LATTICE DYNAMICS OF PERFECT AND IMPERFECT CRYSTALS OF NaCl STRUCTURE

By

Sitaram S. Jaswal

AN ABSTRACT OF A THESIS

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ABSTRACT

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In the atomic theory of solids, both the equilibrium properties and the transport properties of crystals are influenced by vibrations of the crystal lattice into which the atoms are built. The primary concern of the present study is the computation and the application of eigenfrequencies and eigenvectors of normal vibrational modes resulting from the harmonic-approximation treatment of ionic crystals having the NaCl structure. The treatment takes into account short-range overlap forces and long-range Coulomb forces. First the dimensionless Coulomb coupling coefficients for the NaCl structure are evaluated for a moderately fine division of $\underline{k}$-space ($p_x/20$, etc.). Next eigenfrequencies and eigenvectors for NaCl and KCl are computed on both the rigid-ion model and a deformation-dipole model. Since the eigenvectors describe the actual motion of each ion, they have permitted us to classify the normal modes with respect to transversality or longitudinality. The eigenvectors and eigenvalues of the perfect lattice are useful, moreover, in various perturbation calculations for slightly imperfect lattices. We have used the values in a Green's-function computation for the frequencies of local modes and the corresponding amplitudes of impurity-atom vibrations that result from point-mass defects in NaCl and KCl. Finally our results for the frequencies of local modes due to U-centers (substitutional H^- and D^- ions) in NaCl and KCl are compared with experimental findings and with theoretical results by others.

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CHAPTER I

INTRODUCTION

Just two centuries ago Lagrange (1) presented the general theory of small oscillations of a dynamical system with a finite number of degrees of freedom (1762-65). Half a century ago Born and von Kármán (2) applied the theory to the vibrations of the atoms that form a crystal lattice (1912), basing their treatment on quasi-elastic forces between nearest neighbors.* Subsequent developments in the theory, insofar as they concern perfect ionic crystals in the harmonic approximation, are summarized in the section Perfect Lattices.

The effect of changing the masses or the spring constants in an array of coupled particles was studied by Routh (4) in 1877 and by Rayleigh (5) in 1878. The subsequent extension of their ideas to disordered lattices, especially with respect to the effect of substitutional defects on infrared absorption, is described in the section Imperfect Lattices.

Perfect Lattices

To use the atomistic theory one needs to know the nature of forces between the particles of the system. The crystals simplest

*In the same year Debye proposed his continuum theory for the vibrations of a solid. His model was so successful that little attention was paid to the work of Born and von Kármán until 1935, when Blackman (3) made a systematic investigation of dispersion curves and frequency spectra of two- and three-dimensional lattices. He showed that substantial deviations from Debye's theory should occur, especially at very low temperatures, and provided impetus for a renewed attack on lattice vibrations *via* the atomistic approach.

to deal with are ionic crystals, for which the interaction forces between ions were first given by Born (6). The central-force power-law model due to Born works fairly well for ionic crystals. Later an exponential version of short-range forces was given by Born and Mayer (7).

For the Coulomb forces, which are of long range, direct summation over all points is impossible. Born and Thompson (8) using a method developed by Ewald (9), suggested a way of transforming these sums into more rapidly convergent expressions. Thompson (10) gave the final expressions, but he made a slight error in the definition of coefficients. Broch (11) gave the sums for one-dimensional lattices.

Lyddane and Herzfeld (12) extended Madelung's method (13). Their formulas are so complicated that they cannot be used for the whole frequency spectrum, but only for waves propagated along directions of symmetry. They took into account also the free-ion polarizability due to Pauling (14), which gave imaginary frequencies and hence an unstable lattice.

Kellermann (15) used Ewald's method in a new form (16). This modification gave comparatively simple and rapidly converging expressions for the long-range Coulomb terms. Kellermann considered nearest-neighbor short-range forces only. His work put the rigid-ion model in its final form. This model described the elastic constants and the specific-heat data pretty well. The theory is, however, inconsistent with the dielectric properties of the alkali halides, because it neglects the polarizability of the ions. Kellermann's method was extended to other ionic crystals of NaCl structure by Sayre and Beaver (17) and by Karo (18).

Szigeti, in his study of dielectric properties of ionic crystals (19), derived relations connecting empirical static and optical-frequency dielectric constants to the compressibilities and restrahlen frequencies. He found that the apparent charge e^* on an ion, instead of being an electronic charge e, is less than it ($e^* = 0.74e$ for NaCl). Since he took into account the electronic polarization, he attributed the discrepancy to distortion of ions due to overlap forces. Born and Huang (20) used this idea to determine the distortion dipoles due to the overlap forces between nearest neighbors.

Instead of free-ion polarizabilities, Hardy (21) chose the crystal polarizabilities due to Tessman et al. (22) for the study of lattice dynamics of NaCl. He found the frequencies to be real, but the results were worse than with the rigid-ion model. Therefore further modifications would be necessary.

Szigeti's idea of the distortion of ions (19), as exploited by Born and Huang (20), was adapted by Hardy and Karo (23) for NaCl, and by Hardy (24) for KCl. For NaCl only negative ions were considered to be polarizable owing to short-range forces; good agreement was obtained between experiment and theory. For KCl, Hardy tried two models: deformation of negative ions only, and deformation of both kinds of ions. In the latter model he assumed the ratio of the distortion dipoles of the two kinds of ions, $m_-(r)/m_+(r)$, to be equal to the ratio of the square of the corresponding Zachariasen ionic radii, R^2_-/R^2_+. With this choice, though, the results were not so good as with the former model, which did give much improvement over the rigid-ion model.

The connection between the polarization of the ions and the repulsive forces between them has been considered by Yamashita and Kurosawa (25), by Dick and Overhauser (26), and by Hanlon and Lawson (27). The second and third pairs of authors have suggested a shell model for ions having closed-shell electron configurations. A shell model has been used by Cochran (28) to explain inelastic neutron scattering for NaI and Ge. The Chalk River group (29) first took the shell model in its simplest form, where only negative ions are polarizable and only nearest-neighbor short-range forces are considered, in order to explain their neutron-scattering results for NaI. Later (30) they tried more complicated models involving the distortion of both kinds of ions, and including next-nearest-neighbor short-range interactions. They determined the parameters involved by fitting the theory to their neutron-scattering results. Tolpygo (31) took the deformations into account by expressing the perturbation energy as a quadratic function of nuclear displacements and atomic dipole moments, in a way somewhat similar to Hardy's. Maskevich and Tolpygo (31) gave wave-mechanical justification of this treatment by use of the tight-binding approximation. The Chalk River group have compared their simple shell model with the model of Hardy and of Tolpygo. Hardy's method neglects the short-range interaction between an ion and neighboring dipoles; Tolpygo's method neglects short-range dipole-dipole forces.

In the present work the Coulomb coupling coefficients have been computed for a subdivision ($p_x/20$ etc.) of $\underline{k}$-space by summing series given by Kellermann (15). Using Kellermann's subdivision of $\underline{k}$-space as well as our own, we have computed the eigenfrequencies and the associated eigenvectors in NaCl and KCl on the rigid-ion model due to Kellermann, and on the deformation-dipole model due to Hardy. The eigenvectors have been used to classify the normal modes, and to calculate properties of local modes.

Defects

The earliest studies of defects in atomic-lattice vibrations are those of Lifshitz and his collaborators (32). Most of his work went unnoticed by subsequent workers. Montroll and his collaborators (33) carried out a parallel program at the University of Maryland. Other work in this area is that of Litzman (34). Dyson (35) did work on the frequency spectrum of a randomly-disordered linear chain.

Emphasis in these calculations has been on choosing models simple enough that qualitative as well as quantitative answers to certain specific problems can be obtained. Most of the work that has been done is of qualitative nature. Owing to the large number of unknowns involved in the general disordered lattice, it is quite hard to give rigorous quantitative treatment of any realistic problem. Consequently, most of the work has been confined to isotopic impurities where the only parameter that is changed is the mass, though a little work has been done on change of force constants (33). Some study has been made on thermodynamic properties of disordered lattices (33, 36-38).

We are interested in the effect of substitutional defects on infrared absorption. Among the various changes originating from defects, the one that can be treated precisely is change in mass. Accordingly subsequent discussion is limited to this type of defect.

Rosenstock et al. (39) considered a single substitutional mass impurity in a linear monatomic chain with nearest-neighbor short-range forces only, and computed the frequency of the local or out-of-band mode. They showed, moreover, that this mode is optically active. Wallis et al. (40) considered one- and three-dimensional cases with nearest-neighbor central and non-central forces. Some analysis of optical absorption has been given by Maradudin (38).

A general three-dimensional treatment of the problem has been outlined by Maradudin (38) and by Dawber and Elliott (41). They used a Green's-function method originally due to Lifshitz (32).

Based on the theory outlined in references 38 and 41, we have computed the frequencies of local or out-of-band modes which lie above the longitudinal optical branch, as well as the corresponding amplitudes of vibration of the impurity atom, as functions of mass of the impurity in crystals of NaCl structure. We have compared our results with experimental findings (42) and with theoretical calculations by others (39, 40). The present work is not directly concerned with dispersion curves of frequency versus wave numbers for materials studied. Such information is given for the rigid-ion model in reference 18, and for the deformation-dipole model in reference 43.

CHAPTER II

THEORY

A. PERFECT LATTICE

In the harmonic approximation (1) the equation of motion of a periodic lattice may be written as

$$M_\varkappa \ddot{u}_\alpha\binom{\ell}{\varkappa} = \sum_{\ell'\varkappa'\alpha'} \phi_{\alpha\alpha'}\binom{\ell\ell'}{\varkappa\varkappa'}\, u_{\alpha'}\binom{\ell'}{\varkappa'}, \qquad (1.1a)$$

where $M_\varkappa$ is the mass of the $\varkappa$-th particle in the unit cell ($\varkappa$ = 1, . . s, where s is the number of particles in the unit cell); $u_\alpha\binom{\ell}{\varkappa}$ is the α-th component of the displacement from equilibrium of the $\varkappa$-th particle in the ℓ-th cell (α = 1, 2, 3; ℓ = 1, . . . N, where N is the total number of cells in the crystal), and where

$$\phi_{\alpha\alpha'}\binom{\ell\ell'}{\varkappa\varkappa'} \equiv \left[\partial^2\phi/\partial u_\alpha\binom{\ell}{\varkappa}\partial u_{\alpha'}\binom{\ell'}{\varkappa'}\right]_0$$

, with ϕ being the potential energy of the system.

With solutions of the form

$$u_\alpha\binom{\ell}{\varkappa} = M_\varkappa^{-\frac{1}{2}} u_\alpha(\varkappa) \exp\left[-i\omega t + 2\pi i \underline{k}\cdot\underline{x}\binom{\ell}{\varkappa}\right] \qquad (1.2a)$$

we get

$$\omega^2 u_\alpha(\varkappa) = \sum_{\varkappa'\alpha'} D_{\alpha\alpha'}\binom{\underline{k}}{\varkappa\varkappa'}\, u_{\alpha'}(\varkappa'), \qquad (1.3a)$$

where the modified dynamical matrix $D_{\alpha\alpha'}\left(\begin{smallmatrix} & k & \\ \kappa & & \kappa'\end{smallmatrix}\right)$ is given by

$$D_{\alpha\alpha'}\left(\begin{smallmatrix} & k & \\ \kappa & & \kappa'\end{smallmatrix}\right) = -\left(M_\kappa M_{\kappa'}\right)^{-\frac{1}{2}} \sum_{\ell'} \phi_{\alpha\alpha'}\left(\begin{smallmatrix}\ell & \ell' \\ \kappa & \kappa'\end{smallmatrix}\right) \times$$

$$\exp\left[-2\pi i \underline{k}\cdot\left\{\underline{x}\left(\begin{smallmatrix}\ell \\ \kappa\end{smallmatrix}\right) - \underline{x}\left(\begin{smallmatrix}\ell' \\ \kappa'\end{smallmatrix}\right)\right\}\right]. \quad (1.4a)$$

In general, $\underline{\underline{D}}$ is hermitian, and by virtue of the geometric symmetry of the rock-salt structure it is real as well, and hence is symmetric.

For non-trivial solutions of Eqn. (1.3a) to exist, we must have

$$\left|\underline{\underline{D}} - \omega^2 \underline{\underline{1}}\right| = 0 \quad (1.5a)$$

For the rock-salt structure, this equation is of sixth degree in ω^2. Its roots give the eigenfrequencies of normal vibrational modes for a given wavevector $\underline{k}$. These modes correspond to six branches of dispersion curves, which are labeled by $j = 1, \ldots 6$.

With $\underline{\underline{D}}$ evaluated under the assumption of rigid-ion model, and nearest-neighbor short-range interactions, Kellermann (15) solved Eqn. (1.5a) for NaCl. As mentioned in the introduction, other authors (17, 18) applied the same method to some other ionic crystals having the NaCl structure, and later workers (24, 29-31) made similar calculations with models more realistic than the rigid-ion one.

For a given wavevector, corresponding to each branch we can find a vector $\underline{w}$ whose components satisfy the equation

$$\omega_j^2(\underline{k})\, w_\alpha\left(\kappa \middle| \begin{smallmatrix}k \\ j\end{smallmatrix}\right) = \sum_{\kappa'\alpha'} D_{\alpha\alpha'}\left(\begin{smallmatrix} & k & \\ \kappa & & \kappa'\end{smallmatrix}\right) w_{\alpha'}\left(\kappa' \middle| \begin{smallmatrix}k \\ j\end{smallmatrix}\right). \quad (1.6a)$$

These equations determine $\underline{w}$ within a constant factor. The arbitrariness in $\underline{w}$ can be removed by orthonormality conditions:

$$\sum_{\varkappa\alpha} w_\alpha(\varkappa|{}^{k}_{j})\, w^*_\alpha(\varkappa|{}^{k}_{j'}) = \delta_{jj'} \quad ,$$

$$\sum_{j} w_\alpha(\varkappa|{}^{k}_{j})\, w^*_{\alpha'}(\varkappa'|{}^{k}_{j}) = \delta_{\alpha\alpha'}\, \delta_{\varkappa\varkappa'} . \tag{1.7a}$$

This orthonormal set of $\underline{w}$'s is the set of eigenvectors with which we are concerned here.

In matrix form, equation (1.6a) can be written as

$$\underline{\underline{D}}\,\underline{\underline{S}} = \underline{\underline{S}}\,\underline{\underline{\omega}}^2$$

or

$$\tilde{\underline{\underline{S}}}\,\underline{\underline{D}}\,\underline{\underline{S}} = \underline{\underline{\omega}}^2$$

where the columns of $\underline{\underline{S}}$ are the eigenvectors, and $\underline{\underline{\omega}}^2$ is a diagonal matrix with the eigenvalues as the diagonal elements. Since $\underline{\underline{D}}$ is real and symmetric, it can be diagonalized by an orthogonal matrix $\underline{\underline{S}}$.

The general motion of the lattice is given by a superposition of the elementary solutions (1.2a):

$$u_\alpha({}^{l}_{\varkappa}) = N^{-\frac{1}{2}} \sum_{kj} M_\varkappa^{-\frac{1}{2}}\, w_\alpha(\varkappa|{}^{k}_{j})\, Q({}^{k}_{j}) \times$$
$$\times \exp[-i\omega_j(\underline{k})t + 2\pi i\, \underline{k}\cdot\underline{x}({}^{l}_{\varkappa})]. \tag{1.8a}$$

To compute the dynamical matrix we have used two models, the rigid-ion model (RI) due to Kellermann (15), the deformation-dipole (DD) model due to Hardy (24).

1. Rigid-ion model

In this model the ions are treated as point-charges. The interaction potential consists of a short-range central potential between the nearest neighbors, and a long-range Coulomb potential.

The coupling coefficients, which are the elements of the dynamical matrix, are of two kinds: those associated with the motion of the ion under consideration, and those associated with the motion of the rest of the lattice. The coefficients of the first and second kind are given respectively by

$$[\alpha\alpha'\varkappa\varkappa] = -\sum_{\ell\varkappa'} \phi_{\alpha\alpha'}\binom{\ell}{\varkappa\varkappa'} \qquad (1.9a)$$

and

$$(\alpha\alpha'\varkappa\varkappa') = \sum_{\ell} \phi_{\alpha\alpha'}\binom{\ell}{\varkappa\varkappa'} \exp\left(-2\pi i \underline{k}\cdot \underline{r}^{\ell}_{\varkappa\varkappa'}\right), \qquad (1.10a)$$

where $\underline{r}^{\ell}_{\varkappa\varkappa'} = \underline{x}\binom{0}{\varkappa} - \underline{x}\binom{\ell}{\varkappa'}$.

Coupling coefficients due to Coulomb potential

Owing to the symmetry of the NaCl-structure, the contribution to eq. (1.9a) due to the Coulomb terms is zero. The Coulomb part of eq. (1.10a) is given

$$C(\alpha\alpha'\varkappa\varkappa') = \sum_{\ell} \left[\partial^2 \left(e_{\varkappa} e_{\varkappa'} / |\underline{r}^{\ell}_{\varkappa\varkappa'}|\right) / \partial u_{\alpha}\binom{0}{\varkappa} \partial u_{\alpha'}\binom{\ell}{\varkappa'}\right] \exp\left(-2\pi i \underline{k}\cdot \underline{r}^{\ell}_{\varkappa\varkappa'}\right). \qquad (1.11a)$$

This series as it stands is not absolutely convergent. It was evaluated by Kellermann with Ewald's formula for the Theta-function transformation

$$2\pi^{-\frac{1}{2}}\sum_{l}\exp[-\delta^{2}(\mathbf{r}-\mathbf{a}^{l})+2\pi i\mathbf{k}\cdot\mathbf{a}^{l}]$$

$$=\frac{2\pi}{v_a}\sum_{h}\frac{1}{\delta^{3}}\exp[-\pi^{2}/\delta^{2}(\mathbf{b}_h+\mathbf{k})^{2}+2\pi i(\mathbf{b}_h+\mathbf{k})\cdot\mathbf{r}], \qquad (1.12a)$$

where v_a is the volume of unit cell. This transformation makes the series quickly convergent, and maintains the cell neutrality.

Next the summation and the differentiation in eq. (1.11a) are interchanged. Then $1/|r|$ is replaced by $2\pi^{-\frac{1}{2}}\int_0^\infty e^{-\delta^2 r^2}d\delta$. With this substitution in eq. (1.11a), the Ewald transformation can be applied. From eq. (1.12a) we note that the left-hand side converges rapidly for large values of δ, whereas the right-hand side converges rapidly for small values of δ. Hence we break the integration into two parts $\int_0^\infty = \int_0^E + \int_E^\infty$, and use the appropriate integrand from eq. (1.12a).

After integration over δ, differentiation is performed. Going through these mathematical details, Kellermann obtained the final form of the dimensionless coupling coefficients for the NaCl-structure as

$$C(xy\,11)=\frac{v_a}{e^2}C(xy\,11)=-G^{11}_{xy}+H^{l}_{xy}+\frac{8}{3\sqrt{\pi}}\delta^{2}\delta_{xy} \qquad (1.13a)$$

$$C(xy\,12)=\frac{v_a}{e^2}C(xy\,12)=G^{12}_{xy}-H^{m}_{xy} \qquad (1.14a)$$

where

$$G^{11}_{xy} = 4\pi \sum_{h} \frac{(h_x + q_x)(h_y + q_y)}{(\underline{h} + \underline{q})^2} \exp\left[-\frac{\pi^2}{4\delta^2}(\underline{h}+\underline{q})^2\right]$$

$$G^{12}_{xy} = 4\pi \sum_{h} \frac{(h_x + q_x)(h_y + q_y)}{(\underline{h} + \underline{q})^2} \exp\left[-\frac{\pi^2}{4\delta^2}(\underline{h}+\underline{q})^2\right] \times$$

$$\cos\pi(h_x + h_y + h_z)$$

$$H^{\ell}_{xy} = 2 \sum_{\ell} \left[-f(\ell)\,\delta_{xy} + g(\ell)\,\frac{\ell_x \ell_y}{\ell^2}\right] \cos\pi\,\underline{q}\cdot\underline{\ell}$$

$$f(\ell) = (2/\sqrt{\pi})\, e^{-\delta^2\ell^2}/\ell^2 + \frac{\psi(\delta\ell)}{\ell^3}$$

$$g(\ell) = \frac{4}{\sqrt{\pi}}\,\delta^3 e^{-\delta^2\ell^2} + \frac{6}{\sqrt{\pi}}\,\delta\,\frac{e^{-\delta^2\ell^2}}{\ell^2} + \frac{3\psi(\delta\ell)}{\ell^3}$$

$$\psi(\delta\ell) = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\delta\ell} e^{-\xi^2}\,d\xi \;;$$

$$\underline{k} = \frac{1}{2r_0}(q_x, q_y, q_z)$$

$$\ell = (\ell_x^2 + \ell_y^2 + \ell_z^2)^{1/2}.$$

Here (h_x, h_y, h_z) are sets of either all odd or all even integers; (ℓ_x, ℓ_y, ℓ_z) are sets of integers such that $\sum_x \ell_x$ = even, except the (0, 0, 0) set, which is excluded; and (m_x, m_y, m_z) are all sets of integers for which $\sum_x m_x$ = odd. The conditions on these integers arise from the NaCl structure as represented in Cartesian coordinates. These equations hold only for $\underline{k} \neq \underline{0}$. In this case, the 'potential' satisfies Laplace's equation, which gives the condition

$$C(xx\,\kappa\kappa') + C(yy\,\kappa\kappa') + C(zz\,\kappa\kappa') = 0.$$

In performing the summation in equations (1.13a) and (1.14a), Kellermann took $\delta = 1$. We also took $\delta = 1$ for our finer subdivision of $\underline{k}$-space.

For $\underline{k} = \underline{0}$, the 'potential' satisfies Poisson's equation which, in case of cubic symmetry, gives

$$c(\alpha\alpha\kappa\kappa') = -4\pi/3 \quad , \quad c(\alpha\alpha\kappa\kappa) = 4\pi/3$$

and $$c(\alpha\alpha'\kappa\kappa) = c(\alpha\alpha'\kappa\kappa') = 0$$

The coupling coefficients corresponding to longitudinal modes are affected by the polarization on faces of the crystal perpendicular to the direction of motion of the ions; thus there arises an additional contribution of either $+4\pi$ or -4π.

Short-range repulsive forces

The coupling coefficients in this case are given by

$$R[\alpha\alpha'\kappa\kappa] = -\sum_{l}\sum_{\kappa'}\left[\partial^2\varphi(|r^{l}_{\kappa\kappa'}|)/\partial u_{\alpha}\left(\begin{smallmatrix}0\\ \kappa\end{smallmatrix}\right)\partial u_{\alpha'}\left(\begin{smallmatrix}l\\ \kappa'\end{smallmatrix}\right)\right]_0 \qquad (1.15a)$$

$$R(\alpha\alpha'\kappa\kappa') = \sum_{l}\left[\partial^2\varphi(|r^{l}_{\kappa\kappa'}|)/\partial u_{\alpha}\left(\begin{smallmatrix}0\\ \kappa\end{smallmatrix}\right)\partial u_{\alpha'}\left(\begin{smallmatrix}l'\\ \kappa'\end{smallmatrix}\right)\right]_0 \times \exp[-2\pi i\underline{k}\cdot r^{l}_{\kappa\kappa'}]. \qquad (1.16a)$$

With nearest-neighbor interaction in the NaCl structure,

$$R[xy11] = -\sum_{l}\sum_{\kappa'}\left[\varphi''\frac{x^{l}_{1\kappa'}y^{l}_{1\kappa'}}{(r^{l}_{1\kappa'})^2} + \varphi'\left(\frac{\delta_{x}{}^{l}_{1\kappa'}, y^{l}_{1\kappa'}}{r^{l}_{1\kappa'}} - \frac{x^{l}_{1\kappa'}\,y^{l}_{1\kappa'}}{(r_{1\kappa'})^3}\right)\right], \qquad (1.17a)$$

where $\vartheta' = \left.\frac{d\vartheta(r)}{dr}\right]_{r=r_0}$ etc.

In Kellermann's notation,

$$\vartheta' = \frac{r_0}{2}\frac{e^2}{v_a} B \ ; \quad \vartheta'' = \frac{1}{2}\frac{e^2}{v_a} A \, ,$$

where r_0 is the distance between nearest neighbors.

$$R[xy11] = -\frac{1}{2}\frac{e^2}{v_a}\sum_{l}\sum_{\kappa'}\Big[A\,\frac{x^{l}_{1\kappa'}\,y^{l}_{1\kappa'}}{(r^{l}_{1\kappa'})^2} +$$

$$B\Big(\delta_{x^{l}_{1\kappa'}y^{l}_{1\kappa'}} - \frac{x^{l}_{1\kappa'}\,y^{l}_{1\kappa'}}{(r^{l}_{1\kappa'})^2}\Big)\Big]. \qquad (1.18a)$$

With nearest-neighbor interactions,

$$R[xx11] = -(A+2B) \ ; \quad R[xy12] = 0. \qquad (1.19a)$$

Similarly eq. (1.16a) gives

$$R(xy12) = 0 \ ; \quad v_a/e^2 \, R(xx12) = A\cos\pi q_x$$

$$+ B(\cos\pi q_y + \cos\pi q_z). \qquad (1.20a)$$

Now the first Brillouin zone for NaCl structure is defined by the faces

$$q_x \pm q_y \pm q_z = \pm 3/2 \ ; \quad q_x = \pm 1 \ ; \ q_y = \pm 1; \ q_z = \pm 1 \, .$$

If we limit ourselves to the values of $\underline{q}$ given by $0 \leq q_z \leq q_y \leq q_x \leq 1$ and $q_x + q_y + q_z \leq 3/2$, all other points in the zone can be generated by symmetry operations. For actual calculations, one needs to have some kind of subdivision of $\underline{k}$-space such as $q_x = p_x/10$, etc.

To determine the A and B involved in short-range coupling coefficients, one uses the lattice parameter r_o and the compressibility β. The energy per unit cell is given by

$$\phi_o = -\alpha e^2/r_o + 6\,v(r_o) \quad , \tag{1.21a}$$

where α is the Madelung constant, equal to 1.7476 for the NaCl structure. Using the condition of equilibrium, we find

$$d\phi_o/dr_o = o = \alpha e^2/r_o^2 + 6\,v'(r_o). \tag{1.22a}$$

Introducing B in (1.22a), we get

$$B = -2\alpha/3 = -1.165. \tag{1.23a}$$

The compressibility is given by

$$1/\beta = \frac{1}{9 v_a} r_o^2 \frac{d^2\phi_o}{dr_o^2} = \frac{1}{18 r_o} \frac{d^2\phi_o}{dr_o^2}$$

$$= \frac{1}{18 r_o}\left[-2\alpha \frac{e^2}{r_o^3} + \frac{2}{3} A\, e^2/r_o^3\right],$$

$$\text{or} \quad A = \frac{12 r_o^4}{\beta e^2} + 4/3\,\alpha . \tag{1.24a}$$

Finally, the elements of the dynamical matrix are the sum of Coulomb and short-range coupling coefficients:

$$\{\alpha\alpha'\varkappa\varkappa'\} = -(M_\varkappa M_{\varkappa'})^{-1/2}[C\{\alpha\alpha'\varkappa\varkappa'\} + R\{\alpha\alpha\varkappa\varkappa'\}]$$

where $$C\{\ \} \equiv C[\ ] + C(\ ) \qquad \text{etc.} \qquad (1.25a)$$

2. Deformation-Dipole model

In addition to the terms considered in the rigid-ion model, here the crystal polarizabilities and deformation dipoles due to short-range overlap forces are taken into account. We consider only the negative ion polarizable owing to overlap forces. Also, we consider only the distortions occurring between nearest neighbors. Let m(r) be the deformation dipole moment between a positive ion and a negative ion. It is a function of their separation r, and the sign is taken as positive if the moment is directed from the negative towards the positive ion.

To determine the deformation dipole moment to the first order in the displacement, the treatment is parallel to that of the short-range potential considered in part 1. Thus motion of the ion under consideration gives rise to the distortion term $b(\varkappa) = 2(\gamma_\varkappa' + 2\gamma_\varkappa)$, where $\gamma_\varkappa' = [dm_\varkappa(r)/dr]_{r_0}$ and $\gamma_\varkappa = m_\varkappa(r_0)/r_0$.

The distortion due to the motion of neighboring ions is given by

$$a_\beta(\varkappa) = 2[\gamma_\varkappa' \cos\pi q_\beta + \gamma_\varkappa(\cos\pi q_\delta + \cos\pi q_\epsilon)]$$

For the ion $\binom{0}{\varkappa}$, the virtual work involving the field due to the displacement $\underline{U}\binom{0}{\varkappa}$ is given by

$$\Delta W = -[e_\varkappa - b(\varkappa)]\underline{E}\binom{0}{\varkappa}\cdot\underline{U}\binom{0}{\varkappa} - \sum \underline{E}^\alpha \cdot \Delta\mu_D^\alpha, \qquad (1.1b)$$

where $\underline{E}\binom{0}{\varkappa}$ is the field at $\binom{0}{\varkappa}$.

The second term corresponds to the deformation induced on the nearest neighbor by the displacement of $\binom{0}{\varkappa}$. The field $\underline{E}\binom{0}{\varkappa}$ is given by the lattice of dipoles:

$$P_\beta\binom{l'}{\varkappa'} = [e_{\varkappa'} u_\beta(\varkappa') M_{\varkappa'}^{-1/2} + \mu_\beta(\varkappa') + a_\beta(\varkappa') u_\beta(s) M_s^{-1/2}$$

$$- b(\varkappa') u_\beta(\varkappa') M_{\varkappa'}^{-1/2}] \exp[2\pi i \underline{k} \cdot \underline{r}\binom{l}{\varkappa'}] \quad . \qquad (1.2b)$$

Here $\mu_\beta(\varkappa')$ is the component of dipole moment resulting from the crystal polarizability.

Hence the field is given by

$$E_\alpha\binom{0}{\varkappa} = -\sum_{\varkappa',\alpha',s\neq\varkappa'} \frac{\exp[2\pi i \underline{k}\cdot \underline{r}_{\varkappa}^{\circ}]}{e_\varkappa} C(\alpha\alpha'\varkappa\varkappa')[u_{\alpha'}(\varkappa') M_{\varkappa'}^{-1/2}$$

$$+ \mu_{\alpha'}(\varkappa')/e_{\varkappa'} + \frac{1}{e_{\varkappa'}}\left\{\frac{u_{\alpha'}(s)}{M_s^{1/2}} a_{\alpha'}(\varkappa') - b(\varkappa') u_{\alpha'}(\varkappa') M_{\varkappa'}^{-1/2}\right\}] \qquad (1.3b)$$

We can substitute this value of $\underline{E}$ in the expression for ΔW . Then the Coulomb part of the force is given by

$$P_\alpha^c\binom{0}{\varkappa} = -\partial\Delta W/\partial u_\alpha\binom{0}{\varkappa} \qquad (1.4b)$$

After going through various manipulations, Hardy put eq. (1.4b) in matrix form. Adding to the Coulomb part the short-range part, which is the same as that adopted by Kellermann, he arrived at the final form of the dynamical matrix:

$$\underline{\underline{D}} = -\underline{\underline{X}}[\underline{\underline{K}} + \underline{\underline{H}}\,\underline{\underline{U}}\,\underline{\underline{\tilde{S}}} + \underline{\underline{S}}\,\underline{\underline{U}}\,\underline{\underline{H}} + (\underline{\underline{1}} + \underline{\underline{S}}\,\underline{\underline{U}}) \times$$
$$\underline{\underline{H}}\,\underline{\underline{U}}\,\underline{\underline{C}}^{-1}\underline{\underline{A}} + \underline{\underline{S}}\,\underline{\underline{U}}\,\underline{\underline{H}}\,\underline{\underline{U}}\,\underline{\underline{\tilde{S}}}]\underline{\underline{X}} \qquad (1.5b)$$

where

$$\underline{\underline{K}} = R\{\alpha\alpha'\varkappa\varkappa'\} + C\{\alpha\alpha'\varkappa\varkappa'\},$$

$$\underline{\underline{S}} = -b(\varkappa)\,\delta_{\alpha\alpha'}\,\delta_{\varkappa\varkappa'} + a_{\alpha}(\varkappa')\,\delta_{\alpha\alpha'}\,(1-\delta_{\varkappa\varkappa'}),$$

$$\underline{\underline{U}} = \frac{\delta_{\alpha\alpha'}\,\delta_{\varkappa\varkappa'}}{e_{\varkappa}}, \quad \underline{\underline{H}} = C(\alpha\alpha'\varkappa\varkappa'),$$

$$\underline{\underline{X}} = \frac{\delta_{\alpha\alpha'}\,\delta_{\varkappa\varkappa'}}{(m_{\varkappa})^{1/2}},$$

$$\underline{\underline{C}} = \underline{\underline{1}} - \underline{\underline{\alpha}}\,\underline{\underline{U}}\,\underline{\underline{H}}\,\underline{\underline{U}},$$

$$\underline{\underline{\alpha}} = \alpha^{\varkappa}\delta_{\alpha\alpha'}\,\delta_{\varkappa\varkappa'}$$ —(crystal polarizabilities).

The distortion dipoles are computed from a relation given by Born and Huang (20):

$$e^{*} - e = 2\,(\gamma'_{-} + 2\ \gamma_{-}), \tag{1.6b}$$

where the effective charge e^{*} is obtained from the second Szigeti relation (19). If we write $e^{*} \equiv se$, s is given by

$$s = \omega_0\left(\frac{\epsilon_0 - \epsilon_\infty}{4\pi}\right)^{1/2}\left(\frac{3}{\epsilon_\infty + 2}\right)\left(\frac{\overline{M}\,v_a}{e}\right)^{1/2}, \tag{1.7b}$$

with $\overline{M}$, the reduced mass; ϵ_0, the static dielectric constant; ϵ_∞, the high-frequency dielectric constant; and ω_0, the infrared dispersion frequency.

B. IMPERFECT LATTICE

We may write the equation of motion for an imperfect lattice as

$$M_{\kappa}(\ell)\ddot{u}_{\alpha}\binom{\ell}{\kappa}+\sum_{\kappa'\alpha'\ell'}\phi_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}u_{\alpha'}\binom{\ell'}{\kappa'}$$

$$=\Delta M_{\kappa}(\ell)\ddot{u}_{\alpha}\binom{\ell}{\kappa}+\sum_{\kappa'\alpha'\ell'}\Delta\phi_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}u_{\alpha'}\binom{\ell'}{\kappa'}, \qquad (2.1)$$

if we consider only substitutional defects. The first term on the right hand side contains the change in mass due to impurity, ΔM_{κ}, and the second term contains the change in force constants, $\Delta\phi_{\alpha\alpha'}$. If we express $u_{\alpha}\binom{\ell}{\kappa}$ as the superposition of the amplitudes χ of normal modes of imperfect lattice eq. (2.1) becomes

$$-\omega^2 M_{\kappa}\chi_{\alpha}(\kappa/{}^{f}_{\ell})+\sum_{\kappa'\alpha'\ell'}\phi_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}\chi_{\alpha'}(\kappa'/{}^{f}_{\ell'})$$

$$=\sum_{\kappa'\alpha'\ell'}C_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}\chi_{\alpha'}(\kappa'/{}^{f}_{\ell'}) \qquad (2.2)$$

where

$$C_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}=-\Delta M_{\kappa}(\ell)\,\omega^2\delta_{\alpha\alpha'}\delta_{\kappa\kappa'}\delta_{\ell\ell'}+\Delta\phi_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}.$$

The normal modes of the imperfect lattice have been labeled by f, which takes 3sN values.

Eq. (2.2) can be solved by a Green's-function method. The Green's function for this equation is given by

$$-\omega^2 M_{\kappa}\, g_{\alpha\alpha''}\left(\begin{matrix}\ell\ell''\\ \kappa\kappa''\end{matrix};\omega\right)+\sum_{\kappa'\alpha'\ell'}\phi_{\alpha\alpha'}\binom{\ell\ell'}{\kappa\kappa'}g_{\alpha'\alpha''}\left(\begin{matrix}\ell'\ell''\\ \kappa'\kappa''\end{matrix};\omega\right)$$

$$=\delta_{\alpha\alpha''}\,\delta_{\kappa\kappa''}\,\delta_{\ell\ell''}. \qquad (2.3)$$

If we expand $g_{\alpha\alpha'}$ by bilinear expansion in terms of the amplitudes of the normal modes of the perfect lattice, we get

$$g_{\alpha\alpha'}\left({\ell\ell' \atop \varkappa\varkappa'};\omega\right) = \frac{N^{-1/2}}{(M_{\varkappa}M_{\varkappa'})^{1/2}} \sum_{\underline{k}j} \frac{w_{\alpha}(\varkappa|{\underline{k} \atop j})\, w^{*}_{\alpha'}(\varkappa'|{\underline{k} \atop j})}{\omega_j^2(\underline{k}) - \omega^2(f)} \times$$

$$\exp[2\pi i\,\underline{k}\cdot(\underline{x}(\ell) - \underline{x}(\ell'))]. \qquad (2.4)$$

The amplitudes of the normal modes of the imperfect lattice are given by

$$\chi_{\alpha}(\varkappa|{f \atop \ell}) = \sum_{\alpha'\varkappa'\ell'}\sum_{\alpha''\varkappa''\ell''} g_{\alpha\alpha'}\left({\varkappa\varkappa' \atop \ell\ell'};\omega\right)\times$$

$$C_{\alpha\alpha'}\left({\ell'\ell'' \atop \varkappa'\varkappa''}\right)\chi_{\alpha''}(\varkappa''|{f \atop \ell''}). \qquad (2.5)$$

Eq. (2.5) gives the eigenvalue equation

$$\left|\sum_{\alpha'\varkappa'\ell'} g_{\alpha\alpha'}\left({\varkappa\varkappa' \atop \ell\ell'};\omega\right)C_{\alpha'\alpha''}\left({\ell'\ell'' \atop \varkappa'\varkappa''}\right) - \delta_{\alpha\alpha''}\,\delta_{\varkappa\varkappa''}\,\delta_{\ell\ell''}\right| = 0. \qquad (2.6)$$

If we consider a single isotopic impurity, then $\Delta\phi_{\alpha\alpha'}$, is zero, and we have $C_{\alpha\alpha'}\left({\ell'\ell'' \atop \varkappa\varkappa''}\right) = -M_{\varkappa'}\epsilon_{\varkappa'}\,\omega^2\delta_{0\ell'}\,\delta_{\varkappa'\varkappa''}\,\delta_{\alpha'\alpha''}\,\delta_{\ell'\ell''}$

with $\epsilon_{\varkappa} \equiv (M_{\varkappa} - M'_{\varkappa})/M_{\varkappa}$.

With this value of $C_{\alpha'\alpha''}$ eq. (2.6) reduces to

$$\left|M_{\varkappa}\epsilon_{\varkappa}\omega^2 g_{\alpha\alpha'}\left({0\,0 \atop \varkappa\varkappa'};\omega\right) + \delta_{\alpha\alpha'}\,\delta_{\varkappa\varkappa'}\right| = 0. \qquad (2.7)$$

For a diatomic cubic crystal, eq. (2.7) gives us a triply-degenerate equation

$$1 = \frac{\epsilon_\kappa \omega^2(f)}{3N} \sum_{\underline{k}j} \frac{|\underline{W}(\kappa| {\underline{k} \atop j})|^2}{\omega^2(f) - \omega_j^2(\underline{k})} \cdot \tag{2.8}$$

If we apply the normalization condition to the amplitudes of impurity modes and use eq. (2.5), the amplitude of the impurity atom is given by

$$M_\kappa |\chi(\kappa| {f \atop 0})|^2 = \left[\frac{\epsilon_\kappa^2 \omega^4(f)}{3N} \sum_{\underline{k}j} \frac{|\underline{W}(\kappa| {\underline{k} \atop j})|^2}{(\omega_j^2(\underline{k}) - \omega^2(f))^2} - \epsilon \right]^{-1} . \tag{2.9}$$

Eq. (2.8), when solved for $\omega^2(f)$, gives the frequencies of normal modes of the imperfect lattice.

CHAPTER III

COMPUTATION AND RESULTS

A. COULOMB COUPLING COEFFICIENTS

From eqs. (1.13a) and (1.14a) we have computed the Coulomb terms $c\,(\alpha\alpha'\;\kappa\kappa')$ with a finer subdivision of $\underline{k}$-space ($q_x = p_x/20$ etc.) than Kellermann used. This finer subdivision gives 262 distinct points in the first zone, which by symmetry operations generate 8000 points in the first Brillouin zone. These points along with their weights are listed in Table I. The weight is determined by considering whether the point lies inside the zone, on the face, on the edge, or on the corner of the Brillouin zone. If the point lies inside the zone, the weight is given by the total number of permutations which are performed on the sets of p's generated by changing the sign of one of them at a time, two of them at a time, and three of them at a time (including, of course, the original set). For other cases, one has to take into account the neighboring cells. Computed dimensionless Coulomb coupling coefficients have been listed in Tables II (a) and II (b), and in matrix form in Table VIII (Appendix A).

B. EIGENVECTORS AND EIGENFREQUENCIES OF VIBRATIONS FOR THE PERFECT LATTICE

For NaCl and KCl we have made calculations on both the rigid-ion model (RI) and the deformation-dipole (DD) model. Most of the input data for these salts are given in Table III.

Table I Wavevectors for subdivision ($p_x/20$, $p_y/20$, $p_z/20$) of first Brillouin zone and their weight.

Wave Vector			Weight	Wave Vector			Weight
p_x	p_y	p_z		p_x	p_y	p_z	
0.0	0.0	0.0	1	8.0	8.0	4.0	24
2.0	0.0	0.0	6	8.0	6.0	6.0	24
2.0	2.0	0.0	12	8.0	8.0	6.0	24
2.0	2.0	2.0	8	8.0	8.0	8.0	8
4.0	0.0	0.0	6	10.0	0.0	0.0	6
4.0	2.0	0.0	24	10.0	2.0	0.0	24
4.0	4.0	0.0	12	10.0	4.0	0.0	24
4.0	2.0	2.0	24	10.0	6.0	0.0	24
4.0	4.0	2.0	24	10.0	8.0	0.0	24
4.0	4.0	4.0	8	10.0	10.0	0.0	12
6.0	0.0	0.0	6	10.0	2.0	2.0	24
6.0	2.0	0.0	24	10.0	4.0	2.0	48
6.0	4.0	0.0	24	10.0	6.0	2.0	48
6.0	6.0	0.0	12	10.0	8.0	2.0	48
6.0	2.0	2.0	24	10.0	10.0	2.0	24
6.0	4.0	2.0	48	10.0	4.0	4.0	24
6.0	6.0	2.0	24	10.0	6.0	4.0	48
6.0	4.0	4.0	24	10.0	8.0	4.0	48
6.0	6.0	4.0	24	10.0	10.0	4.0	24
6.0	6.0	6.0	8	10.0	6.0	6.0	24
8.0	0.0	0.0	6	10.0	8.0	6.0	48
8.0	2.0	0.0	24	10.0	10.0	6.0	24
8.0	4.0	0.0	24	10.0	8.0	8.0	24
8.0	6.0	0.0	24	10.0	10.0	8.0	24
8.0	8.0	0.0	12	10.0	10.0	10.0	4
8.0	2.0	2.0	24	12.0	0.0	0.0	6
8.0	4.0	2.0	48	12.0	2.0	0.0	24
8.0	6.0	2.0	48	12.0	4.0	0.0	24
8.0	8.0	2.0	24	12.0	6.0	0.0	24
8.0	4.0	4.0	24	12.0	8.0	0.0	24
8.0	6.0	4.0	48	12.0	10.0	0.0	24

Wave Vector p_x	p_y	p_z	Weight	Wave Vector p_x	p_y	p_z	Weight
12.0	12.0	0.0	12	14.0	6.0	4.0	48
12.0	2.0	2.0	24	14.0	8.0	4.0	48
12.0	4.0	2.0	48	14.0	10.0	4.0	48
12.0	6.0	2.0	48	14.0	12.0	4.0	24
12.0	8.0	2.0	48	14.0	6.0	6.0	24
12.0	10.0	2.0	48	14.0	8.0	6.0	48
12.0	12.0	2.0	24	14.0	10.0	6.0	24
12.0	4.0	4.0	24	14.0	8.0	8.0	12
12.0	6.0	4.0	48	16.0	0.0	0.0	6
12.0	8.0	4.0	48	16.0	2.0	0.0	24
12.0	10.0	4.0	48	16.0	4.0	0.0	24
12.0	12.0	4.0	24	16.0	6.0	0.0	24
12.0	6.0	6.0	24	16.0	8.0	0.0	24
12.0	8.0	6.0	48	16.0	10.0	0.0	24
12.0	10.0	6.0	48	16.0	12.0	0.0	24
12.0	12.0	6.0	12	16.0	14.0	0.0	8
12.0	8.0	8.0	24	16.0	2.0	2.0	24
12.0	10.0	8.0	24	16.0	4.0	2.0	48
14.0	0.0	0.0	6	16.0	6.0	2.0	48
14.0	2.0	0.0	24	16.0	8.0	2.0	48
14.0	4.0	0.0	24	16.0	10.0	2.0	48
14.0	6.0	0.0	24	16.0	12.0	2.0	24
14.0	8.0	0.0	24	16.0	4.0	4.0	24
14.0	10.0	0.0	24	16.0	6.0	4.0	48
14.0	12.0	0.0	24	16.0	8.0	4.0	48
14.0	14.0	0.0	12	16.0	10.0	4.0	24
14.0	2.0	2.0	24	16.0	6.0	6.0	24
14.0	4.0	2.0	48	16.0	8.0	6.0	24
14.0	6.0	2.0	48	18.0	0.0	0.0	6
14.0	8.0	2.0	48	18.0	2.0	0.0	24
14.0	10.0	2.0	48	18.0	4.0	0.0	24
14.0	12.0	2.0	48	18.0	6.0	0.0	24
14.0	14.0	2.0	12	18.0	8.0	0.0	24
14.0	4.0	4.0	24	18.0	10.0	0.0	24

Wave Vector			Weight	Wave Vector			Weight
p_x	p_y	p_z		p_x	p_y	p_z	
18.0	12.0	0.0	8	7.0	3.0	1.0	48
18.0	2.0	2.0	24	7.0	5.0	1.0	48
18.0	4.0	2.0	48	7.0	7.0	1.0	24
18.0	6.0	2.0	48	7.0	3.0	3.0	24
18.0	8.0	2.0	48	7.0	5.0	3.0	48
18.0	10.0	2.0	24	7.0	7.0	3.0	24
18.0	4.0	4.0	24	7.0	5.0	5.0	24
18.0	6.0	4.0	48	7.0	7.0	5.0	24
18.0	8.0	4.0	24	7.0	7.0	7.0	8
18.0	6.0	6.0	12	9.0	1.0	1.0	24
20.0	0.0	0.0	3	9.0	3.0	1.0	48
20.0	2.0	0.0	12	9.0	5.0	1.0	48
20.0	4.0	0.0	12	9.0	7.0	1.0	48
20.0	6.0	0.0	12	9.0	9.0	1.0	24
20.0	8.0	0.0	12	9.0	3.0	3.0	24
20.0	10.0	0.0	6	9.0	5.0	3.0	48
20.0	2.0	2.0	12	9.0	7.0	3.0	48
20.0	4.0	2.0	24	9.0	9.0	3.0	24
20.0	6.0	2.0	24	9.0	5.0	5.0	24
20.0	8.0	2.0	16	9.0	7.0	5.0	48
20.0	4.0	4.0	12	9.0	9.0	5.0	24
20.0	6.0	4.0	16	9.0	7.0	7.0	24
1.0	1.0	1.0	8	9.0	9.0	7.0	24
3.0	1.0	1.0	24	9.0	9.0	9.0	8
3.0	3.0	1.0	24	11.0	1.0	1.0	24
3.0	3.0	3.0	8	11.0	3.0	1.0	48
5.0	1.0	1.0	24	11.0	5.0	1.0	48
5.0	3.0	1.0	48	11.0	7.0	1.0	48
5.0	5.0	1.0	24	11.0	9.0	1.0	48
5.0	3.0	3.0	24	11.0	11.0	1.0	24
5.0	5.0	3.0	24	11.0	3.0	3.0	24
5.0	5.0	5.0	8	11.0	5.0	3.0	48
7.0	1.0	1.0	24	11.0	7.0	3.0	48

Wave Vector			Weight	Wave Vector			Weight
p_x	p_y	p_z		p_x	p_y	p_z	
11.0	9.0	3.0	48	15.0	11.0	1.0	48
11.0	11.0	3.0	24	15.0	13.0	1.0	48
11.0	5.0	5.0	24	15.0	3.0	3.0	24
11.0	7.0	5.0	48	15.0	5.0	3.0	48
11.0	9.0	5.0	48	15.0	7.0	3.0	48
11.0	11.0	5.0	24	15.0	9.0	3.0	48
11.0	7.0	7.0	24	15.0	11.0	3.0	48
11.0	9.0	7.0	48	15.0	5.0	5.0	24
11.0	11.0	7.0	24	15.0	7.0	5.0	48
11.0	9.0	9.0	24	15.0	9.0	5.0	48
13.0	1.0	1.0	24	15.0	7.0	7.0	24
13.0	3.0	1.0	48	17.0	1.0	1.0	24
13.0	5.0	1.0	48	17.0	3.0	1.0	48
13.0	7.0	1.0	48	17.0	5.0	1.0	48
13.0	9.0	1.0	48	17.0	7.0	1.0	48
13.0	11.0	1.0	48	17.0	9.0	1.0	48
13.0	13.0	1.0	24	17.0	11.0	1.0	48
13.0	3.0	3.0	24	17.0	3.0	3.0	24
13.0	5.0	3.0	48	17.0	5.0	3.0	48
13.0	7.0	3.0	48	17.0	7.0	3.0	48
13.0	9.0	3.0	48	17.0	9.0	3.0	48
13.0	11.0	3.0	48	17.0	5.0	5.0	24
13.0	13.0	3.0	24	17.0	7.0	5.0	48
13.0	5.0	5.0	24	19.0	1.0	1.0	24
13.0	7.0	5.0	48	19.0	3.0	1.0	48
13.0	9.0	5.0	48	19.0	5.0	1.0	48
13.0	11.0	5.0	48	19.0	7.0	1.0	48
13.0	7.0	7.0	24	19.0	9.0	1.0	48
13.0	9.0	7.0	48	19.0	3.0	3.0	24
15.0	1.0	1.0	24	19.0	5.0	3.0	48
15.0	3.0	1.0	48	19.0	7.0	3.0	48
15.0	5.0	1.0	48	19.0	5.0	5.0	24
15.0	7.0	1.0	48				
15.0	9.0	1.0	48				

TABLE II (a)

COULOMB COUPLING COEFFICIENTS
OF THE FORM c $(\alpha\alpha\varkappa\varkappa')$

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
0.0	0.0	0.0	-8.3776	4.1888	4.1888	8.3776	-4.1888	-4.1888
1.0	1.0	1.0	.0000	.0000	.0000	.0000	.0000	.0000
2.0	.0	.0	-8.2846	4.1423	4.1423	8.5351	-4.2676	-4.2676
2.0	2.0	.0	-2.0470	-2.0470	4.0940	2.1740	2.1740	-4.3479
2.0	2.0	2.0	.0000	.0000	.0000	.0000	.0000	.0000
3.0	1.0	1.0	-5.9078	2.9539	2.9539	6.4051	-3.2026	-3.2026
3.0	3.0	1.0	-1.6676	-1.6676	3.3353	1.9231	1.9231	-3.8462
3.0	3.0	3.0	.0000	.0000	.0000	.0000	.0000	.0000
4.0	.0	.0	-8.0132	4.0066	4.0066	8.9937	-4.4969	-4.4969
4.0	2.0	.0	-5.5427	1.5897	3.9530	6.4048	-1.8228	-4.5820
4.0	4.0	.0	-1.8981	-1.8981	3.7963	2.4151	2.4151	-4.8302
4.0	2.0	2.0	-3.9118	1.9559	1.9559	4.6022	-2.3261	-2.3261
4.0	4.0	2.0	-1.2499	-1.2499	2.4998	1.6350	1.6350	-3.[illegible]
4.0	4.0	4.0	.0000	.0000	.0000	.0000	.0000	.0000
5.0	1.0	1.0	-6.9066	3.4533	3.4533	8.3560	-4.1780	-4.[illegible]
5.0	3.0	1.0	-4.3285	.8823	3.4462	5.5497	-1.0902	-4.[illegible]
5.0	5.0	1.0	-1.6702	-1.6702	3.3403	2.4539	2.4539	-4.9077
5.0	3.0	3.0	-2.7471	1.3736	1.3736	3.7266	-1.8633	-1.8633
5.0	5.0	3.0	-.9373	-.9373	1.8746	1.4530	1.4530	-2.[illegible]
5.0	5.0	5.0	.0000	.0000	.0000	.0000	.0000	.0000
6.0	.0	.0	-7.5855	3.7928	3.7928	9.7125	-4.8563	-4.[illegible]
6.0	2.0	.0	-5.3668	2.6362	3.7306	8.3840	-3.4349	-4.9492
6.0	4.0	.0	-3.8684	.3196	3.5487	5.5654	-.3652	-5.2[illegible]
6.0	6.0	.0	-1.6304	-1.6304	3.2607	2.8235	2.8235	-5.[illegible]
6.0	2.0	2.0	-5.3783	2.6891	2.6891	7.2825	-3.6412	-3.6412
6.0	4.0	2.0	-3.2918	.5374	2.7545	4.8659	-.7111	-4.[illegible]
6.0	6.0	2.0	-1.3530	-1.3530	2.7061	2.4071	2.4071	-4.8142
6.0	4.0	4.0	-1.9985	.9993	.9993	3.2131	-1.6065	-1.6065
6.0	6.0	4.0	-.6987	-.6987	1.3975	1.3453	1.3453	-2.6[illegible]
6.0	6.0	6.0	.0000	.0000	.0000	.0000	.0000	.0000
7.0	1.0	1.0	-6.8486	3.4243	3.4243	9.6220	-4.8110	-4.8110
7.0	3.0	1.0	-5.2811	1.9567	3.3244	7.8467	-2.8692	-5.[illegible]
7.0	5.0	1.0	-3.1906	.0779	3.1128	5.3573	.0964	-5.4[illegible]
7.0	7.0	1.0	-1.3958	-1.3958	2.7915	3.0061	3.0061	-6.0122
7.0	3.0	3.0	-4.1115	2.0557	2.0557	6.4562	-3.2281	-3.2281
7.0	5.0	3.0	-2.4893	.3593	2.1300	4.4097	-.4512	-3.9[illegible]
7.0	7.0	3.0	-1.0403	-1.0403	2.0806	2.3671	2.3671	-4.734[illegible]
7.0	5.0	5.0	-1.4664	.7332	.7332	2.9119	-1.4560	-1.[illegible]
7.0	7.0	5.0	-.5066	-.5066	1.0132	1.2843	1.2843	-2.[illegible]
7.0	7.0	7.0	.0000	.0000	.0000	.0000	.0000	.0000
8.0	.0	.0	-7.0381	3.5190	3.5190	10.6263	-5.3131	-5.313[illegible]
8.0	2.0	.0	-6.3295	2.8838	3.4457	9.8198	-4.4036	-5.41[illegible]
8.0	4.0	.0	-4.6463	1.4155	3.2308	7.8509	-2.1335	-5.71[illegible]
8.0	6.0	.0	-2.7837	-.1057	2.8894	5.5382	.6548	-6.1[illegible]
8.0	8.0	.0	-1.2238	-1.2238	2.4476	3.4018	3.4018	-6.8037
8.0	2.0	2.0	-5.7047	2.8524	2.8524	9.0941	-4.5471	[illegible]

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
8.0	[illegible]	[illegible]	[illegible]	1.4550	[illegible]	7.2992	[illegible]	-4.9450
8.0	6.0	[illegible]	[illegible]	.0037	[illegible]	[illegible]	[illegible]	[illegible]
8.0	[illegible]	[illegible]	-1.0898	1.0890	[illegible]	[illegible]	[illegible]	[illegible]
8.0	4.0	[illegible]	-3.1189	1.5590	[illegible]	[illegible]	[illegible]	[illegible]
8.0	6.0	4.0	-1.8550	.2627	[illegible]	[illegible]	[illegible]	[illegible]
8.0	8.0	4.0	-.7498	-.7498	[illegible]	[illegible]	[illegible]	[illegible]
8.0	6.0	6.0	[illegible]	.8275	[illegible]	[illegible]	[illegible]	-1.3644
8.0	8.0	6.0	.3433	-.3433	[illegible]	[illegible]	[illegible]	[illegible]
8.0	8.0	8.0	.0000	.0000	[illegible]	.0000	[illegible]	.0000
9.0	1.0	1.0	[illegible]	3.2223	[illegible]	10.7947	[illegible]	-6.3974
9.0	3.0	1.0	[illegible]	2.3413	[illegible]	[illegible]	[illegible]	[illegible]
9.0	5.0	1.0	-3.8517	1.0578	[illegible]	[illegible]	-1.6111	[illegible]
9.0	7.0	1.0	-2.2641	-.1208	[illegible]	[illegible]	[illegible]	[illegible]
9.0	9.0	1.0	-.9404	-.9404	[illegible]	[illegible]	[illegible]	[illegible]
9.0	3.0	3.0	[illegible]	2.2874	[illegible]	[illegible]	[illegible]	[illegible]
9.0	5.0	3.0	[illegible]	1.1150	[illegible]	[illegible]	[illegible]	[illegible]
9.0	7.0	3.0	[illegible]	.0156	1.8919	[illegible]	[illegible]	[illegible]
9.0	9.0	3.0	-.7622	-.7622	1.5244	3.2168	3.2168	[illegible]
9.0	5.0	5.0	[illegible]	1.1619	1.1619	[illegible]	-2.7544	[illegible]
9.0	7.0	5.0	-1.3316	.2092	1.1224	[illegible]	[illegible]	[illegible]
9.0	9.0	5.0	-.4799	-.4799	.9599	[illegible]	2.3557	-4.7114
9.0	7.0	7.0	[illegible]	.3584	.3584	[illegible]	[illegible]	[illegible]
9.0	9.0	7.0	-.1976	-.1976	.3952	[illegible]	1.2395	[illegible]
9.0	9.0	9.0	.0000	.0000	.0000	[illegible]	.0000	.0000
10.0	.0	.0	[illegible]	3.2099	3.2099	11.6497	[illegible]	[illegible]
10.0	2.0	.0	[illegible]	2.8337	3.1236	[illegible]	[illegible]	[illegible]
10.0	4.0	.0	[illegible]	1.9000	2.8702	[illegible]	[illegible]	[illegible]
10.0	6.0	.0	[illegible]	.8165	2.4665	[illegible]	[illegible]	[illegible]
10.0	8.0	.0	[illegible]	-.0866	1.9419	[illegible]	[illegible]	[illegible]
10.0	10.0	.0	-.6692	-.6692	1.3384	[illegible]	[illegible]	[illegible]
10.0	2.0	2.0	[illegible]	2.7661	2.7661	[illegible]	[illegible]	[illegible]
10.0	4.0	2.0	[illegible]	1.8749	2.5612	[illegible]	[illegible]	[illegible]
10.0	6.0	2.0	[illegible]	.8338	2.2198	[illegible]	-1.1972	[illegible]
10.0	8.0	2.0	-1.7175	-.0391	1.7565	[illegible]	[illegible]	[illegible]
10.0	10.0	2.0	-.6026	-.6026	1.2052	[illegible]	[illegible]	[illegible]
10.0	4.0	4.0	[illegible]	1.7827	1.7827	[illegible]	[illegible]	[illegible]
10.0	6.0	4.0	[illegible]	.8582	[illegible]	[illegible]	[illegible]	[illegible]
10.0	8.0	4.0	[illegible]	.0733	[illegible]	[illegible]	[illegible]	[illegible]
10.0	10.0	4.0	[illegible]	-.4310	[illegible]	[illegible]	[illegible]	[illegible]
10.0	6.0	6.0	[illegible]	.8303	[illegible]	[illegible]	[illegible]	[illegible]
10.0	8.0	6.0	-.8789	.1799	[illegible]	[illegible]	[illegible]	[illegible]
10.0	10.0	6.0	-.2243	-.2243	.4485	[illegible]	[illegible]	[illegible]
10.0	8.0	8.0	-.4196	.2098	.2098	[illegible]	[illegible]	[illegible]
10.0	10.0	8.0	-.0613	-.0613	.1226	[illegible]	[illegible]	[illegible]
10.0	10.0	10.0	.0000	.0000	.0000	[illegible]	[illegible]	[illegible]
11.0	1.0	1.0	[illegible]	2.9527	2.9527	[illegible]	[illegible]	[illegible]
11.0	3.0	1.0	-5.1814	2.4069	[illegible]	[illegible]	[illegible]	[illegible]
11.0	5.0	1.0	-3.9822	1.5549	2.4273	[illegible]	[illegible]	[illegible]
11.0	7.0	1.0	-2.6320	.6996	1.9324	[illegible]	[illegible]	[illegible]
11.0	9.0	1.0	[illegible]	.0481	1.3253	[illegible]	[illegible]	[illegible]

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
11.0	11.0	1.0	-.3284	-.3284	.6568	4.5093	4.5093	-9.0187
11.0	3.0	3.0	-4.5501	2.2750	2.2750	10.2713	-5.1356	-5.1356
11.0	5.0	3.0	-3.4966	1.4906	2.0059	8.9089	-3.2296	-5.6793
11.0	7.0	3.0	-2.2995	.6989	1.6006	7.2780	-.8524	-6.4255
11.0	9.0	3.0	-1.1755	.0978	1.0776	5.6301	1.6781	-7.3081
11.0	11.0	3.0	-.2388	-.2388	.4776	4.1255	4.1255	-8.2509
11.0	5.0	5.0	-2.6772	1.3386	1.3386	7.7404	-3.8702	-3.8702
11.0	7.0	5.0	-1.7345	.6619	1.0725	6.3035	-1.5682	-4.7352
11.0	9.0	5.0	-.8422	.1568	.6854	4.8078	.9342	-5.7420
11.0	11.0	5.0	-.0998	-.0998	.1997	3.4023	3.4023	-6.8046
11.0	7.0	7.0	-1.0817	.5408	.5408	5.0641	-2.5321	-2.5321
11.0	9.0	7.0	-.4689	.1654	.3035	3.7239	-.0734	-3.6505
11.0	11.0	7.0	.0250	.0250	-.0500	2.4147	2.4147	-4.8295
11.0	9.0	9.0	-.1447	.0724	.0724	2.5007	-1.2504	-1.2504
12.0	.0	.0	-5.7894	2.8947	2.8947	12.6846	-6.3423	-6.3423
12.0	2.0	.0	-5.4581	2.6634	2.7947	12.2862	-5.8165	-6.4698
12.0	4.0	.0	-4.5685	2.0677	2.5008	11.2005	-4.3570	-6.8435
12.0	6.0	.0	-3.3642	1.3328	2.0314	9.6867	-2.2497	-7.4371
12.0	8.0	.0	-2.0964	.6777	1.4187	8.0219	.1840	-8.2059
12.0	10.0	.0	-.9405	.2298	.7106	6.4161	2.6708	-9.0870
12.0	12.0	.0	.0149	.0149	-.0298	5.0000	5.0000	-10.0001
12.0	2.0	2.0	-5.1462	2.5731	2.5731	11.9049	-5.9525	-5.9525
12.0	4.0	2.0	-4.3065	2.0015	2.3050	10.8626	-4.5132	-6.3494
12.0	6.0	2.0	-3.1661	1.2956	1.8705	9.4018	-2.4264	-6.9754
12.0	8.0	2.0	-1.9616	.6676	1.2940	7.7850	-.0045	-7.7805
12.0	10.0	2.0	-.8606	.2435	.6171	6.2153	2.4825	-8.6978
12.0	12.0	2.0	.0501	.0501	-.1003	4.8227	4.8227	-9.6453
12.0	4.0	4.0	-3.5978	1.7989	1.7989	9.9313	-4.9656	-4.9656
12.0	6.0	4.0	-2.6274	1.1732	1.4542	8.6072	-2.9365	-5.6707
12.0	8.0	4.0	-1.5943	.6221	.9722	7.1154	-.5493	-6.5662
12.0	10.0	4.0	-.6457	.2672	.3784	5.6400	1.9368	-7.5767
12.0	12.0	4.0	.1386	.1386	-.2772	4.3075	4.3075	-8.6151
12.0	6.0	6.0	-1.8839	.9419	.9419	7.4536	-3.7268	-3.7268
12.0	8.0	6.0	-1.0882	.5045	.5837	6.1193	-1.3946	-4.7248
12.0	10.0	6.0	-.3594	.2572	.1022	4.7616	1.0856	-5.8472
12.0	12.0	6.0	.2342	.2342	-.4683	3.5005	3.5005	-7.0011
12.0	8.0	8.0	-.5533	.2766	.2766	4.9298	-2.4649	-2.4649
12.0	10.0	8.0	-.0805	.1610	-.0805	3.6749	.0000	-3.6749
13.0	1.0	1.0	-5.3430	2.6715	2.6715	12.9980	-6.4990	-6.4990
13.0	3.0	1.0	-4.7919	2.3285	2.4634	12.3292	-5.5621	-6.7671
13.0	5.0	1.0	-3.8325	1.7738	2.0586	11.1435	-3.8586	-7.2850
13.0	7.0	1.0	-2.6738	1.1920	1.4818	9.6686	-1.6532	-8.0154
13.0	9.0	1.0	-1.5066	.7332	.7734	8.1218	.7802	-8.9020
13.0	11.0	1.0	-.4607	.4695	-.0089	6.6671	3.2022	-9.8693
13.0	13.0	1.0	.3953	.3953	-.7906	5.4126	5.4126	-10.8253
13.0	3.0	3.0	-4.2934	2.1467	2.1467	11.7055	-5.8527	-5.8527
13.0	5.0	3.0	-3.4223	1.6350	1.7873	10.5931	-4.1819	-6.4112
13.0	7.0	3.0	-2.3654	1.1017	1.2637	9.1974	-2.0033	-7.1940
13.0	9.0	3.0	-1.2965	.6913	.6052	7.7191	.4204	-8.1395
13.0	11.0	3.0	-.3365	.4753	-.1388	6.3149	2.8535	-9.1684

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
13.0	13.0	3.0	.4488	.4488	-.8977	5.0927	5.0927	-10.1858
13.0	5.0	5.0	-2.7016	1.3508	1.3508	9.6008	-4.8004	-4.8004
13.0	7.0	5.0	-1.8216	.9044	.9171	8.3356	-2.6727	-5.6629
13.0	9.0	5.0	-.9276	.5833	.3443	6.9706	-.2694	-6.7012
13.0	11.0	5.0	-.1252	.4586	-.3333	5.6488	2.1327	-7.8316
13.0	7.0	7.0	-1.1561	.5780	.5780	7.2134	-3.6067	-3.6067
13.0	9.0	7.0	-.4832	.3721	.1110	5.9712	-1.2367	-4.7345
14.0	.0	.0	-5.2099	2.6050	2.6050	13.6281	-6.8141	-6.8141
14.0	2.0	.0	-4.9522	2.4601	2.4921	13.3192	-6.3658	-6.9534
14.0	4.0	.0	-4.2400	2.0802	2.1598	12.4577	-5.0952	-7.3625
14.0	6.0	.0	-3.2264	1.5986	1.6278	11.2088	-3.1945	-8.0142
14.0	8.0	.0	-2.0910	1.1599	.9311	9.7718	-.9102	-8.8616
14.0	10.0	.0	-.9860	.8636	.1224	8.3257	1.5113	-9.8370
14.0	12.0	.0	-.0146	.7418	-.7272	7.0054	3.8477	-10.8531
14.0	14.0	.0	.7656	.7656	-1.5311	5.9035	5.9035	-11.8071
14.0	2.0	2.0	-4.7055	2.3527	2.3527	13.0199	-6.5099	-6.5099
14.0	4.0	2.0	-4.0232	1.9877	2.0355	12.1837	-5.2510	-6.9327
14.0	6.0	2.0	-3.0505	1.5265	1.5240	10.9680	-3.3632	-7.6048
14.0	8.0	2.0	-1.9588	1.1106	.8482	9.5642	-1.0866	-8.4776
14.0	10.0	2.0	-.8949	.8386	.0563	8.1458	1.3363	-9.4821
14.0	12.0	2.0	.0410	.7420	-.7830	6.6459	3.8833	-10.5292
14.0	14.0	2.0	.7925	.7925	-1.5850	5.7571	5.7571	-11.5142
14.0	4.0	4.0	-3.4220	1.7110	1.7110	11.4148	-5.7074	-5.7074
14.0	6.0	4.0	-2.5612	1.3060	1.2552	10.2876	-3.8366	-6.4510
14.0	8.0	4.0	-1.5911	.9543	.6368	8.9727	-1.6030	-7.3697
14.0	10.0	4.0	-.6428	.7519	-.1091	7.6286	.8222	-8.4508
14.0	12.0	4.0	.1916	.7311	-.9226	6.3824	3.2002	-9.5826
14.0	6.0	6.0	-1.8578	.9289	.9289	9.2784	-4.6392	-4.6392
14.0	8.0	6.0	-1.0625	.6695	.3929	8.0812	-2.4251	-5.6562
14.0	10.0	6.0	-.2858	.5715	-.2858	6.8347	.0000	-6.8347
14.0	8.0	8.0	-.4683	.2342	.2342	7.0011	-3.5005	-3.5005
15.0	1.0	1.0	-4.8406	2.4203	2.4203	13.8946	-6.9473	-6.9473
15.0	3.0	1.0	-4.3891	2.2022	2.1869	13.3558	-6.1195	-7.2363
15.0	5.0	1.0	-3.5777	1.8451	1.7326	12.3766	-4.5808	-7.7958
15.0	7.0	1.0	-2.5516	1.4675	1.0841	11.1167	-2.5286	-8.5882
15.0	9.0	1.0	-1.4621	1.1765	.2857	9.7475	-.1928	-9.5547
15.0	11.0	1.0	-.4329	1.0319	-.5990	8.4180	2.1967	-10.6148
15.0	13.0	1.0	.4511	1.0353	-1.4863	7.2424	4.4257	-11.6681
15.0	3.0	3.0	-3.9702	1.9851	1.9851	12.8446	-6.4223	-6.4223
15.0	5.0	3.0	-3.2156	1.6569	1.5587	11.9131	-4.9046	-7.0085
15.0	7.0	3.0	-2.2590	1.3169	.9421	10.7063	-2.8697	-7.8366
15.0	9.0	3.0	-1.2408	1.0700	.1708	9.3914	-.5306	-8.8608
15.0	11.0	3.0	-.2774	.9757	-.6983	8.1051	1.8639	-9.9690
15.0	5.0	5.0	-2.5615	1.2807	1.2807	11.0625	-5.5313	-5.5313
15.0	7.0	5.0	-1.7292	1.0070	.7222	9.9527	-3.5319	-6.4208
15.0	9.0	5.0	-.8407	.8399	.0008	8.7259	-1.2129	-7.5130
15.0	7.0	7.0	-1.0537	.5268	.5268	8.9538	-4.4769	-4.4769
16.0	.0	.0	-4.7427	2.3713	2.3713	14.3837	-7.1919	-7.1919
16.0	2.0	.0	-4.5259	2.2780	2.2478	14.1295	-6.7884	-7.3411
16.0	4.0	.0	-3.9162	2.0323	1.8839	[illegible]	[illegible]	-7.7797

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
16.0	6.0	.0	-3.0204	1.7206	1.2999	12.3435	-3.8637	-8.4798
16.0	8.0	.0	-1.9759	1.4428	.5330	11.0802	-1.6875	-9.3927
16.0	10.0	.0	-.9146	1.2746	-.3600	9.7728	.6748	-10.4476
16.0	12.0	.0	.0577	1.2440	-1.3017	8.5502	3.0007	-11.5510
16.0	14.0	.0	.8675	1.3286	-2.1961	7.5109	5.0800	-12.5910
16.0	2.0	2.0	-4.3161	2.1580	2.1580	13.8814	-6.9407	-6.9407
16.0	4.0	2.0	-3.7258	1.9223	1.8035	13.1794	-5.7910	-7.3884
16.0	6.0	2.0	-2.8578	1.6257	1.2321	12.1357	-4.0322	-8.1035
16.0	8.0	2.0	-1.8444	1.3675	.4769	10.8977	-1.8606	-9.0370
16.0	10.0	2.0	-.8137	1.2229	-.4092	9.6135	.5046	-10.1181
16.0	12.0	2.0	.1312	1.2199	-1.3511	8.4098	2.8424	-11.2522
16.0	4.0	4.0	-3.1894	1.5947	1.5947	12.5236	-6.2618	-6.2618
16.0	6.0	4.0	-2.3986	1.3395	1.0591	11.5441	-4.5289	-7.0152
16.0	8.0	4.0	-1.4727	1.1353	.3374	10.3754	-2.3724	-8.0031
16.0	10.0	4.0	-.5289	1.0579	-.5289	9.1549	.0000	-9.1549
16.0	6.0	6.0	-1.7196	.8598	.8598	10.6544	-5.3272	-5.3272
16.0	8.0	6.0	-.9226	.7311	.1916	9.5826	-3.2003	-6.3824
17.0	1.0	1.0	-4.4649	2.2324	2.2324	14.5462	-7.2731	-7.2731
17.0	3.0	1.0	-4.0679	2.0875	1.9804	14.0854	-6.5072	-7.5781
17.0	5.0	1.0	-3.3405	1.8513	1.4892	13.2360	-5.0661	-8.1698
17.0	7.0	1.0	-2.3945	1.6074	.7871	12.1208	-3.1109	-9.0099
17.0	9.0	1.0	-1.3568	1.4362	-.0794	10.8820	-.8441	-10.0379
17.0	11.0	1.0	-.3434	1.3854	-1.0420	9.6546	1.5151	-11.1697
17.0	3.0	3.0	-3.6931	1.8465	1.8465	13.6445	-6.8222	-6.8222
17.0	5.0	3.0	-3.0054	1.6315	1.3739	12.8303	-5.3962	-7.4341
17.0	7.0	3.0	-2.1097	1.4184	.6913	11.7585	-3.4531	-8.3054
17.0	9.0	3.0	-1.1252	1.2876	-.1624	10.5641	-1.1875	-9.3767
17.0	5.0	5.0	-2.3895	1.1947	1.1947	12.0786	-6.0393	-6.0393
17.0	7.0	5.0	-1.5849	1.0345	.5504	11.0841	-4.1234	-6.9607
18.0	.0	.0	-4.4392	2.2196	2.2196	14.8722	-7.4361	-7.4361
18.0	2.0	.0	-4.2431	2.1540	2.0891	14.6479	-7.0560	-7.5918
18.0	4.0	.0	-3.6862	1.9821	1.7041	14.0091	-5.9591	-8.0500
18.0	6.0	.0	-2.8534	1.7678	1.0857	13.0484	-4.2662	-8.7822
18.0	8.0	.0	-1.8601	1.5879	.2722	11.8930	-2.1540	-9.7390
18.0	10.0	.0	-.8258	1.5031	-.6773	10.6779	.1692	-10.8472
18.0	12.0	.0	.1445	1.5364	-1.6809	9.5256	2.4836	-12.0092
18.0	2.0	2.0	-4.0521	2.0260	2.0260	14.4283	-7.2142	-7.2142
18.0	4.0	2.0	-3.5094	1.8616	1.6477	13.8027	-6.1232	-7.6795
18.0	6.0	2.0	-2.6973	1.6596	1.0377	12.8610	-4.4367	-8.4244
18.0	8.0	2.0	-1.7279	1.4972	.2307	11.7273	-2.3274	-9.3999
18.0	10.0	2.0	-.7177	1.4354	-.7177	10.5335	.0000	-10.5334
18.0	4.0	4.0	-3.0066	1.5033	1.5033	13.2139	-6.6069	-6.6069
18.0	6.0	4.0	-2.2529	1.3345	.9184	12.3254	-4.9410	-7.3844
18.0	8.0	4.0	-1.3511	1.2199	.1312	11.2523	-2.8424	-8.4098
18.0	6.0	6.0	-1.5850	.7925	.7925	11.5142	-5.7571	-5.7571
19.0	1.0	1.0	-4.2642	2.1321	2.1321	14.8893	-7.4446	-7.4446
19.0	3.0	1.0	-3.8912	2.0212	1.8701	14.4654	-6.7070	-7.7584
19.0	5.0	1.0	-3.2016	1.8424	1.3592	13.6789	-5.3113	-8.3676
19.0	7.0	1.0	-2.2927	1.6645	.6283	12.6364	-3.4028	-9.2337
19.0	9.0	1.0	-1.2799	1.5550	-.2750	11.4662	-1.1710	-10.2952

p_x	p_y	p_z	c(xx11)	c(yy11)	c(zz11)	c(xx12)	c(yy12)	c(zz12)
19.0	3.0	3.0	-3.5359	1.7680	1.7680	14.0584	-7.0292	-7.0292
19.0	5.0	3.0	-2.8783	1.6069	1.2714	13.3023	-5.6462	-7.6561
19.0	7.0	3.0	-2.0105	1.4564	.5541	12.2986	-3.7476	-8.5509
19.0	5.0	5.0	-2.2791	1.1395	1.1395	12.6013	-6.3007	-6.3007
20.0	.0	.0	-4.3340	2.1670	2.1670	15.0411	-7.5205	-7.5205
20.0	2.0	.0	-4.1442	2.1102	2.0340	14.8264	-7.1478	-7.6786
20.0	4.0	.0	-3.6035	1.9619	1.6417	14.2135	-6.0699	-8.1435
20.0	6.0	.0	-2.7904	1.7793	1.0112	13.2879	-4.4008	-8.8871
20.0	8.0	.0	-1.8134	1.6321	.1813	12.1691	-2.3097	-9.8593
20.0	10.0	.0	-.7880	1.5761	-.7880	10.9863	.0000	-10.9862
20.0	2.0	2.0	-3.9589	1.9794	1.9794	14.6160	-7.3080	-7.3080
20.0	4.0	2.0	-3.4308	1.8379	1.5930	14.0153	-6.2356	-7.7797
20.0	6.0	2.0	-2.6363	1.6667	.9696	13.1075	-4.5723	-8.5352
20.0	8.0	2.0	-1.6808	1.5364	.1445	12.0093	-2.4836	-9.5256
20.0	4.0	4.0	-2.9383	1.4692	1.4692	13.4487	-6.7243	-6.7243
20.0	6.0	4.0	-2.1961	1.3286	.8675	12.5910	-5.0800	-7.5109

TABLE II (b)

COULOMB COUPLING COEFFICIENTS OF THE FORM c $(\alpha\alpha'\kappa\kappa')$

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
0.0	0.0	0.0	.0000	.0000	.0000	.0000	.0000	.0000
1.0	1.0	1.0	-4.1746	-4.1746	-4.1746	4.1402	4.1402	4.1402
2.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
2.0	2.0	.0	-6.2246	.0000	.0000	6.0909	.0000	.0000
2.0	2.0	2.0	-4.1335	-4.1335	-4.1335	3.9950	3.9950	3.9950
3.0	1.0	1.0	-3.3836	-3.3836	-1.1299	3.2831	3.2831	1.0931
3.0	3.0	1.0	-5.8187	-1.9455	-1.9455	5.5252	1.8378	1.8378
3.0	3.0	3.0	-4.0695	-4.0695	-4.0695	3.7549	3.7549	3.7549
4.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
4.0	2.0	.0	-4.9052	.0000	.0000	4.6486	.0000	.0000
4.0	4.0	.0	-6.0331	.0000	.0000	5.5403	.0000	.0000
4.0	2.0	2.0	-4.0739	-4.0739	-2.0469	3.8079	3.8079	1.3962
4.0	4.0	2.0	-5.3477	-2.6969	-2.6969	4.8365	2.4030	2.4030
4.0	4.0	4.0	-3.9892	-3.9892	-3.9892	3.4234	3.4234	3.4234
5.0	1.0	1.0	-2.2508	-2.2508	-.4561	2.0925	2.0925	.4146
5.0	3.0	1.0	-5.1525	-1.7269	-1.0481	4.6898	1.5570	.9265
5.0	5.0	1.0	-5.7571	-1.1794	-1.1794	5.0271	.9868	.9868
5.0	3.0	3.0	-4.1742	-4.1742	-2.5396	3.6773	3.6773	2.1835
5.0	5.0	3.0	-4.9604	-3.0321	-3.0321	4.1749	2.4679	2.4679
5.0	5.0	5.0	-3.9004	-3.9004	-3.9004	3.0057	3.0057	3.0057
6.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
6.0	2.0	.0	-3.5774	.0000	.0000	3.2191	.0000	.0000
6.0	4.0	.0	-5.4057	.0000	.0000	4.7174	.0000	.0000
6.0	6.0	.0	-5.6687	.0000	.0000	4.7062	.0000	.0000
6.0	2.0	2.0	-3.2441	-3.2441	-1.1128	2.8722	2.8722	.9371
6.0	4.0	2.0	-5.0100	-2.5376	-1.7308	4.2950	2.1256	1.3919
6.0	6.0	2.0	-5.3649	-1.8744	-1.8744	4.3640	1.3973	1.3973
6.0	4.0	4.0	-4.1145	-4.1145	-2.8187	3.3207	3.3207	2.1643
6.0	6.0	4.0	-4.6331	-3.1961	-3.1961	3.5179	2.2739	2.2739
6.0	6.0	6.0	-3.8120	-3.8120	-3.8120	2.5098	2.5098	2.5098
7.0	1.0	1.0	-1.6103	-1.6103	-.2418	1.4075	1.4075	.1935
7.0	3.0	1.0	-4.1249	-1.3872	-.6239	3.5319	1.1690	.4822
7.0	5.0	1.0	-5.2691	-1.0902	-.8979	4.3327	.8419	.5827
7.0	7.0	1.0	-5.5524	-.8365	-.8365	4.1498	.5447	.5447
7.0	3.0	3.0	-3.6227	-3.6227	-1.6390	2.9842	2.9842	1.2232
7.0	5.0	3.0	-4.7557	-2.9460	-2.1760	3.7454	2.1982	1.5148
7.0	7.0	3.0	-4.9572	-2.3041	-2.3041	3.6557	1.4465	1.4465
7.0	5.0	5.0	-4.0016	-4.0016	-2.9957	2.8453	2.8453	1.9425
7.0	7.0	5.0	-4.3469	-3.2843	-3.2843	2.8491	1.9150	1.9150
7.0	7.0	7.0	-3.7324	-3.7324	-3.7324	1.9464	1.9464	1.9464
8.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
8.0	2.0	.0	-2.6801	.0000	.0000	2.2513	.0000	.0000
8.0	4.0	.0	-4.4649	.0000	.0000	3.6403	.0000	.0000
8.0	6.0	.0	-5.1673	.0000	.0000	4.0132	.0000	.0000
8.0	8.0	.0	-5.0866	.0000	.0000	3.7007	.0000	.0000
8.0	2.0	2.0	-2.5277	-2.5277	-.6898	2.0821	2.0821	.4837

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
8.0	4.0	2.0	-4.2489	-2.1641	-1.1744	3.3913	1.6685	.7756
8.0	6.0	2.0	-4.9694	-1.7513	-1.4013	3.7672	1.1844	.8374
8.0	8.0	2.0	-4.9395	-1.4288	-1.4288	3.4931	.7428	.7428
8.0	4.0	4.0	-3.7201	-3.7201	-2.0391	2.7640	2.7640	1.2566
8.0	6.0	4.0	-4.4710	-3.1116	-2.4896	3.1253	1.9944	1.3955
8.0	8.0	4.0	-4.5611	-2.5914	-2.5914	2.9333	1.2572	1.2572
8.0	6.0	6.0	-3.8729	-3.8729	-3.1256	2.2912	2.2912	1.5725
8.0	8.0	6.0	-4.0932	-3.3421	-3.3421	2.1650	1.4399	1.4399
8.0	8.0	8.0	-3.6695	-3.6695	-3.6695	1.3291	1.3291	1.3291
9.0	1.0	1.0	-1.2022	-1.2022	-.1528	.9728	.9728	.0961
9.0	3.0	1.0	-3.2437	-1.0952	-.4169	2.5730	.8479	.2502
9.0	5.0	1.0	-4.4648	-.9348	-.5862	3.4046	.6520	.3203
9.0	7.0	1.0	-4.8672	-.7781	-.6583	3.5037	.4438	.3120
9.0	9.0	1.0	-4.6797	-.6556	-.6556	3.1312	.2563	.2563
9.0	3.0	3.0	-2.9807	-2.9807	-1.1459	2.2565	2.2565	.6558
9.0	5.0	3.0	-4.1597	-2.5794	-1.6299	3.0121	1.7496	.8473
9.0	7.0	3.0	-4.6038	-2.1803	-1.8523	3.1227	1.1962	.8314
9.0	9.0	3.0	-4.4901	-1.8642	-1.8642	2.8004	.6847	.6847
9.0	5.0	5.0	-3.6828	-3.6828	-2.3611	2.3619	2.3619	1.1088
9.0	7.0	5.0	-4.1836	-3.1958	-2.7368	2.4677	1.6202	1.0980
9.0	9.0	5.0	-4.1851	-2.8039	-2.8039	2.2120	.9031	.9031
9.0	7.0	7.0	-3.7461	-3.7461	-3.2437	1.6823	1.6823	1.0894
9.0	9.0	7.0	-3.8693	-3.3946	-3.3946	1.4715	.8811	.8811
9.0	9.0	9.0	-3.6292	-3.6292	-3.6292	.6742	.6742	.6742
10.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
10.0	2.0	.0	-2.0384	.0000	.0000	1.5783	.0000	.0000
10.0	4.0	.0	-3.5721	.0000	.0000	2.6867	.0000	.0000
10.0	6.0	.0	-4.3886	.0000	.0000	3.1479	.0000	.0000
10.0	8.0	.0	-4.5596	.0000	.0000	3.0672	.0000	.0000
10.0	10.0	.0	-4.2651	.0000	.0000	2.6551	.0000	.0000
10.0	2.0	2.0	-1.9626	-1.9626	-.4827	1.4837	1.4837	.2409
10.0	4.0	2.0	-3.4547	-1.7706	-.8659	2.5323	1.2359	.3965
10.0	6.0	2.0	-4.2697	-1.5379	-1.1022	2.9748	.9117	.4354
10.0	8.0	2.0	-4.4639	-1.3287	-1.1963	2.9029	.5790	.3802
10.0	10.0	2.0	-4.2003	-1.1739	-1.1739	2.5119	.2758	.2758
10.0	4.0	4.0	-3.1543	-3.1543	-1.5677	2.1212	2.1212	.6556
10.0	6.0	4.0	-3.9622	-2.7850	-2.0200	2.5051	1.5701	.7213
10.0	8.0	4.0	-4.2153	-2.4494	-2.2197	2.4477	.9875	.6251
10.0	10.0	4.0	-4.0335	-2.2021	-2.2021	2.1075	.4410	.4410
10.0	6.0	6.0	-3.5791	-3.5791	-2.6454	1.8535	1.8535	.7892
10.0	8.0	6.0	-3.9058	-3.2300	-2.9567	1.7930	1.1361	.6661
10.0	10.0	6.0	-3.8328	-2.9800	-2.9800	1.5056	.4346	.4346
10.0	8.0	8.0	-3.6314	-3.6314	-3.3670	1.0390	1.0390	.5204
10.0	10.0	8.0	-3.6747	-3.4561	-3.4561	.7810	.2655	.2655
10.0	10.0	10.0	-3.6153	-3.6153	-3.6153	.0000	.0000	.0000
11.0	1.0	1.0	-.9073	-.9073	-.1104	.6732	.6732	.0443
11.0	3.0	1.0	-2.5153	-.8530	-.3108	1.8302	.5998	.1162
11.0	5.0	1.0	-3.6142	-.7663	-.4597	2.5301	.4753	.1482
11.0	7.0	1.0	-4.1245	-.6755	-.5462	2.7281	.3293	.1383
11.0	9.0	1.0	-4.1290	-.6005	-.5735	2.5401	.1841	.1002

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
11.0	11.0	1.0	-3.7615	-.5495	-.5495	2.1275	.0525	.0525
11.0	3.0	3.0	-2.3756	-2.3756	-.8778	1.6336	1.6336	.3045
11.0	5.0	3.0	-3.4411	-2.1517	-1.3062	2.2634	1.2967	.3871
11.0	7.0	3.0	-3.9658	-1.9160	-1.5626	2.4426	.6950	.3567
11.0	9.0	3.0	-4.0113	-1.7218	-1.6517	2.2689	.4890	.2489
11.0	11.0	3.0	-3.6905	-1.5921	-1.5921	1.8884	.1149	.1149
11.0	5.0	5.0	-3.1617	-3.1617	-1.9633	1.7977	1.7977	.4856
11.0	7.0	5.0	-3.7098	-2.8671	-2.3768	1.9321	1.2272	.4303
11.0	9.0	5.0	-3.8250	-2.6284	-2.5430	1.7724	.6326	.2670
11.0	11.0	5.0	-3.5858	-2.4791	-2.4791	1.4404	.0679	.0679
11.0	7.0	7.0	-3.4438	-3.4438	-2.9201	1.2853	1.2853	.3407
11.0	9.0	7.0	-3.6437	-3.2414	-3.1733	1.1203	.5843	.1337
11.0	11.0	7.0	-3.5060	-3.1406	-3.1406	.8309	-.1089	-.1089
11.0	9.0	9.0	-3.5341	-3.5341	-3.5083	.3824	.3824	-.1104
12.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
12.0	2.0	.0	-1.5366	.0000	.0000	1.0900	.0000	.0000
12.0	4.0	.0	-2.7697	.0000	.0000	1.9098	.0000	.0000
12.0	6.0	.0	-3.5291	.0000	.0000	2.3224	.0000	.0000
12.0	8.0	.0	-3.8018	.0000	.0000	2.3480	.0000	.0000
12.0	10.0	.0	-3.6690	.0000	.0000	2.0976	.0000	.0000
12.0	12.0	.0	-3.2346	.0000	.0000	1.6976	.0000	.0000
12.0	2.0	2.0	-1.4977	-1.4977	-.3764	1.0321	1.0321	.0967
12.0	4.0	2.0	-2.7068	-1.3961	-.6973	1.8093	.8741	.1527
12.0	6.0	2.0	-3.4621	-1.2677	-.9267	2.2003	.6527	.1497
12.0	8.0	2.0	-3.7464	-1.1478	-1.0528	2.2221	.4065	.0961
12.0	10.0	2.0	-3.6323	-1.0588	-1.0774	1.9796	.1644	.0177
12.0	12.0	2.0	-3.2164	-1.0073	-1.0073	1.5945	-.0554	-.0554
12.0	4.0	4.0	-2.5423	-2.5423	-1.2981	1.5324	1.5324	.2364
12.0	6.0	4.0	-3.2876	-2.3342	-1.7377	1.8599	1.1385	.2184
12.0	8.0	4.0	-3.6035	-2.1421	-1.9900	1.8662	.6920	.1122
12.0	10.0	4.0	-3.5410	-2.0047	-2.0533	1.6410	.2436	-.0365
12.0	12.0	4.0	-3.1767	-1.9344	-1.9344	1.2949	-.1722	-.1722
12.0	6.0	6.0	-3.0688	-3.0688	-2.3504	1.3646	1.3646	.1658
12.0	8.0	6.0	-3.4311	-2.8741	-2.7242	1.3348	.7869	.0066
12.0	10.0	6.0	-3.4441	-2.7506	-2.8462	1.1217	.1677	-.2024
12.0	12.0	6.0	-3.1553	-2.7142	-2.7142	.8227	-.3866	-.3866
12.0	8.0	8.0	-3.2950	-3.2950	-3.2034	.6930	.6930	-.2078
12.0	10.0	8.0	-3.4001	-3.2438	-3.4000	.4703	.0000	-.4703
13.0	1.0	1.0	-.6709	-.6709	-.0891	.4554	.4554	.0136
13.0	3.0	1.0	-1.8682	-.6430	-.2555	1.2575	.4094	.0327
13.0	5.0	1.0	-2.7831	-.5974	-.3902	1.7340	.3275	.0324
13.0	7.0	1.0	-3.2704	-.5482	-.4818	1.9815	.2251	.0110
13.0	9.0	1.0	-3.3664	-.5075	-.5256	1.8969	.1163	-.0227
13.0	11.0	1.0	-3.1398	-.4813	-.5213	1.6255	.0113	-.0591
13.0	13.0	1.0	-2.6694	-.4699	-.4699	1.2630	-.0823	-.0823
13.0	3.0	3.0	-1.8152	-1.8152	-.7341	1.1299	1.1299	.0765
13.0	5.0	3.0	-2.5902	-1.6957	-1.1253	1.6011	.9020	.0671
13.0	7.0	3.0	-3.1840	-1.5680	-1.3954	1.7723	.6138	.0000
13.0	9.0	3.0	-3.3043	-1.4644	-1.5300	1.6851	.3036	-.1036
13.0	11.0	3.0	-3.1079	-1.4018	-1.5250	1.4280	.0000	-.2073

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
13.0	13.0	3.0	-2.6635	-1.3812	-1.3812	1.0925	-.2733	-.2733
13.0	5.0	5.0	-2.5392	-2.5392	-1.7360	1.2700	1.2700	.0275
13.0	7.0	5.0	-3.0469	-2.3814	-2.1707	1.3872	.8435	-.0936
13.0	9.0	5.0	-3.2124	-2.2616	-2.4025	1.2879	.3737	-.2654
13.0	11.0	5.0	-3.0719	-2.2045	-2.4161	1.0504	-.0969	-.4323
13.0	7.0	7.0	-2.9130	-2.9130	-2.7446	.8786	.8786	-.2759
13.0	9.0	7.0	-3.1413	-2.8317	-3.0775	.7475	.3002	-.5200
14.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
14.0	2.0	.0	-1.1107	.0000	.0000	.7238	.0000	.0000
14.0	4.0	.0	-2.0350	.0000	.0000	1.2894	.0000	.0000
14.0	6.0	.0	-2.6514	.0000	.0000	1.6039	.0000	.0000
14.0	8.0	.0	-2.9246	.0000	.0000	1.6606	.0000	.0000
14.0	10.0	.0	-2.8842	.0000	.0000	1.5153	.0000	.0000
14.0	12.0	.0	-2.5887	.0000	.0000	1.2472	.0000	.0000
14.0	14.0	.0	-2.1002	.0000	.0000	.9272	.0000	.0000
14.0	2.0	2.0	-1.0910	-1.0910	-.3217	.6871	.6871	.0057
14.0	4.0	2.0	-2.0026	-1.0390	-.6079	1.2232	.5843	-.0087
14.0	6.0	2.0	-2.6167	-.9725	-.8313	1.5193	.4338	-.0521
14.0	8.0	2.0	-2.8966	-.9111	-.9746	1.5683	.2575	-.1185
14.0	10.0	2.0	-2.8677	-.8635	-1.0284	1.4243	.0748	-.1895
14.0	12.0	2.0	-2.5841	-.8500	-.9878	1.1641	-.0992	-.2410
14.0	14.0	2.0	-2.1042	-.8520	-.8520	.8580	-.2517	-.2517
14.0	4.0	4.0	-1.9177	-1.9177	-1.1528	1.0369	1.0369	-.0528
14.0	6.0	4.0	-2.5269	-1.8106	-1.5842	1.2788	.7611	-.1468
14.0	8.0	4.0	-2.8266	-1.7154	-1.8689	1.3035	.4333	-.2854
14.0	10.0	4.0	-2.8314	-1.6566	-1.9859	1.1596	.0875	-.4264
14.0	12.0	4.0	-2.5821	-1.6434	-1.9213	.9198	-.2478	-.5302
14.0	6.0	6.0	-2.4180	-2.4180	-2.1941	.9172	.9172	-.3114
14.0	8.0	6.0	-2.7512	-2.3316	-2.6142	.8966	.4777	-.5254
14.0	10.0	6.0	-2.8095	-2.2989	-2.8095	.7432	.0000	-.7432
14.0	8.0	8.0	-2.7142	-2.7142	-3.1553	.3866	.3866	-.8227
15.0	1.0	1.0	-.4649	-.4649	-.0784	.2911	.2911	-.0056
15.0	3.0	1.0	-1.3200	-.4512	-.2273	.8108	.2621	-.0208
15.0	5.0	1.0	-1.9754	-.4285	-.3542	1.1679	.2092	-.0454
15.0	7.0	1.0	-2.3641	-.4043	-.4483	1.3209	.1403	-.0791
15.0	9.0	1.0	-2.4784	-.3853	-.5021	1.2871	.0635	-.1168
15.0	11.0	1.0	-2.3495	-.3752	-.5102	1.1195	-.0138	-.1471
15.0	13.0	1.0	-2.0240	-.3745	-.4695	.8795	-.0844	-.1591
15.0	3.0	3.0	-1.2838	-1.2838	-.6600	.7290	.7290	-.0737
15.0	5.0	3.0	-1.9295	-1.2247	-1.0313	1.0465	.5791	-.1521
15.0	7.0	3.0	-2.3228	-1.1629	-1.3100	1.1760	.3822	-.2580
15.0	9.0	3.0	-2.4524	-1.1169	-1.4733	1.1339	.1613	-.3727
15.0	11.0	3.0	-2.3427	-1.0975	-1.5041	.9710	-.0654	-.4644
15.0	5.0	5.0	-1.8561	-1.8561	-1.6194	.8216	.8216	-.2989
15.0	7.0	5.0	-2.2608	-1.7840	-2.0711	.9039	.5212	-.4846
15.0	9.0	5.0	-2.4210	-1.7401	-2.3489	.8414	.1786	-.6321
15.0	7.0	7.0	-2.2108	-2.2108	-2.6750	.5335	.5335	[illegible]
16.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
16.0	2.0	.0	-.7248	.0000	.0000	.4355	.0000	[illegible]
16.0	4.0	.0	-1.3406	.0000	.0000	.7900	[illegible]	[illegible]

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
16.0	6.0	.0	-1.7700	.0000	.0000	.9965	.0000	.0000
16.0	8.0	.0	-1.9812	.0000	.0000	1.0466	.0000	.0000
16.0	10.0	.0	-1.9813	.0000	.0000	.9677	.0000	.0000
16.0	12.0	.0	-1.7998	.0000	.0000	.8049	.0000	.0000
16.0	14.0	.0	-1.4741	.0000	.0000	.6028	.0000	.0000
16.0	2.0	2.0	-.7154	-.7154	-.2945	.4173	.4173	-.0517
16.0	4.0	2.0	-1.3252	-.6908	-.5635	.7495	.3541	-.1133
16.0	6.0	2.0	-1.7539	-.6597	-.7842	.9423	.2590	-.1884
16.0	8.0	2.0	-1.9693	-.6326	-.9382	.9855	.1439	-.2701
16.0	10.0	2.0	-1.9765	-.6171	-1.0104	.9053	.0204	-.3422
16.0	12.0	2.0	-1.8023	-.6163	-.9885	.7463	-.1009	-.3828
16.0	4.0	4.0	-1.2854	-1.2854	-1.0809	.6324	.6324	-.2453
16.0	6.0	4.0	-1.7136	-1.2369	-1.5107	.7867	.4549	-.4025
16.0	8.0	4.0	-1.9421	-1.1982	-1.8176	.8081	.2373	-.5721
16.0	10.0	4.0	-1.9705	-1.1835	-1.9705	.7221	.0000	-.7221
16.0	6.0	6.0	-1.6687	-1.6687	-2.1261	.5474	.5474	-.6520
16.0	8.0	6.0	-1.9213	-1.6434	-2.5820	.5302	.2478	-.9198
17.0	1.0	1.0	-.2744	-.2744	-.0732	.1614	.1614	-.0171
17.0	3.0	1.0	-.7826	-.2683	-.2138	.4517	.1452	-.0534
17.0	5.0	1.0	-1.1816	-.2583	-.3372	.6562	.1150	-.0942
17.0	7.0	1.0	-1.4293	-.2480	-.4332	.7498	.0749	-.1382
17.0	9.0	1.0	-1.5150	-.2408	-.4928	.7380	.0291	-.1794
17.0	11.0	1.0	-1.4508	-.2387	-.5085	.6475	-.0182	-.2082
17.0	3.0	3.0	-.7668	-.7668	-.6249	.4054	.4054	-.1661
17.0	5.0	3.0	-1.1616	-.7412	-.9876	.5860	.3190	-.2920
17.0	7.0	3.0	-1.4128	-.7158	-1.2729	.6638	.2031	-.4274
17.0	9.0	3.0	-1.5074	-.7003	-1.4542	.6447	.0696	-.5547
17.0	5.0	5.0	-1.1315	-1.1315	-1.5677	.4541	.4541	-.5113
17.0	7.0	5.0	-1.3909	-1.1053	-2.0336	.5003	.2745	-.7470
18.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
18.0	2.0	.0	-.3585	.0000	.0000	.2071	.0000	.0000
18.0	4.0	.0	-.6663	.0000	.0000	.3743	.0000	.0000
18.0	6.0	.0	-.8860	.0000	.0000	.4751	.0000	.0000
18.0	8.0	.0	-.9997	.0000	.0000	.5027	.0000	.0000
18.0	10.0	.0	-1.0076	.0000	.0000	.4681	.0000	.0000
18.0	12.0	.0	-.9217	.0000	.0000	.3915	.0000	.0000
18.0	2.0	2.0	-.3548	-.3548	-.2824	.1965	.1965	-.0839
18.0	4.0	2.0	-.6604	-.3453	-.5439	.3545	.1661	-.1731
18.0	6.0	2.0	-.8801	-.3336	-.7643	.4485	.1197	-.2680
18.0	8.0	2.0	-.9959	-.3243	-.9247	.4722	.0625	-.3611
18.0	10.0	2.0	-1.0073	-.3207	-1.0073	.4363	.0000	-.4363
18.0	4.0	4.0	-.6453	-.6453	-1.0499	.2976	.2976	-.3569
18.0	6.0	4.0	-.8658	-.6279	-1.4814	.3715	.2101	-.5529
18.0	8.0	4.0	-.9885	-.6163	-1.8022	.3828	.1009	-.7463
18.0	6.0	6.0	-.8520	-.8520	-2.1042	.2517	.2517	-.8580
19.0	1.0	1.0	-.0908	-.0908	-.0712	.0516	.0516	-.0226
19.0	3.0	1.0	-.2596	-.0891	-.2056	.1448	.0464	-.0690
19.0	5.0	1.0	-.3934	-.0863	-.3307	.2111	.0365	-.1179
19.0	7.0	1.0	-.4782	-.0836	-.4277	.2423	.0233	-.1673
19.0	9.0	1.0	-.5096	-.0820	-.4903	.2396	.0080	-.2110

p_x	p_y	p_z	c(xy11)	c(xz11)	c(yz11)	c(xy12)	c(xz12)	c(yz12)
19.0	3.0	3.0	-.2552	-.2552	-.8113	.1297	.1297	-.2108
19.0	5.0	3.0	-.3881	-.2483	-.9713	.1680	.1014	-.3602
19.0	7.0	3.0	-.4742	-.2418	-1.2604	.2138	.0630	-.5118
19.0	5.0	5.0	-.3803	-.3803	-1.5498	.1444	.1444	-.6167
20.0	.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	2.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	4.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	6.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	8.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	10.0	.0	.0000	.0000	.0000	.0000	.0000	.0000
20.0	2.0	2.0	.0000	.0000	-.2790	.0000	.0000	-.0943
20.0	4.0	2.0	.0000	.0000	-.5385	.0000	.0000	-.1925
20.0	6.0	2.0	.0000	.0000	-.7590	.0000	.0000	-.2943
20.0	8.0	2.0	.0000	.0000	-.9216	.0000	.0000	-.3915
20.0	4.0	4.0	.0000	.0000	-1.0416	.0000	.0000	-.3936
20.0	6.0	4.0	.0000	.0000	-1.4741	.0000	.0000	-.6028

Table III. Input Data for Calculations

	Compressibility (10^{-12}dynes/cm^2) β	Effective Charge e^*/e	Lattice Constant (10^{-8} cm) r_o	Crystal Polarizabilities (10^{-24} (cm)^3) α^+	α^-
NaCl	4.27	0.74	2.814	0.255	2.974
KCl	5.63	0.80	3.139	1.20	2.97

For the RI model, we need only β and r_o. For the DD model, we need as well e^*/e, the effective charge ratio, and α^+ and α^-, the crystal polarizabilities of the two ions involved. The short-range coupling coefficients are computed with eqs. (1.19a) and (1.20a). To form the dynamical matrix, eq. (1.25a) is used for the RI model, and eq. (1.5b) for the DD model.

The dynamical matrix has been taken in the following form:

$$\begin{pmatrix} \{xx11\} & \{xy11\} & \{xz11\} & \{xx12\} & \{xy12\} & \{xz12\} \\ \{xy11\} & \{yy11\} & \{yz11\} & \{xy12\} & \{yy12\} & \{yz12\} \\ \{xz11\} & \{yz11\} & \{zz11\} & \{xz12\} & \{yz12\} & \{zz12\} \\ \{xx12\} & \{xy12\} & \{xz12\} & \{xx22\} & \{xy22\} & \{xz22\} \\ \{xy12\} & \{yy12\} & \{yz12\} & \{xy22\} & \{yy22\} & \{yz22\} \\ \{xz12\} & \{yz12\} & \{zz12\} & \{xz22\} & \{yz22\} & \{zz22\} \end{pmatrix}$$

Once we have the dynamical matrix on either model, our next step is to find the matrix $\underline{\underline{S}}$ which diagonalises the dynamical matrix to give the diagonal matrix $\underline{\underline{\omega}}^2$. Diagonalization has been performed on the CDC-3600 computer at Michigan State University, with an adaptation of 704-709 Fortran program number 664, 00-OP ID: F4 UCSD 1 EIGEN. This subroutine is based on the Jacobi method to diagonalize real symmetric matrices. In this method the largest off-diagonal element is selected, and rotation is performed on the dynamical matrix so that that element becomes zero. This process is repeated successively till all the off-diagonal elements are smaller than a chosen limit. At the same time, the matrices which perform the rotation are multiplied together to give the final diagonalizing matrix $\underline{\underline{S}}$. Thus in the end we get both the eigenvalues ω^2 and the eigenvector matrix $\underline{\underline{S}}$, with each column of $\underline{\underline{S}}$ representing the eigenvector corresponding to its appropriate eigenvalue.

We have done calculations with our subdivision of $\underline{k}$-space as well as Kellermann's. His subdivision amounts to considering 48 points in the first zone in $\underline{k}$-space. These 48 points generate in all 1000 points by symmetry operations in the NaCl structure. In order to give examples of the eigenvectors and to illustrate their application in classification of normal modes, we give in this section the results for Kellermann's subdivision for the rigid-ion model.

To see what typical eigenvectors look like, we have chosen two wavevectors for NaCl, one in a direction of symmetry and the other in a general direction, and have presented the corresponding eigenvectors in Table IV and Table V, respectively. These eigenvectors, when normalized through division by $(NM_{\varkappa})^{\frac{1}{2}}$, give the amplitudes of vibration for the two kinds of ions in a given mode. Each column gives the eigenvectors for a given mode (whose frequency is indicated at the top), the first three elements corresponding to the Cartesian components of displacement of one kind of ion, and the last three of those of the other.

For all the NaCl eigenvectors we have computed the ratio of the amplitudes of vibration for the two kinds of ions. We have calculated also the angle (Na, Cl) between the directions of motion for the two kinds of ions, and the angles (Na, $\underline{k}$) and (Cl, $\underline{k}$) between the directions of motion for each kind of ion and the direction of propagation of the wave. The results are given in Table VI.

For $\underline{k} = \underline{0}$, the ratio of the amplitudes of lighter to heavier atom is inversely proportional to their masses, in the optical branch; in general it increases with increasing $\underline{k}$. The corresponding ratio in the acoustical branch is equal to unity; it decreases with increasing $\underline{k}$. Then, by continuity, we can classify the normal modes into various branches, and state their character as to longitudinality, transversality, or neither. The results for NaCl are shown in Table VI. We see that for $\underline{k}$ along [100], [110], and [111], the waves are purely transverse or longitudinal, and the direction of vibration of both kinds of ions is the same, as is apparent from the symmetry of the crystal structure. Also, in certain directions of somewhat lower symmetry, viz., either when one of the components of wavevector is zero, or when two components are equal, there exists a pair of transverse waves, one optical and one acoustic. In all other cases, the waves are neither transverse nor longitudinal, and the directions of vibrations of two ions are different.

C. Impurity Modes

A substitutional impurity in an otherwise perfect lattice changes the normal mode of vibration. The new modes are of two kinds, in-band modes, and out-of-band or local modes. An in-band mode corresponds to a frequency which is shifted up or down from the frequency of perfect lattice by no more than the separation of consecutive frequencies on either side. Out-of-band or local mode frequencies lie in gaps or regions forbidden in the perfect lattice.

The impurity modes of concern here are the local modes which lie above the longitudinal optical branch, and which are optically active.

They have been observed experimentally by infrared absorption in alkali halides containing U-centers. We consider a substitutional impurity for a Cl^- ion in NaCl and KCl. Examination of eq. (2.8) shows that it has solutions for $\omega(f) > \omega_L$, the largest frequency of the perfect lattice, for positive values of ϵ_{Cl} which are above a certain critical value ϵ critical. To solve eq. (2.8) for these modes, one needs to know the eigenvectors and eigenfrequencies of the perfect lattice. These were obtained as indicated in part B. We have solved eq. (2.8) numerically in the case of NaCl and KCl for the values of ϵ_{Cl} lying between 0 and 1 with proper consideration of the weight of each point in k-space. Weights for Kellermann's subdivision of k-space are given in Table IX (Appendix B). We have solved this equation on both 10 and 20-fold subdivisions of k-space; the results are essentially the same. The frequencies of local mode vs ϵ_{Cl} for NaCl and KCl are shown in Figs. 1 and 2 respectively. On the graphs are shown also the experimental findings (42) for U-centers, and results of theoretical calculations by others (39, 40) who treated U-centers as isotopic impurities.

Knowledge of the frequency of the local mode has been used in eq. (2.9) to find the amplitude of the impurity atom in that mode. Results for the amplitude of vibration of the impurity atom in a local mode, as a function of ϵ_{Cl}, for NaCl and KCl are shown in Figs. 3 and 4 respectively.

With respect to our own results, we note first from Figs. 1 and 2 that the RI model gives somewhat higher frequencies for the local modes than the DD model, as would be expected. Next we see that there are critical values of ϵ_{Cl} for local modes to occur above the longitudinal optical branch in both crystals. Table VII gives the results from our calculations for the frequencies of local modes, and their ratio, corresponding to ϵ_{Cl} equal to 0.972 and 0.943, the values for H^- and D^-, respectively. It contains as well the experimental results for the absorption frequencies observed for H^- and D^- in NaCl and KCl. The ratio given by our calculations is about the same as that of Wallis and Maradudin (40), i.e., $\sim\sqrt{2}$. It is seen that experimental values are far lower than the calculated values on both models and for both crystals. On the other hand, the experimental ratio, available only for KCl, does agree quite well with the theory.

Amplitude of vibration of impurity atom, given by Figs. 3 and 4, increases with the decrease of mass of the impurity as expected.

Since the DD model gives good results for the perfect lattice, the poor agreement between our results and the experimental findings for U-centers indicates that the U-center cannot be treated as a simple isotopic impurity. The changes in force constants, polarization, and effective charge are large enough to have significant effect on the frequencies of defect modes. Unfortunately it would be extremely complicated to take these changes into account.

Table IV NaCl lattice-vibration eigenvectors for wave propagation along the symmetry direction [10,0,0]/10

j		1	2	3	4	5	6
ω_j (10^{13}/sec)		4.198	3.099	3.093	3.093	1.776	1.776
Na^+	w_x	-0.9284	-0.3716	0	0	0	0
	w_y	0	0	-0.8435	0	0	-0.5372
	w_z	0	0	0	-0.8435	-0.5372	0
Cl^-	w_x	0.3716	-0.9284	0	0	0	0
	w_y	0	0	0.5372	0	0	-0.8435
	w_z	0	0	0	0.5372	-0.8435	0

Table V. NaCl lattice-vibration eigenvectors for wave propagation along the non-symmetry direction [9,5,1]/10

j		1	2	3	4	5	6
ω_j (10^{13}/sec)		3.596	3.356	2.896	2.882	2.596	2.229
Na^+	w_x	-0.6435	-0.7022	-0.0052	-0.2421	-0.1651	-0.0830
	w_y	-0.4145	0	0	0.7465	0.5206	0
	w_z	-0.6435	-0.7022	0.0052	-0.2421	-0.1652	-0.0830
Cl^-	w_x	-0.0024	-0.0291	-0.6641	-0.4035	0.5807	0.2902
	w_y	0	0.1101	-0.4125	0	0	-0.9044
	w_z	-0.0032	-0.0291	-0.6441	0.4034	-0.5807	0.2902

Table VI. Properties of lattice-vibration eigenvectors for NaCl on rigid-ion model.

Wavevector p_x	p_y	p_z	Eigenfreq. ω_j (10^{12}/sec)	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
10	4	0	36.27	0	21.80	21.80	11.49		o
			32.83	0	90.00	90.00	4.060	t	o
			29.46	0	68.20	68.20	4.391		o
			29.06	0	21.80	21.80	0.134		a
			25.24	0	90.00	90.00	0.380	t	a
			22.81	0	68.20	68.20	0.351		a
10	2	2	38.78	0	15.79	15.79	4.564		o
			32.54	0	74.21	74.21	3.447		o
			30.13	0	15.79	15.79	0.338		a
			29.36	0	90.00	90.00	2.097	t	o
			24.49	0	74.21	74.21	0.447		a
			18.24	0	90.00	90.00	0.735	t	a

Wavevector			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
p_x	p_y	p_z	$\omega_j(10^{12}/\text{sec})$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
10	2	0	40.32	0	11.31	11.31	3.645		o
			31.34	0	90.00	90.00	2.192	t	o
			30.59	0	11.31	11.31	0.423		a
			30.55	0	78.69	78.69	2.181		o
			20.16	0	90.00	90.00	0.703	t	a
			19.58	0	78.69	78.69	0.707		a
10	0	0	41.98	0	0	0	3.102	ℓ	o
			30.99	0	0	0	0.497	ℓ	a
			30.93	0	90.00	90.00	1.950	t	o
			30.93	0	90.00	90.00	1.950	t	o
			17.76	0	90.00	90.00	0.791	t	a
			17.76	0	90.00	90.00	0.791	t	a
9	5	1	35.96	82.98	34.67	63.24	313.8		o
			33.56	90.00	56.85	77.69	10.49		o
			28.96	89.98	56.87	34.70	0.009		a
			28.82	90.00	81.12	56.84	1.787		o
			25.96	90.00	80.72	56.85	0.863		a
			22.29	90.00	56.85	80.93	0.147		a

Wavevector			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
P_x	P_y	P_z	$\omega_j (10^{12}/sec)$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
9	3	3	37.86	21.01	16.08	4.926	10.35		o
			33.21	65.04	74.82	40.14	6.629		o
			30.21	57.03	40.97	16.06	0.256		a
			27.50	0	90.00	90.00	2.421	t	o
			26.58	30.95	75.56	73.49	0.107		a
			18.75	0	90.00	90.00	0.637	t	a
9	3	1	38.96	7.621	4.838	4.252	3.986		o
			32.10	28.66	87.49	66.87	3.217		o
			30.16	73.33	65.58	11.45	0.771		a
			29.00	57.28	75.86	47.39	1.586		o
			24.16	12.06	80.25	84.22	0.426		a
			19.84	28.00	80.46	81.99	0.650		a
9	1	1	41.67	2.728	2.806	0.077	3.010		o
			31.27	48.61	82.17	49.22	1.810		o
			30.47	0	90.00	90.00	1.963	t	o
			30.47	56.53	37.97	18.55	0.642		a
			19.58	0.922	82.88	83.80	0.726		a
			17.66	0	90.00	90.00	0.785	t	a

Wavevector P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
8	6	0	35.22	0	90.00	90.00	75.68	t	o
			35.20	29.45	0.982	28.47	13.76		o
			28.65	70.43	85.25	14.81	0.816		a
			28.36	0	90.00	90.00	0.020	t	a
			27.47	55.62	84.40	28.78	1.391		o
			20.36	3.466	85.33	88.80	0.521		a
8	4	2	39.72	8.703	15.15	7.555	4.926		o
			31.73	81.64	86.20	15.63	1.573		o
			30.62	78.09	58.50	22.18	1.050		a
			27.61	69.73	88.98	79.13	1.965		o
			24.28	68.15	84.27	73.89	0.538		a
			19.73	11.04	78.98	83.60	0.530		a
8	4	0	39.35	7.961	0.233	8.194	3.188		o
			32.37	0	90.00	90.00	3.350	t	o
			29.79	50.38	52.94	2.555	0.793		a
			26.92	68.55	81.39	30.06	2.469		o
			24.25	0	90.00	90.00	0.460	t	a
			21.61	20.49	63.44	83.93	0.266		a

Wavevector P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
8	2	2	41.77	3.462	4.503	7.964	2.724		o
			30.91	70.08	72.90	37.02	2.268		o
			29.62	64.25	51.55	12.70	0.777		a
			29.17	0	90.00	90.00	2.026	t	o
			22.99	5.586	83.14	88.72	0.461		a
			17.52	0	90.00	90.00	0.761	t	a
8	2	0	42.56	4.076	0.471	4.547	2.538		o
			31.07	0	90.00	90.00	2.086	t	o
			29.99	81.83	61.39	20.43	0.812		a
			28.15	76.94	65.98	37.08	1.573		o
			19.21	0	90.00	90.00	0.739	t	a
			16.92	2.185	80.75	82.93	0.769		a
8	0	0	43.83	0	0	0	2.422	ℓ	o
			30.69	0	90.00	90.00	1.890	t	o
			30.69	0	90.00	90.00	1.890	t	o
			29.89	0	0	0	0.637	ℓ	a
			16.85	0	90.00	90.00	0.816	t	a
			16.85	0	90.00	90.00	0.816	t	a

Wavevector			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*
P_x	P_y	P_z	$\omega_j (10^{12}/\mathrm{sec})$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.	
7	7	1	37.95	21.32	42.48	63.79	9.764	o
			33.29	70.16	46.45	23.71	6.438	o
			30.25	57.94	80.03	42.04	0.273	a
			27.39	0	90.00	90.00	2.440	t o
			26.66	39.85	84.15	48.26	0.094	a
			18.74	0	90.00	90.00	0.632	t a
7	5	3	42.27	89.99	18.11	71.93	19.73	o
			34.24	90.00	71.91	18.09	0.268	a
			28.14	90.00	71.91	48.52	4.024	o
			25.81	90.00	88.98	71.91	2.339	o
			21.52	90.00	82.81	71.91	0.667	a
			19.63	90.00	71.91	87.75	0.264	a
7	5	1	40.41	7.310	11.27	6.298	3.246	o
			32.31	59.77	86.36	28.34	3.105	o
			30.02	53.20	30.12	24.93	0.587	a
			26.31	64.45	86.03	80.97	1.969	o
			23.99	64.02	77.93	68.61	0.892	a
			20.39	37.36	71.55	89.26	0.207	a

Wavevector P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
7	3	3	43.25	2.898	10.44	7.539	2.983		o
			31.75	21.93	34.65	12.72	0.564		a
			28.37	70.71	75.90	33.40	7.279		o
			27.22	o	90.00	90.00	2.241	t	o
			22.87	29.44	48.07	77.51	0.085		a
			17.78	0	90.00	90.00	0.688	t	a
7	3	1	43.95	2.669	5.195	7.084	2.252		o
			30.73	7.707	85.81	86.96	2.373		o
			29.14	41.62	36.55	5.404	0.889		a
			27.21	49.09	82.62	51.66	2.002		o
			21.55	13.97	88.17	88.46	0.514		a
			18.30	4.836	82.04	84.54	0.670		a
7	1	1	45.63	1.787	2.577	4.364	2.092		o
			30.21	26.72	79.85	73.43	1.998		o
			30.05	0	90.00	90.00	1.855	t	o
			28.29	27.07	15.65	11.42	0.728		a
			17.66	1.329	84.82	86.15	0.780		a
			15.98	0	90.00	90.00	0.831	t	a

Wavevector P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
6	6	2	41.73	17.71	16.57	1.135	5.401		o
			33.29	61.31	77.42	16.11	0.560		a
			29.61	49.79	70.07	60.14	2.347		o
			25.29	0	90.00	90.00	3.862	t	o
			22.90	10.24	57.56	67.80	0.414		a
			19.33	0	90.00	90.00	0.399	t	a
6	6	0	40.46	0	0	0	2.742	ℓ	o
			33.04	0	90.00	90.00	5.030	t	o
			28.94	0	0	0	0.562	ℓ	a
			25.85	0	90.00	90.00	0.306	t	a
			25.38	0	90.00	90.00	4.235	t	o
			19.59	0	90.00	90.00	0.364	t	a
6	4	4	44.72	7.856	8.237	0.382	4.985		o
			35.05	20.98	30.90	9.919	0.330		a
			25.35	62.39	80.29	17.89	11.41		o
			25.09	0	90.00	90.00	3.177	t	o
			20.43	37.69	61.40	80.91	0.078		a
			18.62	0	90.00	90.00	0.485	t	a

Wavevector P_x	P_y	P_z	Eigenfreq. $\omega_j (10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
6	4	2	45.23	2.353	6.416	4.769	2.326		o
			30.54	53.03	50.96	5.045	0.942		a
			29.24	54.68	70.72	54.62	1.699		o
			25.15	36.65	85.74	88.02	5.956		o
			20.70	40.34	75.57	79.58	0.424		a
			19.25	19.86	80.70	86.08	0.504		a
6	4	0	45.40	1.490	2.464	3.955	2.043		o
			31.35	0	90.00	90.00	2.400	t	o
			27.71	23.04	23.22	0.188	0.835		a
			24.93	39.82	85.65	54.52	3.327		o
			21.29	0	90.00	90.00	0.642	t	a
			19.34	8.484	78.93	87.41	0.367		a
6	2	2	47.67	0.635	5.556	6.190	1.955		o
			28.67	0	90.00	90.00	1.875	t	o
			28.28	37.18	75.06	67.76	2.304		o
			27.43	34.10	27.52	6.589	0.830		a
			19.37	1.645	89.42	87.77	0.629		a
			15.53	0	90.00	90.00	0.822	t	a

Wavevector			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
P_x	P_y	P_z	$\omega_j(10^{12}/\text{sec})$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
6	2	0	48.11	1.397	3.150	4.547	1.880		o
			30.41	0	90.00	90.00	1.875	t	o
			28.31	28.51	78.30	73.19	2.008		o
			26.25	28.41	14.55	13.86	0.794		a
			16.47	0	90.00	90.00	0.822	t	a
			16.22	1.724	83.03	84.76	0.794		a
6	0	0	48.74	0	0	0	1.856	ℓ	o
			30.10	0	90.00	90.00	1.762	t	o
			30.10	0	90.00	90.00	1.762	t	o
			25.93	0	0	0	0.831	ℓ	a
			14.24	0	90.00	90.00	0.875	t	a
			14.24	0	90.00	90.00	0.875	t	a
5	5	5	45.22		0	—	∞	ℓ	o
			36.42		—	0	0	ℓ	a
			23.97		90.00	—	∞	t	o
			23.97		90.00	—	∞	t	o
			19.30		—	90.00	0	t	a
			19.30		—	90.00	0	t	a

Wavevector P_x	P_y	P_z	Eigenfreq. ω_j (10^{12}/sec)	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
5	5	3	45.92	4.137	6.676	2.542	2.935		o
			33.60	16.50	25.21	8.716	0.551		a
			26.72	15.27	81.46	83.27	2.599		o
			24.04	0	90.00	90.00	12.34	t	o
			19.27	0	90.00	90.00	0.125	t	a
			19.13	3.459	74.64	79.09	0.568		a
5	5	1	46.07	1.903	4.576	2.673	2.074		o
			30.82	28.78	87.56	63.66	2.444		o
			28.36	28.04	8.049	19.99	0.727		a
			24.12	0	90.00	90.00	7.603	t	o
			20.88	3.429	73.76	77.19	0.647		a
			19.19	0	90.00	90.00	0.203	t	a
5	3	3	49.08	0.726	4.521	3.795	2.023		o
			29.48	8.670	14.38	5.706	0.773		a
			26.81	0	90.00	90.00	2.024	t	o
			25.71	11.66	83.13	85.21	2.780		o
			18.60	2.068	80.81	82.88	0.543		a
			16.09	0	90.00	90.00	0.762	t	a

Wavevector			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*
P_x	P_y	P_z	$\omega_j (10^{12}/sec)$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.	
5	3	1	50.08	0.628	3.483	3.729	1.805	o
			29.77	4.104	88.97	85.32	1.915	o
			26.04	43.19	74.93	61.89	2.070	o
			25.25	40.72	27.33	15.20	0.894	a
			17.45	4.820	88.05	87.62	0.712	a
			15.74	3.104	83.74	84.99	0.798	a
5	1	1	51.43	0.280	2.341	2.621	1.737	o
			30.23	0	90.00	90.00	1.647	t o
			28.28	3.133	86.58	89.71	1.908	o
			23.35	3.361	1.020	2.340	0.885	a
			15.68	0.629	88.30	88.93	0.811	a
			10.77	0	90.00	90.00	0.936	t a
4	4	4	48.59	0	0	0	2.291	ℓ o
			32.17	0	0	0	0.673	ℓ a
			24.97	0	90.00	90.00	2.650	t o
			24.97	0	90.00	90.00	2.650	t o
			17.66	0	89.97	89.97	0.582	t a
			17.66	0	90.00	90.00	0.582	t a

Wavevectors			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
P_x	P_y	P_z	$\omega_j (10^{12}/\text{sec})$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
4	4	2	50.66	0.845	3.146	2.301	1.861		o
			28.29	31.57	83.56	64.87	1.935		o
			27.06	31.24	13.51	17.73	0.834		a
			24.90	0	90.00	90.00	2.382	t	o
			16.84	0	90.00	90.00	0.647	t	a
			16.21	1.091	80.72	81.81	0.792		a
4	4	0	50.93	0	0	0	1.757	ℓ	o
			30.35	0	90.00	90.00	1.907	t	o
			24.88	0	90.00	90.00	2.293	t	o
			23.92	0	0	0	0.877	ℓ	a
			16.89	0	90.00	90.00	0.809	t	a
			16.48	0	90.00	90.00	0.673	t	a
4	2	2	53.45	0.047	2.761	2.807	1.704		o
			28.10	0	90.00	90.00	1.736	t	o
			27.04	0.675	87.00	87.68	1.869		o
			22.62	0.719	2.547	1.828	0.905		a
			14.57	0.116	88.02	87.90	0.825		a
			12.72	0	90.00	90.00	0.888	t	a

Wavevectors P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/\text{sec})$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
4	2	0	53.93	0.338	1.949	2.287	1.662		o
			29.65	0	90.00	90.00	1.700	t	o
			27.31	3.136	86.85	89.99	1.762		o
			20.40	3.428	2.428	5.856	0.921		a
			12.70	0.689	84.87	85.56	0.882		a
			12.42	0	90.00	90.00	0.907	t	a
4	0	0	54.38	0	0	0	1.642	ℓ	o
			29.40	0	90.00	90.00	1.642	t	o
			29.40	0	90.00	90.00	1.642	t	o
			18.98	0	0	0	0.939	ℓ	a
			10.27	0	90.00	90.00	0.939	t	a
			10.27	0	90.00	90.00	0.939	t	a
3	3	3	53.34	0	0	0	1.751	ℓ	o
			26.47	0	90.00	90.00	1.867	t	o
			26.47	0	90.00	90.00	1.867	t	o
			24.78	0	0	0	0.881	ℓ	a
			14.23	0	90.00	90.00	0.826	t	a
			14.23	0	89.97	89.97	0.826	t	a

Wavevectors P_x	P_y	P_z	Eigenfreq. $\omega_j(10^{12}/sec)$	Angle (degrees) (Na, Cl)	(Na, k)	(Cl, k)	Na/Cl Mod. Ampl. Rat.	Class.*	
3	3	1	54.84	0.156	1.176	1.020	1.654		o
			29.03	0.899	89.20	88.30	1.706		o
			26.27	0	90.00	90.00	1.790	t	o
			20.10	0.973	3.233	4.206	0.931		a
			12.96	0	90.00	90.00	0.862	t	a
			12.32	0.214	86.02	86.21	0.904		a
3	1	1	56.69	0.115	1.426	1.541	1.602		o
			28.77	0	90.00	90.00	1.617	t	o
			28.28	0.693	88.28	88.97	1.638		o
			15.94	0.783	2.578	3.361	0.961		a
			9.642	0.211	86.80	87.01	0.942		a
			8.886	0	90.00	90.00	0.954	t	a
2	2	2	57.08	0	0	0	1.608	ℓ	o
			27.66	0	90.00	90.00	1.649	t	o
			27.66	0	90.00	90.00	1.649	t	o
			16.71	0	0	0	0.959	ℓ	a
			9.948	0	90.00	90.00	0.935	t	a
			9.948	0	90.00	90.00	0.935	t	a

Wavevectors			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
P_x	P_y	P_z	$\omega_j (10^{12}/sec)$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
2	2	0	57.86	0	0	0	1.582	ℓ	o
			29.07	0	90.00	90.00	1.597	t	o
			27.49	0	90.00	90.00	1.618	t	o
			13.45	0	0	0	0.975	ℓ	a
			8.537	0	90.00	90.00	0.953	t	a
			7.844	0	90.00	90.00	0.965	t	a
2	0	0	58.69	0	0	0	1.563	ℓ	o
			28.85	0	90.00	90.00	1.567	t	o
			28.85	0	90.00	90.00	1.567	t	o
			10.13	0	0	0	0.986	ℓ	a
			5.376	0	90.00	90.00	0.984	t	a
			5.376	0	90.00	90.00	0.984	t	a
1	1	1	59.43	0	0	0	1.556	ℓ	o
			28.38	0	90.00	90.00	1.565	t	o
			28.38	0	89.99	89.99	1.565	t	o
			8.396	0	0	0	0.991	ℓ	a
			5.109	0	89.96	89.96	0.985	t	a
			5.109	0	90.00	90.00	0.985	t	a

Wavevectors			Eigenfreq.	Angle (degrees)			Na/Cl Mod.	Class.*	
P_x	P_y	P_z	$\omega_j(10^{12}/\text{sec})$	(Na, Cl)	(Na, k)	(Cl, k)	Ampl. Rat.		
0	0	0	60.2				1.542	ℓ	o
			28.61				1.542	t	o
			28.61				1.542	t	o
			0				1.000	ℓ	a
			0				1.000	t	a
			0				1.000	t	a

*Classification: o, optical; a, acoustic; t, transverse; ℓ, longitudinal

Table VII. Angular frequencies (in 10^{13} rad/sec) for impurity vibrations in NaCl and KCl.

		Calculated Eigenfrequencies				U-Center Absorption		
		NaCl		KCl			NaCl	KCl
Impurity		RI	DD	RI	DD	Impur-		
Mass	ϵ_{cl}	ω(f)	ω(f)	ω(f)	ω(f)	ity Ion	ω_0	ω_0
1.009	0.972	15.9	15.1	14.2	13.5	H^-	10.52	9.36
2.015	0.943	11.2	10.6	10.1	9.4	D^-	-	6.73
Ratio		1.42	1.42	1.41	1.43			1.39

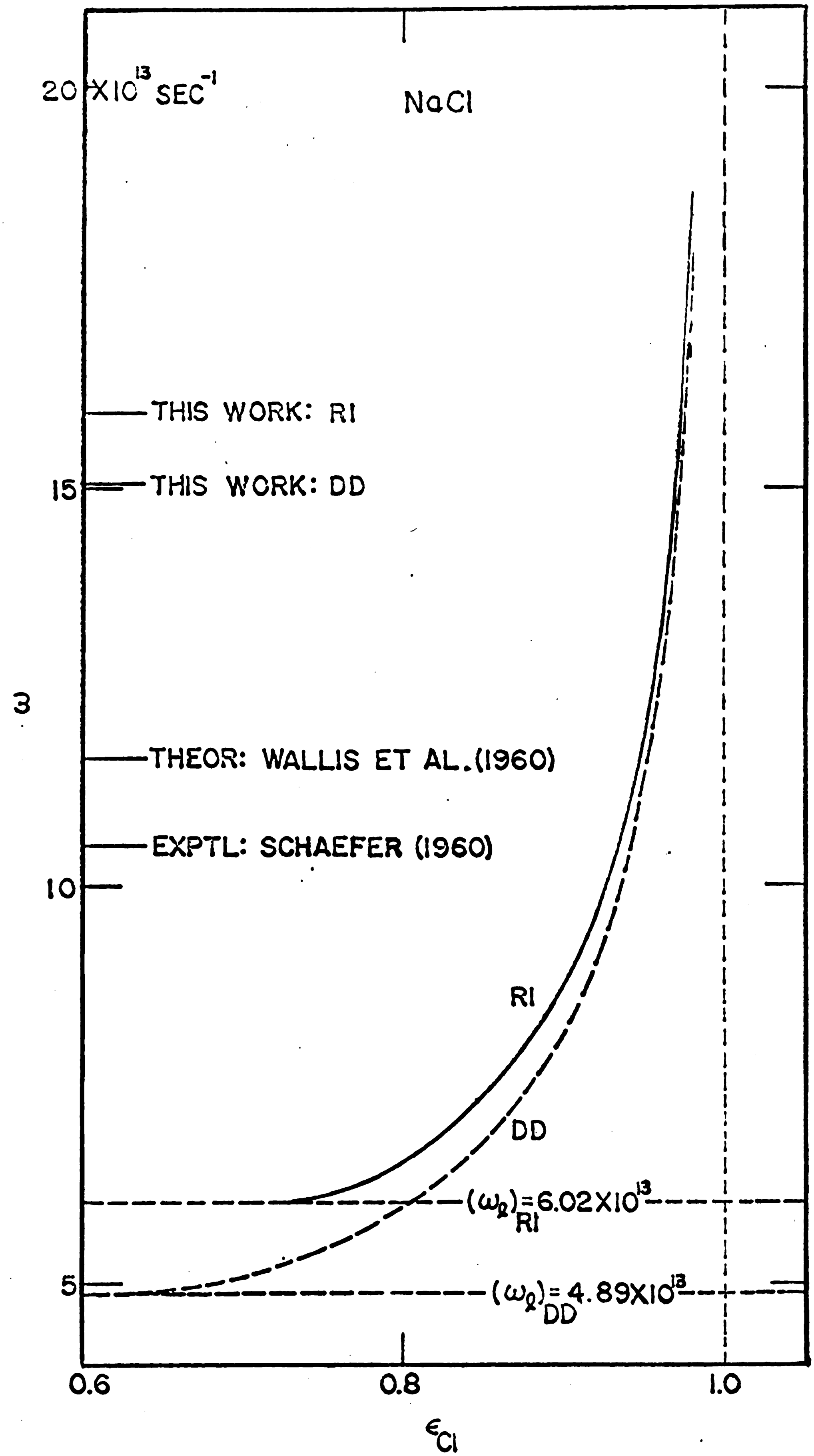

Fig. 1. Frequency of local modes in NaCl as a function of ϵ_{Cl}, on the basis of RI and DD models.

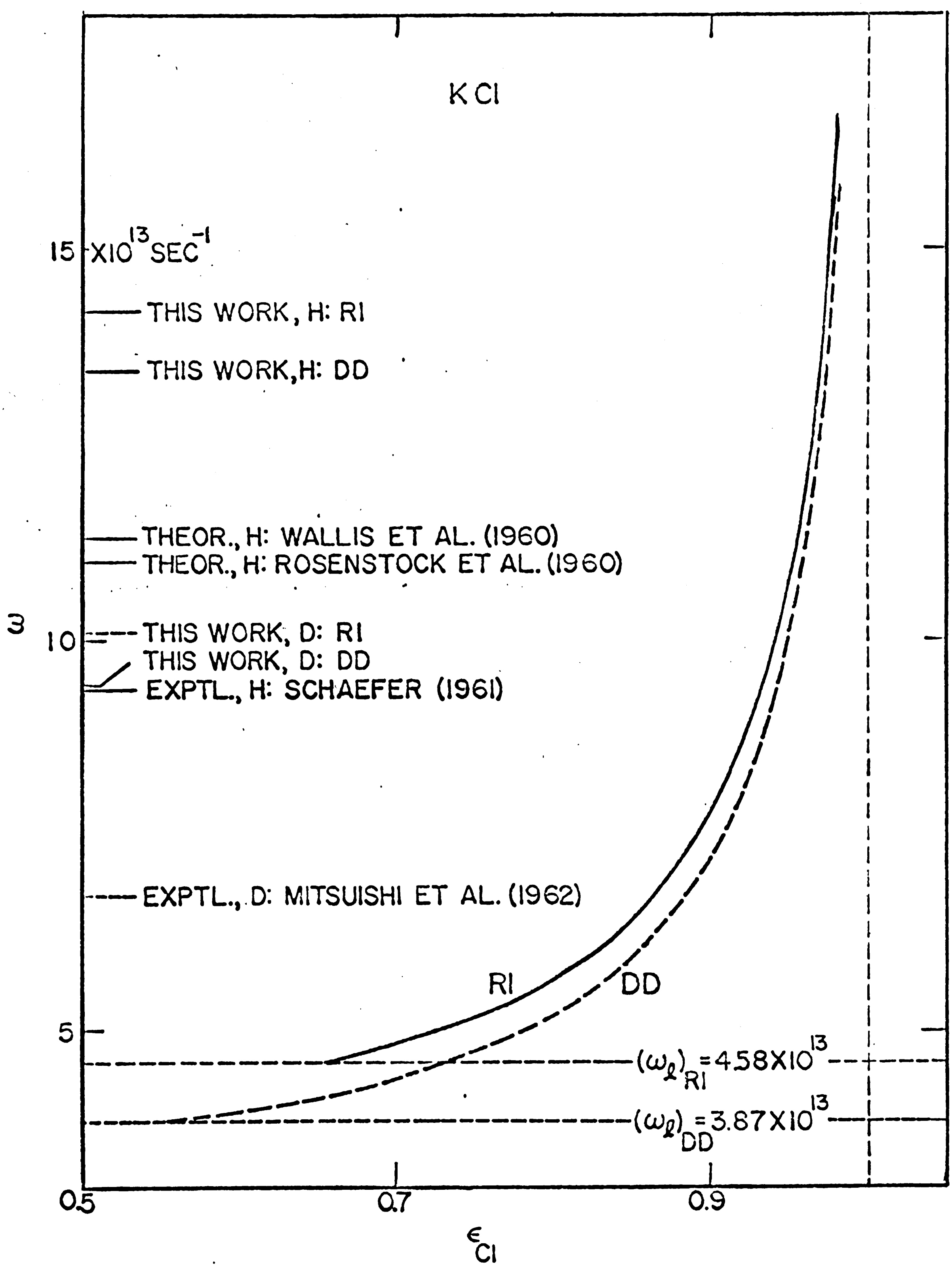

Fig. 2. Frequencies of local modes in KCl as a function of ϵ_{Cl}, on the basis of RI and DD models

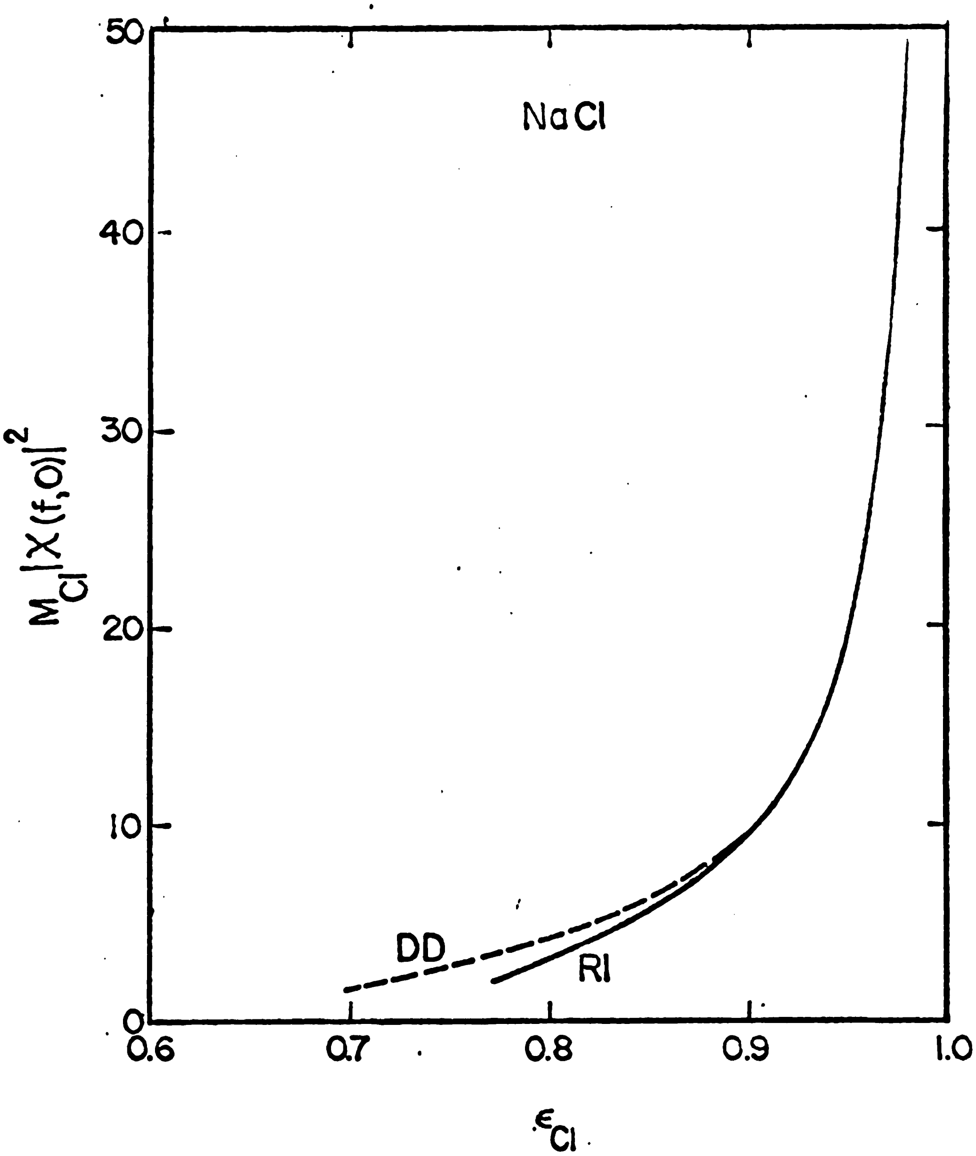

Fig. 3. Amplitude of vibration of impurity atom in NaCl, in terms of $M_{Cl}|\chi(f, 0)|^2$, as a function of ϵ_{Cl}, on the basis of RI and DD models.

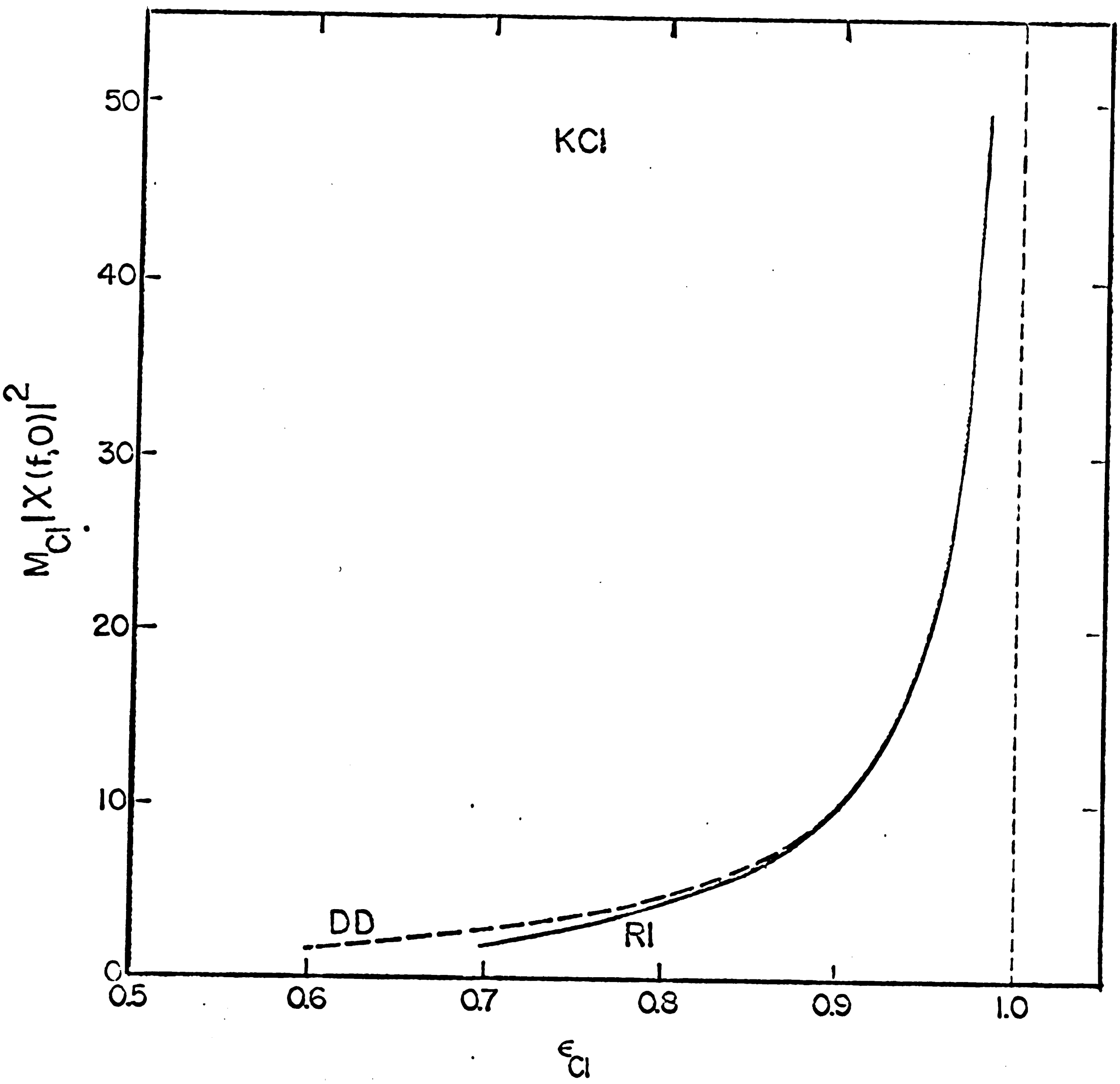

Fig. 4. Amplitude of vibration of impurity atom in KCl, in terms of $M_{Cl} |\chi(f, 0)|^2$, as a function of ϵ_{Cl}, on the basis of RI and DD models.

CHAPTER IV

DISCUSSION

We have seen that for wavevectors directed along axes of symmetry in the perfect rock-salt structure, the lattice vibration waves are either purely transverse or purely longitudinal. For directions of somewhat lower symmetry, viz., when either one component of the wavevector is zero or two of them are equal, there is a pair of transverse waves. But for all other wavevectors, the waves are neither transverse nor longitudinal. We have seen also that when isotopic impurities are introduced in the rock-salt lattice, local modes will appear above the optical branches for mass differences beyond a certain critical value.

From earlier theoretical calculations based on simplified models, it appeared as if U-centers in NaCl and KCl behave quite like isotopic impurities. But evidently it is inadequate to treat them as simple isotopic impurities harmonically coupled to the lattice, without considering changes in force constants, polarization, and effective charge. Unfortunately there is no way to introduce these quantities explicitly. One can, however, take the frequency of the local mode as a known parameter, and make some estimate of the change in short-range force constants between nearest neighbors. One can assume that r_o remains unchanged, and hence that the first derivative of the short-range potential is unchanged from that given by eq. (1.23a). If we assume that there is partial compensation among some of these quantities, and that changes in short-range potential absorb some of them, the only parameter which changes is the quantity A given by eq. (1.24a). With these simplifying assumptions, it is possible to

write a $C_{\alpha\alpha'}\left(\begin{smallmatrix} \ell & \ell' \\ \kappa & \kappa' \end{smallmatrix}\right)$ which would include change in mass and in A. In general this quantity would be a 21x21 matrix, with the only unknown the change in A. Thereby one can find the change in A, and get some idea of the change in force constants produced by the impurity. The computations involved are not prohibitive, but neither are they brief: they are probably worth undertaking.

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Appendix A TABLE VIII

COULOMB COUPLING COEFFICIENTS IN MATRIX FORM

0.0 0.0 0.0

-8.3776	.0000	.0000	8.3776	.0000	.0000
.0000	4.1888	.0000	.0000	-4.1888	.0000
.0000	.0000	4.1888	.0000	.0000	-4.1888
8.3776	.0000	.0000	-8.3776	.0000	.0000
.0000	-4.1888	.0000	.0000	4.1888	.0000
.0000	.0000	-4.1888	.0000	.0000	4.1888

2.0 .0 .0

-8.2846	.0000	.0000	8.5351	.0000	.0000
.0000	4.1423	.0000	.0000	-4.2676	.0000
.0000	.0000	4.1423	.0000	.0000	-4.2676
8.5351	.0000	.0000	-8.2846	.0000	.0000
.0000	-4.2676	.0000	.0000	4.1423	.0000
.0000	.0000	-4.2676	.0000	.0000	4.1423

2.0 2.0 .0

-2.0470	-6.2246	.0000	2.1740	6.0909	.0000
-6.2246	-2.0470	.0000	6.0909	2.1740	.0000
.0000	.0000	4.0940	.0000	.0000	-4.3479
2.1740	6.0909	.0000	-2.0470	-6.2246	.0000
6.0909	2.1740	.0000	-6.2246	-2.0470	.0000
.0000	.0000	-4.3479	.0000	.0000	4.0940

2.0 2.0 2.0

.0000	-4.1335	-4.1335	.0000	3.9950	3.9950
-4.1335	.0000	-4.1335	3.9950	.0000	3.9950
-4.1335	-4.1335	.0000	3.9950	3.9950	.0000
.0000	3.9950	3.9950	.0000	-4.1335	-4.1335
3.9950	.0000	3.9950	-4.1335	.0000	-4.1335
3.9950	3.9950	.0000	-4.1335	-4.1335	.0000

4.0 .0 .0

-8.0132	.0000	.0000	8.9937	.0000	.0000
.0000	4.0066	.0000	.0000	-4.4969	.0000
.0000	.0000	4.0066	.0000	.0000	-4.4969
8.9937	.0000	.0000	-8.0132	.0000	.0000
.0000	-4.4969	.0000	.0000	4.0066	.0000
.0000	.0000	-4.4969	.0000	.0000	4.0066

4.0 2.0 .0

-5.5427	-4.9052	.0000	6.4048	4.6486	.0000
-4.9052	1.5897	.0000	4.6486	-1.8228	.0000
.0000	.0000	3.9530	.0000	.0000	-4.5820
6.4048	4.6485	.0000	-5.5427	-4.9052	.0000
4.6486	-1.8228	.0000	-4.9052	1.5897	.0000
.0000	.0000	-4.5820	.0000	.0000	3.9530

4.0 4.0 .0

-1.8981	-6.0331	.0000	2.4151	5.5403	.0000
-6.0331	-1.8981	.0000	5.5403	2.4151	.0000
.0000	.0000	3.7963	.0000	.0000	-4.8303
2.4151	5.5403	.0000	-1.8981	-6.0331	.0000
5.5403	2.4151	.0000	-6.0331	-1.8981	.0000
.0000	.0000	-4.8303	.0000	.0000	3.7963

[illegible]					
-3.9118	-4.0739	-4.0739	4.6522	3.8079	3.8079
-4.0739	1.9559	-2.0489	3.8079	-2.3261	1.8962
-4.0739	-2.0489	1.9559	3.8079	1.8962	-2.3261
4.6522	3.8079	3.8079	-3.9118	-4.0739	-4.0739
3.8079	-2.3261	1.8962	-4.0739	1.9559	-2.0489
3.8079	1.8962	-2.3261	-4.0739	-2.0489	1.9559
4.0 4.0 2.0					
-1.2499	-5.3477	-2.6969	1.6350	4.8365	2.4030
-5.3477	-1.2499	-2.6969	4.8365	1.6350	2.4030
-2.6969	-2.6969	2.4998	2.4030	2.4030	-3.2701
1.6350	4.8365	2.4030	-1.2499	-5.3477	-2.6969
4.8365	1.6350	2.4030	-5.3477	-1.2499	-2.6969
2.4030	2.4030	-3.2701	-2.6969	-2.6969	2.4998
4.0 4.0 4.0					
.0000	-3.9892	-3.9892	.0000	3.4234	3.4234
-3.9892	.0000	-3.9892	3.4234	.0000	3.4234
-3.9892	-3.9892	.0000	3.4234	3.4234	.0000
.0000	3.4234	3.4234	.0000	-3.9892	-3.9892
3.4234	.0000	3.4234	-3.9892	.0000	-3.9892
3.4234	3.4234	.0000	-3.9892	-3.9892	.0000
6.0 .0 .0					
-7.5855	.0000	.0000	9.7125	.0000	.0000
.0000	3.7928	.0000	.0000	-4.8563	.0000
.0000	.0000	3.7928	.0000	.0000	-4.8563
9.7125	.0000	.0000	-7.5855	.0000	.0000
.0000	-4.8563	.0000	.0000	3.7928	.0000
.0000	.0000	-4.8563	.0000	.0000	3.7928
6.0 2.0 .0					
-6.3668	-3.5774	.0000	8.3840	3.2191	.0000
-3.5774	2.6362	.0000	3.2191	-3.4349	.0000
.0000	.0000	3.7306	.0000	.0000	-4.9492
8.3840	3.2191	.0000	-6.3668	-3.5774	.0000
3.2191	-3.4349	.0000	-3.5774	2.6362	.0000
.0000	.0000	-4.9492	.0000	.0000	3.7306
6.0 4.0 .0					
-3.8684	-5.4057	.0000	5.5654	4.7174	.0000
-5.4057	.3196	.0000	4.7174	-.3452	.0000
.0000	.0000	3.5487	.0000	.0000	-5.2203
5.5654	4.7174	.0000	-3.8684	-5.4057	.0000
4.7174	-.3452	.0000	-5.4057	.3196	.0000
.0000	.0000	-5.2203	.0000	.0000	3.5487
6.0 6.0 .0					
-1.6304	-5.6687	.0000	2.8235	4.7062	.0000
-5.6687	-1.6304	.0000	4.7062	2.8235	.0000
.0000	.0000	3.2607	.0000	.0000	-5.6470
2.8235	4.7062	.0000	-1.6304	-5.6687	.0000
4.7062	2.8235	.0000	-5.6687	-1.6304	.0000
.0000	.0000	-5.6470	.0000	.0000	3.2607

6.0 2.0 2.0

-5.3783	-3.2441	-3.2441	7.2825	2.8722	2.8722
-3.2441	2.6891	-1.1128	2.8722	-3.6412	.9371
-3.2441	-1.1128	2.6891	2.8722	.9371	-3.6412
7.2825	2.8722	2.8722	-5.3783	-3.2441	-3.2441
2.8722	-3.6412	.9371	-3.2441	2.6891	-1.1128
2.8722	.9371	-3.6412	-3.2441	-1.1128	2.6891

6.0 4.0 2.0

-3.2918	-5.0100	-2.5376	4.8659	4.2950	2.1256
-5.0100	.5374	-1.7308	4.2950	-.7111	1.3919
-2.5376	-1.7308	2.7545	2.1256	1.3919	-4.1548
4.8659	4.2950	2.1256	-3.2918	-5.0100	-2.5376
4.2950	-.7111	1.3919	-5.0100	.5374	-1.7308
2.1256	1.3919	-4.1548	-2.5376	-1.7308	2.7545

6.0 6.0 2.0

-1.3530	-5.3649	-1.8744	2.4071	4.3640	1.3973
-5.3649	-1.3530	-1.8744	4.3640	2.4071	1.3973
-1.8744	-1.8744	2.7061	1.3973	1.3973	-4.8142
2.4071	4.3640	1.3973	-1.3530	-5.3649	-1.8744
4.3640	2.4071	1.3973	-5.3649	-1.3530	-1.8744
1.3973	1.3973	-4.8142	-1.8744	-1.8744	2.7061

6.0 4.0 4.0

-1.9985	-4.1145	-4.1145	3.2131	3.3207	3.3207
-4.1145	.9993	-2.8187	3.3207	-1.6065	2.1643
-4.1145	-2.8187	.9993	3.3207	2.1643	-1.6065
3.2131	3.3207	3.3207	-1.9985	-4.1145	-4.1145
3.3207	-1.6065	2.1643	-4.1145	.9993	-2.8187
3.3207	2.1643	-1.6065	-4.1145	-2.8187	.9993

6.0 6.0 4.0

-.6987	-4.6331	-3.1961	1.3453	3.5179	2.2739
-4.6331	-.6987	-3.1961	3.5179	1.3453	2.2739
-3.1961	-3.1961	1.3975	2.2739	2.2739	-2.6907
1.3453	3.5179	2.2739	-.6987	-4.6331	-3.1961
3.5179	1.3453	2.2739	-4.6331	-.6987	-3.1961
2.2739	2.2739	-2.6907	-3.1961	-3.1961	1.3975

6.0 6.0 6.0

.0000	-3.8120	-3.8120	.0000	2.5098	2.5098
-3.8120	.0000	-3.8120	2.5098	.0000	2.5098
-3.8120	-3.8120	.0000	2.5098	2.5098	.0000
.0000	2.5098	2.5098	.0000	-3.8120	-3.8120
2.5098	.0000	2.5098	-3.8120	.0000	-3.8120
2.5098	2.5098	.0000	-3.8120	-3.8120	.0000

8.C .0 .0

-7.0381	.0000	.0000	10.6263	.0000	.0000
.0000	3.5190	.0000	.0000	-5.3131	.0000
.0000	.0000	3.5190	.0000	.0000	-5.3131
10.6263	.0000	.0000	-7.0381	.0000	.0000
.0000	-5.3131	.0000	.0000	3.5190	.0000
.0000	.0000	-5.3131	.0000	.0000	3.5190

8.0 2.0 .0

-6.3295	-2.6801	.0000	9.8198	2.2513	.0000
-2.6801	2.8838	.0000	2.2513	-4.4036	.0000
.0000	.0000	3.4457	.0000	.0000	-5.4162
9.8198	2.2513	.0000	-6.3295	-2.6801	.0000
2.2513	-4.4036	.0000	-2.6801	2.8838	.0000
.0000	.0000	-5.4162	.0000	.0000	3.4457

8.0 4.0 .0

-4.6463	-4.4649	.0000	7.8509	3.6403	.0000
-4.4649	1.4155	.0000	3.6403	-2.1335	.0000
.0000	.0000	3.2308	.0000	.0000	-5.7174
7.8509	3.6403	.0000	-4.6463	-4.4649	.0000
3.6403	-2.1335	.0000	-4.4649	1.4155	.0000
.0000	.0000	-5.7174	.0000	.0000	3.2308

8.0 6.0 .0

-2.7837	-5.1673	.0000	5.5382	4.0132	.0000
-5.1673	-.1057	.0000	4.0132	.6548	.0000
.0000	.0000	2.8894	.0000	.0000	-6.1929
5.5382	4.0132	.0000	-2.7837	-5.1673	.0000
4.0132	.6548	.0000	-5.1673	-.1057	.0000
.0000	.0000	-6.1929	.0000	.0000	2.8894

8.0 8.0 .0

-1.2238	-5.0866	.0000	3.4018	3.7007	.0000
-5.0866	-1.2238	.0000	3.7007	3.4018	.0000
.0000	.0000	2.4476	.0000	.0000	-6.8037
3.4018	3.7007	.0000	-1.2238	-5.0866	.0000
3.7007	3.4018	.0000	-5.0866	-1.2238	.0000
.0000	.0000	-6.8037	.0000	.0000	2.4476

8.0 2.0 2.0

-5.7047	-2.5277	-2.5277	9.0941	2.0821	2.0821
-2.5277	2.8524	-.6898	2.0821	-4.5471	.4837
-2.5277	-.6898	2.8524	2.0821	.4837	-4.5471
9.0941	2.0821	2.0821	-5.7047	-2.5277	-2.5277
2.0821	-4.5471	.4837	-2.5277	2.8524	-.6898
2.0821	.4837	-4.5471	-2.5277	-.6898	2.8524

8.0 4.0 2.0

-4.2049	-4.2489	-2.1641	7.2992	3.3913	1.6685
-4.2489	1.4655	-1.1744	3.3913	-2.3533	.7756
-2.1641	-1.1744	2.7394	1.6685	.7756	-4.9459
7.2992	3.3913	1.6685	-4.2049	-4.2489	-2.1641
3.3913	-2.3533	.7756	-4.2489	1.4655	-1.1744
1.6685	.7756	-4.9459	-2.1641	-1.1744	2.7394

8.0 6.0 2.0

-2.5199	-4.9694	-1.7613	5.1487	3.7672	1.1844
-4.9694	.0037	-1.4013	3.7672	.3848	.8374
-1.7613	-1.4013	2.5162	1.1844	.8374	-5.5335
5.1487	3.7672	1.1844	-2.5199	-4.9694	-1.7613
3.7672	.3848	.8374	-4.9694	.0037	-1.4013
1.1844	.8374	-5.5335	-1.7613	-1.4013	2.5162

8.0 8.0 2.0

-1.0898	-4.9395	-1.4288	3.1215	3.4931	.7428
-4.9395	-1.0898	-1.4288	3.4931	3.1215	.7428
-1.4288	-1.4288	2.1795	.7428	.7428	-6.2430
3.1215	3.4931	.7428	-1.0898	-4.9395	-1.4288
3.4931	3.1215	.7428	-4.9395	-1.0898	-1.4288
.7428	.7428	-6.2430	-1.4288	-1.4288	2.1795

8.0 4.0 4.0

-3.1189	-3.7201	-3.7201	5.8903	2.7640	2.7640
-3.7201	1.5595	-2.0391	2.7640	-2.9452	1.2666
-3.7201	-2.0391	1.5595	2.7640	1.2666	-2.9452
5.8903	2.7640	2.7640	-3.1189	-3.7201	-3.7201
2.7640	-2.9452	1.2666	-3.7201	1.5595	-2.0391
2.7640	1.2666	-2.9452	-3.7201	-2.0391	1.5595

8.0 6.0 4.0

-1.8550	-4.4710	-3.1116	4.1151	3.1253	1.9944
-4.4710	.2627	-2.4896	3.1253	-.3462	1.3955
-3.1116	-2.4896	1.5923	1.9944	1.3955	-3.7689
4.1151	3.1253	1.9944	-1.8550	-4.4710	-3.1116
3.1253	-.3462	1.3955	-4.4710	.2627	-2.4896
1.9944	1.3955	-3.7689	-3.1116	-2.4896	1.5923

8.0 8.0 4.0

-.7498	-4.5611	-2.5914	2.3505	2.9333	1.2572
-4.5611	-.7498	-2.5914	2.9333	2.3505	1.2572
-2.5914	-2.5914	1.4996	1.2572	1.2572	-4.7009
2.3505	2.9333	1.2572	-.7498	-4.5611	-2.5914
2.9333	2.3505	1.2572	-4.5611	-.7498	-2.5914
1.2572	1.2572	-4.7009	-2.5914	-2.5914	1.4996

8.0 6.0 6.0

-1.0559	-3.8729	-3.8729	2.7287	2.2912	2.2912
-3.8729	.5279	-3.1266	2.2912	-1.3644	1.5725
-3.8729	-3.1266	.5279	2.2912	1.5725	-1.3644
2.7287	2.2912	2.2912	-1.0559	-3.8729	-3.8729
2.2912	-1.3644	1.5725	-3.8729	.5279	-3.1266
2.2912	1.5725	-1.3644	-3.8729	-3.1266	.5279

8.0 8.0 6.0

-.3433	-4.0932	-3.3421	1.2524	2.1650	1.4399
-4.0932	-.3433	-3.3421	2.1650	1.2524	1.4399
-3.3421	-3.3421	.6867	1.4399	1.4399	-2.5049
1.2524	2.1650	1.4399	-.3433	-4.0932	-3.3421
2.1650	1.2524	1.4399	-4.0932	-.3433	-3.3421
1.4399	1.4399	-2.5049	-3.3421	-3.3421	.6867

8.0 8.0 8.0

.0000	-3.6695	-3.6695	.0000	1.3291	1.3291
-3.6695	.0000	-3.6695	1.3291	.0000	1.3291
-3.6695	-3.6695	.0000	1.3291	1.3291	.0000
.0000	1.3291	1.3291	.0000	-3.6695	-3.6695
1.3291	.0000	1.3291	-3.6695	.0000	-3.6695
1.3291	1.3291	.0000	-3.6695	-3.6695	.0000

10.0 .0 .0						
	-6.4198	.0000	.0000	11.6497	.0000	.0000
	.0000	3.2099	.0000	.0000	-5.8249	.0000
	.0000	.0000	3.2099	.0000	.0000	-5.8249
	11.6497	.0000	.0000	-6.4198	.0000	.0000
	.0000	-5.8249	.0000	.0000	3.2099	.0000
	.0000	.0000	-5.8249	.0000	.0000	3.2099
10.0 2.0 .0						
	-5.9573	-2.0384	.0000	11.1039	1.5783	.0000
	-2.0384	2.8337	.0000	1.5783	-5.1642	.0000
	.0000	.0000	3.1236	.0000	.0000	-5.9398
	11.1039	1.5783	.0000	-5.9573	-2.0384	.0000
	1.5783	-5.1642	.0000	-2.0384	2.8337	.0000
	.0000	.0000	-5.9398	.0000	.0000	3.1236
10.0 4.0 .0						
	-4.7702	-3.5721	.0000	9.6736	2.6867	.0000
	-3.5721	1.9000	.0000	2.6867	-3.3973	.0000
	.0000	.0000	2.8702	.0000	.0000	-6.2762
	9.6736	2.6867	.0000	-4.7702	-3.5721	.0000
	2.6867	-3.3973	.0000	-3.5721	1.9000	.0000
	.0000	.0000	-6.2762	.0000	.0000	2.8702
10.0 6.0 .0						
	-3.2831	-4.3886	.0000	7.8028	3.1479	.0000
	-4.3886	.8165	.0000	3.1479	-.9937	.0000
	.0000	.0000	2.4665	.0000	.0000	-6.8090
	7.8028	3.1479	.0000	-3.2831	-4.3886	.0000
	3.1479	-.9937	.0000	-4.3886	.8165	.0000
	.0000	.0000	-6.8090	.0000	.0000	2.4665
10.0 8.0 .0						
	-1.8553	-4.5596	.0000	5.8830	3.0672	.0000
	-4.5596	-.0866	.0000	3.0672	1.6132	.0000
	.0000	.0000	1.9419	.0000	.0000	-7.4962
	5.8830	3.0672	.0000	-1.8553	-4.5596	.0000
	3.0672	1.6132	.0000	-4.5596	-.0866	.0000
	.0000	.0000	-7.4962	.0000	.0000	1.9419
10.010.0 .0						
	-.6692	-4.2651	.0000	4.1398	2.6551	.0000
	-4.2651	-.6692	.0000	2.6551	4.1398	.0000
	.0000	.0000	1.3384	.0000	.0000	-8.2796
	4.1398	2.6551	.0000	-.6692	-4.2651	.0000
	2.6551	4.1398	.0000	-4.2651	-.6692	.0000
	.0000	.0000	-8.2796	.0000	.0000	1.3384
10.0 2.0 2.0						
	-5.5321	-1.9626	-1.9626	10.5927	1.4837	1.4837
	-1.9626	2.7661	-.4827	1.4837	-5.2964	.2409
	-1.9626	-.4827	2.7661	1.4837	.2409	-5.2964
	10.5927	1.4837	1.4837	-5.5321	-1.9626	-1.9626
	1.4837	-5.2964	.2409	-1.9626	2.7661	-.4827
	1.4837	.2409	-5.2964	-1.9626	-.4827	2.7661

10.0 4.0 2.0					
-4.4361	-3.4547	-1.7706	9.2452	2.5323	1.2359
-3.4547	1.8749	-.8659	2.5323	-3.5675	.3965
-1.7706	-.8659	2.5612	1.2359	.3965	-5.6777
9.2452	2.5323	1.2359	-4.4361	-3.4547	-1.7706
2.5323	-3.5675	.3965	-3.4547	1.8749	-.8659
1.2359	.3965	-5.6777	-1.7706	-.8659	2.5612
10.0 6.0 2.0					
-3.0536	-4.2697	-1.5379	7.4654	2.9748	.9117
-4.2697	.8338	-1.1022	2.9748	-1.1972	.4354
-1.5379	-1.1022	2.2198	.9117	.4354	-6.2682
7.4654	2.9748	.9117	-3.0536	-4.2697	-1.5379
2.9748	-1.1972	.4354	-4.2697	.8338	-1.1022
.9117	.4354	-6.2682	-1.5379	-1.1022	2.2198
10.0 8.0 2.0					
-1.7175	-4.4639	-1.3287	5.6186	2.9029	.5790
-4.4639	-.0391	-1.1963	2.9029	1.3944	.3802
-1.3287	-1.1963	1.7565	.5790	.3802	-7.0131
5.6186	2.9029	.5790	-1.7175	-4.4639	-1.3287
2.9029	1.3944	.3802	-4.4639	-.0391	-1.1963
.5790	.3802	-7.0131	-1.3287	-1.1963	1.7565
10.010.0 2.0					
-.6026	-4.2003	-1.1739	3.9238	2.5119	.2758
-4.2003	-.6026	-1.1739	2.5119	3.9238	.2758
-1.1739	-1.1739	1.2052	.2758	.2758	-7.8477
3.9238	2.5119	.2758	-.6026	-4.2003	-1.1739
2.5119	3.9238	.2758	-4.2003	-.6026	-1.1739
.2758	.2758	-7.8477	-1.1739	-1.1739	1.2052
10.0 4.0 4.0					
-3.5653	-3.1543	-3.1543	8.0982	2.1212	2.1212
-3.1543	1.7827	-1.5677	2.1212	-4.0491	.6556
-3.1543	-1.5677	1.7827	2.1212	.6556	-4.0491
8.0982	2.1212	2.1212	-3.5653	-3.1543	-3.1543
2.1212	-4.0491	.6556	-3.1543	1.7827	-1.5677
2.1212	.6556	-4.0491	-3.1543	-1.5677	1.7827
10.0 6.0 4.0					
-2.4487	-3.9622	-2.7850	6.5432	2.5051	1.5701
-3.9622	.8582	-2.0200	2.5051	-1.7707	.7213
-2.7850	-2.0200	1.5904	1.5701	.7213	-4.7725
6.5432	2.5051	1.5701	-2.4487	-3.9622	-2.7850
2.5051	-1.7707	.7213	-3.9622	.8582	-2.0200
1.5701	.7213	-4.7725	-2.7850	-2.0200	1.5904
10.0 8.0 4.0					
-1.3529	-4.2153	-2.4494	4.8802	2.4477	.9875
-4.2153	.0733	-2.2197	2.4477	.7753	.6251
-2.4494	-2.2197	1.2796	.9875	.6251	-5.6555
4.8802	2.4477	.9875	-1.3529	-4.2153	-2.4494
2.4477	.7753	.6251	-4.2153	.0733	-2.2197
.9875	.6251	-5.6555	-2.4494	-2.2197	1.2796

```
10.010.0 4.0
     -.4310    -4.0335    -2.2021     3.3085     2.1075      .4410
    -4.0335     -.4310    -2.2021     2.1075     3.3085      .4410
    -2.2021    -2.2021      .8619      .4410      .4410    -6.6171
     3.3085     2.1075      .4410     -.4310    -4.0335    -2.2021
     2.1075     3.3085      .4410    -4.0335     -.4310    -2.2021
      .4410      .4410    -6.6171    -2.2021    -2.2021      .8619
10.0 6.0 6.0
    -1.6606    -3.5791    -3.5791     5.2480     1.8535     1.8535
    -3.5791      .8303    -2.6454     1.8535    -2.6240      .7892
    -3.5791    -2.6454      .8303     1.8535      .7892    -2.6240
     5.2480     1.8535     1.8535    -1.6606    -3.5791    -3.5791
     1.8535    -2.6240      .7892    -3.5791      .8303    -2.6454
     1.8535      .7892    -2.6240    -3.5791    -2.6454      .8303
10.0 8.0 6.0
     -.8789    -3.9058    -3.2300     3.8030     1.7930     1.1361
    -3.9058      .1799    -2.9567     1.7930     -.1511      .6661
    -3.2300    -2.9567      .6990     1.1361      .6661    -3.6519
     3.8030     1.7930     1.1361     -.8789    -3.9058    -3.2300
     1.7930     -.1511      .6661    -3.9058      .1799    -2.9567
     1.1361      .6661    -3.6519    -3.2300    -2.9567      .6990
10.010.0 6.0
     -.2243    -3.8328    -2.9800     2.3782     1.5056      .4346
    -3.8328     -.2243    -2.9800     1.5056     2.3782      .4346
    -2.9800    -2.9800      .4485      .4346      .4346    -4.7564
     2.3782     1.5056      .4346     -.2243    -3.8328    -2.9800
     1.5056     2.3782      .4346    -3.8328     -.2243    -2.9800
      .4346      .4346    -4.7564    -2.9800    -2.9800      .4485
10.0 8.0 8.0
     -.4196    -3.6314    -3.6314     2.5437     1.0390     1.0390
    -3.6314      .2098    -3.3670     1.0390    -1.2718      .5204
    -3.6314    -3.3670      .2098     1.0390      .5204    -1.2718
     2.5437     1.0390     1.0390     -.4196    -3.6314    -3.6314
     1.0390    -1.2718      .5204    -3.6314      .2098    -3.3670
     1.0390      .5204    -1.2718    -3.6314    -3.3670      .2098
10.010.0 8.0
     -.0613    -3.6747    -3.4561     1.2397      .7810      .2655
    -3.6747     -.0613    -3.4561      .7810     1.2397      .2655
    -3.4561    -3.4561      .1226      .2655      .2655    -2.4794
     1.2397      .7810      .2655     -.0613    -3.6747    -3.4561
      .7810     1.2397      .2655    -3.6747     -.0613    -3.4561
      .2655      .2655    -2.4794    -3.4561    -3.4561      .1226
10.010.010.0
      .0000    -3.6153    -3.6153      .0000      .0000      .0000
    -3.6153      .0000    -3.6153      .0000      .0000      .0000
    -3.6153    -3.6153      .0000      .0000      .0000      .0000
      .0000      .0000      .0000      .0000    -3.6153    -3.6153
      .0000      .0000      .0000    -3.6153      .0000    -3.6153
      .0000      .0000      .0000    -3.6153    -3.6153      .0000
```

12.0 .0 .0					
-5.7894	.0000	.0000	12.6846	.0000	.0000
.0000	2.8947	.0000	.0000	-6.3423	.0000
.0000	.0000	2.8947	.0000	.0000	-6.3423
12.6846	.0000	.0000	-5.7894	.0000	.0000
.0000	-6.3423	.0000	.0000	2.8947	.0000
.0000	.0000	-6.3423	.0000	.0000	2.8947
12.0 2.0 .0					
-5.4581	-1.5366	.0000	12.2862	1.0900	.0000
-1.5366	2.6634	.0000	1.0900	-5.8165	.0000
.0000	.0000	2.7947	.0000	.0000	-6.4698
12.2862	1.0900	.0000	-5.4581	-1.5366	.0000
1.0900	-5.8165	.0000	-1.5366	2.6634	.0000
.0000	.0000	-6.4698	.0000	.0000	2.7947
12.0 4.0 .0					
-4.5685	-2.7697	.0000	11.2005	1.9098	.0000
-2.7697	2.0677	.0000	1.9098	-4.3570	.0000
.0000	.0000	2.5008	.0000	.0000	-6.8435
11.2005	1.9098	.0000	-4.5685	-2.7697	.0000
1.9098	-4.3570	.0000	-2.7697	2.0677	.0000
.0000	.0000	-6.8435	.0000	.0000	2.5008
12.0 6.0 .0					
-3.3642	-3.5291	.0000	9.6867	2.3224	.0000
-3.5291	1.3328	.0000	2.3224	-2.2497	.0000
.0000	.0000	2.0314	.0000	.0000	-7.4371
9.6867	2.3224	.0000	-3.3642	-3.5291	.0000
2.3224	-2.2497	.0000	-3.5291	1.3328	.0000
.0000	.0000	-7.4371	.0000	.0000	2.0314
12.0 8.0 .0					
-2.0964	-3.8018	.0000	8.0219	2.3480	.0000
-3.8018	.6777	.0000	2.3480	.1840	.0000
.0000	.0000	1.4187	.0000	.0000	-8.2059
8.0219	2.3480	.0000	-2.0964	-3.8018	.0000
2.3480	.1840	.0000	-3.8018	.6777	.0000
.0000	.0000	-8.2059	.0000	.0000	1.4187
12.010.0 .0					
-.9405	-3.6690	.0000	6.4161	2.0976	.0000
-3.6690	.2298	.0000	2.0976	2.6708	.0000
.0000	.0000	.7106	.0000	.0000	-9.0870
6.4161	2.0976	.0000	-.9405	-3.6690	.0000
2.0976	2.6708	.0000	-3.6690	.2298	.0000
.0000	.0000	-9.0870	.0000	.0000	.7106
12.012.0 .0					
.0149	-3.2346	.0000	5.0000	1.6976	.0000
-3.2346	.0149	.0000	1.6976	5.0000	.0000
.0000	.0000	-.0298	.0000	.0000	-10.0001
5.0000	1.6976	.0000	.0149	-3.2346	.0000
1.6976	5.0000	.0000	-3.2346	.0149	.0000
.0000	.0000	-10.0001	.0000	.0000	-.0298

12.0 2.0 2.0

-5.1462	-1.4977	-1.4977	11.9049	1.0321	1.0321
-1.4977	2.5731	-.3764	1.0321	-5.9525	.0967
-1.4977	-.3764	2.5731	1.0321	.0967	-5.9525
11.9049	1.0321	1.0321	-5.1462	-1.4977	-1.4977
1.0321	-5.9525	.0967	-1.4977	2.5731	-.3764
1.0321	.0967	-5.9525	-1.4977	-.3764	2.5731

12.0 4.0 2.0

-4.3065	-2.7068	-1.3961	10.8626	1.8093	.8741
-2.7068	2.0015	-.6973	1.8093	-4.5132	.1527
-1.3961	-.6973	2.3050	.8741	.1527	-6.3494
10.8626	1.8093	.8741	-4.3065	-2.7068	-1.3961
1.8093	-4.5132	.1527	-2.7068	2.0015	-.6973
.8741	.1527	-6.3494	-1.3961	-.6973	2.3050

12.0 6.0 2.0

-3.1661	-3.4621	-1.2677	9.4018	2.2003	.6527
-3.4621	1.2956	-.9267	2.2003	-2.4264	.1497
-1.2677	-.9267	1.8705	.6527	.1497	-6.9754
9.4018	2.2003	.6527	-3.1661	-3.4621	-1.2677
2.2003	-2.4264	.1497	-3.4621	1.2956	-.9267
.6527	.1497	-6.9754	-1.2677	-.9267	1.8705

12.0 8.0 2.0

-1.9616	-3.7464	-1.1478	7.7850	2.2221	.4065
-3.7464	.6675	-1.0528	2.2221	-.0045	.0961
-1.1478	-1.0528	1.2940	.4065	.0961	-7.7805
7.7850	2.2221	.4065	-1.9616	-3.7464	-1.1478
2.2221	-.0045	.0961	-3.7464	.6676	-1.0528
.4065	.0961	-7.7805	-1.1478	-1.0528	1.2940

12.010.0 2.0

-.8606	-3.6323	-1.0588	6.2153	1.9796	.1644
-3.6323	.2435	-1.0774	1.9796	2.4825	.0177
-1.0588	-1.0774	.6171	.1644	.0177	-8.6978
6.2153	1.9796	.1644	-.8606	-3.6323	-1.0588
1.9796	2.4825	.0177	-3.6323	.2435	-1.0774
.1644	.0177	-8.6978	-1.0588	-1.0774	.6171

12.012.0 2.0

.0501	-3.2164	-1.0073	4.8227	1.5945	-.0554
-3.2164	.0501	-1.0073	1.5945	4.8227	-.0554
-1.0073	-1.0073	-.1003	-.0554	-.0554	-9.6453
4.8227	1.5945	-.0554	.0501	-3.2164	-1.0073
1.5945	4.8227	-.0554	-3.2164	.0501	-1.0073
-.0554	-.0554	-9.6453	-1.0073	-1.0073	-.1003

12.0 4.0 4.0

-3.5978	-2.5423	-2.5423	9.9313	1.5324	1.5324
-2.5423	1.7989	-1.2981	1.5324	-4.9656	.2364
-2.5423	-1.2981	1.7989	1.5324	.2364	-4.9656
9.9313	1.5324	1.5324	-3.5978	-2.5423	-2.5423
1.5324	-4.9656	.2364	-2.5423	1.7989	-1.2981
1.5324	.2364	-4.9656	-2.5423	-1.2981	1.7989

12.0 6.0 4.0

-2.6274	-3.2876	-2.3342	8.6072	1.8599	1.1385
-3.2876	1.1732	-1.7377	1.8599	-2.9365	.2184
-2.3342	-1.7377	1.4542	1.1385	.2184	-5.6707
8.6072	1.8599	1.1385	-2.6274	-3.2876	-2.3342
1.8599	-2.9365	.2184	-3.2876	1.1732	-1.7377
1.1385	.2184	-5.6707	-2.3342	-1.7377	1.4542

12.0 8.0 4.0

-1.5943	-3.6035	-2.1421	7.1154	1.8662	.6920
-3.6035	.6221	-1.9900	1.8662	-.5493	.1122
-2.1421	-1.9900	.9722	.6920	.1122	-6.5662
7.1154	1.8662	.6920	-1.5943	-3.6035	-2.1421
1.8662	-.5493	.1122	-3.6035	.6221	-1.9900
.6920	.1122	-6.5662	-2.1421	-1.9900	.9722

12.010.0 4.0

-.6457	-3.5410	-2.0047	5.6400	1.6410	.2436
-3.5410	.2672	-2.0533	1.6410	1.9368	-.0365
-2.0047	-2.0533	.3784	.2436	-.0365	-7.5767
5.6400	1.6410	.2436	-.6457	-3.5410	-2.0047
1.6410	1.9368	-.0365	-3.5410	.2672	-2.0533
.2436	-.0365	-7.5767	-2.0047	-2.0533	.3784

12.012.0 4.0

.1386	-3.1767	-1.9344	4.3075	1.2949	-.1722
-3.1767	.1386	-1.9344	1.2949	4.3075	-.1722
-1.9344	-1.9344	-.2772	-.1722	-.1722	-8.6151
4.3075	1.2949	-.1722	.1386	-3.1767	-1.9344
1.2949	4.3075	-.1722	-3.1767	.1386	-1.9344
-.1722	-.1722	-8.6151	-1.9344	-1.9344	-.2772

12.0 6.0 6.0

-1.8839	-3.0688	-3.0688	7.4536	1.3646	1.3646
-3.0688	.9419	-2.3504	1.3646	-3.7268	.1658
-3.0688	-2.3504	.9419	1.3646	.1658	-3.7268
7.4536	1.3646	1.3646	-1.8839	-3.0688	-3.0688
1.3646	-3.7268	.1658	-3.0688	.9419	-2.3504
1.3646	.1658	-3.7268	-3.0688	-2.3504	.9419

12.0 8.0 6.0

-1.0882	-3.4311	-2.8741	6.1193	1.3348	.7869
-3.4311	.5045	-2.7242	1.3348	-1.3946	.0066
-2.8741	-2.7242	.5837	.7869	.0066	-4.7248
6.1193	1.3348	.7869	-1.0882	-3.4311	-2.8741
1.3348	-1.3946	.0066	-3.4311	.5045	-2.7242
.7869	.0066	-4.7248	-2.8741	-2.7242	.5837

12.010.0 6.0

-.3594	-3.4441	-2.7506	4.7616	1.1217	.1877
-3.4441	.2572	-2.8462	1.1217	1.0856	-.2024
-2.7506	-2.8462	.1022	.1877	-.2024	-5.8472
4.7616	1.1217	.1877	-.3594	-3.4441	-2.7506
1.1217	1.0856	-.2024	-3.4441	.2572	-2.8462
.1877	-.2024	-5.8472	-2.7506	-2.8462	.1022

12.012.0 6.0

.2342	-3.1553	-2.7142	3.5005	.8227	-.3866
-3.1553	.2342	-2.7142	.8227	3.5005	-.3866
-2.7142	-2.7142	-.4683	-.3866	-.3866	-7.0011
3.5005	.8227	-.3866	.2342	-3.1553	-2.7142
.8227	3.5005	-.3866	-3.1553	.2342	-2.7142
-.3866	-.3866	-7.0011	-2.7142	-2.7142	-.4683

12.0 8.0 8.0

-.5533	-3.2950	-3.2950	4.9298	.6930	.6930
-3.2950	.2766	-3.2034	.6930	-2.4649	-.2078
-3.2950	-3.2034	.2766	.6930	-.2078	-2.4649
4.9298	.6930	.6930	-.5533	-3.2950	-3.2950
.6930	-2.4649	-.2078	-3.2950	.2766	-3.2034
.6930	-.2078	-2.4649	-3.2950	-3.2034	.2766

12.010.0 8.0

-.0805	-3.4001	-3.2438	3.6749	.4703	.0000
-3.4001	.1610	-3.4000	.4703	.0000	-.4703
-3.2438	-3.4000	-.0805	.0000	-.4703	-3.6749
3.6749	.4703	.0000	-.0805	-3.4001	-3.2438
.4703	.0000	-.4703	-3.4001	.1610	-3.4000
.0000	-.4703	-3.6749	-3.2438	-3.4000	-.0805

14.0 .0 .0

-5.2099	.0000	.0000	13.6281	.0000	.0000
.0000	2.6050	.0000	.0000	-6.8141	.0000
.0000	.0000	2.6050	.0000	.0000	-6.8141
13.6281	.0000	.0000	-5.2099	.0000	.0000
.0000	-6.8141	.0000	.0000	2.6050	.0000
.0000	.0000	-6.8141	.0000	.0000	2.6050

14.0 2.0 .0

-4.9522	-1.1107	.0000	13.3192	.7238	.0000
-1.1107	2.4601	.0000	.7238	-6.3658	.0000
.0000	.0000	2.4921	.0000	.0000	-6.9534
13.3192	.7238	.0000	-4.9522	-1.1107	.0000
.7238	-6.3658	.0000	-1.1107	2.4601	.0000
.0000	.0000	-6.9534	.0000	.0000	2.4921

14.0 4.0 .0

-4.2400	-2.0350	.0000	12.4577	1.2894	.0000
-2.0350	2.0802	.0000	1.2894	-5.0952	.0000
.0000	.0000	2.1598	.0000	.0000	-7.3626
12.4577	1.2894	.0000	-4.2400	-2.0350	.0000
1.2894	-5.0952	.0000	-2.0350	2.0802	.0000
.0000	.0000	-7.3626	.0000	.0000	2.1598

14.0 6.0 .0

-3.2264	-2.6514	.0000	11.2088	1.6039	.0000
-2.6514	1.5986	.0000	1.6039	-3.1945	.0000
.0000	.0000	1.6278	.0000	.0000	-8.0142
11.2088	1.6039	.0000	-3.2264	-2.6514	.0000
1.6039	-3.1945	.0000	-2.6514	1.5986	.0000
.0000	.0000	-8.0142	.0000	.0000	1.6278

14.0 8.0 .0					
-2.0910	-2.9246	.0000	9.7718	1.6606	.0000
-2.9246	1.1599	.0000	1.6606	-.9102	.0000
.0000	.0000	.9311	.0000	.0000	-8.8616
9.7718	1.6606	.0000	-2.0910	-2.9246	.0000
1.6606	-.9102	.0000	-2.9246	1.1599	.0000
.0000	.0000	-8.8616	.0000	.0000	.9311
14.010.0 .0					
-.9860	-2.8842	.0000	8.3257	1.5153	.0000
-2.8842	.8636	.0000	1.5153	1.5113	.0000
.0000	.0000	.1224	.0000	.0000	-9.8370
8.3257	1.5153	.0000	-.9860	-2.8842	.0000
1.5153	1.5113	.0000	-2.8842	.8636	.0000
.0000	.0000	-9.8370	.0000	.0000	.1224
14.012.0 .0					
-.0146	-2.5887	.0000	7.0054	1.2472	.0000
-2.5887	.7418	.0000	1.2472	3.8477	.0000
.0000	.0000	-.7272	.0000	.0000	-10.8531
7.0054	1.2472	.0000	-.0146	-2.5887	.0000
1.2472	3.8477	.0000	-2.5887	.7418	.0000
.0000	.0000	-10.8531	.0000	.0000	-.7272
14.014.0 .0					
.7656	-2.1002	.0000	5.9035	.9272	.0000
-2.1002	.7656	.0000	.9272	5.9035	.0000
.0000	.0000	-1.5311	.0000	.0000	-11.8071
5.9035	.9272	.0000	.7656	-2.1002	.0000
.9272	5.9035	.0000	-2.1002	.7656	.0000
.0000	.0000	-11.8071	.0000	.0000	-1.5311
14.0 2.0 2.0					
-4.7055	-1.0910	-1.0910	13.0199	.6871	.6871
-1.0910	2.3527	-.3217	.6871	-6.5099	.0057
-1.0910	-.3217	2.3527	.6871	.0057	-6.5099
13.0199	.6871	.6871	-4.7055	-1.0910	-1.0910
.6871	-6.5099	.0057	-1.0910	2.3527	-.3217
.6871	.0057	-6.5099	-1.0910	-.3217	2.3527
14.0 4.0 2.0					
-4.0232	-2.0026	-1.0390	12.1837	1.2232	.5843
-2.0026	1.9877	-.6079	1.2232	-5.2511	-.0087
-1.0390	-.6079	2.0355	.5843	-.0087	-6.9327
12.1837	1.2232	.5843	-4.0232	-2.0026	-1.0390
1.2232	-5.2511	-.0087	-2.0026	1.9877	-.6079
.5843	-.0087	-6.9327	-1.0390	-.6079	2.0355
14.0 6.0 2.0					
-3.0505	-2.6167	-.9725	10.9680	1.5193	.4338
-2.6167	1.5265	-.8313	1.5193	-3.3632	-.0521
-.9725	-.8313	1.5240	.4338	-.0521	-7.6048
10.9680	1.5193	.4338	-3.0505	-2.6167	-.9725
1.5193	-3.3632	-.0521	-2.6167	1.5265	-.8313
.4338	-.0521	-7.6048	-.9725	-.8313	1.5240

14.0 8.0 2.0

-1.9588	-2.8966	-.9111	9.5642	1.5683	.2575
-2.8966	1.1106	-.9746	1.5683	-1.0865	-.1185
-.9111	-.9746	.8482	.2575	-.1185	-8.4776
9.5642	1.5683	.2575	-1.9588	-2.8966	-.9111
1.5683	-1.0865	-.1185	-2.8966	1.1106	-.9746
.2575	-.1185	-8.4776	-.9111	-.9746	.8482

14.010.0 2.0

-.8949	-2.8677	-.8685	8.1458	1.4243	.0748
-2.8677	.8386	-1.0284	1.4243	1.3363	-.1895
-.8685	-1.0284	.0563	.0748	-.1895	-9.4821
8.1458	1.4243	.0748	-.8949	-2.8677	-.8685
1.4243	1.3363	-.1895	-2.8677	.8386	-1.0284
.0748	-.1895	-9.4821	-.8685	-1.0284	.0563

14.012.0 2.0

.0410	-2.5841	-.8500	6.8459	1.1641	-.0992
-2.5841	.7425	-.9878	1.1641	3.6833	-.2410
-.8500	-.9878	-.7835	-.0992	-.2410	-10.5292
6.8459	1.1641	-.0992	.0410	-2.5841	-.8500
1.1641	3.6833	-.2410	-2.5841	.7425	-.9878
-.0992	-.2410	-10.5292	-.8500	-.9878	-.7835

14.014.0 2.0

.7925	-2.1042	-.8520	5.7571	.8580	-.2517
-2.1042	.7925	-.8520	.8580	5.7571	-.2517
-.8520	-.8520	-1.5850	-.2517	-.2517	-11.5142
5.7571	.8580	-.2517	.7925	-2.1042	-.8520
.8580	5.7571	-.2517	-2.1042	.7925	-.8520
-.2517	-.2517	-11.5142	-.8520	-.8520	-1.5850

14.0 4.0 4.0

-3.4220	-1.9177	-1.9177	11.4148	1.0369	1.0369
-1.9177	1.7110	-1.1528	1.0369	-5.7074	-.0528
-1.9177	-1.1528	1.7110	1.0369	-.0528	-5.7074
11.4148	1.0369	1.0369	-3.4220	-1.9177	-1.9177
1.0369	-5.7074	-.0528	-1.9177	1.7110	-1.1528
1.0369	-.0528	-5.7074	-1.9177	-1.1528	1.7110

14.0 6.0 4.0

-2.5612	-2.5269	-1.8106	10.2878	1.2788	.7611
-2.5269	1.3060	-1.5842	1.2788	-3.8566	-.1488
-1.8106	-1.5842	1.2552	.7611	-.1488	-6.4312
10.2878	1.2788	.7611	-2.5612	-2.5269	-1.8106
1.2788	-3.8566	-.1488	-2.5269	1.3060	-1.5842
.7611	-.1488	-6.4312	-1.8106	-1.5842	1.2552

14.0 8.0 4.0

-1.5911	-2.8266	-1.7154	8.9727	1.3035	.4333
-2.8266	.9543	-1.8689	1.3035	-1.6030	-.2856
-1.7154	-1.8689	.6368	.4333	-.2856	-7.3697
8.9727	1.3035	.4333	-1.5911	-2.8266	-1.7154
1.3035	-1.6030	-.2856	-2.8266	.9543	-1.8689
.4333	-.2856	-7.3697	-1.7154	-1.8689	.6368

14.010.0 4.0

-.6428	-2.8314	-1.6566	7.6286	1.1596	.0875
-2.8314	.7519	-1.9859	1.1596	.8222	-.4284
-1.6566	-1.9859	-.1091	.0875	-.4284	-8.4508
7.6286	1.1596	.0875	-.6428	-2.8314	-1.6566
1.1596	.8222	-.4284	-2.8314	.7519	-1.9859
.0875	-.4284	-8.4508	-1.6566	-1.9859	-.1091

14.012.0 4.0

.1916	-2.5821	-1.6434	6.3824	.9198	-.2478
-2.5821	.7311	-1.9213	.9198	3.2002	-.5302
-1.6434	-1.9213	-.9226	-.2478	-.5302	-9.5826
6.3824	.9198	-.2478	.1916	-2.5821	-1.6434
.9198	3.2002	-.5302	-2.5821	.7311	-1.9213
-.2478	-.5302	-9.5826	-1.6434	-1.9213	-.9226

14.0 6.0 6.0

-1.8578	-2.4180	-2.4180	9.2784	.9172	.9172
-2.4180	.9289	-2.1941	.9172	-4.6392	-.3114
-2.4180	-2.1941	.9289	.9172	-.3114	-4.6392
9.2784	.9172	.9172	-1.8578	-2.4180	-2.4180
.9172	-4.6392	-.3114	-2.4180	.9289	-2.1941
.9172	-.3114	-4.6392	-2.4180	-2.1941	.9289

14.0 8.0 6.0

-1.0625	-2.7512	-2.3316	8.0812	.8966	.4772
-2.7512	.6695	-2.6142	.8966	-2.4251	-.5254
-2.3316	-2.6142	.3929	.4772	-.5254	-5.6562
8.0812	.8966	.4772	-1.0625	-2.7512	-2.3316
.8966	-2.4251	-.5254	-2.7512	.6695	-2.6142
.4772	-.5254	-5.6562	-2.3316	-2.6142	.3929

14.010.0 6.0

-.2858	-2.8095	-2.2989	6.8347	.7432	.0000
-2.8095	.5715	-2.8095	.7432	.0000	-.7432
-2.2989	-2.8095	-.2858	.0000	-.7432	-6.8347
6.8347	.7432	.0000	-.2858	-2.8095	-2.2989
.7432	.0000	-.7432	-2.8095	.5715	-2.8095
.0000	-.7432	-6.8347	-2.2989	-2.8095	-.2858

14.0 8.0 8.0

-.4683	-2.7142	-2.7142	7.0011	.3866	.3866
-2.7142	.2342	-3.1553	.3866	-3.5005	-.8227
-2.7142	-3.1553	.2342	.3866	-.8227	-3.5005
7.0011	.3866	.3866	-.4683	-2.7142	-2.7142
.3866	-3.5005	-.8227	-2.7142	.2342	-3.1553
.3866	-.8227	-3.5005	-2.7142	-3.1553	.2342

16.0 .0 .0

-4.7427	.0000	.0000	14.3837	.0000	.0000
.0000	2.3713	.0000	.0000	-7.1919	.0000
.0000	.0000	2.3713	.0000	.0000	-7.1919
14.3837	.0000	.0000	-4.7427	.0000	.0000
.0000	-7.1919	.0000	.0000	2.3713	.0000
.0000	.0000	-7.1919	.0000	.0000	2.3713

16.0 2.0 .0

-4.5259	-.7248	.0000	14.1295	.4395	.0000
-.7248	2.2780	.0000	.4395	-6.7884	.0000
.0000	.0000	2.2478	.0000	.0000	-7.3411
14.1295	.4395	.0000	-4.5259	-.7248	.0000
.4395	-6.7884	.0000	-.7248	2.2780	.0000
.0000	.0000	-7.3411	.0000	.0000	2.2478

16.0 4.0 .0

-3.9162	-1.3406	.0000	13.4106	.7905	.0000
-1.3406	2.0323	.0000	.7905	-5.6310	.0000
.0000	.0000	1.8838	.0000	.0000	-7.7797
13.4106	.7905	.0000	-3.9162	-1.3406	.0000
.7905	-5.6310	.0000	-1.3406	2.0323	.0000
.0000	.0000	-7.7797	.0000	.0000	1.8838

16.0 6.0 .0

-3.0204	-1.7700	.0000	12.3435	.9965	.0000
-1.7700	1.7206	.0000	.9965	-3.8637	.0000
.0000	.0000	1.2999	.0000	.0000	-8.4798
12.3435	.9965	.0000	-3.0204	-1.7700	.0000
.9965	-3.8637	.0000	-1.7700	1.7206	.0000
.0000	.0000	-8.4798	.0000	.0000	1.2999

16.0 8.0 .0

-1.9759	-1.9812	.0000	11.0802	1.0466	.0000
-1.9812	1.4428	.0000	1.0466	-1.6875	.0000
.0000	.0000	.5330	.0000	.0000	-9.3927
11.0802	1.0466	.0000	-1.9759	-1.9812	.0000
1.0466	-1.6875	.0000	-1.9812	1.4428	.0000
.0000	.0000	-9.3927	.0000	.0000	.5330

16.010.0 .0

-.9146	-1.9813	.0000	9.7728	.9677	.0000
-1.9813	1.2746	.0000	.9677	.6748	.0000
.0000	.0000	-.3600	.0000	.0000	-10.4476
9.7728	.9677	.0000	-.9146	-1.9813	.0000
.9677	.6748	.0000	-1.9813	1.2746	.0000
.0000	.0000	-10.4476	.0000	.0000	-.3600

16.012.0 .0

.0577	-1.7998	.0000	8.5502	.8049	.0000
-1.7998	1.2440	.0000	.8049	3.0007	.0000
.0000	.0000	-1.3017	.0000	.0000	-11.5510
8.5502	.8049	.0000	.0577	-1.7998	.0000
.8049	3.0007	.0000	-1.7998	1.2440	.0000
.0000	.0000	-11.5510	.0000	.0000	-1.3017

16.014.0 .0

.8675	-1.4741	.0000	7.5109	.6028	.0000
-1.4741	1.3286	.0000	.6028	5.0800	.0000
.0000	.0000	-2.1961	.0000	.0000	-12.5910
7.5109	.6028	.0000	.8675	-1.4741	.0000
.6028	5.0800	.0000	-1.4741	1.3286	.0000
.0000	.0000	-12.5910	.0000	.0000	-2.1961

16.0 2.0 2.0

-4.3161	-.7154	-.7154	13.8814	.4173	.4173
-.7154	2.1580	-.2945	.4173	-6.9407	-.0517
-.7154	-.2945	2.1580	.4173	-.0517	-6.9407
13.8814	.4173	.4173	-4.3161	-.7154	-.7154
.4173	-6.9407	-.0517	-.7154	2.1580	-.2945
.4173	-.0517	-6.9407	-.7154	-.2945	2.1580

16.0 4.0 2.0

-3.7258	-1.3252	-.6908	13.1794	.7495	.3541
-1.3252	1.9223	-.5635	.7495	-5.7910	-.1133
-.6908	-.5635	1.8035	.3541	-.1133	-7.3884
13.1794	.7495	.3541	-3.7258	-1.3252	-.6908
.7495	-5.7910	-.1133	-1.3252	1.9223	-.5635
.3541	-.1133	-7.3884	-.6908	-.5635	1.8035

16.0 6.0 2.0

-2.8578	-1.7539	-.6597	12.1357	.9423	.2590
-1.7539	1.6257	-.7842	.9423	-4.0322	-.1884
-.6597	-.7842	1.2321	.2590	-.1884	-8.1035
12.1357	.9423	.2590	-2.8578	-1.7539	-.6597
.9423	-4.0322	-.1884	-1.7539	1.6257	-.7842
.2590	-.1884	-8.1035	-.6597	-.7842	1.2321

16.0 8.0 2.0

-1.8444	-1.9693	-.6326	10.8977	.9855	.1439
-1.9693	1.3675	-.9382	.9855	-1.8606	-.2701
-.6326	-.9382	.4769	.1439	-.2701	-9.0370
10.8977	.9855	.1439	-1.8444	-1.9693	-.6326
.9855	-1.8606	-.2701	-1.9693	1.3675	-.9382
.1439	-.2701	-9.0370	-.6326	-.9382	.4769

16.010.0 2.0

-.8137	-1.9765	-.6171	9.6135	.9053	.0204
-1.9765	1.2229	-1.0104	.9053	.5046	-.3422
-.6171	-1.0104	-.4092	.0204	-.3422	-10.1181
9.6135	.9053	.0204	-.8137	-1.9765	-.6171
.9053	.5046	-.3422	-1.9765	1.2229	-1.0104
.0204	-.3422	-10.1181	-.6171	-1.0104	-.4092

16.012.0 2.0

.1312	-1.8023	-.6163	8.4098	.7463	-.1009
-1.8023	1.2199	-.9885	.7463	2.8424	-.3828
-.6163	-.9885	-1.3511	-.1009	-.3828	-11.2522
8.4098	.7463	-.1009	.1312	-1.8023	-.6163
.7463	2.8424	-.3828	-1.8023	1.2199	-.9885
-.1009	-.3828	-11.2522	-.6163	-.9885	-1.3511

16.0 4.0 4.0

-3.1894	-1.2854	-1.2854	12.5236	.6324	.6324
-1.2854	1.5947	-1.0809	.6324	-6.2618	-.2453
-1.2854	-1.0809	1.5947	.6324	-.2453	-6.2618
12.5236	.6324	.6324	-3.1894	-1.2854	-1.2854
.6324	-6.2618	-.2453	-1.2854	1.5947	-1.0809
.6324	-.2453	-6.2618	-1.2854	-1.0809	1.5947

16.0 6.0 4.0						
	-2.3986	-1.7136	-1.2369	11.5441	.7867	.4549
	-1.7136	1.3395	-1.5107	.7867	-4.5289	-.4025
	-1.2369	-1.5107	1.0591	.4549	-.4025	-7.0152
	11.5441	.7867	.4549	-2.3986	-1.7136	-1.2369
	.7867	-4.5289	-.4025	-1.7136	1.3395	-1.5107
	.4549	-.4025	-7.0152	-1.2369	-1.5107	1.0591
16.0 8.0 4.0						
	-1.4727	-1.9421	-1.1982	10.3754	.8081	.2373
	-1.9421	1.1353	-1.8176	.8081	-2.3724	-.5721
	-1.1982	-1.8176	.3374	.2373	-.5721	-8.0031
	10.3754	.8081	.2373	-1.4727	-1.9421	-1.1982
	.8081	-2.3724	-.5721	-1.9421	1.1353	-1.8176
	.2373	-.5721	-8.0031	-1.1982	-1.8176	.3374
16.010.0 4.0						
	-.5289	-1.9705	-1.1835	9.1549	.7221	.0000
	-1.9705	1.0579	-1.9705	.7221	.0000	-.7221
	-1.1835	-1.9705	-.5289	.0000	-.7221	-9.1549
	9.1549	.7221	.0000	-.5289	-1.9705	-1.1835
	.7221	.0000	-.7221	-1.9705	1.0579	-1.9705
	.0000	-.7221	-9.1549	-1.1835	-1.9705	-.5289
16.0 6.0 6.0						
	-1.7196	-1.6687	-1.6687	10.6544	.5474	.5474
	-1.6687	.8598	-2.1261	.5474	-5.3272	-.6520
	-1.6687	-2.1261	.8598	.5474	-.6520	-5.3272
	10.6544	.5474	.5474	-1.7196	-1.6687	-1.6687
	.5474	-5.3272	-.6520	-1.6687	.8598	-2.1261
	.5474	-.6520	-5.3272	-1.6687	-2.1261	.8598
16.0 8.0 6.0						
	-.9226	-1.9213	-1.6434	9.5826	.5302	.2478
	-1.9213	.7311	-2.5820	.5302	-3.2003	-.9198
	-1.6434	-2.5820	.1916	.2478	-.9198	-6.3824
	9.5826	.5302	.2478	-.9226	-1.9213	-1.6434
	.5302	-3.2003	-.9198	-1.9213	.7311	-2.5820
	.2478	-.9198	-6.3824	-1.6434	-2.5820	.1916
18.0 .0 .0						
	-4.4392	.0000	.0000	14.8722	.0000	.0000
	.0000	2.2196	.0000	.0000	-7.4361	.0000
	.0000	.0000	2.2196	.0000	.0000	-7.4361
	14.8722	.0000	.0000	-4.4392	.0000	.0000
	.0000	-7.4361	.0000	.0000	2.2196	.0000
	.0000	.0000	-7.4361	.0000	.0000	2.2196
18.0 2.0 .0						
	-4.2431	-.3585	.0000	14.6479	.2071	.0000
	-.3585	2.1540	.0000	.2071	-7.0560	.0000
	.0000	.0000	2.0891	.0000	.0000	-7.5918
	14.6479	.2071	.0000	-4.2431	-.3585	.0000
	.2071	-7.0560	.0000	-.3585	2.1540	.0000
	.0000	.0000	-7.5918	.0000	.0000	2.0891

18.0 4.0 .0

-3.6862	-.6663	.0000	14.0091	.3743	.0000
-.6663	1.9821	.0000	.3743	-5.9591	.0000
.0000	.0000	1.7041	.0000	.0000	-8.0500
14.0091	.3743	.0000	-3.6862	-.6663	.0000
.3743	-5.9591	.0000	-.6663	1.9821	.0000
.0000	.0000	-8.0500	.0000	.0000	1.7041

18.0 6.0 .0

-2.8534	-.8860	.0000	13.0484	.4751	.0000
-.8860	1.7678	.0000	.4751	-4.2662	.0000
.0000	.0000	1.0857	.0000	.0000	-8.7822
13.0484	.4751	.0000	-2.8534	-.8860	.0000
.4751	-4.2662	.0000	-.8860	1.7678	.0000
.0000	.0000	-8.7822	.0000	.0000	1.0857

18.0 8.0 .0

-1.8601	-.9997	.0000	11.8930	.5027	.0000
-.9997	1.5879	.0000	.5027	-2.1540	.0000
.0000	.0000	.2722	.0000	.0000	-9.7390
11.8930	.5027	.0000	-1.8601	-.9997	.0000
.5027	-2.1540	.0000	-.9997	1.5879	.0000
.0000	.0000	-9.7390	.0000	.0000	.2722

18.0 10.0 .0

-.8258	-1.0076	.0000	10.6779	.4681	.0000
-1.0076	1.5031	.0000	.4681	.1692	.0000
.0000	.0000	-.6773	.0000	.0000	-10.8472
10.6779	.4681	.0000	-.8258	-1.0076	.0000
.4681	.1692	.0000	-1.0076	1.5031	.0000
.0000	.0000	-10.8472	.0000	.0000	-.6773

18.0 12.0 .0

.1445	-.9217	.0000	9.5256	.3915	.0000
-.9217	1.5364	.0000	.3915	2.4836	.0000
.0000	.0000	-1.6809	.0000	.0000	-12.0092
9.5256	.3915	.0000	.1445	-.9217	.0000
.3915	2.4836	.0000	-.9217	1.5364	.0000
.0000	.0000	-12.0092	.0000	.0000	-1.6809

18.0 2.0 2.0

-4.0521	-.3548	-.3548	14.4283	.1965	.1965
-.3548	2.0260	-.2824	.1965	-7.2142	-.0839
-.3548	-.2824	2.0260	.1965	-.0839	-7.2142
14.4283	.1965	.1965	-4.0521	-.3548	-.3548
.1965	-7.2142	-.0839	-.3548	2.0260	-.2824
.1965	-.0839	-7.2142	-.3548	-.2824	2.0260

18.0 4.0 2.0

-3.5094	-.6604	-.3453	13.8027	.3545	.1661
-.6604	1.8616	-.5439	.3545	-6.1232	-.1731
-.3453	-.5439	1.6477	.1661	-.1731	-7.6795
13.8027	.3545	.1661	-3.5094	-.6604	-.3453
.3545	-6.1232	-.1731	-.6604	1.8616	-.5439
.1661	-.1731	-7.6795	-.3453	-.5439	1.6477

18.0 6.0 2.0					
-2.6973	-.8801	-.3336	12.8610	.4485	.1197
-.8801	1.6596	-.7643	.4485	-4.4367	-.2680
-.3336	-.7643	1.0377	.1197	-.2680	-8.4244
12.8610	.4485	.1197	-2.6973	-.8801	-.3336
.4485	-4.4367	-.2680	-.8801	1.6596	-.7643
.1197	-.2680	-8.4244	-.3336	-.7643	1.0377
18.0 8.0 2.0					
-1.7279	-.9959	-.3243	11.7273	.4722	.0625
-.9959	1.4972	-.9247	.4722	-2.3274	-.3611
-.3243	-.9247	.2307	.0625	-.3611	-9.3999
11.7273	.4722	.0625	-1.7279	-.9959	-.3243
.4722	-2.3274	-.3611	-.9959	1.4972	-.9247
.0625	-.3611	-9.3999	-.3243	-.9247	.2307
18.010.0 2.0					
-.7177	-1.0073	-.3207	10.5335	.4363	.0000
-1.0073	1.4354	-1.0073	.4363	.0000	-.4363
-.3207	-1.0073	-.7177	.0000	-.4363	-10.5334
10.5335	.4363	.0000	-.7177	-1.0073	-.3207
.4363	.0000	-.4363	-1.0073	1.4354	-1.0073
.0000	-.4363	-10.5334	-.3207	-1.0073	-.7177
18.0 4.0 4.0					
-3.0066	-.6453	-.6453	13.2139	.2976	.2976
-.6453	1.5033	-1.0499	.2976	-6.6069	-.3569
-.6453	-1.0499	1.5033	.2976	-.3569	-6.6069
13.2139	.2976	.2976	-3.0066	-.6453	-.6453
.2976	-6.6069	-.3569	-.6453	1.5033	-1.0499
.2976	-.3569	-6.6069	-.6453	-1.0499	1.5033
18.0 6.0 4.0					
-2.2529	-.8658	-.6279	12.3254	.3715	.2101
-.8658	1.3345	-1.4814	.3715	-4.9410	-.5528
-.6279	-1.4814	.9184	.2101	-.5528	-7.3844
12.3254	.3715	.2101	-2.2529	-.8658	-.6279
.3715	-4.9410	-.5528	-.8658	1.3345	-1.4814
.2101	-.5528	-7.3844	-.6279	-1.4814	.9184
18.0 8.0 4.0					
-1.3511	-.9885	-.6163	11.2523	.3828	.1009
-.9885	1.2199	-1.8022	.3828	-2.8424	-.7463
-.6163	-1.8022	.1312	.1009	-.7463	-8.4098
11.2523	.3828	.1009	-1.3511	-.9885	-.6163
.3828	-2.8424	-.7463	-.9885	1.2199	-1.8022
.1009	-.7463	-8.4098	-.6163	-1.8022	.1312
18.0 6.0 6.0					
-1.5850	-.8520	-.8520	11.5142	.2517	.2517
-.8520	.7925	-2.1042	.2517	-5.7571	-.8580
-.8520	-2.1042	.7925	.2517	-.8580	-5.7571
11.5142	.2517	.2517	-1.5850	-.8520	-.8520
.2517	-5.7571	-.8580	-.8520	.7925	-2.1042
.2517	-.8580	-5.7571	-.8520	-2.1042	.7925

20.0 .0 .0

-4.3340	.0000	.0000	15.0411	.0000	.0000
.0000	2.1670	.0000	.0000	-7.5205	.0000
.0000	.0000	2.1670	.0000	.0000	-7.5205
15.0411	.0000	.0000	-4.3340	.0000	.0000
.0000	-7.5205	.0000	.0000	2.1670	.0000
.0000	.0000	-7.5205	.0000	.0000	2.1670

20.0 2.0 .0

-4.1442	.0000	.0000	14.8264	.0000	.0000
.0000	2.1102	.0000	.0000	-7.1478	.0000
.0000	.0000	2.0340	.0000	.0000	-7.6786
14.8264	.0000	.0000	-4.1442	.0000	.0000
.0000	-7.1478	.0000	.0000	2.1102	.0000
.0000	.0000	-7.6786	.0000	.0000	2.0340

20.0 4.0 .0

-3.6035	.0000	.0000	14.2135	.0000	.0000
.0000	1.9619	.0000	.0000	-6.0699	.0000
.0000	.0000	1.6417	.0000	.0000	-8.1435
14.2135	.0000	.0000	-3.6035	.0000	.0000
.0000	-6.0699	.0000	.0000	1.9619	.0000
.0000	.0000	-8.1435	.0000	.0000	1.6417

20.0 6.0 .0

-2.7904	.0000	.0000	13.2879	.0000	.0000
.0000	1.7793	.0000	.0000	-4.4008	.0000
.0000	.0000	1.0112	.0000	.0000	-8.8871
13.2879	.0000	.0000	-2.7904	.0000	.0000
.0000	-4.4008	.0000	.0000	1.7793	.0000
.0000	.0000	-8.8871	.0000	.0000	1.0112

20.0 8.0 .0

-1.8134	.0000	.0000	12.1691	.0000	.0000
.0000	1.6321	.0000	.0000	-2.3097	.0000
.0000	.0000	.1813	.0000	.0000	-9.8593
12.1691	.0000	.0000	-1.8134	.0000	.0000
.0000	-2.3097	.0000	.0000	1.6321	.0000
.0000	.0000	-9.8593	.0000	.0000	.1813

20.010.0 .0

-.7880	.0000	.0000	10.9863	.0000	.0000
.0000	1.5761	.0000	.0000	.0000	.0000
.0000	.0000	-.7880	.0000	.0000	-10.9862
10.9863	.0000	.0000	-.7880	.0000	.0000
.0000	.0000	.0000	.0000	1.5761	.0000
.0000	.0000	-10.9862	.0000	.0000	-.7880

20.0 2.0 2.0

-3.9589	.0000	.0000	14.6160	.0000	.0000
.0000	1.9794	-.2790	.0000	-7.3080	-.0943
.0000	-.2790	1.9794	.0000	-.0943	-7.3080
14.6160	.0000	.0000	-3.9589	.0000	.0000
.0000	-7.3080	-.0943	.0000	1.9794	-.2790
.0000	-.0943	-7.3080	.0000	-.2790	1.9794

20.0 4.0 2.0

-3.4308	.0000	.0000	14.0153	.0000	.0000
.0000	1.8379	-.5385	.0000	-6.2356	-.1925
.0000	-.5385	1.5930	.0000	-.1925	-7.7797
14.0153	.0000	.0000	-3.4308	.0000	.0000
.0000	-6.2356	-.1925	.0000	1.8379	-.5385
.0000	-.1925	-7.7797	.0000	-.5385	1.5930

20.0 6.0 2.0

-2.6363	.0000	.0000	13.1075	.0000	.0000
.0000	1.6667	-.7590	.0000	-4.5723	-.2943
.0000	-.7590	.9696	.0000	-.2943	-8.5352
13.1075	.0000	.0000	-2.6363	.0000	.0000
.0000	-4.5723	-.2943	.0000	1.6667	-.7590
.0000	-.2943	-8.5352	.0000	-.7590	.9696

20.0 8.0 2.0

-1.6808	.0000	.0000	12.0093	.0000	.0000
.0000	1.5364	-.9216	.0000	-2.4836	-.3915
.0000	-.9216	.1445	.0000	-.3915	-9.5256
12.0093	.0000	.0000	-1.6808	.0000	.0000
.0000	-2.4836	-.3915	.0000	1.5364	-.9216
.0000	-.3915	-9.5256	.0000	-.9216	.1445

20.0 4.0 4.0

-2.9383	.0000	.0000	13.4487	.0000	.0000
.0000	1.4692	-1.0416	.0000	-6.7243	-.3936
.0000	-1.0416	1.4692	.0000	-.3936	-6.7243
13.4487	.0000	.0000	-2.9383	.0000	.0000
.0000	-6.7243	-.3936	.0000	1.4692	-1.0416
.0000	-.3936	-6.7243	.0000	-1.0416	1.4692

20.0 6.0 4.0

-2.1961	.0000	.0000	12.5910	.0000	.0000
.0000	1.3286	-1.4741	.0000	-5.0800	-.6028
.0000	-1.4741	.8675	.0000	-.6028	-7.5109
12.5910	.0000	.0000	-2.1961	.0000	.0000
.0000	-5.0800	-.6028	.0000	1.3286	-1.4741
.0000	-.6028	-7.5109	.0000	-1.4741	.8675

1.0 1.0 1.0

.0000	-4.1746	-4.1746	.0000	4.1402	4.1402
-4.1746	.0000	-4.1746	4.1402	.0000	4.1402
-4.1746	-4.1746	.0000	4.1402	4.1402	.0000
.0000	4.1402	4.1402	.0000	-4.1746	-4.1746
4.1402	.0000	4.1402	-4.1746	.0000	-4.1746
4.1402	4.1402	.0000	-4.1746	-4.1746	.0000

3.0 1.0 1.0

-5.9078	-3.3836	-3.3836	6.4051	3.2831	3.2831
-3.3836	2.9539	-1.1299	3.2831	-3.2026	1.0931
-3.3836	-1.1299	2.9539	3.2831	1.0931	-3.2026
6.4051	3.2831	3.2831	-5.9078	-3.3836	-3.3836
3.2831	-3.2026	1.0931	-3.3836	2.9539	-1.1299
3.2831	1.0931	-3.2026	-3.3836	-1.1299	2.9539

3.0 3.0 1.0

-1.6676	-5.8187	-1.9455	1.9231	5.5252	1.8378
-5.8187	-1.6676	-1.9455	5.5252	1.9231	1.8378
-1.9455	-1.9455	3.3353	1.8378	1.8378	-3.8462
1.9231	5.5252	1.8378	-1.6676	-5.8187	-1.9455
5.5252	1.9231	1.8378	-5.8187	-1.6676	-1.9455
1.8378	1.8378	-3.8462	-1.9455	-1.9455	3.3353

3.0 3.0 3.0

.0000	-4.0695	-4.0695	.0000	3.7549	3.7549
-4.0695	.0000	-4.0695	3.7549	.0000	3.7549
-4.0695	-4.0695	.0000	3.7549	3.7549	.0000
.0000	3.7549	3.7549	.0000	-4.0695	-4.0695
3.7549	.0000	3.7549	-4.0695	.0000	-4.0695
3.7549	3.7549	.0000	-4.0695	-4.0695	.0000

5.0 1.0 1.0

-6.9066	-2.2508	-2.2508	8.3560	2.0925	2.0925
-2.2508	3.4533	-.4561	2.0925	-4.1780	.4146
-2.2508	-.4561	3.4533	2.0925	.4146	-4.1780
8.3560	2.0925	2.0925	-6.9066	-2.2508	-2.2508
2.0925	-4.1780	.4146	-2.2508	3.4533	-.4561
2.0925	.4146	-4.1780	-2.2508	-.4561	3.4533

5.0 3.0 1.0

-4.3285	-5.1525	-1.7269	5.5497	4.6898	1.5570
-5.1525	.8823	-1.0481	4.6898	-1.0902	.9265
-1.7269	-1.0481	3.4462	1.5570	.9265	-4.4595
5.5497	4.6898	1.5570	-4.3285	-5.1525	-1.7269
4.6898	-1.0902	.9265	-5.1525	.8823	-1.0481
1.5570	.9265	-4.4595	-1.7269	-1.0481	3.4462

5.0 5.0 1.0

-1.6702	-5.7571	-1.1794	2.4539	5.0271	.9868
-5.7571	-1.6702	-1.1794	5.0271	2.4539	.9868
-1.1794	-1.1794	3.3403	.9868	.9868	-4.9077
2.4539	5.0271	.9868	-1.6702	-5.7571	-1.1794
5.0271	2.4539	.9868	-5.7571	-1.6702	-1.1794
.9868	.9868	-4.9077	-1.1794	-1.1794	3.3403

5.0 3.0 3.0

-2.7471	-4.1742	-4.1742	3.7266	3.6773	3.6773
-4.1742	1.3736	-2.5396	3.6773	-1.8633	2.1835
-4.1742	-2.5396	1.3736	3.6773	2.1835	-1.8633
3.7266	3.6773	3.6773	-2.7471	-4.1742	-4.1742
3.6773	-1.8633	2.1835	-4.1742	1.3736	-2.5396
3.6773	2.1835	-1.8633	-4.1742	-2.5396	1.3736

5.0 5.0 3.0

-.9373	-4.9604	-3.0321	1.4530	4.1749	2.4679
-4.9604	-.9373	-3.0321	4.1749	1.4530	2.4679
-3.0321	-3.0321	1.8746	2.4679	2.4679	-2.9060
1.4530	4.1749	2.4679	-.9373	-4.9604	-3.0321
4.1749	1.4530	2.4679	-4.9604	-.9373	-3.0321
2.4679	2.4679	-2.9060	-3.0321	-3.0321	1.8746

5.0 5.0 5.0					
.0000	-3.9004	-3.9004	.0000	3.0057	3.0057
-3.9004	.0000	-3.9004	3.0057	.0000	3.0057
-3.9004	-3.9004	.0000	3.0057	3.0057	.0000
.0000	3.0057	3.0057	.0000	-3.9004	-3.9004
3.0057	.0000	3.0057	-3.9004	.0000	-3.9004
3.0057	3.0057	.0000	-3.9004	-3.9004	.0000
7.0 1.0 1.0					
-6.8486	-1.6103	-1.6103	9.6220	1.4075	1.4075
-1.6103	3.4243	-.2418	1.4075	-4.8110	.1935
-1.6103	-.2418	3.4243	1.4075	.1935	-4.8110
9.6220	1.4075	1.4075	-6.8486	-1.6103	-1.6103
1.4075	-4.8110	.1935	-1.6103	3.4243	-.2418
1.4075	.1935	-4.8110	-1.6103	-.2418	3.4243
7.0 3.0 1.0					
-5.2811	-4.1249	-1.3872	7.8467	3.5319	1.1690
-4.1249	1.9567	-.6239	3.5319	-2.8092	.4822
-1.3872	-.6239	3.3244	1.1690	.4822	-5.0375
7.8467	3.5319	1.1690	-5.2811	-4.1249	-1.3872
3.5319	-2.8092	.4822	-4.1249	1.9567	-.6239
1.1690	.4822	-5.0375	-1.3872	-.6239	3.3244
7.0 5.0 1.0					
-3.1906	-5.2691	-1.0902	5.3573	4.3327	.8419
-5.2691	.0779	-.8079	4.3327	.0964	.5827
-1.0902	-.8079	3.1128	.8419	.5827	-5.4537
5.3573	4.3327	.8419	-3.1906	-5.2691	-1.0902
4.3327	.0964	.5827	-5.2691	.0779	-.8079
.8419	.5827	-5.4537	-1.0902	-.8079	3.1128
7.0 7.0 1.0					
-1.3958	-5.3524	-.8365	3.0061	4.1498	.5447
-5.3524	-1.3958	-.8365	4.1498	3.0061	.5447
-.8365	-.8365	2.7915	.5447	.5447	-6.0122
3.0061	4.1498	.5447	-1.3958	-5.3524	-.8365
4.1498	3.0061	.5447	-5.3524	-1.3958	-.8365
.5447	.5447	-6.0122	-.8365	-.8365	2.7915
7.0 3.0 3.0					
-4.1115	-3.6227	-3.6227	6.4562	2.9842	2.9842
-3.6227	2.0557	-1.6390	2.9842	-3.2281	1.2232
-3.6227	-1.6390	2.0557	2.9842	1.2232	-3.2281
6.4562	2.9842	2.9842	-4.1115	-3.6227	-3.6227
2.9842	-3.2281	1.2232	-3.6227	2.0557	-1.6390
2.9842	1.2232	-3.2281	-3.6227	-1.6390	2.0557
7.0 5.0 3.0					
-2.4893	-4.7557	-2.9260	4.4097	3.7454	2.1982
-4.7557	.3593	-2.1760	3.7454	-.4912	1.5148
-2.9260	-2.1760	2.1300	2.1982	1.5148	-3.9185
4.4097	3.7454	2.1982	-2.4893	-4.7557	-2.9260
3.7454	-.4912	1.5148	-4.7557	.3593	-2.1760
2.1982	1.5148	-3.9185	-2.9260	-2.1760	2.1300

7.0 7.0 3.0						
	-1.0403	-4.9572	-2.3041	2.3671	3.6557	1.4465
	-4.9572	-1.0403	-2.3041	3.6557	2.3671	1.4465
	-2.3041	-2.3041	2.0806	1.4465	1.4465	-4.7341
	2.3671	3.6557	1.4465	-1.0403	-4.9572	-2.3041
	3.6557	2.3671	1.4465	-4.9572	-1.0403	-2.3041
	1.4465	1.4465	-4.7341	-2.3041	-2.3041	2.0806
7.0 5.0 5.0						
	-1.4664	-4.0016	-4.0016	2.9119	2.8453	2.8453
	-4.0016	.7332	-2.9957	2.8453	-1.4560	1.9425
	-4.0016	-2.9957	.7332	2.8453	1.9425	-1.4560
	2.9119	2.8453	2.8453	-1.4664	-4.0016	-4.0016
	2.8453	-1.4560	1.9425	-4.0016	.7332	-2.9957
	2.8453	1.9425	-1.4560	-4.0016	-2.9957	.7332
7.0 7.0 5.0						
	-.5066	-4.3469	-3.2843	1.2843	2.8491	1.9150
	-4.3469	-.5066	-3.2843	2.8491	1.2843	1.9150
	-3.2843	-3.2843	1.0132	1.9150	1.9150	-2.5685
	1.2843	2.8491	1.9150	-.5066	-4.3469	-3.2843
	2.8491	1.2843	1.9150	-4.3469	-.5066	-3.2843
	1.9150	1.9150	-2.5685	-3.2843	-3.2843	1.0132
7.0 7.0 7.0						
	.0000	-3.7324	-3.7324	.0000	1.9464	1.9464
	-3.7324	.0000	-3.7324	1.9464	.0000	1.9464
	-3.7324	-3.7324	.0000	1.9464	1.9464	.0000
	.0000	1.9464	1.9464	.0000	-3.7324	-3.7324
	1.9464	.0000	1.9464	-3.7324	.0000	-3.7324
	1.9464	1.9464	.0000	-3.7324	-3.7324	.0000
9.0 1.0 1.0						
	-6.4446	-1.2022	-1.2022	10.7947	.9728	.9728
	-1.2022	3.2223	-.1528	.9728	-5.3974	.0961
	-1.2022	-.1528	3.2223	.9728	.0961	-5.3974
	10.7947	.9728	.9728	-6.4446	-1.2022	-1.2022
	.9728	-5.3974	.0961	-1.2022	3.2223	-.1528
	.9728	.0961	-5.3974	-1.2022	-.1528	3.2223
9.0 3.0 1.0						
	-5.4193	-3.2437	-1.0952	9.5880	2.5730	.8479
	-3.2437	2.3413	-.4169	2.5730	-3.9621	.2502
	-1.0952	-.4169	3.0780	.8479	.2502	-5.6260
	9.5880	2.5730	.8479	-5.4193	-3.2437	-1.0952
	2.5730	-3.9621	.2502	-3.2437	2.3413	-.4169
	.8479	.2502	-5.6260	-1.0952	-.4169	3.0780
9.0 5.0 1.0						
	-3.8517	-4.4648	-.9348	7.6721	3.4046	.6520
	-4.4648	1.0578	-.5862	3.4046	-1.6111	.3203
	-.9348	-.5862	2.7939	.6520	.3203	-6.0610
	7.6721	3.4046	.6520	-3.8517	-4.4648	-.9348
	3.4046	-1.6111	.3203	-4.4648	1.0578	-.5862
	.6520	.3203	-6.0610	-.9348	-.5862	2.7939

9.0 7.0 1.0					
-2.2641	-4.8672	-.7781	5.5978	3.5037	.4438
-4.8672	-.1208	-.6583	3.5037	1.0656	.3120
-.7781	-.6583	2.3850	.4438	.3120	-6.6635
5.5978	3.5037	.4438	-2.2641	-4.8672	-.7781
3.5037	1.0656	.3120	-4.8672	-.1208	-.6583
.4438	.3120	-6.6635	-.7781	-.6583	2.3850
9.0 9.0 1.0					
-.9404	-4.6797	-.6556	3.6908	3.1312	.2563
-4.6797	-.9404	-.6556	3.1312	3.6908	.2563
-.6556	-.6556	1.8808	.2563	.2563	-7.3816
3.6908	3.1312	.2563	-.9404	-4.6797	-.6556
3.1312	3.6908	.2563	-4.6797	-.9404	-.6556
.2563	.2563	-7.3816	-.6556	-.6556	1.8808
9.0 3.0 3.0					
-4.5748	-2.9807	-2.9807	8.5503	2.2565	2.2565
-2.9807	2.2874	-1.1459	2.2565	-4.2751	.6558
-2.9807	-1.1459	2.2874	2.2565	.6558	-4.2751
8.5503	2.2565	2.2565	-4.5748	-2.9807	-2.9807
2.2565	-4.2751	.6558	-2.9807	2.2874	-1.1459
2.2565	.6558	-4.2751	-2.9807	-1.1459	2.2874
9.0 5.0 3.0					
-3.2620	-4.1597	-2.5794	6.8657	3.0121	1.7496
-4.1597	1.1150	-1.6299	3.0121	-2.0221	.8473
-2.5794	-1.6299	2.1470	1.7496	.8473	-4.8436
6.8657	3.0121	1.7496	-3.2620	-4.1597	-2.5794
3.0121	-2.0221	.8473	-4.1597	1.1150	-1.6299
1.7496	.8473	-4.8436	-2.5794	-1.6299	2.1470
9.0 7.0 3.0					
-1.9075	-4.6038	-2.1803	4.9899	3.1227	1.1962
-4.6038	.0156	-1.8523	3.1227	.5984	.8314
-2.1803	-1.8523	1.8919	1.1962	.8314	-5.5883
4.9899	3.1227	1.1962	-1.9075	-4.6038	-2.1803
3.1227	.5984	.8314	-4.6038	.0156	-1.8523
1.1962	.8314	-5.5883	-2.1803	-1.8523	1.8919
9.0 9.0 3.0					
-.7622	-4.4901	-1.8642	3.2168	2.8004	.6847
-4.4901	-.7622	-1.8642	2.8004	3.2168	.6847
-1.8642	-1.8642	1.5244	.6847	.6847	-6.4335
3.2168	2.8004	.6847	-.7622	-4.4901	-1.8642
2.8004	3.2168	.6847	-4.4901	-.7622	-1.8642
.6847	.6847	-6.4335	-1.8642	-1.8642	1.5244
9.0 5.0 5.0					
-2.3239	-3.6828	-3.6828	5.5089	2.3619	2.3619
-3.6828	1.1619	-2.3611	2.3619	-2.7544	1.1088
-3.6828	-2.3611	1.1619	2.3619	1.1088	-2.7544
5.5089	2.3619	2.3619	-2.3239	-3.6828	-3.6828
2.3619	-2.7544	1.1088	-3.6828	1.1619	-2.3611
2.3619	1.1088	-2.7544	-3.6828	-2.3611	1.1619

[illegible].0 7.0 5.0					
-1.3316	-4.1836	-3.1958	3.9255	2.4677	1.6202
-4.1836	.2092	-2.7368	2.4677	-.2388	1.0980
-3.1958	-2.7368	1.1224	1.6202	1.0980	-3.6867
3.9255	2.4677	1.6202	-1.3316	-4.1836	-3.1958
2.4677	-.2388	1.0980	-4.1836	.2092	-2.7368
1.6202	1.0980	-3.6867	-3.1958	-2.7368	1.1224
[illegible].0 9.0 5.0					
-.4799	-4.1851	-2.8039	2.3557	2.2120	.9031
-4.1851	-.4799	-2.8039	2.2120	2.3557	.9031
-2.8039	-2.8039	.9599	.9031	.9031	-4.7114
2.3557	2.2120	.9031	-.4799	-4.1851	-2.8039
2.2120	2.3557	.9031	-4.1851	-.4799	-2.8039
.9031	.9031	-4.7114	-2.8039	-2.8039	.9599
[illegible].0 7.0 7.0					
-.7167	-3.7461	-3.7461	2.6149	1.6823	1.6823
-3.7461	.3584	-3.2437	1.6823	-1.3074	1.0894
-3.7461	-3.2437	.3584	1.6823	1.0894	-1.3074
2.6149	1.6823	1.6823	-.7167	-3.7461	-3.7461
1.6823	-1.3074	1.0894	-3.7461	.3584	-3.2437
1.6823	1.0894	-1.3074	-3.7461	-3.2437	.3584
[illegible].[illegible] [illegible].0 7.0					
-.1976	-3.8693	-3.3946	1.2395	1.4715	.8811
-3.8693	-.1976	-3.3946	1.4715	1.2395	.8811
-3.3946	-3.3946	.3952	.8811	.8811	-2.4791
1.2395	1.4715	.8811	-.1976	-3.8693	-3.3946
1.4715	1.2395	.8811	-3.8693	-.1976	-3.3946
.8811	.8811	-2.4791	-3.3946	-3.3946	.3952
[illegible].[illegible] [illegible].0 9.0					
.0000	-3.6292	-3.6292	.0000	.6742	.6742
-3.6292	.0000	-3.6292	.6742	.0000	.6742
-3.6292	-3.6292	.0000	.6742	.6742	.0000
.0000	.6742	.6742	.0000	-3.6292	-3.6292
.6742	.0000	.6742	-3.6292	.0000	-3.6292
.6742	.6742	.0000	-3.6292	-3.6292	.0000
11.0 1.0 1.0					
-5.9054	-.9073	-.9073	11.9374	.6732	.6732
-.9073	2.9527	-.1104	.6732	-5.9687	.0443
-.9073	-.1104	2.9527	.6732	.0443	-5.9687
11.9374	.6732	.6732	-5.9054	-.9073	-.9073
.6732	-5.9687	.0443	-.9073	2.9527	-.1104
.6732	.0443	-5.9687	-.9073	-.1104	2.9527
[illegible].0 3.0 1.0					
-5.1814	-2.5153	-.8530	11.0629	1.8302	.5998
-2.5153	2.4069	-.3108	1.8302	-4.8480	.1162
-.8530	-.3108	2.7744	.5998	.1162	-6.2149
11.0629	1.8302	.5998	-5.1814	-2.5153	-.8530
1.8302	-4.8480	.1162	-2.5153	2.4069	-.3108
.5998	.1162	-6.2149	-.8530	-.3108	2.7744

11.0 5.0 1.0

-3.9822	-3.6142	-.7663	9.5748	2.5301	.4753
-3.6142	1.5549	-.4597	2.5301	-2.8865	.1482
-.7663	-.4597	2.4273	.4753	.1482	-6.6884
9.5748	2.5301	.4753	-3.9822	-3.6142	-.7663
2.5301	-2.8865	.1482	-3.6142	1.5549	-.4597
.4753	.1482	-6.6884	-.7663	-.4597	2.4273

11.0 7.0 1.0

-2.6320	-4.1245	-.6755	7.8205	2.7281	.3293
-4.1245	.6996	-.5462	2.7281	-.4684	.1383
-.6755	-.5462	1.9324	.3293	.1383	-7.3521
7.8205	2.7281	.3293	-2.6320	-4.1245	-.6755
2.7281	-.4684	.1383	-4.1245	.6996	-.5462
.3293	.1383	-7.3521	-.6755	-.5462	1.9324

11.0 9.0 1.0

-1.3734	-4.1290	-.6005	6.0768	2.5401	.1841
-4.1290	.0481	-.5735	2.5401	2.0753	.1002
-.6005	-.5735	1.3253	.1841	.1002	-8.1521
6.0768	2.5401	.1841	-1.3734	-4.1290	-.6005
2.5401	2.0753	.1002	-4.1290	.0481	-.5735
.1841	.1002	-8.1521	-.6005	-.5735	1.3253

11.011.0 1.0

-.3284	-3.7615	-.5495	4.5093	2.1275	.0525
-3.7615	-.3284	-.5495	2.1275	4.5093	.0525
-.5495	-.5495	.6568	.0525	.0525	-9.0187
4.5093	2.1275	.0525	-.3284	-3.7615	-.5495
2.1275	4.5093	.0525	-3.7615	-.3284	-.5495
.0525	.0525	-9.0187	-.5495	-.5495	.6568

11.0 3.0 3.0

-4.5501	-2.3756	-2.3756	10.2713	1.6336	1.6336
-2.3756	2.2750	-.8778	1.6336	-5.1356	.3045
-2.3756	-.8778	2.2750	1.6336	.3045	-5.1356
10.2713	1.6336	1.6336	-4.5501	-2.3756	-2.3756
1.6336	-5.1356	.3045	-2.3756	2.2750	-.8778
1.6336	.3045	-5.1356	-2.3756	-.8778	2.2750

11.0 5.0 3.0

-3.4966	-3.4411	-2.1517	8.9089	2.2634	1.2967
-3.4411	1.4906	-1.3062	2.2634	-3.2296	.3871
-2.1517	-1.3062	2.0059	1.2967	.3871	-5.6793
8.9089	2.2634	1.2967	-3.4966	-3.4411	-2.1517
2.2634	-3.2296	.3871	-3.4411	1.4906	-1.3062
1.2967	.3871	-5.6793	-2.1517	-1.3062	2.0059

11.0 7.0 3.0

-2.2995	-3.9658	-1.9160	7.2780	2.4426	.8950
-3.9658	.6989	-1.5626	2.4426	-.8524	.3567
-1.9160	-1.5626	1.6006	.8950	.3567	-6.4255
7.2780	2.4426	.8950	-2.2995	-3.9658	-1.9160
2.4426	-.8524	.3567	-3.9658	.6989	-1.5626
.8950	.3567	-6.4255	-1.9160	-1.5626	1.6006

11.0 9.0 3.0

-1.1755	-4.0113	-1.7218	5.6301	2.2689	.4890
-4.0113	.0978	-1.6517	2.2689	1.6781	.2489
-1.7218	-1.6517	1.0776	.4890	.2489	-7.3081
5.6301	2.2689	.4890	-1.1755	-4.0113	-1.7218
2.2689	1.6781	.2489	-4.0113	.0978	-1.6517
.4890	.2489	-7.3081	-1.7218	-1.6517	1.0776

11.011.0 3.0

-.2388	-3.6905	-1.5921	4.1255	1.8884	.1149
-3.6905	-.2388	-1.5921	1.8884	4.1255	.1149
-1.5921	-1.5921	.4776	.1149	.1149	-8.2509
4.1255	1.8884	.1149	-.2388	-3.6905	-1.5921
1.8884	4.1255	.1149	-3.6905	-.2388	-1.5921
.1149	.1149	-8.2509	-1.5921	-1.5921	.4776

11.0 5.0 5.0

-2.6772	-3.1617	-3.1617	7.7404	1.7977	1.7977
-3.1617	1.3386	-1.9633	1.7977	-3.8702	.4856
-3.1617	-1.9633	1.3386	1.7977	.4856	-3.8702
7.7404	1.7977	1.7977	-2.6772	-3.1617	-3.1617
1.7977	-3.8702	.4856	-3.1617	1.3386	-1.9633
1.7977	.4856	-3.8702	-3.1617	-1.9633	1.3386

11.0 7.0 5.0

-1.7345	-3.7098	-2.8671	6.3035	1.9321	1.2272
-3.7098	.6619	-2.3768	1.9321	-1.5682	.4303
-2.8671	-2.3768	1.0725	1.2272	.4303	-4.7352
6.3035	1.9321	1.2272	-1.7345	-3.7098	-2.8671
1.9321	-1.5682	.4303	-3.7098	.6619	-2.3768
1.2272	.4303	-4.7352	-2.8671	-2.3768	1.0725

11.0 9.0 5.0

-.8422	-3.8250	-2.6284	4.8078	1.7724	.6326
-3.8250	.1568	-2.5430	1.7724	.9342	.2670
-2.6284	-2.5430	.6854	.6326	.2670	-5.7420
4.8078	1.7724	.6326	-.8422	-3.8250	-2.6284
1.7724	.9342	.2670	-3.8250	.1568	-2.5430
.6326	.2670	-5.7420	-2.6284	-2.5430	.6854

11.011.0 5.0

-.0998	-3.5858	-2.4791	3.4023	1.4404	.0679
-3.5858	-.0998	-2.4791	1.4404	3.4023	.0679
-2.4791	-2.4791	.1997	.0679	.0679	-6.8046
3.4023	1.4404	.0679	-.0998	-3.5858	-2.4791
1.4404	3.4023	.0679	-3.5858	-.0998	-2.4791
.0679	.0679	-6.8046	-2.4791	-2.4791	.1997

11.0 7.0 7.0

-1.0817	-3.4438	-3.4438	5.0641	1.2853	1.2853
-3.4438	.5408	-2.9201	1.2853	-2.5321	.3407
-3.4438	-2.9201	.5408	1.2853	.3407	-2.5321
5.0641	1.2853	1.2853	-1.0817	-3.4438	-3.4438
1.2853	-2.5321	.3407	-3.4438	.5408	-2.9201
1.2853	.3407	-2.5321	-3.4438	-2.9201	.5408

11.0 9.0 7.0

-.4689	-3.6437	-3.2414	3.7239	1.1203	.5843
-3.6437	.1654	-3.1733	1.1203	-.0734	.1337
-3.2414	-3.1733	.3035	.5843	.1337	-3.6505
3.7239	1.1203	.5843	-.4689	-3.6437	-3.2414
1.1203	-.0734	.1337	-3.6437	.1654	-3.1733
.5843	.1337	-3.6505	-3.2414	-3.1733	.3035

11.011.0 7.0

.0250	-3.5060	-3.1406	2.4147	.8309	-.1089
-3.5060	.0250	-3.1406	.8309	2.4147	-.1089
-3.1406	-3.1406	-.0500	-.1089	-.1089	-4.8295
2.4147	.8309	-.1089	.0250	-3.5060	-3.1406
.8309	2.4147	-.1089	-3.5060	.0250	-3.1406
-.1089	-.1089	-4.8295	-3.1406	-3.1406	-.0500

11.0 9.0 9.0

-.1447	-3.5341	-3.5341	2.5007	.3824	.3824
-3.5341	.0724	-3.5083	.3824	-1.2504	-.1104
-3.5341	-3.5083	.0724	.3824	-.1104	-1.2504
2.5007	.3824	.3824	-.1447	-3.5341	-3.5341
.3824	-1.2504	-.1104	-3.5341	.0724	-3.5083
.3824	-.1104	-1.2504	-3.5341	-3.5083	.0724

13.0 1.0 1.0

-5.3430	-.6709	-.6709	12.9980	.4554	.4554
-.6709	2.6715	-.0891	.4554	-6.4990	.0136
-.6709	-.0891	2.6715	.4554	.0136	-6.4990
12.9980	.4554	.4554	-5.3430	-.6709	-.6709
.4554	-6.4990	.0136	-.6709	2.6715	-.0891
.4554	.0136	-6.4990	-.6709	-.0891	2.6715

13.0 3.0 1.0

-4.7919	-1.8882	-.6430	12.3292	1.2575	.4094
-1.8882	2.3285	-.2555	1.2575	-5.5621	.0327
-.6430	-.2555	2.4634	.4094	.0327	-6.7671
12.3292	1.2575	.4094	-4.7919	-1.8882	-.6430
1.2575	-5.5621	.0327	-1.8882	2.3285	-.2555
.4094	.0327	-6.7671	-.6430	-.2555	2.4634

13.0 5.0 1.0

-3.8325	-2.7831	-.5974	11.1435	1.7840	.3275
-2.7831	1.7738	-.3902	1.7840	-3.8586	.0324
-.5974	-.3902	2.0586	.3275	.0324	-7.2850
11.1435	1.7840	.3275	-3.8325	-2.7831	-.5974
1.7840	-3.8586	.0324	-2.7831	1.7738	-.3902
.3275	.0324	-7.2850	-.5974	-.3902	2.0586

13.0 7.0 1.0

-2.6738	-3.2704	-.5482	9.6686	1.9815	.2251
-3.2704	1.1920	-.4818	1.9815	-1.6532	.0110
-.5482	-.4818	1.4818	.2251	.0110	-8.0154
9.6686	1.9815	.2251	-2.6738	-3.2704	-.5482
1.9815	-1.6532	.0110	-3.2704	1.1920	-.4818
.2251	.0110	-8.0154	-.5482	-.4818	1.4818

13.0 9.0 1.0

-1.5066	-3.3664	-.5075	8.1218	1.8969	.1163
-3.3664	.7332	-.5256	1.8969	.7802	-.0237
-.5075	-.5256	.7734	.1163	-.0237	-8.9020
8.1218	1.8969	.1163	-1.5066	-3.3664	-.5075
1.8969	.7802	-.0237	-3.3664	.7332	-.5256
.1163	-.0237	-8.9020	-.5075	-.5256	.7734

13.011.0 1.0

-.4607	-3.1398	-.4813	6.6671	1.6255	.0113
-3.1398	.4695	-.5213	1.6255	3.2022	-.0591
-.4813	-.5213	-.0089	.0113	-.0591	-9.8693
6.6671	1.6255	.0113	-.4607	-3.1398	-.4813
1.6255	3.2022	-.0591	-3.1398	.4695	-.5213
.0113	-.0591	-9.8693	-.4813	-.5213	-.0089

13.013.0 1.0

.3953	-2.6694	-.4699	5.4126	1.2630	-.0823
-2.6694	.3953	-.4699	1.2630	5.4126	-.0823
-.4699	-.4699	-.7906	-.0823	-.0823	-10.8253
5.4126	1.2630	-.0823	.3953	-2.6694	-.4699
1.2630	5.4126	-.0823	-2.6694	.3953	-.4699
-.0823	-.0823	-10.8253	-.4699	-.4699	-.7906

13.0 3.0 3.0

-4.2934	-1.8152	-1.8152	11.7055	1.1299	1.1299
-1.8152	2.1467	-.7341	1.1299	-5.8527	.0765
-1.8152	-.7341	2.1467	1.1299	.0765	-5.8527
11.7055	1.1299	1.1299	-4.2934	-1.8152	-1.8152
1.1299	-5.8527	.0765	-1.8152	2.1467	-.7341
1.1299	.0765	-5.8527	-1.8152	-.7341	2.1467

13.0 5.0 3.0

-3.4223	-2.6902	-1.6957	10.5931	1.6011	.9020
-2.6902	1.6350	-1.1253	1.6011	-4.1819	.0671
-1.6957	-1.1253	1.7873	.9020	.0671	-6.4112
10.5931	1.6011	.9020	-3.4223	-2.6902	-1.6957
1.6011	-4.1819	.0671	-2.6902	1.6350	-1.1253
.9020	.0671	-6.4112	-1.6957	-1.1253	1.7873

13.0 7.0 3.0

-2.3654	-3.1840	-1.5680	9.1974	1.7723	.6138
-3.1840	1.1017	-1.3954	1.7723	-2.0033	.0000
-1.5680	-1.3954	1.2637	.6138	.0000	-7.1940
9.1974	1.7723	.6138	-2.3654	-3.1840	-1.5680
1.7723	-2.0033	.0000	-3.1840	1.1017	-1.3954
.6138	.0000	-7.1940	-1.5680	-1.3954	1.2637

13.0 9.0 3.0

-1.2965	-3.3043	-1.4644	7.7191	1.6851	.3036
-3.3043	.6913	-1.5300	1.6851	.4204	-.1036
-1.4644	-1.5300	.6052	.3036	-.1036	-8.1395
7.7191	1.6851	.3036	-1.2965	-3.3043	-1.4644
1.6851	.4204	-.1036	-3.3043	.6913	-1.5300
.3036	-.1036	-8.1395	-1.4644	-1.5300	.6052

13.011.0 3.0

-.3365	-3.1079	-1.4018	6.3149	1.4280	.0000
-3.1079	.4753	-1.5250	1.4280	2.8535	-.2073
-1.4018	-1.5250	-.1388	.0000	-.2073	-9.1684
6.3149	1.4280	.0000	-.3365	-3.1079	-1.4018
1.4280	2.8535	-.2073	-3.1079	.4753	-1.5250
.0000	-.2073	-9.1684	-1.4018	-1.5250	-.1388

13.013.0 3.0

.4488	-2.6635	-1.3812	5.0927	1.0925	-.2733
-2.6635	.4488	-1.3812	1.0925	5.0927	-.2733
-1.3812	-1.3812	-.8977	-.2733	-.2733	-10.1854
5.0927	1.0925	-.2733	.4488	-2.6635	-1.3812
1.0925	5.0927	-.2733	-2.6635	.4488	-1.3812
-.2733	-.2733	-10.1854	-1.3812	-1.3812	-.8977

13.0 5.0 5.0

-2.7016	-2.5392	-2.5392	9.6008	1.2700	1.2700
-2.5392	1.3508	-1.7360	1.2700	-4.8004	.0275
-2.5392	-1.7360	1.3508	1.2700	.0275	-4.8004
9.6008	1.2700	1.2700	-2.7016	-2.5392	-2.5392
1.2700	-4.8004	.0275	-2.5392	1.3508	-1.7360
1.2700	.0275	-4.8004	-2.5392	-1.7360	1.3508

13.0 7.0 5.0

-1.8216	-3.0469	-2.3814	8.3356	1.3872	.8435
-3.0469	.9044	-2.1707	1.3872	-2.6727	-.0936
-2.3814	-2.1707	.9171	.8435	-.0936	-5.6629
8.3356	1.3872	.8435	-1.8216	-3.0469	-2.3814
1.3872	-2.6727	-.0936	-3.0469	.9044	-2.1707
.8435	-.0936	-5.6629	-2.3814	-2.1707	.9171

13.0 9.0 5.0

-.9276	-3.2124	-2.2616	6.9706	1.2879	.3737
-3.2124	.5833	-2.4025	1.2879	-.2694	-.2654
-2.2616	-2.4025	.3443	.3737	-.2654	-6.7012
6.9706	1.2879	.3737	-.9276	-3.2124	-2.2616
1.2879	-.2694	-.2654	-3.2124	.5833	-2.4025
.3737	-.2654	-6.7012	-2.2616	-2.4025	.3443

13.011.0 5.0

-.1252	-3.0719	-2.2045	5.6488	1.0504	-.0969
-3.0719	.4586	-2.4181	1.0504	2.1827	-.4323
-2.2045	-2.4181	-.3333	-.0969	-.4323	-7.8316
5.6488	1.0504	-.0969	-.1252	-3.0719	-2.2045
1.0504	2.1827	-.4323	-3.0719	.4586	-2.4181
-.0969	-.4323	-7.8316	-2.2045	-2.4181	-.3333

13.0 7.0 7.0

-1.1561	-2.9130	-2.9130	7.2134	.8786	.8786
-2.9130	.5780	-2.7446	.8786	-3.6067	-.2789
-2.9130	-2.7446	.5780	.8786	-.2789	-3.6067
7.2134	.8786	.8786	-1.1561	-2.9130	-2.9130
.8786	-3.6067	-.2789	-2.9130	.5780	-2.7446
.8786	-.2789	-3.6067	-2.9130	-2.7446	.5780

13.0 9.0 7.0					
-.4832	-3.1413	-2.8317	5.9712	.7475	.3002
-3.1413	.3721	-3.0775	.7475	-1.2367	-.5200
-2.8317	-3.0775	.1110	.3002	-.5200	-4.7345
5.9712	.7475	.3002	-.4832	-3.1413	-2.8317
.7475	-1.2367	-.5200	-3.1413	.3721	-3.0775
.3002	-.5200	-4.7345	-2.8317	-3.0775	.1110
15.0 1.0 1.0					
-4.8406	-.4649	-.4649	13.8946	.2911	.2911
-.4649	2.4203	-.0784	.2911	-6.9473	-.0056
-.4649	-.0784	2.4203	.2911	-.0056	-6.9473
13.8946	.2911	.2911	-4.8406	-.4649	-.4649
.2911	-6.9473	-.0056	-.4649	2.4203	-.0784
.2911	-.0056	-6.9473	-.4649	-.0784	2.4203
15.0 3.0 1.0					
-4.3891	-1.3200	-.4512	13.3558	.8108	.2621
-1.3200	2.2022	-.2273	.8108	-6.1195	-.0208
-.4512	-.2273	2.1869	.2621	-.0208	-7.2363
13.3558	.8108	.2621	-4.3891	-1.3200	-.4512
.8108	-6.1195	-.0208	-1.3200	2.2022	-.2273
.2621	-.0208	-7.2363	-.4512	-.2273	2.1869
15.0 5.0 1.0					
-3.5777	-1.9754	-.4285	12.3766	1.1679	.2092
-1.9754	1.8451	-.3542	1.1679	-4.5808	-.0454
-.4285	-.3542	1.7326	.2092	-.0454	-7.7958
12.3766	1.1679	.2092	-3.5777	-1.9754	-.4285
1.1679	-4.5808	-.0454	-1.9754	1.8451	-.3542
.2092	-.0454	-7.7958	-.4285	-.3542	1.7326
15.0 7.0 1.0					
-2.5516	-2.3641	-.4043	11.1167	1.3209	.1403
-2.3641	1.4675	-.4483	1.3209	-2.5286	-.0795
-.4043	-.4483	1.0841	.1403	-.0795	-8.5882
11.1167	1.3209	.1403	-2.5516	-2.3641	-.4043
1.3209	-2.5286	-.0795	-2.3641	1.4675	-.4483
.1403	-.0795	-8.5882	-.4043	-.4483	1.0841
15.0 9.0 1.0					
-1.4621	-2.4784	-.3853	9.7475	1.2871	.0638
-2.4784	1.1765	-.5021	1.2871	-.1928	-.1168
-.3853	-.5021	.2857	.0638	-.1168	-9.5547
9.7475	1.2871	.0638	-1.4621	-2.4784	-.3853
1.2871	-.1928	-.1168	-2.4784	1.1765	-.5021
.0638	-.1168	-9.5547	-.3853	-.5021	.2857
15.011.0 1.0					
-.4329	-2.3495	-.3752	8.4180	1.1195	-.0132
-2.3495	1.0319	-.5102	1.1195	2.1967	-.1471
-.3752	-.5102	-.5990	-.0132	-.1471	-10.6148
8.4180	1.1195	-.0132	-.4329	-2.3495	-.3752
1.1195	2.1967	-.1471	-2.3495	1.0319	-.5102
-.0132	-.1471	-10.6148	-.3752	-.5102	-.5990

15.013.0 1.0					
.4511	-2.0240	-.3745	7.2424	.8795	-.0844
-2.0240	1.0353	-.4695	.8795	4.4257	-.1590
-.3745	-.4695	-1.4863	-.0844	-.1590	-11.6681
7.2424	.8795	-.0844	.4511	-2.0240	-.3745
.8795	4.4257	-.1590	-2.0240	1.0353	-.4695
-.0844	-.1590	-11.6681	-.3745	-.4695	-1.4863
15.0 3.0 3.0					
-3.9702	-1.2838	-1.2838	12.8447	.7290	.7290
-1.2838	1.9851	-.6600	.7290	-6.4223	-.0733
-1.2838	-.6600	1.9851	.7290	-.0733	-6.4223
12.8447	.7290	.7290	-3.9702	-1.2838	-1.2838
.7290	-6.4223	-.0733	-1.2838	1.9851	-.6600
.7290	-.0733	-6.4223	-1.2838	-.6600	1.9851
15.0 5.0 3.0					
-3.2156	-1.9295	-1.2247	11.9130	1.0465	.5790
-1.9295	1.6569	-1.0313	1.0465	-4.9045	-.1524
-1.2247	-1.0313	1.5587	.5790	-.1524	-7.0085
11.9130	1.0465	.5790	-3.2156	-1.9295	-1.2247
1.0465	-4.9045	-.1524	-1.9295	1.6569	-1.0313
.5790	-.1524	-7.0085	-1.2247	-1.0313	1.5587
15.0 7.0 3.0					
-2.2590	-2.3228	-1.1629	10.7083	1.1760	.3820
-2.3228	1.3169	-1.3100	1.1760	-2.8697	-.2580
-1.1629	-1.3100	.9421	.3820	-.2580	-7.8386
10.7083	1.1760	.3820	-2.2590	-2.3228	-1.1629
1.1760	-2.8697	-.2580	-2.3228	1.3169	-1.3100
.3820	-.2580	-7.8386	-1.1629	-1.3100	.9421
15.0 9.0 3.0					
-1.2408	-2.4524	-1.1169	9.3914	1.1339	.1610
-2.4524	1.0700	-1.4733	1.1339	-.5388	-.3722
-1.1169	-1.4733	.1708	.1610	-.3722	-8.8527
9.3914	1.1339	.1610	-1.2408	-2.4524	-1.1169
1.1339	-.5388	-.3722	-2.4524	1.0700	-1.4733
.1610	-.3722	-8.8527	-1.1169	-1.4733	.1708
15.011.0 3.0					
-.2774	-2.3427	-1.0975	8.1051	.9710	-.0639
-2.3427	.9757	-1.5041	.9710	1.8639	-.4644
-1.0975	-1.5041	-.6983	-.0639	-.4644	-9.9690
8.1051	.9710	-.0639	-.2774	-2.3427	-1.0975
.9710	1.8639	-.4644	-2.3427	.9757	-1.5041
-.0639	-.4644	-9.9690	-1.0975	-1.5041	-.6983
15.0 5.0 5.0					
-2.5615	-1.8561	-1.8561	11.0625	.8216	.8216
-1.8561	1.2807	-1.6194	.8216	-5.5313	-.2989
-1.8561	-1.6194	1.2807	.8216	-.2989	-5.5313
11.0625	.8216	.8216	-2.5615	-1.8561	-1.8561
.8216	-5.5313	-.2989	-1.8561	1.2807	-1.6194
.8216	-.2989	-5.5313	-1.8561	-1.6194	1.2807

15.0 7.0 5.0						
	-1.7292	-2.2608	-1.7840	9.9527	.9039	.5218
	-2.2608	1.0070	-2.0711	.9039	-3.5319	-.4846
	-1.7840	-2.0711	.7222	.5218	-.4846	-6.4208
	9.9527	.9039	.5218	-1.7292	-2.2608	-1.7840
	.9039	-3.5319	-.4846	-2.2608	1.0070	-2.0711
	.5218	-.4846	-6.4208	-1.7840	-2.0711	.7222
15.0 9.0 5.0						
	-.8407	-2.4210	-1.7401	8.7259	.8414	.1786
	-2.4210	.8399	-2.3489	.8414	-1.2129	-.6821
	-1.7401	-2.3489	.0000	.1786	-.6821	-7.5130
	8.7259	.8414	.1786	-.8407	-2.4210	-1.7401
	.8414	-1.2129	-.6821	-2.4210	.8399	-2.3489
	.1786	-.6821	-7.5130	-1.7401	-2.3489	.0000
15.0 7.0 7.0						
	-1.0537	-2.2108	-2.2108	8.9538	.5335	.5335
	-2.2108	.5268	-2.6750	.5335	-4.4769	-.7603
	-2.2108	-2.6750	.5268	.5335	-.7603	-4.4769
	8.9538	.5335	.5335	-1.0537	-2.2108	-2.2108
	.5335	-4.4769	-.7603	-2.2108	.5268	-2.6750
	.5335	-.7603	-4.4769	-2.2108	-2.6750	.5268
17.0 1.0 1.0						
	-4.4649	-.2744	-.2744	14.5462	.1614	.1614
	-.2744	2.2324	-.0732	.1614	-7.2731	-.0171
	-.2744	-.0732	2.2324	.1614	-.0171	-7.2731
	14.5462	.1614	.1614	-4.4649	-.2744	-.2744
	.1614	-7.2631	-.0171	-.2744	2.2324	-.0732
	.1614	-.0171	-7.2731	-.2744	-.0732	2.2324
17.0 3.0 1.0						
	-4.0679	-.7828	-.2683	14.0854	.4517	.1452
	-.7828	2.0875	-.2138	.4517	-6.5072	-.0534
	-.2683	-.2138	1.9804	.1452	-.0534	-7.5781
	14.0854	.4517	.1452	-4.0679	-.7828	-.2683
	.4517	-6.5072	-.0534	-.7828	2.0875	-.2138
	.1452	-.0534	-7.5781	-.2683	-.2138	1.9804
17.0 5.0 1.0						
	-3.3405	-1.1816	-.2583	13.2360	.6562	.1150
	-1.1816	1.8513	-.3372	.6562	-5.0661	-.0942
	-.2583	-.3372	1.4892	.1150	-.0942	-8.1698
	13.2360	.6562	.1150	-3.3405	-1.1816	-.2583
	.6562	-5.0661	-.0942	-1.1816	1.8513	-.3372
	.1150	-.0942	-8.1698	-.2583	-.3372	1.4892
17.0 7.0 1.0						
	-2.3945	-1.4293	-.2480	12.1208	.7498	.0749
	-1.4293	1.6074	-.4332	.7498	-3.1109	-.1382
	-.2480	-.4332	.7871	.0749	-.1382	-9.0099
	12.1208	.7498	.0749	-2.3945	-1.4293	-.2480
	.7498	-3.1109	-.1382	-1.4293	1.6074	-.4332
	.0749	-.1382	-9.0099	-.2480	-.4332	.7871

17.0 9.0 1.0

-1.3568	-1.5150	-.2408	10.8820	.7380	.0291
-1.5150	1.4362	-.4928	.7380	-.8441	-.1794
-.2408	-.4928	-.0794	.0291	-.1794	-10.0379
10.8820	.7380	.0291	-1.3568	-1.5150	-.2408
.7380	-.8441	-.1794	-1.5150	1.4362	-.4928
.0291	-.1794	-10.0379	-.2408	-.4928	-.0794

17.011.0 1.0

-.3434	-1.4508	-.2387	9.6546	.6475	-.0182
-1.4508	1.3854	-.5085	.6475	1.5151	-.2082
-.2387	-.5085	-1.0420	-.0182	-.2082	-11.1697
9.6546	.6475	-.0182	-.3434	-1.4508	-.2387
.6475	1.5151	-.2082	-1.4508	1.3854	-.5085
-.0182	-.2082	-11.1697	-.2387	-.5085	-1.0420

17.0 3.0 3.0

-3.6931	-.7668	-.7668	13.6445	.4054	.4054
-.7668	1.8465	-.6249	.4054	-6.8222	-.1661
-.7668	-.6249	1.8465	.4054	-.1661	-6.8222
13.6445	.4054	.4054	-3.6931	-.7668	-.7668
.4054	-6.8222	-.1661	-.7668	1.8465	-.6249
.4054	-.1661	-6.8222	-.7668	-.6249	1.8465

17.0 5.0 3.0

-3.0054	-1.1618	-.7412	12.8303	.5860	.3190
-1.1618	1.6315	-.9876	.5860	-5.3962	-.2920
-.7412	-.9876	1.3739	.3190	-.2920	-7.4341
12.8303	.5860	.3190	-3.0054	-1.1618	-.7412
.5860	-5.3962	-.2920	-1.1618	1.6315	-.9876
.3190	-.2920	-7.4341	-.7412	-.9876	1.3739

17.0 7.0 3.0

-2.1097	-1.4128	-.7158	11.7585	.6638	.2031
-1.4128	1.4184	-1.2729	.6638	-3.4531	-.4274
-.7158	-1.2729	.6913	.2031	-.4274	-8.3054
11.7585	.6638	.2031	-2.1097	-1.4128	-.7158
.6638	-3.4531	-.4274	-1.4128	1.4184	-1.2729
.2031	-.4274	-8.3054	-.7158	-1.2729	.6913

17.0 9.0 3.0

-1.1252	-1.5074	-.7003	10.5641	.6447	.0696
-1.5074	1.2876	-1.4542	.6447	-1.1875	-.5547
-.7003	-1.4542	-.1624	.0696	-.5547	-9.3767
10.5641	.6447	.0696	-1.1252	-1.5074	-.7003
.6447	-1.1875	-.5547	-1.5074	1.2876	-1.4542
.0696	-.5547	-9.3767	-.7003	-1.4542	-.1624

17.0 5.0 5.0

-2.3895	-1.1315	-1.1315	12.0786	.4541	.4541
-1.1315	1.1947	-1.5677	.4541	-6.0393	-.5113
-1.1315	-1.5677	1.1947	.4541	-.5113	-6.0393
12.0786	.4541	.4541	-2.3895	-1.1315	-1.1315
.4541	-6.0393	-.5113	-1.1315	1.1947	-1.5677
.4541	-.5113	-6.0393	-1.1315	-1.5677	1.1947

17.0 7.0 5.0

-1.5849	-1.3909	-1.1053	11.0841	.5003	.2745
-1.3909	1.0345	-2.0336	.5003	-4.1234	-.7470
-1.1053	-2.0336	.5504	.2745	-.7470	-6.9607
11.0841	.5003	.2745	-1.5849	-1.3909	-1.1053
.5003	-4.1234	-.7470	-1.3909	1.0345	-2.0336
.2745	-.7470	-6.9607	-1.1053	-2.0336	.5504

19.0 1.0 1.0

-4.2642	-.0908	-.0908	14.8893	.0516	.0516
-.0908	2.1321	-.0712	.0516	-7.4446	-.0226
-.0908	-.0712	2.1321	.0516	-.0226	-7.4446
14.8893	.0516	.0516	-4.2642	-.0908	-.0908
.0516	-7.4446	-.0226	-.0908	2.1321	-.0712
.0516	-.0226	-7.4446	-.0908	-.0712	2.1321

19.0 3.0 1.0

-3.8912	-.2596	-.0891	14.4654	.1448	.0464
-.2596	2.0212	-.2086	.1448	-6.7070	-.0690
-.0891	-.2086	1.8701	.0464	-.0690	-7.7584
14.4654	.1448	.0464	-3.8912	-.2596	-.0891
.1448	-6.7070	-.0690	-.2596	2.0212	-.2086
.0464	-.0690	-7.7584	-.0891	-.2086	1.8701

19.0 5.0 1.0

-3.2016	-.3934	-.0863	13.6789	.2111	.0365
-.3934	1.8424	-.3307	.2111	-5.3113	-.1179
-.0863	-.3307	1.3592	.0365	-.1179	-8.3676
13.6789	.2111	.0365	-3.2016	-.3934	-.0863
.2111	-5.3113	-.1179	-.3934	1.8424	-.3307
.0365	-.1179	-8.3676	-.0863	-.3307	1.3592

19.0 7.0 1.0

-2.2927	-.4782	-.0836	12.6364	.2423	.0233
-.4782	1.6645	-.4277	.2423	-3.4028	-.1673
-.0836	-.4277	.6283	.0233	-.1673	-9.2337
12.6364	.2423	.0233	-2.2927	-.4782	-.0836
.2423	-3.4028	-.1673	-.4782	1.6645	-.4277
.0233	-.1673	-9.2337	-.0836	-.4277	.6283

19.0 9.0 1.0

-1.2799	-.5096	-.0820	11.4662	.2396	.0080
-.5096	1.5550	-.4903	.2396	-1.1710	-.2110
-.0820	-.4903	-.2750	.0080	-.2110	-10.2952
11.4662	.2396	.0080	-1.2799	-.5096	-.0820
.2396	-1.1710	-.2110	-.5096	1.5550	-.4903
.0080	-.2110	-10.2952	-.0820	-.4903	-.2750

19.0 3.0 3.0

-3.5359	-.2552	-.2552	14.0584	.1297	.1297
-.2552	1.7680	-.6113	.1297	-7.0292	-.2108
-.2552	-.6113	1.7680	.1297	-.2108	-7.0292
14.0584	.1297	.1297	-3.5359	-.2552	-.2552
.1297	-7.0292	-.2108	-.2552	1.7680	-.6113
.1297	-.2108	-7.0292	-.2552	-.6113	1.7680

19.0 5.0 3.0

-2.8783	-.3881	-.2483	13.3023	.1880	.1014
-.3881	1.6069	-.9713	.1880	-5.6462	-.3602
-.2483	-.9713	1.2714	.1014	-.3602	-7.6561
13.3023	.1880	.1014	-2.8783	-.3881	-.2483
.1880	-5.6462	-.3602	-.3881	1.6069	-.9713
.1014	-.3602	-7.6561	-.2483	-.9713	1.2714

19.0 7.0 3.0

-2.0105	-.4742	-.2418	12.2986	.2138	.0630
-.4742	1.4564	-1.2604	.2138	-3.7476	-.5118
-.2418	-1.2604	.5541	.0630	-.5118	-8.5509
12.2986	.2138	.0630	-2.0105	-.4742	-.2418
.2138	-3.7476	-.5118	-.4742	1.4564	-1.2604
.0630	-.5118	-8.5509	-.2418	-1.2604	.5541

19.0 5.0 5.0

-2.2791	-.3803	-.3803	12.6013	.1444	.1444
-.3803	1.1395	-1.5498	.1444	-6.3007	-.6167
-.3803	-1.5498	1.1395	.1444	-.6167	-6.3007
12.6013	.1444	.1444	-2.2791	-.3803	-.3803
.1444	-6.3007	-.6167	-.3803	1.1395	-1.5498
.1444	-.6167	-6.3007	-.3803	-1.5498	1.1395

Appendix B

Table IX

Wavevectors for subdivision ($p_x/10$, $p_y/10$, $p_z/10$) of first Brillouin zone and their weights.

WAVEVECTOR			WEIGHT	WAVEVECTOR			WEIGHT
p_x	p_y	p_z		p_x	p_y	p_z	
10	4	0	12	6	4	0	24
10	2	2	12	6	2	2	24
10	2	0	12	6	2	0	24
10	0	0	3	6	0	0	6
9	5	1	24	5	5	5	4
9	3	3	12	5	5	3	24
9	3	1	48	5	5	1	24
9	1	1	24	5	3	3	24
8	6	0	24	5	3	1	48
8	4	2	48	5	1	1	24
8	4	0	24	4	4	4	8
8	2	2	24	4	4	2	24
8	2	0	24	4	4	0	12
8	0	0	6	4	2	2	24
7	7	1	12	4	2	0	24
7	5	3	24	4	0	0	6
7	5	1	48	3	3	3	8
7	3	3	24	3	3	1	24
7	3	1	48	3	1	1	24
7	1	1	24	2	2	2	8
6	6	2	24	2	2	0	12
6	6	0	12	2	0	0	6
6	4	4	24	1	1	1	8
6	4	2	48	0	0	0	1