	5	1	5	3	3	35.807	-0.002	0.28	78
5	3	2	3	3	0	125.095	0.000	0.02	78
5	4	2	3	2	2	142.889	-0.008	0.02	78
5	4	2	4	4	0	62.825	-0.003	0.41	78
5	3	2	4	3	2	77.864	0.002	4.25	78
5	4	2	4	2	2	80.031	-0.002	1.42	78
5	3	2	5	1	4	47.140	0.000	2.76	78
5	4	2	5	2	4	48.638	0.001	0.55	78
5	2	3	3	2	1	111.495	0.001	5.27	78
5	3	3	3	3	1	108.917	-0.006	0.02	78
5	2	3	3	0	3	142.527	0.004	0.10	78
5	2	3	4	4	1	44.445	0.000	6.71	78
5	3	3	4	3	1	48.970	0.002	0.85	78
5	2	3	4	2	3	79.065	0.000	7.18	78
5	3	3	4	1	3	79.195	-0.002	0.08	78
5	2	3	5	0	5	64.247	-0.003	3.68	78
5	1	4	3	1	2	94.492	0.005	0.10	78
5	1	4	4	3	2	30.728	0.007	0.20	78
5	2	4	4	2	2	31.393	-0.003	0.24	78
5	1	4	4	1	4	79.272	-0.001	5.05	78
5	0	5	3	0	3	78.271	-0.002	2.00	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	0	5	4	2	3	14.831	0.017	0.82	78
6	6	0	4	2	2	192.762	0.000	0.08	78
6	6	0	5	4	2	112.725	-0.004	0.73	78
6	6	0	6	4	2	20.398	-0.002	0.41	78
6	6	1	4	4	1	176.620	-0.003	5.21	78
6	5	1	5	5	1	87.381	0.008	0.01	78
6	6	1	5	4	1	102.776	-0.004	5.13	78
6	6	1	5	2	3	132.168	-0.010	0.02	78
6	5	1	6	3	3	28.680	-0.005	0.02	78
6	6	1	6	4	3	37.260	-0.006	0.10	78
6	5	2	4	3	2	174.514	0.007	0.08	78
6	5	2	5	5	0	78.193	0.002	1.67	78
6	4	2	5	4	2	92.326	-0.004	2.48	78
6	5	2	5	3	2	96.644	-0.001	6.58	78
6	4	2	5	2	4	140.967	0.000	0.25	78
6	5	2	5	1	4	143.784	-0.001	2.00	78
6	4	2	6	2	4	46.073	-0.001	1.27	78
6	5	2	6	3	4	48.873	-0.003	5.18	78
6	3	3	4	3	1	143.470	0.004	0.42	78
6	4	3	4	4	1	139.356	-0.001	1.25	78
6	3	3	4	1	3	173.695	0.000	0.25	78
6	4	3	4	2	3	173.976	0.000	1.29	78
6	3	3	5	5	1	58.699	0.010	0.10	78
6	4	3	5	4	1	65.513	0.000	7.24	78
6	3	3	5	3	3	94.502	0.004	0.10	78
6	4	3	5	2	3	94.911	0.000	7.91	78
6	4	3	5	0	5	159.173	0.011	0.41	78
6	3	3	6	1	5	63.765	-0.004	0.41	78
6	4	3	6	2	5	64.078	0.001	2.18	78
6	3	4	5	3	2	47.771	0.001	0.58	78
6	3	4	5	1	4	94.912	0.002	0.35	78
6	3	4	6	1	6	80.341	0.004	0.60	78
6	2	5	4	2	3	109.899	0.000	0.25	78
6	2	5	5	2	3	30.837	0.003	1.90	78
6	2	5	5	0	5	95.083	-0.002	2.84	78
6	1	6	4	1	4	93.847	0.001	5.00	78
6	1	6	5	1	4	14.573	0.000	10.10	78
7	7	0	5	5	0	207.453	-0.003	2.00	78
7	7	0	5	3	2	225.907	-0.003	2.00	78
7	7	0	6	5	2	129.264	-0.001	0.48	78
7	6	1	5	4	1	203.423	-0.002	0.50	78
7	6	1	6	6	1	100.647	0.002	5.18	78
7	7	1	6	5	1	120.933	-0.013	0.34	78
7	6	1	6	4	3	137.912	0.001	1.02	78
7	6	1	7	4	3	28.294	-0.001	5.16	78
7	5	2	6	5	2	106.210	0.003	2.00	78
7	6	2	6	4	2	113.693	0.000	0.19	78
7	5	2	6	3	4	155.083	0.001	2.00	78
7	6	2	6	2	4	159.771	0.003	0.02	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	5	2	7	3	4	44.710	0.000	5.00	78
7	6	2	7	4	4	49.334	0.006	0.10	78
7	4	3	5	4	1	175.122	-0.008	0.25	78
7	5	3	5	5	1	169.353	-0.002	0.25	78
7	5	3	5	3	3	205.158	-0.006	0.08	78
7	4	3	6	4	3	109.627	0.011	0.10	78
7	5	3	6	3	3	110.668	0.001	0.17	78
7	4	3	6	2	5	173.698	0.005	0.08	78
7	5	3	6	1	5	174.429	-0.007	0.08	78
7	4	3	7	2	5	63.065	0.002	6.36	78
7	5	3	7	3	5	63.807	0.004	0.16	78
7	3	4	5	3	2	158.136	-0.005	5.30	78
7	4	4	5	4	2	156.693	-0.002	0.48	78
7	3	4	5	1	4	205.277	-0.004	2.00	78
7	4	4	5	2	4	205.330	-0.001	0.25	78
7	3	4	6	5	2	61.493	-0.003	5.08	78
7	4	4	6	4	2	64.366	0.001	0.34	78
7	3	4	6	3	4	110.370	-0.002	0.50	78
7	4	4	6	2	4	110.445	0.006	0.10	78
7	3	4	6	3	5	110.371	-0.015	0.25	78
7	3	4	6	1	6	190.703	-0.005	0.34	78
7	3	4	7	1	6	79.833	-0.002	0.89	78
7	2	5	5	2	3	141.473	0.008	0.60	78
7	2	5	5	0	5	205.714	-0.001	0.13	78
7	2	5	6	4	3	46.564	0.010	0.42	78
7	3	5	6	3	3	46.861	-0.003	0.47	78
7	2	5	6	2	5	110.640	0.009	0.76	78
7	3	5	6	1	5	110.626	-0.007	0.25	78
7	2	5	7	0	7	96.309	0.003	1.72	78
7	1	6	5	1	4	125.446	0.000	0.48	78
7	1	6	6	3	4	30.538	0.002	0.12	78
7	1	6	6	3	5	30.537	-0.014	0.41	78
7	1	6	6	1	6	110.873	0.000	1.45	78
7	0	7	5	0	5	109.408	-0.002	2.07	78
7	0	7	6	2	5	14.321	-0.004	6.34	78
8	8	1	6	6	1	239.767	0.001	2.25	78
8	8	1	7	6	1	139.121	0.000	2.48	78
8	7	1	7	5	3	152.770	0.009	0.41	78
8	8	1	7	4	3	167.419	0.003	0.48	78
8	7	1	8	5	3	28.481	-0.001	0.41	78
8	6	2	6	4	2	233.180	0.002	1.25	78
8	7	2	6	5	2	237.418	-0.002	0.48	78
8	6	2	6	2	4	279.258	0.006	0.02	78
8	7	2	7	7	0	108.154	-0.002	0.25	78
8	6	2	7	6	2	119.484	-0.001	0.27	78
8	6	2	8	4	4	43.153	0.004	1.25	78
8	6	3	6	4	3	236.184	-0.003	0.60	78
8	6	3	6	2	5	300.259	-0.004	0.25	78
8	6	3	7	6	1	98.276	0.001	0.33	78



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	5	3	7	5	3	124.285	0.006	0.17	78
8	6	3	7	4	3	126.566	-0.004	2.15	78
8	5	3	7	3	5	188.099	0.017	0.02	78
8	6	3	7	2	5	189.632	-0.001	2.04	78
8	5	3	8	3	5	62.045	0.003	0.42	78
8	6	3	8	4	5	63.581	-0.002	3.34	78
8	4	4	6	4	2	190.027	-0.002	1.25	78
8	5	4	6	5	2	187.367	-0.001	0.10	78
8	4	4	6	2	4	236.105	0.001	0.02	78
8	5	4	6	3	4	236.241	-0.003	0.20	78
8	5	4	6	1	6	316.581	0.001	0.02	78
8	4	4	7	6	2	76.334	-0.002	0.19	78
8	5	4	7	5	2	81.163	0.001	2.34	78
8	5	4	7	3	4	125.873	0.001	2.06	78
8	5	4	7	1	6	205.704	-0.003	0.17	78
8	5	4	8	3	6	79.384	0.003	2.15	78
8	4	5	6	4	3	172.601	-0.003	0.55	78
8	4	5	6	2	5	236.682	0.001	0.41	78
8	4	5	7	4	3	62.988	0.000	3.37	78
8	3	5	7	3	5	126.054	0.015	0.08	78
8	4	5	7	2	5	126.053	0.003	2.62	78
8	4	5	7	0	7	222.354	-0.002	0.51	78
8	4	5	8	2	7	95.717	0.000	1.71	78
8	3	6	6	3	4	156.871	0.009	0.13	78
8	3	6	6	3	5	156.862	-0.015	0.41	78
8	3	6	6	1	6	237.193	-0.006	0.67	78
8	3	6	7	3	4	46.490	-0.001	0.87	78
8	3	6	7	1	6	126.324	-0.002	2.96	78
8	3	6	8	1	8	112.241	0.001	0.50	78
8	2	7	6	2	5	140.964	0.000	5.41	78
8	2	7	7	2	5	30.321	-0.012	0.50	78
8	2	7	7	0	7	126.644	0.005	5.12	78
8	1	8	6	1	6	124.966	0.006	5.15	78
8	1	8	7	1	6	14.090	0.004	0.57	78
9	9	0	7	7	0	270.468	0.003	0.10	78
9	9	0	9	7	2	30.089	-0.013	0.05	78
9	8	1	8	8	1	127.005	0.015	0.10	78
9	8	1	8	6	3	167.834	-0.002	0.57	78
9	8	1	9	6	3	29.504	0.003	0.48	78
9	7	2	8	7	2	132.206	-0.001	1.72	78
9	7	2	9	5	4	41.562	0.000	0.17	78
9	6	3	7	4	3	264.901	-0.004	0.19	78
9	6	3	7	2	5	327.972	0.005	0.06	78
9	6	3	8	6	3	138.341	0.007	0.06	78
9	6	3	8	4	5	201.912	-0.005	0.19	78
9	6	3	9	4	5	60.627	-0.002	2.14	78
9	5	4	7	5	2	221.854	-0.005	0.41	78
9	5	4	7	3	4	266.567	-0.003	0.04	78
9	5	4	7	1	6	346.403	-0.002	0.24	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	5	4	8	7	2	90.643	-0.003	0.10	78
9	5	4	8	5	4	140.692	-0.006	0.80	78
9	6	4	8	4	4	141.260	0.020	-0.08	78
9	5	4	8	3	6	220.076	-0.003	0.55	78
9	5	4	9	3	6	78.448	-0.001	2.04	78
9	6	4	9	4	6	78.834	0.000	0.41	78
9	4	5	7	4	3	204.272	-0.003	0.49	78
9	4	5	7	2	5	267.344	0.006	0.10	78
9	5	5	7	3	5	267.382	0.016	0.41	78
9	4	5	7	0	7	363.646	0.002	0.10	78
9	4	5	8	6	3	77.711	0.006	0.08	78
9	5	5	8	5	3	79.283	-0.001	0.02	78
9	4	5	8	4	5	141.294	0.006	1.10	78
9	5	5	8	3	5	141.328	0.002	0.10	78
9	4	5	8	2	7	237.020	0.015	0.50	78
9	4	5	9	2	7	95.024	0.002	1.78	78
9	4	5	9	0	9	223.139	-0.011	0.06	78
9	3	6	7	3	4	188.126	0.005	0.41	78
9	3	6	7	1	6	267.958	0.002	1.25	78
9	3	6	8	5	4	62.238	-0.011	0.10	78
9	3	6	8	3	6	141.636	0.006	1.46	78
9	3	6	8	1	8	253.874	0.004	0.16	78
9	3	6	9	1	8	111.490	0.000	2.15	78
9	2	7	7	2	5	172.321	0.005	2.00	78
9	2	7	7	0	7	268.624	0.002	2.07	78
9	2	7	8	4	5	46.266	0.000	1.03	78
9	2	7	8	2	7	141.985	0.002	0.98	78
9	2	7	9	0	9	128.132	0.004	0.57	78
9	1	8	7	1	6	156.467	0.001	2.00	78
9	1	8	8	3	6	30.140	0.000	2.01	78
9	1	8	8	1	8	142.380	0.000	0.50	78
9	0	9	7	0	7	140.495	0.001	5.02	78
9	0	9	8	2	7	13.859	0.004	0.25	78
10	9	2	9	9	0	137.422	-0.006	0.10	78
10	8	2	10	6	4	40.196	0.000	0.10	78
10	8	3	9	6	3	159.396	0.004	0.48	78
10	8	3	9	4	5	220.023	0.001	0.41	78
10	7	4	9	7	2	115.052	0.004	0.10	78
10	7	4	9	5	4	156.614	0.004	1.25	78
10	7	4	10	5	6	78.279	-0.002	2.00	78
10	6	5	8	6	3	234.160	-0.005	0.41	78
10	6	5	8	4	5	297.742	-0.005	0.48	78
10	6	5	9	4	5	156.464	0.004	0.10	78
10	6	5	9	2	7	251.484	0.003	0.10	78
10	6	5	10	4	7	94.319	0.004	0.27	78
10	5	6	8	5	4	219.014	-0.013	0.41	78
10	5	6	8	3	6	298.402	-0.006	0.42	78
10	5	6	8	1	8	410.650	0.002	0.26	78
10	5	6	9	5	4	78.328	-0.001	0.17	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	5	6	9	3	6	156.777	-0.001	0.30	78
10	5	6	9	1	8	268.268	0.000	0.10	78
10	5	6	10	3	8	110.665	-0.001	2.12	78
10	4	7	8	4	5	203.436	0.003	1.25	78
10	4	7	8	2	7	299.152	0.002	1.27	78
10	4	7	9	4	5	62.142	-0.003	0.41	78
10	4	7	9	2	7	157.164	-0.003	0.53	78
10	4	7	9	0	9	285.299	0.004	0.17	78
10	4	7	10	2	9	127.200	0.000	0.66	78
10	3	8	8	3	6	187.741	-0.002	5.09	78
10	3	8	8	1	8	299.983	0.001	0.73	78
10	3	8	9	3	6	46.112	0.000	2.18	78
10	3	8	9	1	8	157.601	-0.001	3.32	78
10	2	9	8	2	7	171.948	-0.002	0.55	78
10	2	9	9	2	7	29.962	-0.005	0.57	78
10	2	9	9	0	9	158.095	0.000	1.61	78
10	1	10	8	1	8	156.009	-0.001	5.02	78
10	1	10	9	1	8	13.632	0.002	2.00	78
11	9	2	11	7	4	39.367	-0.004	0.10	78
11	8	3	10	8	3	164.198	-0.003	0.15	78
11	8	3	11	6	5	56.607	0.001	0.41	78
11	7	4	11	5	6	76.060	0.004	0.41	78
11	7	5	10	7	3	112.661	-0.008	0.25	78
11	6	5	11	6	5	.001	0.001	0.10	78
11	6	5	11	4	7	93.297	0.000	0.55	78
11	5	6	9	5	4	250.051	-0.006	0.10	78
11	5	6	9	3	6	328.501	-0.005	0.17	78
11	5	6	10	5	6	171.719	-0.009	0.05	78
11	5	6	11	3	8	109.746	0.003	0.41	78
11	4	7	9	2	7	329.338	-0.003	0.26	78
11	4	7	10	4	7	172.178	0.003	0.12	78
11	4	7	10	2	9	299.384	0.010	0.16	78
11	4	7	11	2	9	126.194	0.002	0.25	78
11	3	8	9	3	6	218.762	0.000	0.10	78
11	3	8	9	1	8	330.251	-0.001	0.51	78
11	3	8	10	5	6	61.985	0.001	0.53	78
11	3	8	10	3	8	172.650	0.000	0.51	78
11	3	8	11	1	10	142.836	-0.004	0.92	78
11	2	9	9	2	7	203.149	0.000	2.00	78
11	2	9	9	0	9	331.281	0.004	0.41	78
11	2	9	10	4	7	45.984	0.002	0.57	78
11	2	9	10	2	9	173.188	0.006	0.92	78
11	1	10	9	1	8	187.411	-0.002	2.00	78
11	1	10	10	3	8	29.811	0.001	0.49	78
11	1	10	10	1	10	173.779	-0.004	1.39	78
11	0	11	9	0	9	171.507	0.001	5.00	78
12	7	6	12	5	8	108.785	0.001	0.10	78
12	6	7	12	4	9	125.112	0.001	0.10	78
12	5	8	10	5	6	249.505	0.009	0.10	78

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	5	8	10	3	8	360.170	0.008	0.10	78
12	5	8	11	5	6	77.765	-0.003	0.10	78
12	5	8	11	3	8	187.516	0.004	0.16	78
12	5	8	12	3	10	141.641	0.010	0.20	78
12	4	9	10	4	7	234.066	0.003	1.25	78
12	4	9	10	2	9	361.259	-0.004	0.10	78
12	4	9	11	2	9	188.083	0.002	0.02	78
12	4	9	12	2	11	158.412	0.002	0.10	78
12	3	10	10	3	8	218.527	-0.003	2.00	78
12	3	10	11	1	10	188.716	-0.004	0.41	78
12	2	11	11	2	9	29.670	-0.001	0.50	78
12	1	12	10	1	10	186.980	-0.001	6.30	78
13	5	8	11	3	8	389.685	-0.001	0.41	78
13	4	9	11	2	9	390.861	-0.002	1.67	78
13	4	9	13	2	11	156.971	-0.006	0.01	78
13	3	10	11	3	8	249.341	0.004	1.35	78
13	3	10	11	1	10	392.175	-0.002	0.50	78
13	3	10	12	5	8	61.825	-0.001	0.10	78
13	3	10	12	3	10	203.463	0.006	0.05	78
13	2	11	11	2	9	233.888	0.003	0.50	78
13	2	11	12	4	9	45.802	-0.003	0.01	78
13	2	11	12	2	11	204.218	0.003	0.25	78
13	1	12	11	1	10	218.266	-0.001	1.25	78
13	0	13	11	0	11	202.434	0.002	5.00	78
13	0	13	12	2	11	12.989	-0.002	0.10	78
14	5	10	12	5	8	279.803	-0.009	0.20	78
14	5	10	12	3	10	421.449	0.006	0.12	78
14	4	11	12	2	11	423.003	0.011	0.02	78
14	2	13	12	2	11	233.657	0.002	0.53	78
14	2	13	13	0	13	220.667	0.003	0.08	78
14	1	14	12	1	12	217.858	0.001	1.25	78
15	2	13	13	0	13	455.733	0.001	0.02	78
15	0	15	13	0	13	233.250	-0.005	1.25	78
16	1	16	14	1	14	248.622	0.000	0.49	78
17	0	17	15	0	15	263.972	0.014	0.10	78
2	2	0	0	0	0	47.699	-0.004	2.09	80
2	2	0	2	0	2	16.251	0.002	2.79	80
2	1	1	1	1	1	30.887	-0.003	4.93	80
2	2	1	1	0	1	32.663	-0.002	8.25	80
2	0	2	0	0	0	31.451	-0.003	2.04	80
2	1	2	1	1	0	15.604	-0.001	7.33	80
3	3	0	1	1	0	79.562	0.000	5.34	80
3	3	0	2	1	2	63.959	0.002	7.74	80
3	3	0	3	1	2	16.520	0.001	10.13	80
3	3	0	4	1	4	1.320	0.008	0.41	80
3	2	1	1	0	1	78.317	-0.002	0.75	80
3	3	1	1	1	1	80.522	0.002	2.09	80
3	2	1	2	2	1	45.655	0.001	6.31	80
3	3	1	2	1	1	49.633	0.002	6.22	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
3	2	1	3	0	3	31.034	0.002	2.95	80
3	3	1	3	1	3	33.673	-0.001	0.50	80
3	1	2	1	1	0	63.040	-0.003	2.34	80
3	2	2	2	2	0	31.458	-0.003	1.40	80
3	1	2	2	1	2	47.439	0.001	4.75	80
3	2	2	2	0	2	47.712	0.003	0.51	80
3	0	3	1	0	1	47.286	-0.001	2.51	80
3	1	3	1	1	1	46.832	-0.014	0.12	80
3	0	3	2	2	1	14.623	0.001	3.81	80
3	1	3	2	1	1	15.961	0.005	2.21	80
4	4	0	2	2	0	111.496	0.004	0.19	80
4	4	0	3	2	2	80.030	-0.002	0.55	80
4	4	0	4	2	2	17.181	0.004	4.09	80
4	3	1	2	1	1	109.618	0.014	0.02	80
4	4	1	2	2	1	112.643	0.002	1.09	80
4	3	1	3	3	1	59.977	0.003	2.26	80
4	4	1	3	2	1	66.986	0.000	7.84	80
4	3	1	3	1	3	93.656	0.008	0.10	80
4	4	1	3	0	3	98.025	0.007	1.00	80
4	3	1	4	1	3	30.237	-0.002	6.52	80
4	4	1	4	2	3	34.578	-0.001	8.41	80
4	4	1	5	0	5	19.771	0.002	0.10	80
4	2	2	2	2	0	94.315	-0.001	2.18	80
4	3	2	2	1	2	111.184	0.006	0.62	80
4	3	2	3	3	0	47.223	0.002	2.93	80
4	2	2	3	2	2	62.855	0.000	2.87	80
4	3	2	3	1	2	63.740	-0.001	3.20	80
4	3	2	4	1	4	48.534	0.000	2.46	80
4	1	3	2	1	1	79.362	-0.004	0.51	80
4	2	3	2	2	1	78.063	0.002	2.92	80
4	1	3	3	3	1	29.731	-0.004	0.50	80
4	2	3	3	2	1	32.408	0.001	9.52	80
4	1	3	3	1	3	63.401	-0.008	0.49	80
4	2	3	3	0	3	63.442	0.003	3.20	80
4	1	4	2	1	2	62.645	0.000	0.51	80
4	1	4	3	1	2	15.210	0.003	0.71	80
5	5	0	3	3	0	143.481	-0.001	5.83	80
5	5	0	3	1	2	160.010	0.009	0.25	80
5	5	0	4	3	2	96.261	0.001	4.94	80
5	5	0	4	1	4	144.805	0.011	0.67	80
5	5	0	5	3	2	18.401	0.000	5.59	80
5	5	0	5	1	4	65.545	0.000	0.05	80
5	4	1	3	2	1	140.865	0.002	0.67	80
5	5	1	3	3	1	144.661	0.002	1.92	80
5	4	1	3	0	3	171.901	0.006	0.20	80
5	5	1	3	1	3	178.335	0.001	0.05	80
5	4	1	4	4	1	73.876	-0.001	6.77	80
5	5	1	4	3	1	84.685	-0.001	4.16	80
5	4	1	4	2	3	108.455	-0.001	6.00	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	5	1	4	1	3	114.931	0.007	1.43	80
5	4	1	5	2	3	29.410	-0.002	8.04	80
5	5	1	5	3	3	35.746	-0.005	0.30	80
5	4	1	5	0	5	93.647	0.001	0.10	80
5	3	2	3	3	0	125.083	0.002	2.67	80
5	3	2	3	1	2	141.607	0.007	0.43	80
5	4	2	3	2	2	142.847	-0.002	0.27	80
5	4	2	4	4	0	62.820	0.003	0.80	80
5	3	2	4	3	2	77.860	0.000	8.87	80
5	4	2	4	2	2	79.993	-0.001	4.06	80
5	3	2	4	1	4	126.394	0.001	2.62	80
5	3	2	5	1	4	47.142	-0.002	3.29	80
5	4	2	5	2	4	48.609	-0.007	0.02	80
5	2	3	3	2	1	111.451	0.000	5.50	80
5	3	3	3	3	1	108.910	0.002	0.02	80
5	2	3	3	0	3	142.486	0.003	0.57	80
5	3	3	3	1	3	142.589	0.007	0.08	80
5	2	3	4	4	1	44.467	0.002	7.93	80
5	3	3	4	3	1	48.932	-0.002	1.75	80
5	2	3	4	2	3	79.045	0.001	11.43	80
5	3	3	4	1	3	79.178	0.005	0.39	80
5	2	3	5	0	5	64.233	-0.001	5.18	80
5	1	4	3	1	2	94.463	0.007	0.10	80
5	1	4	4	3	2	30.717	0.001	1.00	80
5	2	4	4	2	2	31.383	0.005	0.08	80
5	1	4	4	1	4	79.247	-0.002	5.84	80
5	0	5	3	2	1	47.229	0.012	0.05	80
5	0	5	3	0	3	78.247	-0.002	2.31	80
5	0	5	4	2	3	14.811	0.001	1.09	80
6	6	0	4	4	0	175.464	-0.004	1.25	80
6	6	0	4	2	2	192.650	0.005	1.25	80
6	6	0	5	4	2	112.649	-0.002	2.15	80
6	6	0	6	4	2	20.309	-0.001	2.68	80
6	5	1	4	3	1	172.109	0.000	0.92	80
6	6	1	4	4	1	176.532	0.000	3.34	80
6	5	1	4	1	3	202.350	0.002	0.17	80
6	6	1	4	2	3	211.110	-0.002	1.35	80
6	5	1	5	5	1	87.427	0.004	2.53	80
6	6	1	5	4	1	102.654	-0.002	6.99	80
6	5	1	5	3	3	123.174	-0.001	0.64	80
6	6	1	5	2	3	132.066	-0.002	1.07	80
6	5	1	6	3	3	28.697	-0.001	2.39	80
6	6	1	6	4	3	37.186	-0.001	2.04	80
6	6	1	6	2	5	101.262	0.017	0.02	80
6	5	2	4	3	2	174.448	0.002	0.57	80
6	5	2	4	1	4	222.995	0.016	0.08	80
6	5	2	5	5	0	78.182	-0.003	2.45	80
6	4	2	5	4	2	92.340	-0.001	5.37	80
6	5	2	5	3	2	96.586	0.000	7.49	80



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
6	4	2	5	2	4	140.962	0.006	0.05	80
6	5	2	5	1	4	143.728	-0.002	2.01	80
6	4	2	6	2	4	46.095	0.004	1.77	80
6	5	2	6	3	4	48.849	0.001	2.87	80
6	3	3	4	3	1	143.414	0.003	1.43	80
6	4	3	4	4	1	139.347	0.001	3.07	80
6	3	3	4	1	3	173.658	0.008	1.27	80
6	4	3	4	2	3	173.924	-0.001	5.50	80
6	3	3	5	5	1	58.727	0.002	1.46	80
6	4	3	5	4	1	65.469	0.000	11.05	80
6	3	3	5	3	3	94.475	-0.002	0.51	80
6	4	3	5	2	3	94.880	-0.001	10.11	80
6	4	3	5	0	5	159.116	0.001	0.92	80
6	3	3	6	1	5	63.751	-0.007	0.42	80
6	4	3	6	2	5	64.057	-0.002	3.20	80
6	3	3	7	1	7	49.442	0.005	0.02	80
6	4	3	7	0	7	49.742	0.004	0.25	80
6	2	4	4	2	2	126.245	0.002	0.17	80
6	3	4	4	3	2	125.599	0.001	5.12	80
6	3	4	4	1	4	174.132	0.001	2.26	80
6	2	4	5	4	2	46.249	0.000	0.10	80
6	3	4	5	3	2	47.740	0.002	5.71	80
6	2	4	5	2	4	94.866	0.001	0.24	80
6	3	4	5	1	4	94.882	0.000	1.10	80
6	3	4	6	1	6	80.313	-0.001	0.51	80
6	2	5	4	2	3	109.869	0.003	0.48	80
6	2	5	5	2	3	30.825	0.003	5.56	80
6	2	5	5	0	5	95.055	-0.001	10.77	80
6	1	6	4	1	4	93.818	0.000	6.41	80
6	1	6	5	1	4	14.569	0.001	7.18	80
7	7	0	5	5	0	207.342	-0.003	5.12	80
7	7	0	5	3	2	225.746	0.000	2.09	80
7	7	0	6	5	2	129.160	0.000	2.64	80
7	7	0	6	3	4	178.005	-0.003	0.08	80
7	7	0	7	5	2	22.926	0.002	5.91	80
7	6	1	5	4	1	203.362	-0.005	0.51	80
7	7	1	5	5	1	208.208	-0.002	2.06	80
7	6	1	5	2	3	232.775	-0.004	0.10	80
7	7	1	5	3	3	243.951	-0.011	0.02	80
7	6	1	6	6	1	100.712	0.000	1.39	80
7	7	1	6	5	1	120.785	-0.002	1.86	80
7	6	1	6	4	3	137.896	-0.003	2.12	80
7	7	1	6	3	3	149.484	-0.001	0.47	80
7	6	1	7	4	3	28.298	0.000	3.78	80
7	7	1	7	5	3	38.857	-0.001	0.05	80
7	6	1	7	2	5	91.358	-0.001	0.10	80
7	5	2	5	5	0	184.423	0.002	0.08	80
7	5	2	5	3	2	202.826	0.005	0.82	80
7	6	2	5	4	2	205.946	-0.002	0.10	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	5	2	5	1	4	249.968	0.002	0.08	80
7	6	2	6	6	0	93.297	0.001	0.10	80
7	5	2	6	5	2	106.236	0.000	4.40	80
7	6	2	6	4	2	113.610	0.003	0.20	80
7	5	2	6	3	4	155.086	0.003	1.82	80
7	5	2	7	3	4	44.742	0.000	5.36	80
7	4	3	5	4	1	175.066	-0.003	2.18	80
7	5	3	5	5	1	169.359	0.007	0.12	80
7	4	3	5	2	3	204.480	-0.001	1.36	80
7	5	3	5	3	3	205.110	0.006	0.20	80
7	4	3	5	0	5	268.719	0.004	0.41	80
7	4	3	6	6	1	72.418	0.005	1.02	80
7	5	3	6	5	1	81.935	0.006	0.23	80
7	4	3	6	4	3	109.598	-0.002	4.12	80
7	5	3	6	3	3	110.628	0.001	0.55	80
7	4	3	6	2	5	173.659	0.000	1.92	80
7	5	3	6	1	5	174.382	-0.003	1.25	80
7	4	3	7	2	5	63.062	0.002	5.43	80
7	5	3	7	3	5	63.780	-0.004	0.53	80
7	5	3	7	1	7	160.075	0.011	0.08	80
7	4	3	8	2	7	32.740	0.002	0.02	80
7	3	4	5	5	0	139.688	0.009	0.02	80
7	3	4	5	3	2	158.079	0.000	5.21	80
7	3	4	5	1	4	205.221	-0.003	2.03	80
7	4	4	5	2	4	205.279	0.007	0.08	80
7	3	4	6	5	2	61.493	-0.001	5.66	80
7	4	4	6	4	2	64.318	0.002	0.60	80
7	3	4	6	3	4	110.344	0.002	0.94	80
7	4	4	6	2	4	110.411	0.004	0.82	80
7	3	4	6	1	6	190.657	0.002	0.34	80
7	3	4	7	1	6	79.815	0.000	1.15	80
7	3	5	5	5	1	105.570	0.002	0.02	80
7	2	5	5	2	3	141.431	0.010	0.41	80
7	2	5	6	6	1	9.339	-0.014	0.02	80
7	2	5	6	4	3	46.544	0.004	0.55	80
7	3	5	6	3	3	46.852	0.009	0.25	80
7	2	5	6	2	5	110.602	0.004	1.31	80
7	3	5	6	1	5	110.603	0.003	0.41	80
7	2	5	7	0	7	96.279	0.001	2.79	80
7	1	6	5	1	4	125.407	-0.001	0.47	80
7	1	6	6	3	4	30.528	0.002	0.64	80
7	1	6	6	1	6	110.841	0.001	3.79	80
7	0	7	5	0	5	109.375	-0.002	2.43	80
7	0	7	6	2	5	14.320	0.000	7.41	80
8	8	0	6	6	0	238.991	-0.003	2.00	80
8	8	0	7	6	2	145.688	-0.009	0.10	80
8	8	0	8	6	2	26.162	0.000	1.03	80
8	8	1	6	6	1	239.640	0.000	2.54	80
8	8	1	6	4	3	276.825	-0.002	0.19	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	8	1	7	6	1	138.928	0.000	1.11	80
8	7	1	7	5	3	152.741	0.004	2.50	80
8	8	1	7	4	3	167.228	0.001	0.48	80
8	7	1	8	5	3	28.462	0.000	2.18	80
8	8	1	8	6	3	40.715	0.004	0.78	80
8	6	2	6	4	2	233.138	-0.004	1.25	80
8	7	2	6	5	2	237.329	-0.001	0.12	80
8	6	2	6	2	4	279.242	0.009	0.41	80
8	7	2	6	3	4	286.186	0.008	0.25	80
8	7	2	7	7	0	108.169	-0.001	0.08	80
8	6	2	7	6	2	119.524	-0.011	0.10	80
8	7	2	7	5	2	131.090	-0.005	0.47	80
8	7	2	7	3	4	175.829	-0.008	0.12	80
8	6	2	8	4	4	43.192	0.000	2.42	80
8	7	2	8	5	4	50.002	0.000	5.30	80
8	7	2	8	3	6	129.358	-0.005	0.05	80
8	6	3	6	6	1	198.918	-0.011	0.05	80
8	5	3	6	3	3	234.916	0.015	0.01	80
8	6	3	6	4	3	236.114	-0.001	0.76	80
8	5	3	6	1	5	298.658	-0.001	0.01	80
8	6	3	6	2	5	300.167	-0.007	0.08	80
8	6	3	7	6	1	98.216	-0.001	1.00	80
8	5	3	7	5	3	124.275	0.001	0.69	80
8	6	3	7	4	3	126.511	-0.004	3.06	80
8	5	3	7	3	5	188.054	-0.004	0.08	80
8	6	3	7	2	5	189.575	-0.001	2.07	80
8	5	3	8	3	5	62.057	0.002	1.75	80
8	6	3	8	4	5	63.561	-0.001	3.25	80
8	4	4	6	4	2	189.951	0.002	0.85	80
8	5	4	6	5	2	187.326	-0.002	2.04	80
8	4	4	6	2	4	236.048	0.007	0.69	80
8	5	4	6	3	4	236.175	-0.001	1.28	80
8	5	4	6	1	6	316.488	-0.002	0.10	80
8	4	4	7	6	2	76.340	-0.003	0.10	80
8	5	4	7	5	2	81.094	0.001	6.37	80
8	4	4	7	4	4	125.630	-0.004	0.25	80
8	5	4	7	3	4	125.836	0.001	5.41	80
8	5	4	7	1	6	205.653	0.003	0.67	80
8	5	4	8	3	6	79.361	0.000	2.78	80
8	4	5	6	6	1	135.364	-0.003	0.02	80
8	3	5	6	3	3	172.847	0.001	0.08	80
8	4	5	6	4	3	172.554	0.000	5.09	80
8	3	5	6	1	5	236.598	-0.006	0.10	80
8	4	5	6	2	5	236.614	0.002	2.32	80
8	3	5	7	5	3	62.217	-0.002	1.35	80
8	4	5	7	4	3	62.957	0.003	2.43	80
8	3	5	7	3	5	125.999	-0.005	0.20	80
8	4	5	7	2	5	126.014	0.000	4.94	80
8	4	5	7	0	7	222.291	-0.001	1.68	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
8	4	5	8	2	7	95.691	0.000	2.43	80
8	4	5	9	0	9	81.854	0.013	0.02	80
8	3	6	6	3	4	156.818	0.003	0.58	80
8	3	6	6	1	6	237.130	0.001	0.60	80
8	3	6	7	5	2	1.728	-0.004	0.10	80
8	3	6	7	3	4	46.475	0.001	1.10	80
8	3	6	7	1	6	126.290	0.001	5.59	80
8	3	6	8	1	8	112.209	0.002	2.93	80
8	2	7	6	6	1	39.660	-0.016	0.01	80
8	2	7	6	4	3	76.844	-0.018	0.02	80
8	2	7	6	2	5	140.921	0.000	5.46	80
8	2	7	7	2	5	30.321	-0.002	0.85	80
8	2	7	7	0	7	126.602	0.002	5.87	80
8	1	8	6	1	6	124.924	0.002	5.52	80
8	1	8	7	1	6	14.085	0.003	2.20	80
9	9	0	7	7	0	270.317	0.000	0.48	80
9	9	0	7	5	2	293.243	0.002	0.48	80
9	8	1	7	6	1	266.005	-0.004	0.53	80
9	9	1	7	7	1	270.781	0.010	0.10	80
9	8	1	7	4	3	294.307	0.000	0.41	80
9	8	1	8	8	1	127.074	-0.007	1.13	80
9	8	1	8	6	3	167.792	0.000	5.27	80
9	8	1	9	6	3	29.443	0.000	2.43	80
9	7	2	7	5	2	263.373	-0.001	0.41	80
9	7	2	7	3	4	308.109	-0.007	0.19	80
9	8	2	8	8	0	122.870	0.003	0.48	80
9	7	2	8	7	2	132.276	-0.003	2.01	80
9	8	2	8	6	2	149.032	0.002	0.60	80
9	7	2	8	5	4	182.276	-0.005	0.10	80
9	8	2	8	4	4	192.222	0.000	0.10	80
9	7	2	9	5	4	41.610	-0.001	2.42	80
9	8	2	9	6	4	51.026	-0.001	0.10	80
9	6	3	7	6	1	236.562	-0.004	0.53	80
9	6	3	7	4	3	264.862	-0.002	0.60	80
9	6	3	7	2	5	327.919	-0.006	0.42	80
9	6	3	8	8	1	97.635	-0.003	0.33	80
9	6	3	8	6	3	138.351	0.002	0.62	80
9	7	3	8	5	3	142.677	-0.008	0.15	80
9	6	3	8	4	5	201.911	0.000	0.91	80
9	7	3	8	3	5	204.729	-0.010	0.17	80
9	6	3	9	4	5	60.662	0.000	6.75	80
9	7	3	9	5	5	63.450	-0.003	1.29	80
9	6	3	9	2	7	155.662	0.001	0.41	80
9	5	4	7	5	2	221.762	0.000	0.73	80
9	5	4	7	3	4	266.504	0.000	0.80	80
9	5	4	7	1	6	346.326	0.006	0.67	80
9	5	4	8	7	2	90.668	0.000	0.60	80
9	6	4	8	6	2	98.003	0.000	1.25	80
9	5	4	8	5	4	140.671	0.001	1.82	80



UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
9	6	4	8	4	4	141.196	0.001	2.09	80
9	5	4	8	3	6	220.027	-0.004	1.67	80
9	5	4	9	3	6	78.441	0.000	5.22	80
9	6	4	9	4	6	78.815	-0.001	3.25	80
9	4	5	7	4	3	204.203	0.000	0.34	80
9	4	5	7	2	5	267.259	-0.004	0.48	80
9	5	5	7	3	5	267.294	0.004	0.01	80
9	4	5	7	0	7	363.548	0.007	0.23	80
9	4	5	8	6	3	77.686	-0.001	1.50	80
9	5	5	8	5	3	79.244	0.013	0.05	80
9	4	5	8	4	5	141.248	-0.001	2.84	80
9	5	5	8	3	5	141.292	0.006	0.10	80
9	4	5	8	2	7	236.941	0.001	0.50	80
9	4	5	9	2	7	95.002	0.003	2.18	80
9	4	5	9	0	9	223.094	0.004	0.02	80
9	4	5	10	2	9	65.023	-0.020	-0.02	80
9	3	6	7	3	4	188.065	0.002	0.51	80
9	3	6	7	1	6	267.879	0.001	2.18	80
9	3	6	8	5	4	62.230	0.002	0.26	80
9	3	6	8	3	6	141.589	0.000	4.13	80
9	3	6	8	1	8	253.794	-0.002	2.93	80
9	3	6	9	1	8	111.460	0.000	3.53	80
9	2	7	7	2	5	172.263	-0.001	5.50	80
9	2	7	7	0	7	268.542	0.000	2.26	80
9	2	7	8	4	5	46.253	0.003	2.71	80
9	2	7	8	2	7	141.941	0.000	1.45	80
9	2	7	9	0	9	128.092	0.001	2.54	80
9	1	8	7	1	6	156.418	-0.001	5.02	80
9	1	8	8	3	6	30.131	0.001	1.50	80
9	1	8	8	1	8	142.338	0.001	1.85	80
9	0	9	7	2	5	44.165	-0.008	0.02	80
9	0	9	7	0	7	140.450	-0.001	5.12	80
9	0	9	8	2	7	13.852	0.001	0.98	80
10	10	1	8	8	1	301.558	-0.001	0.48	80
10	10	1	9	8	1	174.483	0.005	0.08	80
10	9	1	9	7	3	183.130	-0.001	0.48	80
10	8	2	9	6	4	195.577	-0.005	0.41	80
10	8	2	10	6	4	40.241	0.001	0.51	80
10	8	2	10	4	6	117.669	-0.003	0.41	80
10	8	3	9	6	3	159.285	0.003	0.48	80
10	8	3	9	4	5	219.947	0.003	0.48	80
10	7	3	10	5	5	58.849	-0.002	0.10	80
10	6	4	8	4	4	296.524	-0.013	0.02	80
10	7	4	9	7	2	114.945	0.003	1.25	80
10	6	4	9	6	4	155.358	0.016	0.02	80
10	7	4	9	5	4	156.555	0.001	2.00	80
10	6	4	10	4	6	77.430	-0.002	0.08	80
10	7	4	10	5	6	78.264	0.002	2.01	80
10	6	5	8	6	3	234.103	0.001	0.10	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	6	5	8	4	5	297.667	0.004	0.12	80
10	6	5	8	2	7	393.349	-0.006	1.25	80
10	6	5	9	6	3	95.748	-0.005	0.33	80
10	5	5	9	5	5	156.312	0.009	0.05	80
10	6	5	9	4	5	156.415	0.001	0.62	80
10	6	5	9	2	7	251.411	-0.002	1.25	80
10	6	5	10	4	7	94.292	-0.001	0.75	80
10	6	5	10	2	9	221.448	-0.009	0.19	80
10	5	6	8	5	4	218.960	-0.001	0.48	80
10	5	6	8	3	6	298.321	-0.001	1.17	80
10	5	6	8	1	8	410.525	-0.004	0.85	80
10	4	6	9	6	4	77.911	0.001	0.48	80
10	5	6	9	5	4	78.292	0.001	0.64	80
10	4	6	9	4	6	156.729	0.003	0.41	80
10	5	6	9	3	6	156.733	0.000	1.96	80
10	5	6	9	1	8	268.189	-0.003	1.32	80
10	5	6	10	3	8	110.635	-0.002	5.84	80
10	4	7	8	4	5	203.373	0.002	2.03	80
10	4	7	8	2	7	299.063	0.001	5.52	80
10	4	7	9	4	5	62.124	0.002	2.04	80
10	4	7	9	2	7	157.122	0.001	2.93	80
10	4	7	9	0	9	285.212	0.001	0.55	80
10	4	7	10	2	9	127.164	-0.001	2.62	80
10	3	8	8	3	6	187.683	-0.003	5.16	80
10	3	8	8	1	8	299.892	0.000	2.65	80
10	3	8	9	3	6	46.097	0.001	4.52	80
10	3	8	9	1	8	157.557	0.001	2.48	80
10	3	8	10	1	10	143.929	-0.001	0.55	80
10	2	9	8	4	5	76.224	0.018	0.02	80
10	2	9	8	2	7	171.898	0.001	0.55	80
10	2	9	9	2	7	29.954	-0.002	2.79	80
10	2	9	9	0	9	158.047	0.000	2.59	80
10	1	10	8	1	8	155.962	0.000	6.27	80
10	1	10	9	1	8	13.626	0.000	0.82	80
11	10	1	10	8	3	198.763	0.003	0.41	80
11	10	1	11	8	3	34.489	0.002	0.41	80
11	9	2	11	7	4	39.388	-0.004	0.48	80
11	8	3	10	8	3	164.273	0.000	1.35	80
11	8	3	11	6	5	56.684	-0.001	2.00	80
11	9	3	11	7	5	63.853	-0.008	0.08	80
11	7	4	10	7	4	169.504	0.004	0.10	80
11	7	4	10	5	6	247.768	0.005	0.10	80
11	7	4	11	5	6	76.081	-0.002	2.04	80
11	8	4	11	6	6	77.754	0.003	0.41	80
11	6	5	9	6	3	266.870	0.000	0.10	80
11	6	5	9	4	5	327.532	0.000	0.10	80
11	6	5	10	8	3	107.583	-0.005	0.16	80
11	7	5	10	7	3	112.564	0.003	0.00	80
11	6	5	10	6	5	171.116	-0.001	0.10	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
11	7	5	10	5	5	171.413	0.001	0.00	80
11	6	5	11	4	7	93.288	0.002	2.07	80
11	7	5	11	5	7	93.498	0.001	0.41	80
11	5	6	9	5	4	249.969	-0.002	0.10	80
11	5	6	9	3	6	328.411	-0.001	0.10	80
11	5	6	10	7	4	93.415	-0.002	0.10	80
11	5	6	10	5	6	171.679	0.000	0.33	80
11	5	6	10	3	8	282.320	0.004	0.10	80
11	5	6	11	3	8	109.718	0.001	2.00	80
11	4	7	9	6	3	173.574	-0.010	0.25	80
11	4	7	9	4	5	234.247	0.001	1.60	80
11	4	7	9	2	7	329.246	0.001	2.12	80
11	4	7	9	0	9	457.322	-0.014	0.10	80
11	4	7	10	6	5	77.829	-0.002	1.16	80
11	4	7	10	4	7	172.125	0.001	3.37	80
11	4	7	10	2	9	299.282	-0.007	0.17	80
11	4	7	11	2	9	126.161	0.003	0.60	80
11	3	8	9	3	6	218.695	0.000	1.35	80
11	3	8	9	1	8	330.158	0.003	0.60	80
11	3	8	10	5	6	61.965	0.002	2.07	80
11	3	8	10	3	8	172.601	0.002	2.15	80
11	3	8	10	1	10	316.528	-0.001	0.02	80
11	3	8	11	1	10	142.803	0.003	0.92	80
11	2	9	9	2	7	203.085	-0.002	5.09	80
11	2	9	9	0	9	331.177	0.000	2.00	80
11	2	9	10	4	7	45.964	-0.002	2.48	80
11	2	9	10	2	9	173.131	0.000	3.92	80
11	2	9	11	0	11	159.722	-0.002	1.07	80
11	1	10	9	3	6	75.876	-0.019	0.41	80
11	1	10	9	1	8	187.355	0.000	5.43	80
11	1	10	10	3	8	29.799	0.000	1.10	80
11	1	10	10	1	10	173.730	0.001	1.32	80
11	0	11	9	0	9	171.455	0.001	5.43	80
11	0	11	10	2	9	13.408	0.001	0.41	80
12	12	1	12	10	3	48.187	-0.003	0.05	80
12	7	6	12	5	8	108.763	0.006	0.48	80
12	6	7	10	6	5	264.777	0.002	0.17	80
12	6	7	10	4	7	359.069	0.001	0.08	80
12	6	7	11	6	5	93.662	0.004	0.05	80
12	6	7	11	4	7	186.951	0.008	0.08	80
12	6	7	12	4	9	125.076	-0.001	0.43	80
12	5	8	10	5	6	249.421	0.003	0.56	80
12	5	8	10	3	8	360.054	-0.001	0.89	80
12	5	8	11	5	6	77.740	0.002	0.55	80
12	5	8	11	3	8	187.455	0.000	1.12	80
12	5	8	11	1	10	330.250	-0.006	0.10	80
12	5	8	12	3	10	141.591	-0.001	1.15	80
12	4	9	10	4	7	233.996	0.005	2.06	80
12	4	9	10	2	9	361.160	0.004	1.35	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
12	4	9	11	4	7	61.870	0.003	0.10	80
12	4	9	11	2	9	188.032	0.007	1.25	80
12	4	9	12	2	11	158.370	0.003	0.73	80
12	3	10	10	3	8	218.461	-0.002	5.08	80
12	3	10	10	1	10	362.394	0.001	0.20	80
12	3	10	11	3	8	45.864	0.000	0.30	80
12	3	10	11	1	10	188.666	0.002	0.73	80
12	2	11	10	2	9	202.791	0.002	2.12	80
12	2	11	11	2	9	29.658	0.000	0.53	80
12	2	11	11	0	11	189.382	0.000	0.34	80
12	1	12	10	1	10	186.923	0.000	6.25	80
13	6	7	12	8	5	108.886	-0.003	0.41	80
13	5	8	12	7	6	93.351	-0.003	2.00	80
13	5	8	12	5	8	202.114	0.003	0.41	80
13	4	9	11	4	7	264.579	-0.008	0.10	80
13	4	9	11	2	9	390.747	0.002	1.35	80
13	4	9	13	2	11	156.930	-0.002	0.25	80
13	3	10	11	3	8	249.254	-0.007	0.91	80
13	3	10	11	1	10	392.055	-0.006	0.75	80
13	3	10	12	5	8	61.803	-0.002	0.20	80
13	3	10	12	3	10	203.397	0.000	0.16	80
13	3	10	13	1	12	173.850	-0.013	0.01	80
13	2	11	11	2	9	233.814	0.001	2.12	80
13	2	11	11	0	11	393.536	-0.001	0.66	80
13	2	11	12	4	9	45.790	0.002	0.48	80
13	2	11	12	2	11	204.156	0.001	0.71	80
13	2	11	13	0	13	191.170	0.002	0.08	80
13	1	12	11	1	10	218.201	0.003	2.03	80
13	1	12	12	3	10	29.535	0.002	0.02	80
13	0	13	11	0	11	202.368	-0.001	5.09	80
13	0	13	12	2	11	12.991	0.004	0.10	80
14	5	10	12	5	8	279.728	0.005	0.08	80
14	5	10	12	3	10	421.315	0.001	0.10	80
14	4	11	12	4	9	264.497	-0.004	0.50	80
14	4	11	12	2	11	422.869	0.001	0.48	80
14	4	11	13	2	11	218.706	-0.007	0.08	80
14	3	12	12	3	10	249.131	-0.004	0.50	80
14	3	12	12	1	12	424.607	0.002	0.06	80
14	2	13	12	2	11	233.578	-0.002	2.09	80
14	2	13	13	2	11	29.426	0.001	0.02	80
14	2	13	13	0	13	220.588	-0.005	0.10	80
14	1	14	12	1	12	217.789	0.001	2.10	80
15	3	12	13	3	10	279.710	0.000	0.10	80
15	2	13	13	2	11	264.425	-0.002	0.34	80
15	2	13	13	0	13	455.596	0.001	0.08	80
15	1	14	13	1	12	248.936	0.003	0.76	80
15	1	14	14	3	12	29.332	0.000	0.10	80
15	0	15	13	0	13	233.177	-0.004	0.17	80
15	0	15	14	2	13	12.588	0.000	0.10	80

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
16	4	13	14	4	11	294.882	-0.004	0.41	80
16	3	14	14	3	12	279.690	0.002	1.25	80
16	2	15	14	2	13	264.257	0.000	0.33	80
16	2	15	15	0	15	251.665	-0.004	0.05	80
16	1	16	14	1	14	248.544	0.000	2.03	80
17	3	14	15	3	12	310.033	0.003	0.08	80
17	0	17	15	0	15	263.878	0.000	0.55	80
18	1	18	16	1	16	279.179	-0.001	0.25	80
2	1	1	1	1	1	30.906	0.016	0.08	82
2	2	1	1	0	1	32.642	-0.003	0.41	82
2	1	2	1	1	0	15.601	0.000	1.75	82
3	3	0	1	1	0	79.534	0.000	1.32	82
3	3	0	2	1	2	63.933	0.000	1.39	82
3	3	0	3	1	2	16.508	0.002	1.32	82
3	3	1	1	1	1	80.495	0.012	0.08	82
3	3	1	2	1	1	49.591	-0.003	0.30	82
3	2	1	3	0	3	31.042	0.007	0.08	82
3	1	2	1	1	0	63.028	0.000	0.13	82
3	1	2	2	1	2	47.420	-0.007	0.16	82
3	0	3	1	0	1	47.269	-0.002	0.41	82
3	0	3	2	2	1	14.627	0.001	0.25	82
4	4	1	3	2	1	66.917	-0.010	0.08	82
4	3	1	4	1	3	30.243	-0.005	0.25	82
4	4	1	4	2	3	34.532	-0.009	0.34	82
4	2	2	2	2	0	94.302	0.004	0.10	82
4	3	2	3	3	0	47.210	0.000	1.35	82
4	2	2	3	2	2	62.837	-0.009	0.25	82
4	3	2	3	1	2	63.713	-0.004	1.25	82
4	1	3	3	3	1	29.748	0.005	0.01	82
4	2	3	3	2	1	32.386	0.000	1.06	82
4	2	3	3	0	3	63.419	-0.002	0.21	82
4	1	4	2	1	2	62.631	0.004	0.08	82
5	5	0	3	3	0	143.416	-0.002	0.15	82
5	5	0	4	3	2	96.203	-0.005	0.10	82
5	5	0	5	3	2	18.349	-0.001	0.60	82
5	4	1	4	4	1	73.916	0.008	0.41	82
5	5	1	4	3	1	84.595	-0.004	0.10	82
5	4	1	4	2	3	108.449	0.000	0.42	82
5	4	1	5	2	3	29.423	-0.002	1.25	82
5	3	2	3	3	0	125.073	0.005	0.10	82
5	3	2	4	3	2	77.856	-0.002	1.35	82
5	4	2	4	2	2	79.949	-0.008	0.10	82
5	3	2	5	1	4	47.144	-0.004	0.41	82
5	2	3	3	2	1	111.410	0.000	0.50	82
5	3	3	3	3	1	108.888	-0.005	0.05	82
5	2	3	4	4	1	44.493	0.010	0.50	82
5	2	3	4	2	3	79.025	0.001	0.92	82
5	2	3	5	0	5	64.228	0.009	0.13	82
5	1	4	4	3	2	30.712	0.002	0.41	82

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
5	1	4	4	1	4	79.233	0.006	0.48	82
5	0	5	3	0	3	78.224	-0.002	2.42	82
5	0	5	4	2	3	14.810	0.005	0.21	82
6	6	0	4	4	0	175.384	0.001	0.08	82
6	5	1	4	3	1	172.066	-0.003	0.01	82
6	6	1	5	4	1	102.530	-0.008	0.67	82
6	5	1	6	3	3	28.709	-0.001	0.24	82
6	6	1	6	4	3	37.103	-0.008	0.08	82
6	5	2	5	5	0	78.178	-0.001	2.00	82
6	4	2	5	4	2	92.348	-0.003	0.25	82
6	5	2	5	3	2	96.530	0.001	0.89	82
6	4	2	6	2	4	46.100	-0.008	0.25	82
6	5	2	6	3	4	48.836	0.014	0.01	82
6	3	3	4	3	1	143.355	-0.004	0.02	82
6	4	3	4	4	1	139.347	0.013	0.41	82
6	4	3	4	2	3	173.880	0.005	0.41	82
6	4	3	5	4	1	65.431	0.005	1.38	82
6	4	3	5	2	3	94.854	0.003	1.32	82
6	3	4	4	3	2	125.564	-0.001	0.41	82
6	3	4	5	3	2	47.708	0.001	0.41	82
6	3	4	5	1	4	94.852	-0.003	0.25	82
6	2	5	4	2	3	109.838	0.004	0.10	82
6	2	5	5	0	5	95.027	-0.002	1.72	82
6	1	6	4	1	4	93.790	0.000	3.25	82
6	1	6	5	1	4	14.557	-0.007	0.41	82
7	7	0	5	5	0	207.239	0.001	0.48	82
7	7	0	5	3	2	225.589	0.001	0.25	82
7	7	0	6	5	2	129.061	0.002	0.41	82
7	7	0	7	5	2	22.801	0.003	0.10	82
7	6	1	7	4	3	28.311	0.009	0.41	82
7	5	2	6	5	2	106.257	-0.005	0.20	82
7	5	2	7	3	4	44.774	0.003	2.00	82
7	4	3	5	4	1	175.008	-0.002	0.08	82
7	4	3	5	2	3	204.425	-0.010	0.08	82
7	4	3	5	0	5	268.653	-0.001	0.06	82
7	4	3	6	4	3	109.582	-0.002	0.10	82
7	3	4	5	3	2	158.021	0.002	2.00	82
7	3	4	5	1	4	205.159	-0.008	0.02	82
7	3	4	6	5	2	61.489	-0.001	0.41	82
7	4	4	6	4	2	64.272	0.004	0.08	82
7	4	4	6	2	4	110.372	-0.004	0.08	82
7	3	4	6	1	6	190.610	0.007	0.05	82
7	3	4	7	1	6	79.802	0.006	0.33	82
7	2	5	5	2	3	141.397	0.020	-0.05	82
7	2	5	6	4	3	46.543	0.017	0.05	82
7	1	6	5	1	4	125.377	0.006	0.10	82
7	1	6	6	3	4	30.526	0.010	0.02	82
7	1	6	6	1	6	110.810	0.003	0.17	82
7	0	7	5	0	5	109.344	-0.002	0.48	82

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
7	0	7	6	2	5	14.316	-0.001	1.50	82
8	7	1	7	5	3	152.709	-0.001	0.05	82
8	6	2	8	4	4	43.233	0.001	0.08	82
8	7	2	8	5	4	49.954	0.001	0.08	82
8	6	3	6	2	5	300.083	-0.002	0.41	82
8	6	3	7	4	3	126.466	0.005	0.10	82
8	5	4	6	5	2	187.286	-0.002	0.41	82
8	5	4	7	5	2	81.028	0.001	0.55	82
8	5	4	7	3	4	125.801	0.003	0.41	82
8	5	4	8	3	6	79.345	0.003	0.48	82
8	4	5	6	4	3	172.498	-0.006	0.10	82
8	4	5	7	2	5	125.971	-0.007	0.10	82
8	3	6	6	1	6	237.059	-0.001	0.08	82
8	3	6	7	3	4	46.451	-0.005	0.50	82
8	3	6	7	1	6	126.253	0.001	0.80	82
8	3	6	8	1	8	112.174	0.002	0.10	82
8	2	7	6	2	5	140.878	-0.002	2.00	82
8	2	7	7	0	7	126.562	-0.001	2.00	82
8	1	8	6	1	6	124.890	0.002	5.02	82
8	1	8	7	1	6	14.085	0.005	0.10	82
9	7	2	9	5	4	41.653	0.000	1.25	82
9	6	3	9	4	5	60.690	0.004	0.48	82
9	7	3	9	5	5	63.416	-0.009	0.05	82
9	5	4	9	3	6	78.430	0.000	0.08	82
9	4	5	8	4	5	141.207	-0.003	0.41	82
9	4	5	8	2	7	236.889	0.014	0.02	82
9	4	5	9	2	7	94.955	-0.020	-0.02	82
9	3	6	8	5	4	62.205	-0.003	0.10	82
9	3	6	8	3	6	141.549	-0.001	0.10	82
9	3	6	8	1	8	253.725	0.003	0.02	82
9	3	6	9	1	8	111.429	0.001	0.48	82
9	2	7	7	2	5	172.212	-0.001	0.48	82
9	2	7	7	0	7	268.454	-0.009	0.08	82
9	2	7	8	4	5	46.241	0.006	0.08	82
9	2	7	8	2	7	141.910	0.010	0.32	82
9	1	8	7	1	6	156.375	0.001	2.00	82
9	1	8	8	1	8	142.292	-0.001	0.01	82
9	0	9	7	0	7	140.411	-0.004	5.00	82
10	7	4	10	5	6	78.250	0.012	0.05	82
10	5	6	9	5	4	78.259	-0.001	0.05	82
10	5	6	9	3	6	156.689	-0.002	0.08	82
10	5	6	10	3	8	110.610	0.002	0.20	82
10	4	7	8	2	7	298.977	-0.001	0.25	82
10	4	7	9	4	5	62.107	0.004	0.10	82
10	4	7	9	2	7	157.064	-0.014	0.25	82
10	4	7	10	2	9	127.118	-0.011	0.02	82
10	3	8	8	3	6	187.633	0.001	0.48	82
10	3	8	8	1	8	299.805	0.000	0.33	82
10	3	8	9	3	6	46.080	-0.003	0.02	82

UPPER			LOWER			OBSERVED	OBS-CALC	WEIGHT	ISO
J	K _a	K _c	J	K _a	K _c	(cm ⁻¹)	(cm ⁻¹)		
10	3	8	9	1	8	157.492	-0.019	0.10	82
10	2	9	9	2	7	29.948	-0.001	0.25	82
10	2	9	9	0	9	158.000	0.003	0.10	82
10	1	10	8	1	8	155.926	0.003	5.00	82
11	4	7	11	2	9	126.122	-0.007	0.01	82
11	3	8	10	5	6	61.955	0.005	0.48	82
11	3	8	10	3	8	172.558	0.000	0.08	82
11	3	8	11	1	10	142.772	0.006	0.01	82
11	2	9	9	2	7	203.035	0.002	0.25	82
11	2	9	10	4	7	45.951	-0.004	0.08	82
11	2	9	10	2	9	173.086	0.002	0.27	82
11	1	10	9	1	8	187.305	0.002	0.48	82
11	1	10	10	3	8	29.813	0.021	-0.08	82
11	0	11	9	0	9	171.406	-0.003	2.00	82
12	3	10	10	1	10	362.286	-0.007	0.02	82
12	2	11	10	2	9	202.731	0.000	0.41	82
12	1	12	10	1	10	186.867	0.000	2.06	82



APPENDIX F

SUBROUTINE CONVERT

```

SUBROUTINE CONVERT(PAR,IFREP,HAM,JBAND)
C   THIS SUBROUTINE CONVERTS MOLECULAR VIBRATION-ROTATION CONSTANTS
C   BELONGING TO A REDUCED HAMILTONIAN (E.G. WATSONS OR TYPKES)
C   AND CALCULATES THE DETERMINABLE COEFFICIENTS DEFINED BY WATSON,
C   WHICH ARE INDEPENDENT OF WHICH REDUCTION OF THE HAMILTONIAN IS
C   USED. IF THE I-R ROTATIONAL REPRESENTATION WAS USED, THE
C   COEFFICIENTS ARE CYCLICALLY PERMUTED TO CORRESPOND TO THE
C   COEFFICIENTS OBTAINED IN THE III-R REPRESENTATION.
DIMENSION C(19),D(15),PAR(24)
C   PAR IS AN ARRAY CONTAINING THE REDUCED HAMILTONIAN CONSTANTS.
C   C IS AN ARRAY CONTAINING THE CARTESIAN COEFFICIENTS CALCULATED
C   FROM THE REDUCED COEFFICIENTS USING THE FORMULAS DERIVED BY
C   W. F. MURPHY, J. MOLEC. SPECTROSC., 89, 561-565 (1981).
C   D IS AN ARRAY CONTAINING THE DETERMINABLE COEFFICIENTS.
TYPE INTEGER HAM
CALL NOBLANK
DO 15 I=1,15
D(I)=0.0
15 CONTINUE
DO 25 I=1,19
C(I)=0.0
25 CONTINUE
IF(HAM.EQ.3) GO TO 100
C   CARTESIAN COEFFICIENTS FROM TYPKES REDUCED COEFFICIENTS.
C(1)=PAR(1)
C(2)=PAR(2)
C(3)=PAR(3)
C(4)=-PAR(4)-2*PAR(7)+2*PAR(8)
C(5)=-PAR(4)+2*PAR(7)+2*PAR(8)
C(6)=-PAR(4)-PAR(5)-PAR(6)
C(7)=-PAR(4)-6*PAR(8)
C(8)=-PAR(4)-0.5*PAR(5)-PAR(7)

```



```

C(9)=-PAR(4)-0.5*PAR(5)+PAR(7)
C(10)=PAR(9)+PAR(13)+0.5*PAR(14)+PAR(15)
C(11)=PAR(9)-PAR(13)+0.5*PAR(14)-PAR(15)
C(12)=PAR(9)+PAR(10)+PAR(11)+PAR(12)
C(13)=1.5*PAR(9)+0.5*PAR(13)-1.25*PAR(14)-1.5*PAR(15)
C(14)=1.5*PAR(9)-0.5*PAR(13)-1.25*PAR(14)+1.5*PAR(15)
C(15)=1.5*PAR(9)+0.5*PAR(10)+PAR(13)+0.25*PAR(14)
C(16)=1.5*PAR(9)+PAR(10)+0.5*PAR(11)+0.5*PAR(13)
C(17)=1.5*PAR(9)+0.5*PAR(10)-PAR(13)+0.25*PAR(14)
C(18)=1.5*PAR(9)+PAR(10)+0.5*PAR(11)-0.5*PAR(13)
C(19)=3*PAR(9)+PAR(10)-1.5*PAR(14)
GO TO 200

```

100 CONTINUE

C CARTESIAN COEFFICIENTS FROM WATSONS REDUCED COEFFICIENTS.

```

C(1)=PAR(1)
C(2)=PAR(2)
C(3)=PAR(3)
C(4)=-PAR(4)-2*PAR(7)
C(5)=-PAR(4)+2*PAR(7)
C(6)=-PAR(4)-PAR(5)-PAR(6)
C(7)=-PAR(4)
C(8)=-PAR(4)-0.5*PAR(5)-PAR(7)-PAR(8)
C(9)=-PAR(4)-0.5*PAR(5)+PAR(7)+PAR(8)
C(10)=PAR(9)+2*PAR(13)
C(11)=PAR(9)-2*PAR(13)
C(12)=PAR(9)+PAR(10)+PAR(11)+PAR(12)
C(13)=1.5*PAR(9)+PAR(13)
C(14)=1.5*PAR(9)-PAR(13)
C(15)=1.5*PAR(9)+0.5*PAR(10)+2*PAR(13)+PAR(14)
C(16)=1.5*PAR(9)+PAR(10)+0.5*PAR(11)+PAR(13)+PAR(14)+PAR(15)
C(17)=1.5*PAR(9)+0.5*PAR(10)-2*PAR(13)-PAR(14)
C(18)=1.5*PAR(9)+PAR(10)+0.5*PAR(11)-PAR(13)-PAR(14)-PAR(15)
C(19)=3*PAR(9)+PAR(10)

```

200 CONTINUE

IF (IFREP.EQ.1) GO TO 300

C CALCULATION OF DETERMINABLE COEFFICIENTS IN THE III-R ROTATIONAL

C REPRESENTATION (X=A, Y=B, AND Z= C).

$$D(1)=C(1)-2*C(9)$$

$$D(2)=C(2)-2*C(8)$$

$$D(3)=C(3)-2*C(7)$$

$$D(4)=C(4)$$

$$D(5)=C(5)$$

$$D(6)=C(6)$$

$$D(7)=C(9)+C(8)+C(7)$$

$$D(8)=C(1)*C(9)+C(2)*C(8)+C(3)*C(7)$$

$$D(9)=C(10)$$

$$D(10)=C(11)$$

$$D(11)=C(12)$$

$$D(12)=3*(C(13)+C(14)+C(15)+C(16)+C(17)+C(18))+C(19)$$

$$D(13)=(C(1)-C(3))*C(13)+(C(1)-C(2))*C(15)-2*(C(4)-C(7))$$

$$1*(C(4)-C(8))$$

$$D(14)=(C(2)-C(1))*C(17)+(C(2)-C(3))*C(14)-2*(C(5)-C(9))$$

$$1*(C(5)-C(7))$$

$$D(15)=(C(3)-C(2))*C(16)+(C(3)-C(1))*C(18)-2*(C(6)-C(8))$$

$$1*(C(6)-C(9))$$

GO TO 400

300 CONTINUE

C DETERMINABLE COEFFICIENTS FROM REDUCED COEFFICIENTS FIT IN THE I-R

C REPRESENTATION BY CYCLIC PERMUTATION OF THE CARTESIAN

C COEFFICIENTS (X=B, Y=C, Z=A).

$$D(1)=C(3)-2*C(7)$$

$$D(2)=C(1)-2*C(9)$$

$$D(3)=C(2)-2*C(8)$$

$$D(4)=C(6)$$

$$D(5)=C(4)$$

$$D(6)=C(5)$$

$$D(7)=C(9)+C(8)+C(7)$$

$$D(8)=C(1)*C(9)+C(2)*C(8)+C(3)*C(7)$$

$$D(9)=C(12)$$

$$D(10)=C(10)$$

$$D(11)=C(11)$$

$$D(12)=3*(C(13)+C(14)+C(15)+C(16)+C(17)+C(18))+C(19)$$

```

      D(13)=(C(3)-C(2))*C(16)+(C(3)-C(1))*C(18)-2*(C(6)-C(8))
1*(C(6)-C(9))
      D(14)=(C(1)-C(3))*C(13)+(C(1)-C(2))*C(15)-2*(C(4)-C(7))
1*(C(4)-C(8))
      D(15)=(C(2)-C(1))*C(17)+(C(2)-C(3))*C(14)-2*(C(5)-C(9))
1*(C(5)-C(7))
400 CONTINUE
      PRINT 10
      PRINT 20,JBAND
      PRINT 30,(D(I),I=1,3)
      PRINT 40,(D(I),I=4,8)
      PRINT 50,(D(I),I=9,15)
10 FORMAT(*0 WATSONS DETERMINABLE COEFFICIENTS,CALCULATED USING
1 RELATIONS DEVELOPED BY W.F. MURPHY,J.M.S.,89,561 (1981).*)
20 FORMAT(*0*,A8,* STATE DETERMINABLE COEFFICIENTS*)
30 FORMAT(/** A = *,F15.9,/* B = *,F15.9,/* C = *,F15.9/**)
40 FORMAT(/** TXX = *,1PE15.8,/* TYY = *,E15.8,/* TZZ = *,E15.8,
1 /* T1 = *,E15.8,/* T2 = *,E15.8/**)
50 FORMAT(/** HXXX = *,1PE15.8,/* HYYY = *,E15.8,/* HZZZ = *,E15.8,
1 /* H1 = *,E15.8,/* H2 = *,E15.8,/* H3 = *,E15.8,
2 /* H4 = *,E15.8)
      RETURN
      END

```



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