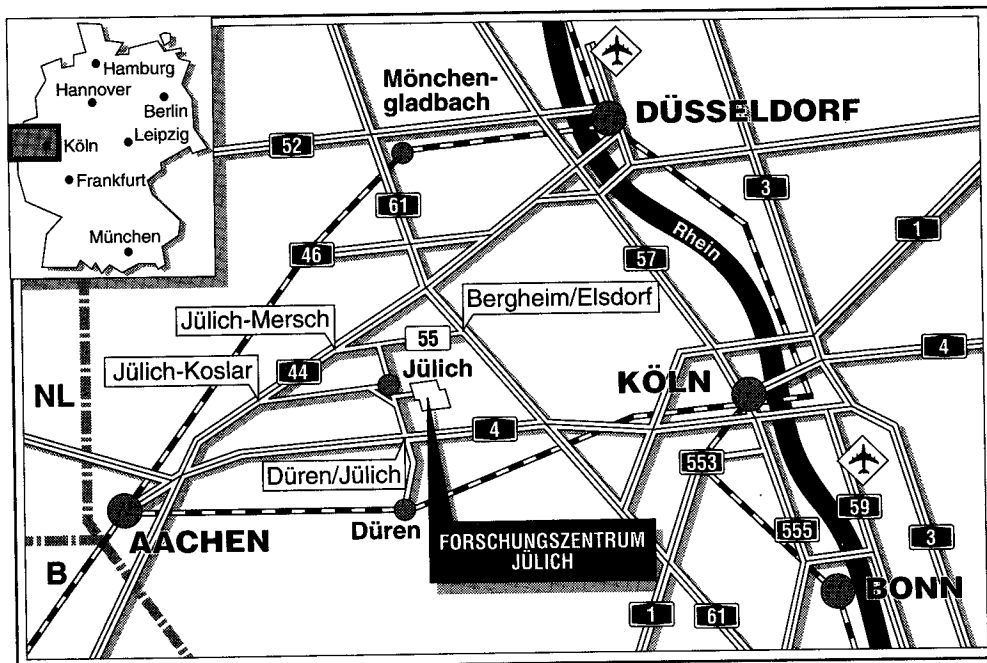*Institut für Festkörperforschung*

U N I S O F T –

A PROGRAM PACKAGE FOR
LATTICE–DYNAMICAL CALCULATIONS:
USER MANUAL

SECOND, REVISED EDITION

Götz Eckold

UNISOFT -

A PROGRAM PACKAGE FOR LATTICE-DYNAMICAL CALCULATIONS: USER MANUAL

SECOND, REVISED EDITION OF JÜL-SPEZ-366

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Preface

The program package UNISOFT for lattice-dynamical calculations was developed in 1986. After the publication of the User Manual (KFA report, Jül-Spez-366 (1986)) and an article in the Journal of Applied Crystallography (Vol.20, page 134-139 (1987)) the source code of the programs was sent out to users all around the world. In the meantime some minor errors were detected and corrected. In this respect, I am particularly grateful to J. Bethke (Aachen) and D. Strauch (Regensburg) for helpful comments. Furthermore, a number of small improvements have been made until now. The whole concept of the program package, however, remained unchanged. The rather old-fashioned formatted input, in particular, is still used because it seems to be the most general input form available on all types of computers. Thus, the basic version of UNISOFT, which is the subject of this manual, is almost independent of any particular operating system.

Based on UNISOFT, a workshop on 'lattice dynamics' was held in Jülich in autumn 1991. Hands on the computer, the participants (crystallographers, mineralogists, chemists, physicists) became familiar with the fundamentals of this subject. The success of this workshop proved that computer assisted teaching may be a powerful tool in order to convey even theoretical subjects. UNISOFT thus turned out to be useful not only for the interpretation of experimental data but also for the education of students and graduates.

The brisk demand for the User Manual, which is meanwhile out of print, led us to prepare a second edition. This was a good opportunity to correct some mistakes in the formulae and to include several updates.

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1.0 Introduction

Lattice-dynamical investigations provide a powerful tool for the determination of interatomic forces and chemical bonding in crystals. In general the extraction of, say, potential parameters from phonon dispersion curves, as determined experimentally, is possible with the help of model calculations only. Phonons which are cooperative excitations in many-body systems provide informations about interactions within the whole crystal. A quantitative interpretation of single phonons is therefore restricted to very simple crystal structures. In general, however, unambigious statements about interatomic forces require the knowledge of a good number of the phonon branches, at least in the symmetry directions.

Often, the determination of phonon dispersion curves is a rather hard task since a crystal with N particles per unit cell exhibits as many as 3N phonon branches. The only experimental method which allows the detection of phonons at arbitrary points within the Brillouin zone is the inelastic neutron scattering. Again, model calculations are very useful and sometimes even necessary in order to find phonons experimentally since phonon intensities vary strongly from one Brillouin zone to another and are determined by the corresponding eigenvectors. For complex structures, model calculations and neutron scattering experiments are thus complementary. The determination of interatomic forces in crystals requires both, the theoretical and the experimental approach which need to go hand in hand.

The three-axes spectrometer UNIDAS at the FRJ-2 reactor at Jülich is available to external users and is especially designed to meet the requirements for phonon investigations. Details of this machine are described in the UNIDAS-Handbuch [1]. In the present paper we report on the complement to this spectrometer, namely the computer program package UNISOFT which allows to perform model calculations on phonon dispersion in general structures with up to 20 particles per primitive cell.

UNISOFT has been developed in order to provide a tool for the optimization of experiments as well as for a first interpretation of the results. Certainly, a general lattice-dynamical program cannot deal with the most complex models for interatomic interactions. Until now the standard models such as

- Born-von Kármán model (longitudinal and transverse springs)

- Born-Mayer potential

- Lennard-Jones potential

- van der Waals potential

- Coulomb potential (Ewald's method of summation)

- shell model

are implemented. The interaction between each pair of atoms can be chosen individually as an arbitrary combination of these model potentials. More sophisticated

models must be developed by the user and are beyond the scope of UNISOFT as a universally applicable lattice-dynamical program.

Special attention has been paid to the handling of this program package by external users. Offering the possibility of a tailored interatomic interaction set-up for each individual substance under consideration, the system is rather complex, of course. Universality of the programs, however, does not exclude an easy mode of operation. Thus, UNISOFT can indeed be used in combination with UNIDAS by experimenters which are not familiar with details of lattice-dynamical calculations and the interpretation of phonon dispersion curves. This combination of software and hardware is able to simplify the determination of interatomic forces in crystals even for non-specialists.

Chapter 2 of this report briefly reviews the theoretical background of lattice dynamics in the harmonic approximation along with group-theoretical considerations and symmetry constraints to the dynamical matrix. The response of a phonon system in neutron scattering experiments is also discussed. In section 3 the global structure of the program package is displayed before a detailed description of the individual programs is given in chapter 4. Section 5 deals with computer requirements. Some possible extensions of this program system are discussed in chapter 6. In order to illustrate all information available with UNISOFT, an example for a complete treatment of a crystal structure within this program system is presented in appendix A. Finally, a comprehensive list of all input cards, the alphabetical list of subroutines, the subroutine reference list and the list of symbols used in this manual are given in the appendices B, C, D and E.

Concerning the notation, matrices are denoted by bold printed capital letters and vectors are represented by bold printed lower case letters.

2.0 Fundamentals of Lattice Dynamics

In this chapter we give a brief summary of the theoretical basis used for lattice-dynamical calculations. For a detailed treatment the reader is referred to the review articles by LEIBFRIED [2], COCHRAN and COWLEY [3], MARADUDIN and VOSKO [4] and the references therein.

2.1 Lattice Dynamics in the Harmonic Approximation

Lattice dynamics in the harmonic approximation describes the modes of motion in a crystalline solid in the case of small displacements of the atoms from their respective equilibrium positions. If there are N particles per primitive cell and N_c cells per crystal the (time-dependent) position of the κ-th atom ($\kappa = 1 \ldots N$) within the l-th primitive cell ($l = 1 \ldots N_c$) is given by

$$r_{\kappa l}(t) = r_\kappa + r_l . \tag{2.1}$$

r_l is the vector to the origin of the l-th cell. $r^0_{\kappa l}$ and r^0_κ denote the corresponding equilibrium values. The displacement of atom (κl) is thus:

$$u_{\kappa l}(t) = r_{\kappa l}(t) - r^0_{\kappa l} . \tag{2.2}$$

The Hamiltonian for this crystal system may be represented by

$$H = \sum_\kappa \sum_l \frac{p^2_{\kappa l}}{2m_\kappa} + \sum_\kappa \sum_l \sum_{\kappa'} \sum_{l'} V(\kappa l, \kappa' l') , \tag{2.3}$$

m_κ and $p_{\kappa l}$ being the mass and the momentum of particle (κl), respectively. $V(\kappa l, \kappa' l')$ is the interaction potential between particles (κl) and ($\kappa' l'$). Three-body forces and higher-order interactions are neglected. In equilibrium the second term in equation (2.3) takes the constant value V_0. If only small displacements of the atoms from their equilibrium positions are considered the potential energy may be expanded in powers of $u_{\kappa l}$. Retaining the terms up to the second order in the displacements and dropping the constant V_0 one obtains for the Hamiltonian:

$$H = \frac{1}{2} \sum_\kappa \sum_l m_\kappa \dot{u}^2_{\kappa l} + \frac{1}{2} \sum_\kappa \sum_l \sum_{\kappa'} \sum_{l'} u_{\kappa l} V(\kappa l, \kappa' l') u_{\kappa' l'} . \tag{2.4}$$

All first-order terms vanish since the potential energy is minimized in the equilibrium position. For (κl) $\neq$ ($\kappa' l'$), $V(\kappa l, \kappa' l')$ is the matrix of second derivatives of the pair potential $V(\kappa l, \kappa' l')$ taken at the equilibrium positions:

$$V_{\alpha\beta}(\kappa l, \kappa' l') = - \frac{\partial^2 V(\kappa l, \kappa' l')}{\partial r_\alpha \partial r_\beta} \Big|_{r = r^0_{\kappa' l'} - r^0_{\kappa l}} . \tag{2.5}$$

$- V(\kappa l, \kappa' l') u_{\kappa' l'}$ is the force acting upon the atom (κl) when ($\kappa' l'$) is displaced by $u_{\kappa' l'}$. Thus V is a force constant matrix. The self term $V(\kappa l, \kappa l)$ describes the restoring force

if only atom (κl) is displaced and all the other atoms are at rest. $V(\kappa l, \kappa l)$ is *not* the second-derivative matrix of a self potential but is given by:

$$V(\kappa l, \kappa l) = - \sum_{(\kappa'l') \neq (\kappa l)} V(\kappa l, \kappa'l') .$$ (2.6)

Equation (2.6) is a consequence of the fact that there cannot be a force on any atom if the crystal as a whole is translated. From equation (2.4) one obtains the equations of motion:

$$m_\kappa \ddot{u}_{\kappa l} = - \sum_{\kappa'} \sum_{l'} V(\kappa l, \kappa'l') \, u_{\kappa'l'} .$$ (2.7)

Solutions of this set of coupled differential equations are of the form:

$$u_\pm(\kappa l \mid qj) = \frac{1}{\sqrt{Nm_\kappa}} \, e(\kappa \mid qj) \, e^{i(\mathbf{qr}_l \pm \omega_{qj}t)}$$ (2.8)

which are plane waves with wave vector $\mathbf{q}$ and polarization vector $e(\kappa \mid qj)$. Due to periodic boundary conditions $\mathbf{q}$ is restricted to a sequence of discrete values which, however, are very close to each other. Thus, for practical work $\mathbf{q}$ can be treated as a continuous variable. For each $\mathbf{q}$ there are $3N$ different modes of vibration or *phonons* represented by different polarization vectors $e(\kappa \mid qj)$ and frequencies ω_{qj} $(j = 1 ... 3N)$. The actual displacement of the atom (κl) is a linear combination

$$u_{\kappa l} = \sum_{q} \sum_{j} [A_{qj} u_+(\kappa l \mid qj) + A'_{qj} u_-(\kappa l \mid qj)] .$$ (2.9)

Since $u(\kappa l)$ is a real vector equation (2.9) can be transformed into:

$$u_{\kappa l} = \frac{1}{\sqrt{Nm_\kappa}} \sum_{q} \sum_{j} Q_{qj} e(\kappa \mid qj) \, e^{i\mathbf{qr}_l}$$ (2.10)

where

$$Q_{qj} = A_{qj} e^{-i\omega_{qj}t} + A^*_{-qj} e^{i\omega_{qj}t}$$ (2.11)

are the *Normal Coordinates.* * denotes the complex conjugate. These normal coordinates determine the amplitude of the lattice vibrations or, in other words, the number of phonons which are excited at a given temperature. The average values may be calculated by statistical methods (see section 2.7).

The Hamiltonian (2.4) can be expressed in terms of the normal coordinates as:

$$H = \frac{1}{2N} \sum_{q} \sum_{j} [\, |\dot{Q}_{qj}|^2 + \omega^2_{qj} |Q_{qj}|^2]$$ (2.12)

which is just the superposition of the Hamiltonians of $3N$ independent harmonic oscillators for each $\mathbf{q}$.

The polarization vectors $e(\kappa|qj)$ and the frequencies ω_{qj} are obtained as eigenvectors and eigenfrequencies of the Fourier transformed force constant matrix multiplied by the square root of the masses:

The (3×3) submatrices

$$D(\kappa\kappa'|q) = \frac{1}{\sqrt{m_\kappa m_{\kappa'}}} \sum_{l'} V(\kappa l, \kappa'l')e^{iq(r_{l'} - r_l)}$$ (2.13)

are assembled within a (3N×3N) matrix:

$$D(q) = \begin{pmatrix} D(11|q) & \cdots & D(1N|q) \\ \vdots & & \vdots \\ D(N1|q) & \cdots & D(NN|q) \end{pmatrix}$$ (2.14)

which is called the *Dynamical Matrix*.[1] It should be noticed that the right hand side of equation (2.13) is independent of l since only the differences $r_{l'} - r_l$ enter in $V(\kappa l, \kappa'l')$ as well as in the phase factor.

Collecting the polarization vectors $e(\kappa|qj)$ in an analogous manner:

$$e(qj) = \begin{pmatrix} e(1|qj) \\ \vdots \\ e(N|qj) \end{pmatrix}$$ (2.15)

it can immediately be seen from equation (7) that the following eigenvector equation holds:

$$\omega_{qj}^2\, e(qj) = D(q)\, e(qj)\,.$$ (2.16)

Usually, the eigenvectors $e(qj)$ are chosen to be orthonormalized and to have the property:

$$e^*(qj) = e(-qj)\,.$$ (2.17)

Once the Dynamical Matrix is known, the displacement pattern and the frequency of each of the 3N phonons can be calculated. Inspection of the definition, equation (9), leads to the fact that D must be hermitian and, consequently, the eigenvalues ω^2 are real quantities.

For later use it is convenient to introduce the notation $F(q)$ for the Fourier transformed force constant matrix which is built from the (3×3) submatrices $F(\kappa\kappa'|q)$ in the same way as $D(q)$ is built from $D(\kappa\kappa'|q)$:

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[1] This is the D-definition of the Dynamical Matrix in the notation of *MARADUDIN* and *VOSKO* [4]. Another definition, the C-definition, is obtained if the phase factors $e^{iq(r_{\kappa'} - r_\kappa)}$ are included.

$$F(\kappa\kappa'\,|\,\mathbf{q}) = \sum_{l'} V(\kappa l,\, \kappa'l')e^{i\mathbf{q}(\mathbf{r}_{l'} - \mathbf{r}_l)}\,. \tag{2.18}$$

The Dynamical Matrix can now be expressed as:

$$D(\mathbf{q}) = M\ F(\mathbf{q})\ M \tag{2.19}$$

where **M** is the diagonal matrix of the inverse square roots of the atomic masses:

$$M_{\alpha\beta}(\kappa\kappa') = \frac{1}{\sqrt{m_\kappa}}\,\delta_{\alpha\beta}\delta_{\kappa\kappa'}\,. \tag{2.20}$$

Modelling the vibrational properties of a crystal within the harmonic approximation obviously implies the construction of the Dynamical Matrix. There are several approaches which are commonly used:

1. The force constants, *i.e.* the elements of $V(\kappa l,\kappa'l')$, are used as adjustable parameters directly. Known as the *Born-von Kármán model*, this approach is suitable only for cases in which short range forces dominate. Otherwise the number of model parameters becomes too large.

2. Interatomic potentials are put forward and the force constants are calculated as second derivatives of these model potentials according to equation (2.5). In the case of long-range potentials, such as the Coulomb potential, special tricks are needed in order to overcome the problem of slow convergence of the Fourier series in equation (2.13) (Ewald-summation [5] or Bertaut-approach [6]).

3. Other degrees of freedom such as the motion of electron shells may be introduced in order to simulate electrical polarization effects.

More complicated and sometimes sophisticated models have been devised for special crystals. Here, however, we restrict ourselves to rather simple interatomic force models which are applicable as standard models to a variety of different materials and which, therefore, are suitable for the use in a general lattice-dynamical program like UNISOFT. It should be mentioned, however, that even on the basis of a few simple interatomic interaction types a rather complex model set-up can be generated simply by combining two or more of these types.

In the following, the three principal approaches for the construction of the Dynamical Matrix are discussed in some detail.

2.2   Born-von Kármán model

In the Born-von Kármán model the force constants are treated as model parameters. They are *not* interpreted in terms of a special interatomic potential. Due to the symmetry of the force constant matrix each interaction is described by six force constants:

$$V(\kappa l,\, \kappa' l') = \begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix}.$$ (2.21)

Assuming the forces to be central forces, the number of parameters is reduced to two, namely the

Longitudinal Force Constant

$$L = \frac{d^2 V(\kappa l,\, \kappa' l')}{dr^2} \Big|_{r \,=\, |r^o_{\kappa' l'} - r^o_{\kappa l}|}$$ (2.22)

and the

Transverse Force Constant

$$T = \frac{1}{r} \frac{dV(\kappa l,\, \kappa' l')}{dr} \Big|_{r \,=\, |r^o_{\kappa' l'} - r^o_{\kappa l}|}.$$ (2.23)

In terms of these parameters the elements of $V(\kappa l,\, \kappa' l')$ are:

$$V_{\alpha\beta}(\kappa l,\, \kappa' l') = -(L-T)\frac{r_\alpha r_\beta}{r^2} - T\,\delta_{\alpha\beta}$$ (2.24)

where r_α is the cartesian component of $r = r^o_{\kappa' l'} - r^o_{\kappa l}$ in direction α and r is the modulus of r.

Obviously, this description of interatomic forces is restricted to short-range interactions. These interactions can be visualized by springs. L corresponds to the ordinary longitudinal spring producing restoring forces if the distance between the atoms (κl) and $(\kappa' l')$ is altered. T, on the other hand, corresponds to a transverse spring producing restoring forces if one atom is displaced in a direction perpendicular to the bond.

2.3 Explicit Interatomic Potentials

If two types of atoms κ and κ' are coupled via a potential which can be formulated explicitly and which is valid over a certain range of interatomic distances then the force constants for all pairs (κl) and $(\kappa' l')$ can be calculated from this potential. In this case, the number of parameters is reduced and long-range interactions such as Coulomb forces are feasible. Several model potentials are commonly used and included in UNISOFT:

BORN-MAYER:

$$V_{\kappa\kappa'}(r) = V_0 \exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right)$$ (2.25)

$$L = \frac{V_0}{(\sigma_\kappa + \sigma_{\kappa'})^2} \exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right)$$ (2.26)

$$T = -\frac{V_o}{(\sigma_\kappa + \sigma_{\kappa'})r}\exp\left(-\frac{r}{\sigma_\kappa + \sigma_{\kappa'}}\right)$$

(2.27)

LENNARD-JONES:

$$V_{\kappa\kappa'}(r) = V_o\left[\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - \left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6\right]$$

(2.28)

$$L = 6\frac{V_o}{r^2}\left[26\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - 7\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6\right]$$

(2.29)

$$T = -6\frac{V_o}{r^2}\left[2\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^{12} - \left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6\right]$$

(2.30)

van der WAALS:

$$V_{\kappa\kappa'}(r) = -V_o\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6$$

(2.31)

$$L = -42\frac{V_o}{r^2}\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6$$

(2.32)

$$T = 6\frac{V_o}{r^2}\left(\frac{\sigma_\kappa + \sigma_{\kappa'}}{r}\right)^6$$

(2.33)

COULOMB:

$$V_{\kappa\kappa'} = \frac{Z_\kappa Z_{\kappa'}}{4\pi\varepsilon_0 r} \ .$$

(2.34)

The first three potentials are short ranged and the Dynamical Matrix can be calculated by direct summation according to equation (2.13). The Coulomb interaction, however, requires a special treatment since the series in equation (2.13) is non-convergent due to the fact that we are dealing with point charges. Replacing the point charges by charge distributions, however, the Fourier transform of the second derivatives of this potential can be given explicitly. For a Gaussian charge distribution, *e.g.*,

$$\rho_\kappa = Z_\kappa\sqrt{\frac{p}{\pi}}^3 e^{-pr^2}$$

(2.35)

as introduced by *EWALD* [5], the Fourier transform of the second derivatives is:

$$F^G_{\alpha\beta}(\kappa\kappa'\,|\,q) = \frac{Z_\kappa Z_{\kappa'}}{\varepsilon_0 V}\sum_g \frac{(g + q)_\alpha(g + q)_\beta}{|g + q|^2}\, e^{-|g+q|^2/4p}\, e^{ig(r^o_\kappa - r^o_{\kappa'})}\ .$$

(2.36)

The summation runs over all reciprocal lattice vectors **g** and is rapidly convergent due to the Gaussian damping factor. v is the volume of the primitive cell.[2] The over-

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[2] In numerical calculations **q** must not be set exactly equal to zero since then the **q**=0 term cannot be evaluated. Due to the neglect of retardation effects very long phonon wavelenghts cannot be treated in this way. The Γ-point phonons are approximated in

lap of the charge distributions of different atoms requires a correction term taking into account the difference between the potential of point charges and Gaussian charge distributions. This term can be written as:

$$V_{\kappa\kappa'}^{overlap}(r) = 2\sqrt{\frac{p}{\pi}} \frac{Z_\kappa Z_{\kappa'}}{4\pi\varepsilon_0 r} \int_r^\infty e^{-px^2} dx .$$ (2.37)

The error function guarantees the corresponding Fourier series of the second derivatives being rapidly convergent in direct space:

$$F_{\alpha\beta}^{overlap}(\kappa\kappa' | \mathbf{q}) = - \sum_{l'} \frac{\partial^2 V_{\kappa\kappa'}^{overlap}(r)}{\partial r_\alpha \partial r_\beta} e^{i\mathbf{q}r} \Big|_{r = r_{\kappa l}^0 - r_{\kappa' l'}^0} .$$ (2.38)

The parameter p which determines the width of the Gaussian charge distribution can be adjusted in order to optimize the convergence of both series, in direct and reciprocal space, simultaneously. The entire Coulomb part of the Fourier transformed force constant matrix is the sum:

$$F^C(\kappa\kappa' | \mathbf{q}) = F^G(\kappa\kappa' | \mathbf{q}) + F^{overlap}(\kappa\kappa' | \mathbf{q}) .$$ (2.39)

The self term corresponding to $V(\kappa l, \kappa l)$ which is *not* the second derivative of the self potential, as pointed out earlier, must be taken into account by:

$$F^C(\kappa\kappa | \mathbf{q}) = F^G(\kappa\kappa | \mathbf{q}) + F^{overlap}(\kappa\kappa | \mathbf{q}) - \sum_{\kappa'} [F^G(\kappa\kappa' | 0) + F^{overlap}(\kappa\kappa' | 0)] .$$ (2.40)

It is convenient to introduce the *matrix of Coulomb coefficients* C as:

$$C(\kappa\kappa' | \mathbf{q}) = \frac{1}{Z_\kappa Z_{\kappa'}} F^C(\kappa\kappa' | \mathbf{q}) .$$ (2.41)

C is independent of the atomic properties and is entirely determined by the crystal structure. Defining the diagonal matrix of the charges Z by:

$$Z_{\alpha\beta}(\kappa\kappa') = Z_\kappa \delta_{\alpha\beta}\delta_{\kappa\kappa'}$$ (2.42)

and collecting the full (3N×3N) matrix C(q) in analogy to equation (2.14), equation (2.41) can be rewritten as:

$$F^C(\mathbf{q}) = Z \, C(\mathbf{q}) \, Z$$ (2.43)

and the Coulomb part of the Dynamical Matrix is given by:

$$D^C(\mathbf{q}) = M \, Z \, C(\mathbf{q}) \, Z \, M .$$ (2.44)

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lattice-dynamical calculations by the consideration of small but non-zero wavevectors. The LO-TO-splitting is obtained as the difference of phonon frequencies if the Γ-point is approached from different directions.

Another method to deal with the Coulomb potential has been introduced by *BERTAUT* [6]. Here, the point charges are replaced by charge distributions which, on the one hand, are broad enough to guarantee a rapid convergence of the Fourier series corresponding to equation (2.36), but which, on the other hand, do not overlap. Charge distributions of this kind may be described by polynomials in $|r - r^0_{\kappa l}|$ the coefficients of which are determined by the nearest neighbour distances. This method, however, is not used within UNISOFT. Therefore, details of the Bertaut-approach are not given here.

2.4 Combination of Different Interactions

Sometimes, a particular interaction between atoms of type κ and κ' is to be described as a superposition of several model potentials m. In this case, the corresponding submatrices $D(\kappa\kappa'|q)$ and $F(\kappa\kappa'|q)$ of the Dynamical Matrix and of the Fourier transformed force constant matrix can be calculated as a sum

$$D(\kappa\kappa'|q) = \sum_m D^{(m)}(\kappa\kappa'|q)$$

$$F(\kappa\kappa'|q) = \sum_m F^{(m)}(\kappa\kappa'|q)$$

(2.45)

where $D^{(m)}(\kappa\kappa'|q)$ and $F^{(m)}(\kappa\kappa'|q)$ are entirely determined by the potential m. The interaction between other atoms λ and λ' may be modelled by another combination of potentials. Thus, for each individual crystal a very specific interaction set-up can be provided. The linear combination of the different contributions $D^{(m)}(\kappa\kappa'|q)$ finally gives the total dynamical matrix $D(q)$.

The model in which the Coulomb interaction is combined with the short range repulsive Born-Mayer potential for all atoms is known as the *Rigid Ion Model*.

2.5 Shell Model

In all models for interatomic interactions discussed so far, the atoms are assumed to be hard spheres. The existence of a deformable electron shell is neglected and, hence, effects due to electronic polarization cannot be accounted for. In a large number of crystals, however, the polarizability plays an important role and a proper lattice-dynamical treatment requires the consideration of the motion of electron shells.

The *shell model* introduced by *DICK* and *OVERHAUSER* [7] provides one of the simplest methods to deal with this problem: Each atom (κl) is divided into a sherically-symmetrical outer electron shell and a core consisting of the nucleus and the inner electrons. If the shell and the core carry the charges Y_κ and X_κ, respectively, the total charge of particle (κl) is given by $Z_\kappa = X_\kappa + Y_\kappa$. In equilibrium, the shell is centered at the position of the corresponding atom core, $r^0_{\kappa l}$. The shell may be displaced from the core and its momentary position is denoted by $w_{\kappa l}$. The electric dipole moment of the atom (κl) is thus:

$$p^e_{\kappa l} = Y_\kappa(w_{\kappa l} - u_{\kappa l}) = Y_\kappa \overline{w}_{\kappa l} \,, \tag{2.46}$$

$\overline{w}_{\kappa l}$ being the relative displacement of the shell with respect to the core $\overline{w}_{\kappa l} = w_{\kappa l} - u_{\kappa l}$. The electron shell can now be regarded as an additional particle interacting with neighbouring atoms and neighbouring shells. Usually, these interactions are described in terms of the rigid ion model: In addition to their Coulomb interaction, represented by the matrix of second derivatives V^c, shells and cores are considered to be interconnected by (longitudinal and transverse) springs. The direct core-core interactions is treated just as in the preceeding sections. For each two atoms (κl) and $(\kappa' l')$ the short-range coupling is illustrated schematically in Fig. 1.

Fig. 1. The interactions of two atoms according to the shell model.
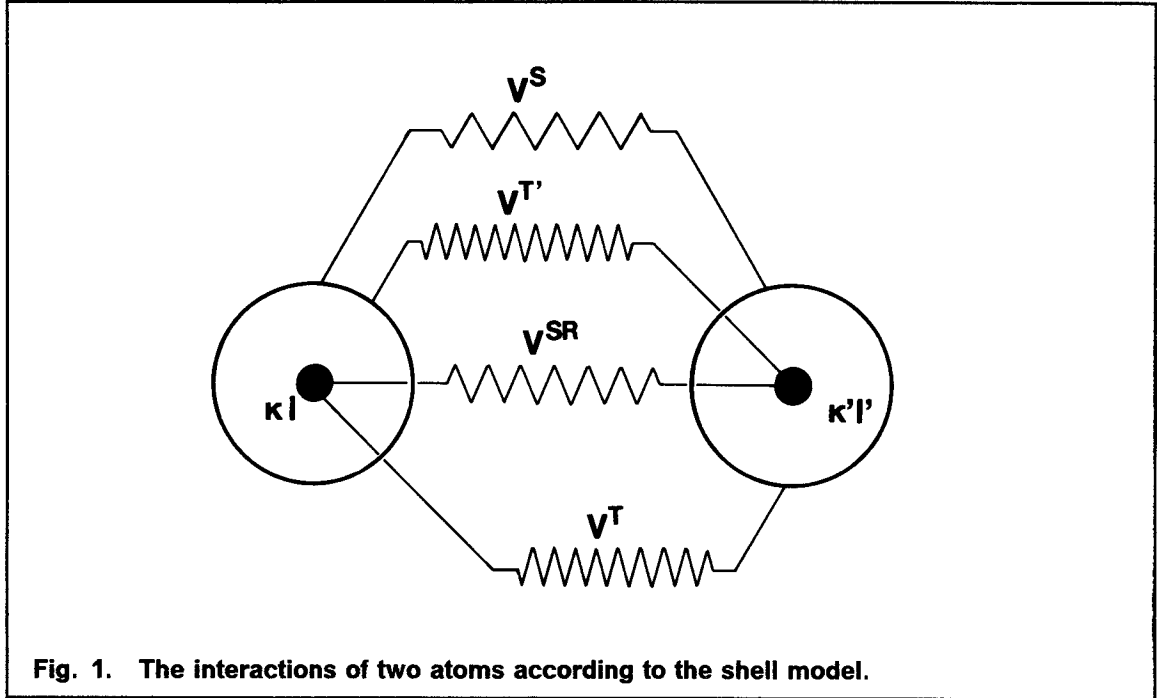
Mathematically, the short-range interactions of the shell model are represented by the force constant matrices $V^{SR}(\kappa l, \kappa' l')$, $V^S(\kappa l, \kappa' l')$, $V^T(\kappa l, \kappa' l')$ and $V^{T'}(\kappa l, \kappa' l')$. V^{SR} is associated with the direct core-core coupling as discussed previously. $V^S(\kappa l, \kappa' l')$ describes the shell-shell interaction. $V^T(\kappa l, \kappa' l')$ is the force constant matrix for the coupling between core(κl) and shell($\kappa' l'$) and $V^{T'}(\kappa l, \kappa' l')$ is the corresponding matrix for the interaction between shell(κl) and core($\kappa' l'$) of different particles (κl) and $(\kappa' l')$. Obviously, the following equation holds:

$$V^T_{\alpha\beta}(\kappa l, \kappa' l') = V^{T'}_{\beta\alpha}(\kappa' l', \kappa l) \,. \tag{2.47}$$

Special attention has to be paid to the the proper consideration of the self terms which are calculated according to equation (2.6):

$$V^T(\kappa l, \kappa l) = - \sum_{(\kappa' l') \neq (\kappa l)} V^T(\kappa l, \kappa' l') \tag{2.48}$$

$$\mathbf{V}^{T'}(\kappa l, \kappa l) = -\sum_{(\kappa' l') \neq (\kappa l)} \mathbf{V}^{T'}(\kappa l, \kappa' l') \qquad (2.49)$$

$$\mathbf{V}^{S}(\kappa l, \kappa l) = -\sum_{(\kappa' l') \neq (\kappa l)} \mathbf{V}^{S}(\kappa l, \kappa' l') \; . \qquad (2.50)$$

Note that $\mathbf{V}^T$ and $\mathbf{V}^{T'}$ do not include the coupling between core and shell within the same atom. This interaction is described by an extra force constant K_κ which may be represented by the shell charge Y_κ and the free ion polarizability α_κ:

$$K_\kappa = \frac{Y_\kappa^2}{\alpha_\kappa} \; . \qquad (2.51)$$

Collecting all interactions visualized in Fig. 1 on page 11, the following equations of motion are obtained:

For the cores:

$$\begin{aligned}
m_\kappa \ddot{\mathbf{u}}_{\kappa l} = &- X_\kappa \sum_{\kappa'} \sum_{l'} \mathbf{V}^C(\kappa l, \kappa' l') \, [X_{\kappa'} \mathbf{u}_{\kappa' l'} + Y_{\kappa'} \mathbf{w}_{\kappa' l'}] - \\
&- \sum_{(\kappa' l') \neq (\kappa l)} [\mathbf{V}^{SR}(\kappa l, \kappa' l') \mathbf{u}_{\kappa' l'} + \mathbf{V}^T(\kappa l, \kappa' l') \mathbf{w}_{\kappa' l'}] + \\
&+ K_\kappa \mathbf{w}_{\kappa l} - [\mathbf{V}^{SR}(\kappa l, \kappa l) + \mathbf{V}^T(\kappa l, \kappa l) + K_\kappa] \, \mathbf{u}_{\kappa l}
\end{aligned} \qquad (2.52)$$

and for the shells:

$$\begin{aligned}
m_S \ddot{\mathbf{w}}_{\kappa l} = &- Y_\kappa \sum_{\kappa'} \sum_{l'} \mathbf{V}^C(\kappa l, \kappa' l') \, [X_{\kappa'} \mathbf{u}_{\kappa' l'} + Y_{\kappa'} \mathbf{w}_{\kappa' l'}] - \\
&- \sum_{(\kappa' l') \neq (\kappa l)} [\mathbf{V}^{T'}(\kappa l, \kappa' l') \mathbf{u}_{\kappa' l'} + \mathbf{V}^{S}(\kappa l, \kappa' l') \mathbf{w}_{\kappa' l'}] + \\
&+ K_\kappa \mathbf{u}_{\kappa l} - [\mathbf{V}^{T'}(\kappa l, \kappa l) + \mathbf{V}^{S}(\kappa l, \kappa l) + K_\kappa] \, \mathbf{w}_{\kappa l} \; .
\end{aligned} \qquad (2.53)$$

The mass m_S of the electron shell is negligible compared to the ionic mass m_κ. Therefore, the left hand side of equation (2.53) is approximately zero:

$$m_S \ddot{\mathbf{w}}_{\kappa l} \simeq 0 \; . \qquad (2.54)$$

This condition is a mathematical formulation of the *adiabatic approximation*: The electron shell instantaneously occupies the position of minimum energy. Thus, equation (2.53) can be used to eliminate the shell coordinates $\mathbf{w}_{\kappa l}$ from the equation of motion for the cores, equation (2.52). Adding equations (2.52) and (2.53) and re-placing the shell coordinates $\mathbf{w}_{\kappa l}$ by the *relative* displacement vectors $\overline{\mathbf{w}}_{\kappa l}$ one obtains:

$$-m_\kappa \ddot{u}_{\kappa l} = Z_\kappa \sum_{\kappa'}\sum_{l'} V^C(\kappa l, \kappa'l') [Z_{\kappa'}u_{\kappa'l'} + Y_{\kappa'}\overline{w}_{\kappa'l'}] +$$

$$+ \sum_{\kappa'}\sum_{l'} [V^{SR}(\kappa l, \kappa'l') + V^T(\kappa l, \kappa'l') + V^{T'}(\kappa l, \kappa'l') + V^S(\kappa l, \kappa'l')]\, u_{\kappa'l'} +$$

$$+ \sum_{\kappa'}\sum_{l'} [V^T(\kappa l, \kappa'l') + V^S(\kappa l, \kappa'l')]\, \overline{w}_{\kappa'l'} +$$

$$+ [V^{T'}(\kappa l, \kappa l) - V^T(\kappa l, \kappa l)]\, \overline{w}_{\kappa l} .$$

(2.55)

Equation (2.53) is transformed into:

$$0 = Y_\kappa \sum_{\kappa'}\sum_{l'} V^C(\kappa l, \kappa'l') [Z_{\kappa'}u_{\kappa'l'} + Y_{\kappa'}\overline{w}_{\kappa'l'}] +$$

$$+ \sum_{\kappa'}\sum_{l'} [V^{T'}(\kappa l, \kappa'l') + V^S(\kappa l, \kappa'l')]\, u_{\kappa'l'} +$$

$$+ \sum_{\kappa'}\sum_{l'} V^S(\kappa l, \kappa'l')\overline{w}_{\kappa'l'} + V^{T'}(\kappa l, \kappa l)\overline{w}_{\kappa l} + K_\kappa \overline{w}_{\kappa l} .$$

(2.56)

The term

$$\sum_{\kappa'}\sum_{l'} V^C(\kappa l, \kappa'l')[Z_{\kappa'}u_{\kappa'l'} + Y_{\kappa'}\overline{w}_{\kappa'l'}]$$

is the dynamical part of the effective electrical field at the equilibrium position of atom (κl).

Remembering the procedure of section 2.1, the equations of motion are solved by plane waves for u as well as for $\overline{w}$. According to equations (2.8) and (2.15) one obtains the eigenvectors e_u and e_w for the motion of the cores and of the shells, respectively, and the last two equations are transformed into [3]:

$$\omega^2\, e_u = [M(ZCZ + F^{SR} + F^T + F^{T'} + F^S)M]\, e_u +$$
$$+ [M(ZCY + F^T + F^S + F_o^{T'} - F_o^T)M]\, e_w$$

(2.57)

and

$$0 = [(YCZ + F^{T'} + F^S)M]\, e_u + [(YCY + F^S + F_o^{T'} + K)M]\, e_w .$$

(2.58)

M being the mass tensor and C the matrix of Coulomb coefficients as defined by equations (2.20) and (2.41). F^{SR}, F^T, $F^{T'}$ and F^S are the Fourier transforms of V^{SR}, V^T, $V^{T'}$ and V^S, respectively. Y and K are the diagonal matrices of the shell charges and the intraatomic shell-core force constants. F_o^T and $F_o^{T'}$ contain the self-terms of the

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[3] For simplicity, the arguments qj labelling the different phonon states are omitted.

shell-core and the core-shell interactions. Both matrices have a block-diagonal form and the (3x3) submatrices along the diagonal are:

$$F_0^T(\kappa\kappa) = V^T(\kappa l, \kappa l) \tag{2.59}$$

and

$$F_0^{T'}(\kappa\kappa) = V^{T'}(\kappa l, \kappa l) . \tag{2.60}$$

It should be noticed that in contrast to all other matrices appearing in the equations (2.57) and (2.58), F^T and $F^{T'}$ in general are *not* hermitian. This is due to the fact that the interaction between core (κl) and shell$(\kappa' l')$ is not necessarily the same as the interaction between core$(\kappa' l')$ and shell(κl). The hermitian conjugate matrix of $F^{T'}$ is given by:

$$(F^{T'})^+ = F^T + F_0^{T'} - F_0^T . \tag{2.61}$$

Inspection of equations (2.57) and (2.58) yields that the *effective* short range contributions to the core-core, the shell-core, the core-shell and the shell-shell interactions are determined by the combinations

$$F^{CC} = F^{SR} + F^T + F^{T'} + F^S , \tag{2.62}$$

$$F^{SC} = F^{T'} + F^S , \tag{2.63}$$

$$F^{CS} = F^T + F^S + F_0^{T'} - F_0^T = (F^{SC})^+ \tag{2.64}$$

and

$$F^{SS} = F^S + F_0^{T'} + K , \tag{2.65}$$

respectively. Combining the two equations (2.57) and (2.58), e_w can be eliminated and one finally obtains the eigenvector equation for the motion of the ionic cores:

$$\omega^2 e_u = M [F^{CC} + ZCZ - (F^{SC} + YCZ)^+(F^{SS} + YCY)^{-1}(F^{SC} + YCZ)] M e_u . \tag{2.66}$$

Thus, by comparison with equation (2.16), the total Dynamical Matrix turns out to be:

$$D = M[ZCZ + F^{CC} - (YCZ + F^{SC})^+(YCY + F^{SS})^{-1}(YCZ + F^{SC})]M . \tag{2.67}$$

$+$ denotes the hermitian conjugate matrix.

From equation (2.67) it can be seen that the shell model requires a special treatment: The polarization term, *i.e.* the third term on the right hand side of equation (2.67) has the form of a hermitian transformation in the 3N-dimensional space. Thus, all (3Nx3N) matrices appearing in equation (2.67) must be set up as a whole before the total Fourier transformed force constant matrix can be completed. It is not possible to calculate the (3x3) submatrices $D(\kappa\kappa' | q)$ individually.

2.6 Constraints for the Elements of the Dynamical Matrix

The number of model parameters may become rather large if a complex structure or a complex interaction set-up is considered. There are, however, constraints for the force constant matrix and, hence, for the model parameters. These constraints arise from:

- the condition of translational invariance

- the condition of rotational invariance

- the condition of zero strain

- symmetry transformations.

2.6.1 Translational Invariance

A rigid translation of the crystal as a whole does not affect the interatomic potentials. As a consequence, there cannot be any force on any atom. In terms of the force constants this condition reads:

$$\sum_{\kappa'}\sum_{l'} V(\kappa l, \kappa' l') = 0 \qquad \forall \ (\kappa l) . \tag{2.68}$$

Usually, this condition is used to determine the self term $V(\kappa l, \kappa l)$, as pointed out in section 2.1. In the shell model, equation (2.68) applies to all individual matrices describing the core-core, the core-shell, and the shell-shell interactions.

2.6.2 Rotational Invariance

Similarly, a rigid rotation of the crystal as a whole does not affect the interatomic potential. Formally, the force in the direction α acting on the atom (κl) as a result of a rigid rotation around the x-, y- and z-axes can be written as:

$$f_\alpha^x(\kappa l) = \sum_{\kappa'}\sum_{l'} [V_{\alpha y}(\kappa l, \kappa' l') r_z^0(\kappa' l') - V_{\alpha z}(\kappa l, \kappa' l') r_y^0(\kappa' l')] \tag{2.69}$$

$$f_\alpha^y(\kappa l) = \sum_{\kappa'}\sum_{l'} [V_{\alpha z}(\kappa l, \kappa' l') r_x^0(\kappa' l') - V_{\alpha x}(\kappa l, \kappa' l') r_z^0(\kappa' l')] \tag{2.70}$$

$$f_\alpha^z(\kappa l) = \sum_{\kappa'}\sum_{l'} [V_{\alpha x}(\kappa l, \kappa' l') r_y^0(\kappa' l') - V_{\alpha y}(\kappa l, \kappa' l') r_x^0(\kappa' l')] . \tag{2.71}$$

The condition of rotational invariance requires that all of these forces vanish.

In order to test a particular model the sums in equations (2.69)-(2.71) must be calculated numerically what may be difficult for long-range interactions. The invariance conditions can, however, be expressed by the Dynamical Matrix at small phonon

wavevectors: Remembering its definition, equation (2.13), $D(\kappa\kappa'|\mathbf{q})$ may be expanded in a Taylor series of $\mathbf{q}$. Retaining the first-order terms one obtains:

$$\sqrt{m_\kappa m_{\kappa'}}\, e^{i\mathbf{q}(\mathbf{r}^0_{\kappa'} - \mathbf{r}^0_\kappa)} D(\kappa\kappa'|\mathbf{q}) \simeq$$

$$\sum_{l'} V(\kappa l, \kappa'l') + i\mathbf{q} \sum_{l'} (\mathbf{r}^0_{\kappa'l'} - \mathbf{r}^0_{\kappa l}) V(\kappa l, \kappa'l') . \qquad (2.72)$$

Denoting

$$D'(\kappa\kappa'|\mathbf{q}) = \sqrt{m_\kappa m_{\kappa'}}\, e^{i\mathbf{q}(\mathbf{r}^0_{\kappa'} - \mathbf{r}^0_\kappa)} D(\kappa\kappa'|\mathbf{q}) \qquad (2.73)$$

and

$$\begin{aligned}
\delta\mathbf{q}_x &= (\delta q \ \ 0 \ \ 0) \\
\delta\mathbf{q}_y &= (0 \ \ \delta q \ \ 0) \\
\delta\mathbf{q}_z &= (0 \ \ 0 \ \ \delta q) ,
\end{aligned} \qquad (2.74)$$

the following equation is obtained for small δq:

$$D'(\kappa\kappa'|\delta\mathbf{q}_\alpha) = \sum_{l'} V(\kappa l, \kappa'l') + i\,\delta q \sum_{l'} V(\kappa l, \kappa'l')(\mathbf{r}^0_{\kappa'l'} - \mathbf{r}^0_{\kappa l})_\alpha . \qquad (2.75)$$

By comparison with equations (2.69)-(2.71), the conditions of rotational invariance can now be expressed as:

$$f^x_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha y}(\kappa\kappa'|\delta\mathbf{q}_z) - D'_{\alpha z}(\kappa\kappa'|\delta\mathbf{q}_y)] = 0 \qquad (2.76)$$

$$f^y_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha z}(\kappa\kappa'|\delta\mathbf{q}_x) - D'_{\alpha x}(\kappa\kappa'|\delta\mathbf{q}_z)] = 0 \qquad (2.77)$$

$$f^z_\alpha(\kappa l) = \frac{1}{i\delta q} \sum_{\kappa'} [D'_{\alpha x}(\kappa\kappa'|\delta\mathbf{q}_y) - D'_{\alpha y}(\kappa\kappa'|\delta\mathbf{q}_x)] = 0 . \qquad (2.78)$$

These sums can readily be evaluated, thus providing a test of rotational invariance.

For a system with central forces the matrix V can be represented by longitudinal and transverse force constants, equation (2.24). It can easily be shown that in this case the forces $f^z_\alpha(\kappa l)$ vanish identically and $f_\beta(\kappa l)$ is just the force in the direction $\alpha \times \beta$ acting on atom (κl) if all atoms occupy their equilibrium positions. Thus, the condition of rotational invariance is equivalent to the postulate that we are dealing with an equilibrium crystal structure.

This test for rotational invariance fails, however, if the shell model is considered. A rigid rotation of the whole crystal implies that all relative displacements of the shells $(\overline{W}_{\kappa'l'})$ are definitely zero. Thus, the constraints do not apply to the whole Dynamical Matrix but only to those parts which are free from polarization contributions namely the Coulomb term and the effective core-core interaction respresented by F^{c-c}, just like in the rigid ion model.

2.6.3 Condition of Zero Strain

A crystal in its equilibrium state must not have internal strains. The comparison of the microscopic dynamics in the small q regime with the macroscopic description of elasticity leads to the following condition for zero strain:

$$G_{\alpha\beta\gamma\delta} = \sum_{\kappa}\sum_{l}\sum_{\kappa'}\sum_{l'} V_{\alpha\beta}(\kappa l,\, \kappa' l')(r^0_{\kappa l} - r^0_{\kappa' l'})_\gamma (r^0_{\kappa l} - r^0_{\kappa' l'})_\delta -$$
$$- V_{\gamma\delta}(\kappa l,\, \kappa' l')(r^0_{\kappa l} - r^0_{\kappa' l'})_\alpha (r^0_{\kappa l} - r^0_{\kappa' l'})_\beta$$
$$= 0. \tag{2.79}$$

This equation can be expressed in terms of the Dynamical Matrix at small q in analogy to the treatment in the preceeding section. Here, however, the second-order terms in the expansion according to equation (2.72) are involved:

$$G_{\alpha\beta\gamma\delta} = -\frac{1}{\delta q^2} \sum_{\kappa}\sum_{\kappa'} D'_{\alpha\beta}(\kappa\kappa'\,|\,\delta q_\gamma + \delta q_\delta) - D'_{\alpha\beta}(\kappa\kappa'\,|\,\delta q_\gamma) - D'_{\alpha\beta}(\kappa\kappa'\,|\,\delta q_\delta) -$$
$$- D'_{\gamma\delta}(\kappa\kappa'\,|\,\delta q_\alpha + \delta q_\beta) + D'_{\gamma\delta}(\kappa\kappa'\,|\,\delta q_\alpha) + D'_{\gamma\delta}(\kappa\kappa'\,|\,\delta q_\beta) \tag{2.80}$$
$$= 0.$$

The condition of zero strain, however, is not used very frequently for lattice-dynamical calculations.

2.6.4 Constraints Due to Symmetry

Obviously, symmetry operations which transform the crystal into itself provide further constraints to the elements of the force constant matrix and of the Dynamical Matrix. Suppose, there is a symmetry operation $(S\,|\,v)$[4] which sends the atom (κl) into the atom (λm) and simultaneously the atom $(\kappa' l')$ into $(\lambda' m')$. Then the elements $V(\kappa l,\, \kappa' l')$ and $V(\lambda m,\, \lambda' m')$ are no longer independent but can be calculated from one another. By consideration of the whole symmetry group the number of independent interactions can be obtained. The list of these interactions can be used as a guide for a proper model set-up.

For those symmetry operations $(S\,|\,v)$ which leave the phonon wavevector quasi-invariant:

$$S\,q = q + g \tag{2.81}$$

(g being a reciprocal lattice vector) the transformation of the Dynamical Matrix is given by:

$$D(\lambda\lambda'\,|\,q) = S\, D(\kappa\kappa'\,|\,q)\, e^{iq(r^0_\lambda - r^0_{\lambda'} - S(r^0_\kappa - r^0_{\kappa'}))}. \tag{2.82}$$

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4   In this notation S is the rotational matrix and v is a fractional translation defining the symmetry transformation.

2.7 Amplitudes of Lattice Vibrations

According to equation (2.10) the displacement of a particular atom is given as a sum over the different phonon states (qj). In order to calculate phonon intensities as measured in neutron scattering experiments the amplitude of each lattice vibration (qj) at a given temperature has to be known. Especially for the investigation of lattice vibrations with high frequencies or at low temperatures, however, the quantum mechanical description is more adequate. The amplitude of a lattice mode is then obtained from the occupation probability of a phonon state.

In terms of the normal coordinates Q_{qj}, the Hamiltonian of the crystal system is given by equation (2.12) as a sum over the distinct and independent phonon states. Thus, each phonon state (qj) can be considered separately as a one-dimensional harmonic oscillator with respect to the normal coordinate Q_{qj}:

$$H_{qj} = \frac{1}{2N} [\,|\dot{Q}_{qj}|^2 + \omega_{qj}^2 |Q_{qj}|^2\,] \,. \tag{2.83}$$

In quantum mechanical terms Q_{qj} and $\dot{Q}_{qj}$ correspond to the canonical conjugate operators Q and P which, in turn, can be represented by the creation and annihilation operators a^+ and a:

$$Q = \sqrt{\frac{\hbar}{2\omega_{qj}}}\,(a^+_{-qj} + a_{qj}) \tag{2.84}$$

$$P = i\sqrt{\frac{\hbar\omega_{qj}}{2}}\,(a^+_{-qj} - a_{qj}) \,. \tag{2.85}$$

(For a more detailed discussion see textbooks on quantum mechanics.) Inserting these operators in equation (2.83) one gets:

$$H_{qj} = \hbar\omega_{qj}\,(a^+_{qj}a_{qj} + \frac{1}{2}) \,. \tag{2.86}$$

The expectation value of a^+a is just the number of phonons n_{qj} with the energy $\hbar\omega_{qj}$ excited at a given temperature. $\hbar\omega_{qj}/2$ is the zero point energy. Phonons obey Bose-statistics, therefore $< a^+a >$ can be calculated as:

$$n_{qj} = < a^+a > = \frac{1}{\exp(\dfrac{\hbar\omega_{qj}}{k_BT}) - 1} \,. \tag{2.87}$$

The displacement operator for particle (κl) is obtained from equations (2.10) and (2.11) by replacing the coefficients A_{qj} and A^*_{-qj} by the operators a_{qj} and a^+_{-qj}, resp.:

$$u_{\kappa l} = \sqrt{\frac{\hbar}{2Nm_\kappa\omega_{qj}}} \sum_q\sum_j e(\kappa\,|\,qj)\,e^{iqr_l}\,[a_{qj}e^{-i\omega_{qj}t} + a^+_{-qj}e^{i\omega_{qj}t}] \,. \tag{2.88}$$

The mean square displacement of particle (κl) corresponding to a single phonon state (qj) is given by:

$$< u^2_{\kappa l} > = (n_{qj} + \frac{1}{2})\,\frac{\hbar}{Nm_\kappa\omega_{qj}}\,|e(\kappa\,|\,qj)|^2 \,, \tag{2.89}$$

and in the classical limit:

$$n_{qj} \rightarrow \frac{k_B T}{\hbar \omega_{qj}}$$

$$< u^2_{\kappa l} > \rightarrow \frac{k_B T}{N m_{\kappa} \omega^2_{qj}} |e(\kappa | qj)|^2 \,. \tag{2.90}$$

2.8 Phonon Intensities in Neutron Scattering

Inelastic neutron scattering is the unique experimental method for the determination of phonon dispersion curves. Phonon intensities vary, however, from one Brillouin zone to the other, depending on the particular eigenvector. Therefore, it is sometimes a rather hard task to detect special phonons experimentally. In this case, lattice-dynamical calculations may provide a guide for the optimization of experiments.

In neutron scattering experiments a monochromatized beam characterized by the wavevector k_i hits the sample and one asks for the number of neutrons leaving the sample with the wavevector k_f. The scattering probability and, hence, the scattered intensity is essentially determined by the

momentum transfer[5]

$$\hbar Q = \hbar(k_i - k_f) \tag{2.91}$$

and the

energy transfer

$$\hbar \omega = \frac{\hbar^2}{2m_n} (k_i^2 - k_f^2) \,, \tag{2.92}$$

(m_n being the neutron mass). Due to resolution and normalizing effects the intensity does, in fact, depend on the special choice of k_i and k_f but the response of the sample itself can be described in terms of Q and ω. $\hbar Q$ and $\hbar \omega$ are the momentum and the energy, resp., which are transferred to the sample during the scattering process and equations (2.91) and (2.92) are the laws of momentum and energy conservation. We will not give a review of the fundamentals of neutron scattering here. We only want to recall that phonons are collective excitations of the crystal lattice and, hence, it is the coherent part of the scattering which carries the information about the distinct phonon states. For details the reader is referred to the literature, e.g. [8].

The calculation of phonon intensities, of the so-called dynamical structure factor, starts from the following expression for the coherent scattering function S_{coh} which is proportional to the scattered intensity:

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5   Different from the convention followed in the other parts of this manual, here the capital bold printed letter Q denotes a vector rather than a matrix. The reason for this inconsistency is, that in the literature concerning neutron scattering the scattering vector is almost exclusively denoted by Q.

$$S_{coh}(\mathbf{Q}, \omega) = \frac{1}{N} \int \sum_{\kappa} \sum_{l} \sum_{\kappa'} \sum_{l'} b_{\kappa} b_{\kappa'}^{*} e^{-i\mathbf{Q}(\mathbf{r}_{\kappa l}^{0} - \mathbf{r}_{\kappa' l'}^{0})} < e^{-i\mathbf{Q}(\mathbf{u}_{\kappa l}(t) - \mathbf{u}_{\kappa' l'}(0))} > e^{-i\omega t} dt , \qquad (2.93)$$

where b_{κ} and $b_{\kappa'}$ are the coherent scattering lengths of particles of type κ and κ', resp.. Using the results of section 2.7 for the atomic displacements $\mathbf{u}$ of a harmonic crystal and expanding the phase factor in equation (2.93) in powers of $\mathbf{u}_{\kappa l}(t) - \mathbf{u}_{\kappa' l'}(0)$, one obtains after some calculation for the *one-phonon scattering*, *i.e.* the first-order term in the displacements:

$$S_{coh}^{(1)}(\mathbf{Q}, \omega) = \frac{1}{N} \sum_{\mathbf{q}} \sum_{j} S_{coh}^{(\mathbf{q}j)}(\mathbf{Q}, \omega) , \qquad (2.94)$$

$S_{coh}^{(\mathbf{q}j)}$ being the partial scattering function due to the single phonon state $(\mathbf{q}j)$:

$$S_{coh}^{(\mathbf{q}j)}(\mathbf{Q}, \omega) = \frac{\hbar}{\omega_{\mathbf{q}j}} | \sum_{\kappa} \frac{b_{\kappa} e^{-W_{\kappa}}}{\sqrt{m_{\kappa}}} \mathbf{Q} \, \mathbf{e}(\kappa | \mathbf{q}j) \, e^{-i\mathbf{Q}\mathbf{r}_{\kappa}^{0}} |^{2} \cdot$$

$$\cdot \{[n_{\mathbf{q}j} + 1]\delta(\omega - \omega_{\mathbf{q}j}) + n_{\mathbf{q}j}\delta(\omega + \omega_{\mathbf{q}j})\} \sum_{\mathbf{g}} \delta_{\mathbf{Q}, \, \mathbf{g}+\mathbf{q}} . \qquad (2.95)$$

$e^{-W_{\kappa}}$ is the Debye-Waller factor of particles of type κ. The δ-functions on the right hand side of equation (2.95) reflect the energy and momentum conservation since the phonon $(\mathbf{q}j)$ carries the energy $\hbar\omega_{\mathbf{q}j}$ and the momentum $\hbar\mathbf{q}$. In periodic structures, the wavevector of excitations is always defined modulo a reciprocal lattice vector $\mathbf{g}$. Therefore, every phonon can in principle be measured in every Brillouin zone $\mathbf{g}$. This is taken into account by the sum over $\mathbf{g}$ in equation (2.95). Furthermore, a phonon can be created or absorbed by a neutron corresponding to δ-peaks at positive or negative frequency. Obviously, the creation of a phonon is more likely than the absorption, since in the latter case the phonon must already be excited. The phonon intensity is thus larger at $+ \omega_{\mathbf{q}j}$ than at $- \omega_{\mathbf{q}j}$. The asymmetry of the spectra is given by the condition of *Detailed Balance*:

$$\frac{I(\omega_{\mathbf{q}j})}{I(-\omega_{\mathbf{q}j})} = \frac{n_{\mathbf{q}j} + 1}{n_{\mathbf{q}j}} = \exp(\frac{\hbar\omega_{\mathbf{q}j}}{k_{B}T}) . \qquad (2.96)$$

Phonons can only be observed in scattering experiments if their polarization vectors $\mathbf{e}(\mathbf{q}j)$ have non-zero components in the direction of the momentum transfer. Mathematically, this is described by the dot-product $\mathbf{Qe}$ in equation (2.95). Thus, lattice-dynamical calculations which directly yield the frequencies and the polarization vectors can be used to predict phonon intensities which may be obtained in neutron scattering experiments.

2.9 The Symmetry of Lattice Vibrations

The Dynamical Matrix and its eigenvectors are functions of the atomic positions within the crystal and can thus be represented by symmetry-adapted functions. Since $\mathbf{D}$ is also a function of the phonon wavevector $\mathbf{q}$ the following discussion is restricted to symmetry operations which leave the wavevector invariant. These symmetry op-

erations form the *group of the wave vector* G_q which is a subgroup of the total symmetry group G_o. The symmetry adapted functions or *symmetry coordinates* are the basis vectors for the various irreducible multiplier representations (IMR) of G_q. The eigenvectors of the Dynamical Matrix can be represented as a linear combination of the symmetry coordinates of one single representation. Thus, the eigenvectors are labelled according to their symmetry.

The transformation of the Dynamical Matrix under the operations of G_q is given by equation (2.82) and provides a 3N-dimensional (reducible) representation Γ_{3N} of G_q, the set of 3N cartesian coordinates generating the corresponding vector space. As a result from group theory, there is a finite number of irreducible multiplier representations γ_i of G_q and Γ_{3N} may be represented as the direct sum:

$$\Gamma_{3N} = \sum_i m_i \gamma_i \,, \tag{2.97}$$

m_i being the multiplicity of γ_i. Correspondingly, the 3N-dimensional vector space is decomposed into several subspaces of lower dimensions which are invariant under the operations of G_q. A basis of each of these subspaces can be constructed by projector techniques as described in [4]. With respect to these new symmetry coordinates which are linear combinations of the 3N cartesian coordinates, the Dynamical Matrix is block-diagonalized. The dimensions of the individual blocks are given by the multiplicity of the corresponding IMR.

Let x_i^l be a 3N-dimensional vector transforming according to the i-th IMR (l ... m_i). If all the vectors x_i^l are pairwise orthonormal they form the set of symmetry coordinates:

$$X = (x_1^1 \ldots x_1^{m_1} x_2^1 \ldots) \tag{2.98}$$

The block-diagonalized Dynamical Matrix is given by the transformation:

$$D^X = X^{-1} D X \,. \tag{2.99}$$

Each block i of this matrix can now be diagonalized individually. All corresponding eigenvectors e_i^X belong to the same IMR. Thus, the different vibrational modes are automatically arranged according to their symmetry. The eigenvectors are retransformed to cartesian coordinates by:

$$e_i = X e_i^X \,. \tag{2.100}$$

More detailed information about the group-theoretical analysis of lattice vibrations including time-reversal conditions etc. are given in the review article by *MARADUDIN* and *VOSKO* [4].

For the practical work with the program package UNISOFT, however, it is sufficient to know that there is a set of symmetry coordinates which provides the decomposition of the Dynamical Matrix and its eigenvectors according to different symmetries. These symmetry coordinates can be calculated simply on the basis of group theory for each crystal structure without any other assumption.

2.10 Static Electrical Field and Gradients

Within the framework of lattice dynamics based on Coulomb interactions the static electrical field **h** and the field gradient **H** at the position of any atom (κl) may be calculated. **h** is proportional to the gradient of the total electrostatic potential except the self potential and **H** is the matrix of second derivatives:

$$h_\alpha(\kappa l) = -\frac{1}{Z_\kappa} \sum_{\kappa'} \sum_{l'} \frac{\partial V^c_{\kappa\kappa'}(r)}{\partial r_\alpha} \Big|_{r=r^0_{\kappa l}-r^0_{\kappa'l'}} \tag{2.101}$$

$$H_{\alpha\beta}(\kappa l) = -\frac{1}{Z_\kappa} \sum_{\kappa'} \sum_{l'} \frac{\partial^2 V^c_{\kappa\kappa'}(r)}{\partial r_\alpha \partial r_\beta} \Big|_{r=r^0_{\kappa l}-r^0_{\kappa'l'}} . \tag{2.102}$$

Obviously, **H** is closely related to the matrix of Coulomb coefficients defined in section 2.3:

$$H(\kappa l) = \sum_{\kappa'} Z_{\kappa'} C(\kappa\kappa' | q \to 0) - \frac{Z_\kappa}{3\varepsilon_0} \sqrt{\frac{p}{\pi}}^3 I , \tag{2.103}$$

(I being the unit matrix). Note that the sum on the right hand side of equation (2.103) does *not* depend on the direction from which $q = 0$ is approached whereas the Coulomb coefficients itselves do (see footnote [2] on page 8). The second term is due to the self potential of the Gaussian charge distribution which is used for the evaluation of the Coulomb coefficients (compare section 2.3). **C** contains the self term and **H** does not.

The electrical field can be calculated by Ewald's method in analogy to equations (2.34)-(2.39):

$$h_\alpha(\kappa l) = \frac{i}{V\varepsilon_0} \sum_{\kappa'} Z_{\kappa'} \sum_g \frac{g_\alpha}{|g|^2} \exp\left[-\frac{g^2}{4p}\right] \exp\left[ig(r^0_\kappa - r^0_{\kappa'})\right] +$$

$$+ \sum_{\kappa'} \sum_{l'} \frac{1}{Z_{\kappa'}} \frac{\partial V^{overlap}_{\kappa\kappa'}(r)}{\partial r_\alpha} \Big|_{r=r^0_{\kappa l}-r^0_{\kappa'l'}} . \tag{2.104}$$

The last two equations allow to calculate electrostatic properties of crystals quite generally. Thus, lattice-dynamical methods can be applied not only to phonon investigations but also to other experimental techniques such as nuclear quadrupole resonance etc..

3.0 Structure of UNISOFT

The program package UNISOFT in its basic version allows to perform a lattice-dynamical treatment of crystals with up to 20 atoms per primitive cell. There are no restrictions on crystal symmetry and structure and phonon wavevectors can be chosen arbitrarily. At present, UNISOFT consists of nine individual programs originally written in FORTRAN IV and adapted to FORTRAN 77. In particular, these programs deal with the following topics:

Program *Topic*

GROUP Group-theoretical analysis of the crystal structure

IND Determination of independent interactions

NN Neighbourhood analysis of each atom in the crystal

MODEL1 Model calculations

HIST Histogram of dispersion curves

SF Dynamical structure factors

PARDER Partial derivatives of phonon frequencies

ROTINV Test of rotational invariance

EFG Electrical fields and their gradients.

The individual programs communicate with each other via four different disk-datasets:

COORD contains informations about the space group of the crystal and about the group of the wavevector for every **q** selected as well as the symmetry coordinates.

INDDAT contains the number of independent interactions and for each of these a representative pair of atoms.

XNN contains for each pair of atoms the vectors for up to the 10th nearest neighbours arranged in neighbouring shells (pair correlation vectors).

RESULT contains the results of model calculation including the matrix of Coulomb coefficients, eigenvectors and eigenvalues.

Fig. 2 on page 24 displays the structure of UNISOFT and the communication between the different programs. Obviously, for a given crystal structure the programs **IND** and **NN** need to be run only once. **GROUP**, however, has to be invoked whenever a new set of phonon wavevectors is considered since the symmetry coordinates depend on **q** and are needed in subsequent programs.
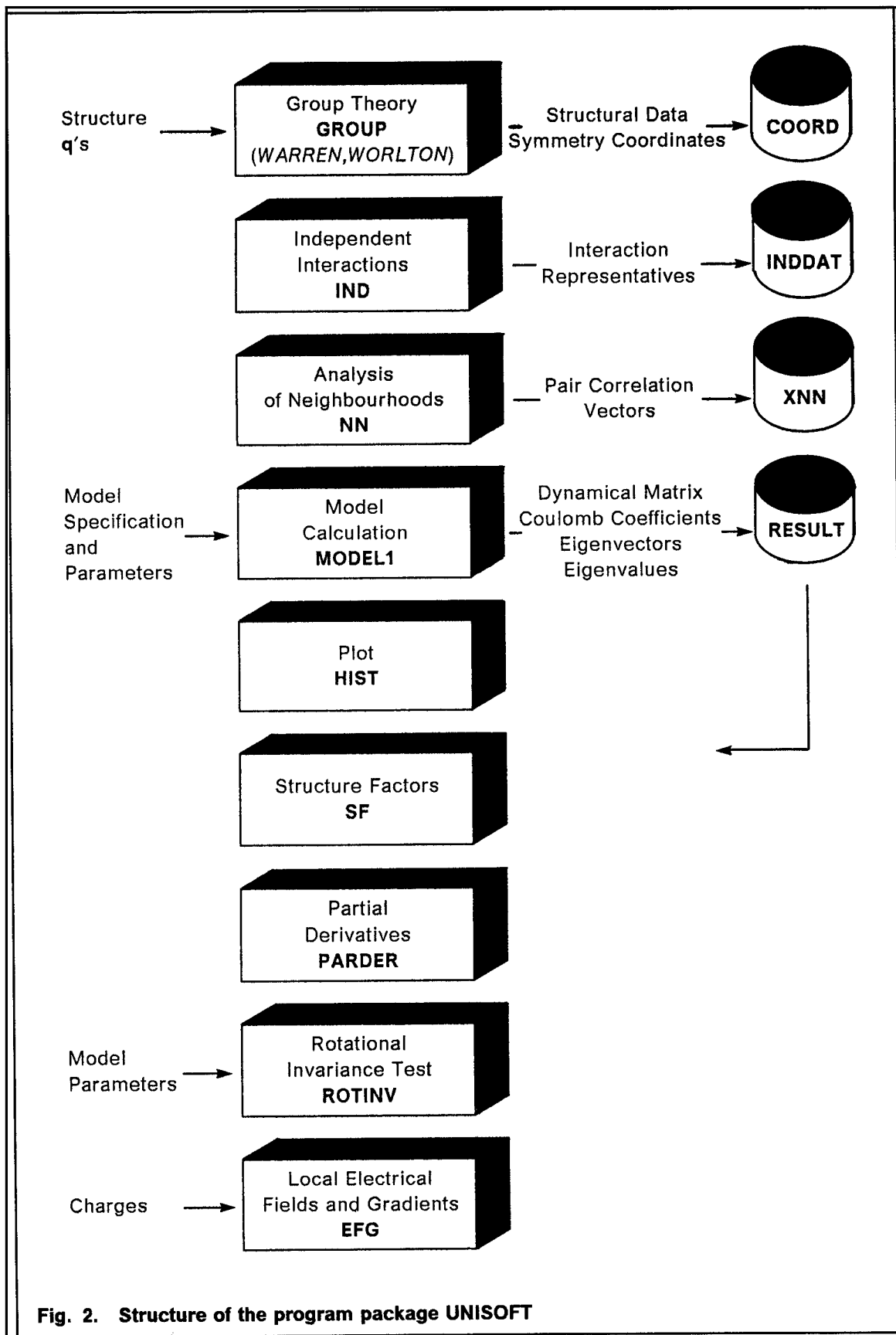
Fig. 2. Structure of the program package UNISOFT

GROUP has been developed by *WARREN* and *WORLTON* [9]. It has been slightly modified in order to be compatible with the communication features of UNISOFT. All the other programs have a rigorous modular structure. They are tailored on the basis of rather small subroutines each of which deals with a very specific task. Therefore, some of the subroutines can be used in different programs. A complete list of all subroutines used within UNISOFT is given in appendix C. The modular structure of UNISOFT offers the possibility to extend this program package rather easily. Thus, in existing programs new features may be implemented such as new interaction potentials in **MODEL1**. On the other hand, separate new programs may be added which make use of previous results and which may contain one or more of the existing general subroutines. Examples for possible extensions are briefly discussed in section 6.

In the following chapter, a detailed description of the purpose of each individual program is given along with the instructions for use.

4.0 Detailed Description of the Individual Programs

4.1 GROUP

4.1.1 General Purpose

The program **GROUP** performes a group-theoretical analysis of a given crystal structure. It is described in detail by *WARREN* and *WORLTON* [9]. Here, we only want to give a short review of the facilities of this program which are important for subsequent lattice-dynamical calculations. **GROUP** has been slightly modified compared to the original version of *WARREN* and *WORLTON* in order to meet the requirements for the communication with the other programs of UNISOFT.

The theoretical foundation of **GROUP** is the review article of *MARADUDIN* and *VOSKO* [4] where the symmetry constraints for the lattice vibrations are investigated in a general way.

Given the basis vectors of the primitive cell and the position vectors of *all* atoms within this cell, the program determines the symmetry operations transforming the infinite crystal into itself, *i.e.* the space group of the lattice. If desired, the atom transformation table and the multiplication table for the symmetry operations are printed.

The set of phonon wavevectors **q** for which lattice-dynamical calculations are to be performed is selected in **GROUP**. For each value of **q** the point group G_q of the rotational parts of symmetry operations which leave **q** invariant (modulo a reciprocal lattice vector) is determined along with the set of irreducible multiplier representations (IMR) of G_q.

For N atoms per primitive cell the vector space of the 3N cartesian coordinates provides a 3N-dimensional representation Γ_{3N} of G_q according to equation (2.82) on page 17. This representation may be written as a direct sum of several of the irreducible representations γ_i:

$$\Gamma_{3N} = \sum_i m_i \gamma_i \, . \tag{4.1}$$

The multiplicity m_i of the i-th IMR in this decomposition is given by the characters χ of Γ and χ_i of γ_i:

$$m_i = \frac{1}{G} \sum_i \chi_i^*(g) \, \chi(g) \, , \tag{4.2}$$

where G is the order of G_q and the sum runs over all elements g of G_q. Basis vectors for the corresponding invariant subspaces are found by projector techniques as described in [4]. These so-called *Symmetry Coordinates* are used for the block diagonalization of the Dynamical Matrix as discussed in section 2.9. By diagonalizing

the individual blocks of the Dynamical Matrix separately, the eigenvectors will be arranged automatically according to their symmetry.

The form of the symmetry-reduced Dynamical Matrix can be obtained without a specific lattice-dynamical model simply from group theory: The number of independent elements of the Dynamical Matrix is given by:

$$n = \frac{1}{2} \sum_i m_i(m_i + 1)$$ (4.3)

as a direct consequence of the irreducible decomposition. This number might, however, be further reduced if there is a symmetry operation which transformes q into $-q$ since $D(-q) = D^*(q)$.

Numerically, independent elements can be found in the following way: Starting from a random hermitian matrix all the symmetry elements of G_q are applied according to equation (2.82). Comparing the resultant and the original matrices, those elements which have to be identical are detected as well as those which have to be zero. Thus, representing different elements by different alphabetical symbols and zero elements by a dot (.), a symbolic symmetry reduced Dynamical Matrix is obtained. This reduction, however, may be incomplete since the computer does not realize if two elements are linked by a well defined factor such as 1/2, 2, -1, $\sqrt{3/2}$ etc.. Nevertheless, the symbolic form of the (partially) reduced Dynamical Matrix which is calculated in **GROUP** may provide some feeling for symmetry constraints since this matrix is defined with respect to the cartesian particle coordinates. Using the symmetry coordinates, the symbolic matrix is transformed into a block diagonalized form. This representation, however, may be less illustrative since it is defined in the vector space of the symmetry coordinates.

For the Γ-point (zero wavevector) G_q obviously is the whole point group of the lattice. The selection rules for Raman and infrared active modes are determined by symmetry and, hence, can be detected simply by the application of group theory.

Note that in systems with Coulomb interactions lattice-dynamical calculations cannot be performed exactly for $q = 0$ without taking into account retardation effects (c.f. footnote 2 on page 8). In these cases, Γ-point modes are calculated by considering very small but non-zero wavevectors δq. The group-theoretical treatment, however, should be based on the whole point group of the lattice even if, striktly speaking, δq is of lower symmetry. Consequently, all wavevectors with moduli smaller than 0.001Å^{-1} are interpreted within **GROUP** as being zero.

4.1.2   The Position of GROUP within the Framework of UNISOFT

In a lattice-dynamical treatment of a crystal structure **GROUP** has to be invoked as the first program. Since the symmetry coordinates depend on the phonon wavevector q the program **GROUP** also has to be run whenever a new set of q-values is selected.

The structural parameters including the position vectors of all atoms per primitive cell and the symmetry operations are written on the disk dataset **COORD** (logical unit 1).

For each value of the phonon wavevector the irreducible representations and the corresponding calculated symmetry coordinates are saved on **COORD** as well and can be used by other programs.

4.1.3 Input

Card 1 **Comment** [18A4]

This comment is used as a header for
the printed output.

Card 2 **NA, IPM, IDC, NCC, NX** [5I5]

NA	= Number of atoms per primitive cell ($\leq$ 20)
IPM	= 1 if printing of multiplication
	table of the space group is desired
IDC	= 0(1) if the D-(C)-definition according to
	MARADUDIN and *VOSKO* of the
	Dynamical Matrix is to be used
	(see footnote [1] on page 5)
	In order to be compatible with other
	programs of UNISOFT use the D-definition,
	IDC = 0, always!
NCC	= Number of comment double-cards given below
NX	= Number of additional atoms (outside the
	primitive cell) the positions of which will
	be given to make sure that the space group
	of the crystal will be determined correctly.
	In most cases NX can be set to zero. Only
	if the proper space group is not found it
	may be necessary to use NX > 0.

Card 3 **(NAME(I), I = 1,NA)** [18A4]

NAME(I) = symbolic name for atom I (in general
the chemical symbol) which is used
to provide a more illustrative output

Card 4 **Comment** [33A4]

NCC (double cards) of format [33A4]
providing more detailed information about the
structure under consideration

Card 5 **((A(I,J), I = 1,3), J = 1,3)** [9F8.5]

A(I,J)	= I-th cartesian coordinate of the
	J-th basis vector of the primitive
	cell in the direct space in $\mathring{A}$

For each of the NA + NX atoms one card of the
following type must be given:

Card 6 **TY, (X(I), I = 1,3), JM**   **[I5,3F10.5,I5]**

TY   = type number of the atom
          This parameter is used to distinguish
          between different kinds of atoms.
          Symmetrical equivalent atoms obviously
          are of the same type. This is, however,
          not necessarily the case for all chemically
          identical atoms: Rather, atoms which are
          expected to have different interaction
          parameters have to be of different types.

X(I)   = I-th cartesian coordinate of
          the position vector in Å

JM   = 1(0) if the unit is a molecule (atom)
          Since in the present version, UNISOFT
          deals with atomic structures only,
          use JM = 0 always!

Card 7 **(QS(I), I = 1,3)**   **[3F10.5]**

QS(I)   = I-th cartesian coordinate in Å^{-1}
          of a vector QS used for scaling
          wavevector input.
          If QS(I) = 0 wavevectors are scaled
          according to the intersection of
          the cartesian axes with the
          Brillouin zone boundary
          (not exactly in the case
          of more complicated structures -
          check by yourself!).

Card 8 **NIR, IT**   **[2I5]**

Control card:

NIR   = 0: program stop
          = 1: program continue
          = -1: program restart

IT   = 0,1,...8: control parameter for output list
          A larger value of IT corresponds to more
          printed informations. Please, check by
          yourself the effect of IT.

Card 9 **Comment**   **[18A4]**

For each value of the phonon wavevector a
separate comment can be given.

```
Card 10 (Q(I), I = 1,3)                                      [3F10.5]
     Q(I)      = I-th cartesian coordinate of the
                 wavevector in units of QS(I) or
                 in units of the zone boundary
                 (see card 7)
```

You may continue the input by giving the cards 8.- 10. for other values of **Q**. The program stops reading further input cards if it detects a card of type 8 with NIT = 0.

4.1.4 Output

The extent of the printed output is determined by the parameter IT (card 8). For larger values of IT even intermediate results during the determination of irreducible representations are printed. The user is recommended to try the different possibilities of output control by himself.

If **GROUP** is run for the first time for a given structure the results of the space group determination should carefully be examined. In some cases it might be necessary to give coordinates of additional atoms outside the first primitive cell in order to make sure that the program will find the correct space group.

An example is given in appendix A.1, page 69.

4.2 IND

The program **IND** determines the number of different types of atoms and the independent interactions in a crystal which has been defined by the input of the program **GROUP**. As pointed out in section 2.6.4 a list of independent, *i.e.* symmetrical inequivalent, interactions as produced by **IND** may serve as a guide for a proper set-up of a lattice-dynamical model. This is especially useful for more complicated structures since a multiple (and perhaps inconsistent) definition of the same interaction can easily be avoided.

IND has to be run only once for a given structure. It does not need any user input but reads the structural information from the disk-dataset **COORD** (logical unit 1). Thus, **GROUP** has to be run first. The output is printed as well as stored on the file **INDDAT** (logical unit 3) for further use by subsequent programs. An example is given in appendix A.2, page 76.

4.3 NN

4.3.1 General Purpose

The program **NN** analyzes the neighbourhood of each atom in the primitive cell. Since the calculation of a Dynamical Matrix requires the evaluation of a lattice sum corresponding to equations (2.18) or (2.38) it is convenient to arrange the neighbours of a given atom in spherical shells. The lattice sums are rapidly convergent and only near neighbours need to be considered. For each pair of atoms κ and κ' up to 10 neighbouring shells are examined: *i.e.*, particles κ' in different primitive cells l' are arranged according to their distance with respect to atom κ in cell 0. All atoms $\kappa'l'$ which exhibit the same or nearly the same distance are said to belong to the same shell (see Fig. 3). Obviously, the interactions between κ and all atoms κ' within a shell are identical at least for central force models.

Fig. 3.   The concept of neighbouring shells:
Atom κ in cell 0 (●) surrounded by atoms κ' in different cells l_i, l_j, ...(o).
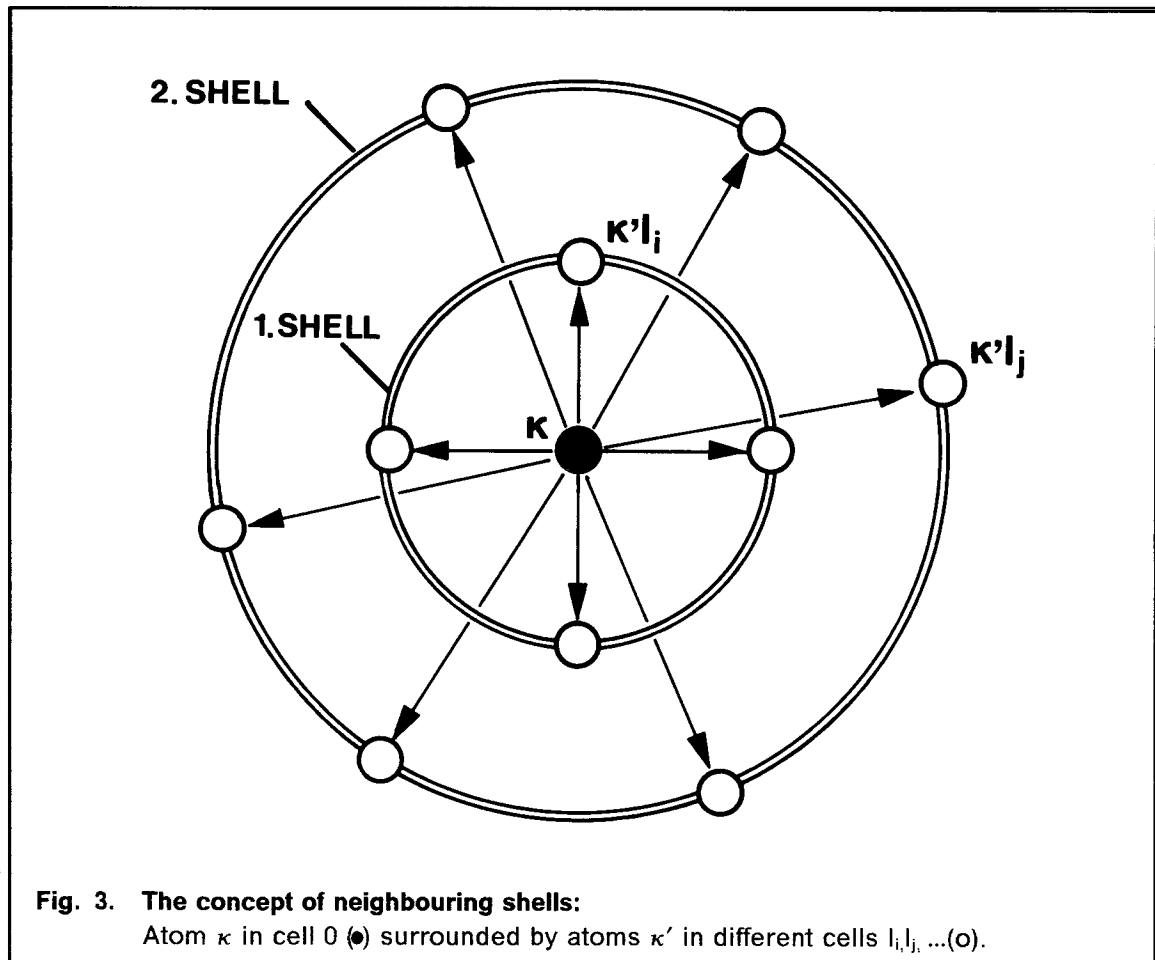
The program **NN** lists the difference vectors $r_{x0} - r_{x'l'}$ for all atoms within these shells. In parallel, the data are stored on the disk-dataset **XNN**. Subsequent programs like **MODEL1, PARDER** or **EFG** make use of the ordered arrangement of the atoms: The lattice sum of equation (2.18) is replaced by the sum over all particles of the first neighbouring shells. Furthermore, for complicated structures also the set-up of a

lattice-dynamical model itself is simplified using the results of **NN**: Since **NN** essentially determines the pair-correlation one can immediately select the most important interactions which have to be specified in the model. In slightly distorted structures, *e.g.*, often two or more shells are rather close to one another. Thus, the neglect of interactions with atoms of one of these shells can lead to unreasonable results.

The number of atoms κ' which are located at a given distance from an atom κ defines the partial pair-correlation function. The program **NN** offers the possibility to display this correlation function as a histogram plot. Remembering that several atoms within the primitive cell might belong to the same type, it can be even more illustrative to plot the *type-dependent correlation function*, *i.e.* the number of particles of the same type located at a given distance.

The number of shells to be examined for each pair of atoms κ and κ' can be chosen between 1 and 10. The thickness of the shells is given in Å. Note, however, that both parameters have to be selected in a way to guarantee that the number of atoms per shell does not exceed 50!

4.3.2 The Position of NN within the Framework of UNISOFT

NN needs to be run only once for a given structure. The structural information is read from the file **COORD** (logical unit 1). If a plot of the type-dependent pair-correlation function is required the information about the different types of atoms is read from **INDDAT** (logical unit 2). Thus, **GROUP** and **IND** have to be run first. The distance vectors of all atoms in the shells examined are written on the disk-dataset **XNN** (logical unit 3). These data provide the input for other programs like **MODEL1, PARDER** or **EFG**.

4.3.3 Input

```
Card 1   (IDIR(I), I=1,3)                                              [3I5]
         Output Control:
         IDIR(1)  = 1 (0): with (without) printout
         IDIR(2)  = 0 no histogram of pair correlation function (pcf)
         IDIR(2)  = 1 histogram of atom specific pcf
         IDIR(2)  = 2 histogram of type specific pcf
                      (may be useful if several atoms
                      within the primitive cell belong
                      to the same type)
         IDIR(3)  = 0 (1): (no) storage of data
```

```
Card 2   NNS                                                          [I5]
         NNS     = maximum number of shells to be examined.
                   NNS ≤ 10 and NNS has to be chosen
                   in a way to guarantee that the number of
                   atoms per shell is not larger than 50.
```

```
Card 3   DELTA, DMAX                                                  [2F10.6]
         DELTA   = thickness of a shell in Å
         DMAX    = maximum shell radius in Å for histogram-plot
```

4.3.4 Output

The output may become rather voluminous especially for more complicated structures with many particles per unit cell. An excerpt of an example is given in appendix A.3, page 77.

4.4 MODEL1

4.4.1 General Purpose

The program **MODEL1** calculates phonon frequencies and eigenvectors for the particular structure analyzed in the preceeding programs **GROUP**, **IND** and **NN**. It can thus be regarded as the heart of UNISOFT wheras the other programs are auxiliary routines. The phonon wavevectors are chosen arbitrarily in **GROUP** since the group-theoretical treatment, *i.e.* the calculation of symmetry coordinates, depends on **q** (see section 2.9).

A lattice-dynamical model set-up requires the specification of all (pair-) interactions within a particular structure. In most cases, interactions (other than Coulomb interactions) will be restricted to near neighbours. Sometimes, force constants may be calculated from interatomic potentials, but if a reliable potential does not exist, *e.g.* for covalent bonds, the force constants itselves are considered as model parameters (Born-von Kármán model). In the latter case, the number of model parameters may become rather large if more neighbouring shells are taken into account. The essential feature of **MODEL1** is the fact that the interaction between each pair of atoms can be modelled individually by selecting one or more of the following interaction types which are implemented presently:

1. Born-von Kármán model (longitudinal and transverse springs)

2. Born-Mayer potential

3. Lennard-Jones potential

4. van der Waals potential

5. Coulomb potential

6. shell model.

This list may be extended rather easily if necessary. The combination of different interactions for different pairs of atoms allows the set-up of very specific force models.

The variety of different models which may be calculated with **MODEL1** does not necessarily lead to a complicated mode of operation. Rather, a formalism is found which reduces the required number of input cards as much as possible and, hence, facilitates the use of this program.

The theoretical basis of **MODEL1** is discussed in chapter 2. Here, we only want to give some additional informations which are important for numerical calculations. The entire model is composed on the basis of pair-interactions. Since we deal with central forces, the interactions between two pairs of atoms belonging to the same neighbouring shell are assumed to be identical. This is definitely true if longitudinal and transverse force constants are deduced from a specific interatomic potential. Whenever an interaction is described by atom-specific parameters like a short-range

repulsion parameter σ (Born-Mayer potential), a charge Z (Coulomb-potential) or a polarizability α (shell model) the same parameter applies to all atoms of the same type as defined in **GROUP**. The range for the validity of a short-range interaction type is always given in numbers of neighbouring shells since these have already been analyzed by **NN**.

As discussed in sections 2.1 and 2.4 the Dynamical Matrix and the Fourier transformed force constant matrix can be collected from (3×3) submatrices $D^{(m)}(\kappa\kappa'|q)$ and $F^{(m)}(\kappa\kappa'|q)$, respectively, which describe the interaction between particles κ and κ' according to the interaction type or model potential m. The shell model, however, requires a hermitian transformation of the full (3N×3N) matrices. Here, the Fourier transformed force constant matrices F^s and F^T, resp. $F^{T'}$, as defined in section 2.5 must be treated separately and these, in turn, can be collected from small submatrices. Thus, the problem of constructing a Dynamical Matrix is reduced to the calculation of the submatrices $F(\kappa\kappa'|q)$, $F^s(\kappa\kappa'|q)$, $F^T(\kappa\kappa'|q)$ and $C(\kappa\kappa'|q)$[6]. We can restrict ourselves to those pairs of atoms κ and κ' which correspond to one of the independent interactions determined by program **IND**. Other submatrices are calculated by means of the transformation (2.82) and, since the matrices F and F^s are hermitian, $F(\kappa'\kappa|q)$, $F^s(\kappa'\kappa|q)$ and $C(\kappa'\kappa|q)$ are obtained immediately. F^T, however, may be non-hermitian. Therefore, another independent submatrix, namely $F^T(\kappa'\kappa|q)$ is considered in the program.

Inserting all these small matrices into the full (3N×3N) matrices and calculating the self terms according to equation (2.6) from the condition of translational invariance, the Fourier transformed force constant matrices are obtained. If the shell model is used, finally the transformation of equation (2.67) is performed and the resultant matrix is combined with F and multiplied by the mass tensor to give the complete Dynamical Matrix.

The Coulomb potential is long-ranged and the corresponding part of the Dynamical Matrix is represented by rapidly converging series in direct and reciprocal space according to *EWALD* [5] as discussed in section 2.3. The maximal radius r_{max} for the summation in direct space can be given as input. The Ewald-parameter p corresponding to the width of the Gaussian charge distribution (see equation (2.35)) is calculated from r_{max} by

$$x = r_{max}\sqrt{p} = 4.17 \tag{4.4}$$

as proposed by *NÜSSLEIN* [9]. This choice is convenient since both damping factors entering in the two series are sufficiently small for this value of x:

$$e^{-x^2} \simeq 2.8 \times 10^{-8} \quad \text{and} \quad 1 - erf(x) \simeq 3.8 \times 10^{-9}.$$

The program checks whether the choice of r_{max} is suitable or not: First, r_{max} should not be too large in order to be able to use the results of program **NN**; *i.e.* r_{max} has to be smaller than the radius of the last neighbouring shell examined in **NN**. Second, if two

---

6   In the present context, F denotes that part of the Fourier transformed force constant matrix which does not contain polarization effects.

neighbouring shells are very close to one another, the consideration of only one of these shells may lead to wrong results. In this case, r_{max} will automatically be reduced until a gap of more than 0.5 Å between two shells is reached. If the corresponding radii are d_n and d_{n+1}, r_{max} is calculated as:

$$r_{max} = 0.2\,d_n + 0.8\,d_{n+1} \, . \tag{4.5}$$

The actual values used within a calculation can be printed if desired (see control parameters, section 4.4.7).

Note that the phonon wavevector must not be set exactly equal to zero if Coulomb interaction is used (see footnote [2] on page 8 and section 4.1.1)

If the Dynamical Matrix is completed, the symmetry coordinates determined in **GROUP** are used for the block-diagonalization according to equation (2.99). The diagonalization of the individual blocks yields the eigenvalues and eigenvectors. The latter are retransformed to the cartesian coordinate system by multiplication with the symmetry coordinates (equation (2.100)).

4.4.2 The Position of MODEL1 within the Framework of UNISOFT

MODEL1 is the central program of UNISOFT. It uses all the results of programs **GROUP**, **IND** and **NN** which have to be run first. The data are read from the files **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **XNN** (logical unit 4). The calculated Dynamical Matrices, Coulomb coefficients, eigenvectors and eigenvalues may be stored on the disk-dataset **RESULT** (logical unit 2), if desired. Via this dataset the results of the model calculation can be transferred to other programs like **HIST**, **PARDER** or **SF**.

4.4.3 The Structure of MODEL1

A schematic block-diagram of **MODEL1** is given in Fig. 4 on page 39. Obviously, the most specific and complex work is done in the two subroutines GETPAR and DYN2. These routines dealing with the definition of the model and with the set-up of the Dynamical Matrix, respectively, are therefore discussed in separate sections. All the other blocks in Fig. 4 represent rather simple activities and need not be described in detail. For the diagonalization of the Dynamical Matrix the standard IMSL routine E2CHF is used which is embedded in subroutine EIGEN. If necessary, it can easily be replaced.

A complete list of all subroutines is given in appendix C.
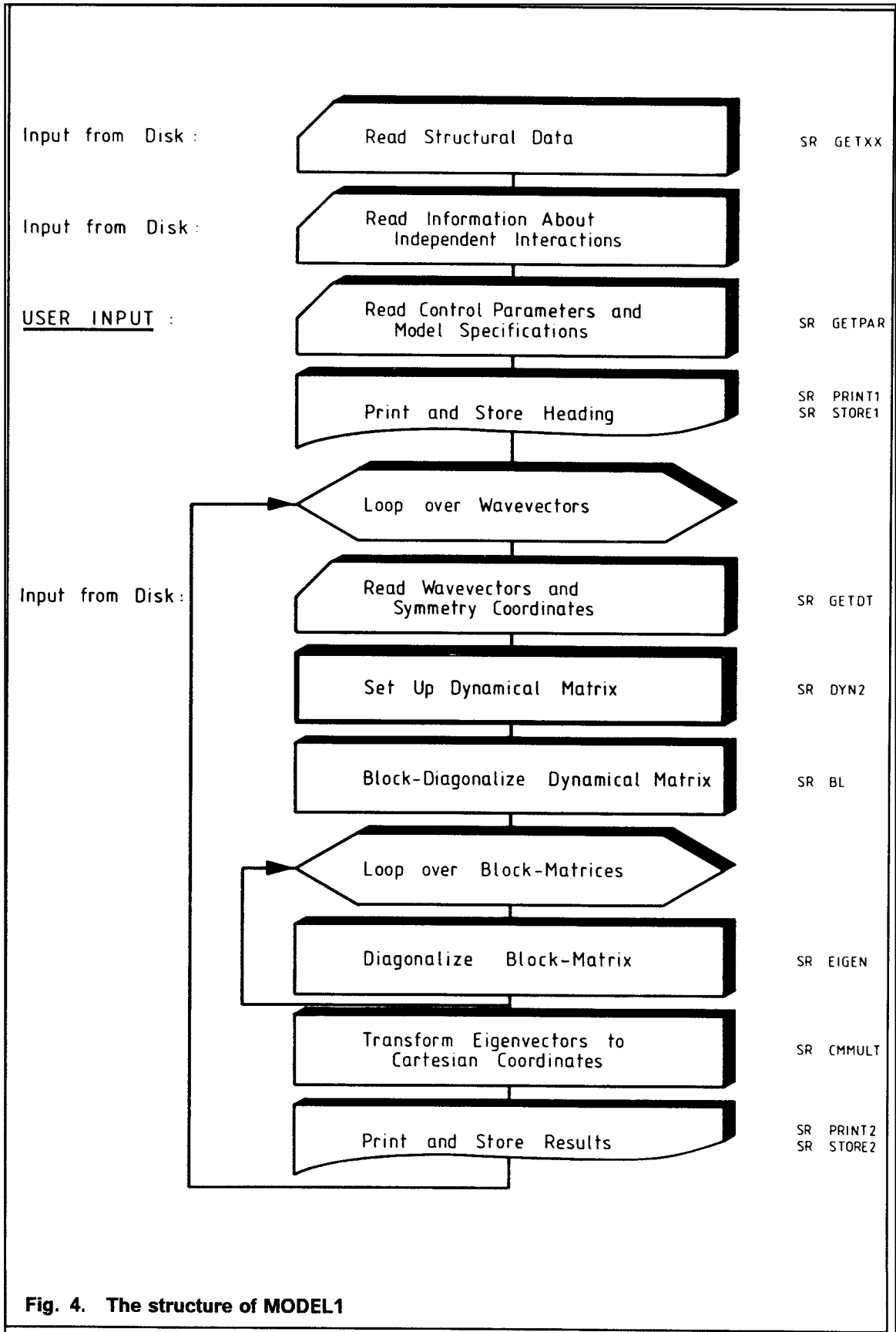
Fig. 4.   The structure of MODEL1

4.4.4 How to Define a Model Set-Up

In this section the input procedure is described which is governed by subroutine GETPAR. As mentioned earlier, each independent interaction can be modelled by an arbitrary superposition of the different interaction types collected in Tab. 1.

Interaction type		General Parameters		Atom Specific Parameters		Interaction Specific Parameters	
#	Specification	No.	Symbol [unit]	No. per atom type	Symbol [unit]	No. per neighb. shell	Symbol [unit]
1	Force constant model (Born - von Kármán)	-		-		2	$L\,[Nm^{-1}]$ $T\,[Nm^{-1}]$
2	Born-Mayer potential	1	$V_0\,[eV]$	1	$\sigma\,[\text{Å}]$	-	
3	Lennard-Jones potential	1	$V_0\,[eV]$	1	$\sigma\,[\text{Å}]$	-	
4	van der Waals potential	1	$V_0\,[eV]$	1	$\sigma\,[\text{Å}]$	-	
5	Coulomb potential	-		1	$Z\,[e]$	-	
6	shell model	-		2	$Y\,[e]$ $\alpha\,[\text{Å}^3]$	6	$L^{c-s}[Nm^{-1}]$ $T^{c-s}[Nm^{-1}]$ $L^{s-c}[Nm^{-1}]$ $T^{s-c}[Nm^{-1}]$ $L^{s-s}[Nm^{-1}]$ $T^{s-s}[Nm^{-1}]$

V_0	strength of potential
σ	short-range interaction parameter
Z	ionic charge
Y	shell charge
α	free ion polarizability
L	longitudinal force constant
T	transverse force constant

Tab. 1. Interaction types (model potentials) supported by UNISOFT

Each interaction type is represented by a running number and specified by a certain number of parameters. In order to simplify the input procedure which has to take into

account all the different types of interactions, three groups of parameters are introduced:

Atom-Specific Parameters (ASP's)

These parameters depend on the nature of the distinguishable types of atoms only. Examples are the Born-Mayer radius, the ionic charge, the electronic polarizability, etc..

General Parameters (GP's)

These parameters are independent of atomic properties. The prefactors V_o in the Born-Mayer, Lennard-Jones or van der Waals potentials are examples.

Interaction-Specific Parameters (ISP's)

These parameters in general depend on a particular *pair* of atoms and not only on the nature of each individual one. Examples are force constants in the Born-von Kármán model or in the shell model. It is assumed that the same ISP's hold for all pairs of atoms κ and κ' which exhibit the same interatomic spacing, *i.e.* for all atoms within the same neighbouring shell.

The corresponding parameters for the individual interaction types supported by UNISOFT are included in Tab. 1.

Within the model set-up all the different parameters are labelled by a running integer. Actual values are assigned to the various parameters at the end of the input. Thus different interactions may be described by the same parameters, *e.g.*, and the modification of parameter values is independent of the model set-up.

Example: Suppose you have two pairs of atoms (κ,κ') and (λ,λ') the interaction of which is modelled by longitudinal (L) and transverse (T) springs (Born-von Kármán model). These parameters may be labelled by the numbers 1, 2, 3, 4 where the parameters 1 and 2 correspond to L and T for the κ-κ' interaction while the parameters 3 and 4 describe the λ-λ' interaction. After having completed the model set-up for all interactions the actual parameter values are given as a series like:

100.   17.   50.   19.   ...

assigning $L(\kappa\kappa') = 100\,Nm^{-1}$, $T(\kappa\kappa') = 17\,Nm^{-1}$, $L(\lambda\lambda') = 50\,Nm^{-1}$ and $T(\lambda\lambda') = 19\,Nm^{-1}$. For the calculation of phonon frequencies for other sets of parameter values only this last line must be modified. If the λ-λ' interaction is to be identical with the κ-κ' interaction (in spite of being symmetrical inequivalent) the same parameter number can be used for both and parameters 3 and 4 are dropped.

The specification of a particular interaction model is achieved in the following manner:

1. **Give the number N of an interaction type.**

2. **Give the numbers for ASP's and GP's for interaction type N, if any.**

3. **Select those pairs of atoms I,J to which the interaction type N is applied and give the number of neighbouring shells NS until which this interaction is extended. (In the case of Coulomb interaction, N=5, all atoms in the whole crystal are automatically considered.)**

4. **For each of the NS shells give the numbers for ISP's, if any.**

5. **Repeat steps 3 and 4 until all *independent* pair-interactions are worked through.**

6. **Repeat the whole sequence, 1.-5., for different interaction types until the model set-up is completed.**

7. **Assign values to all the parameters used in the set-up.**

Further examples might illustrate this procedure (the input numbers are printed in bold):

a)   Born-von Kármán interactions between atoms 1 and 4 up to the second nearest neighbours and between atoms 2 and 5 up to the third nearest neighbours:
Interaction type **1**
No ASP's and GP's
Pair **1 4** considering **2** neighbouring shells
ISP's **1**(L) **2**(T) for the first shell
ISP's **3**(L) **4**(T) for the second shell
Pair **2 5** considering **3** neighbouring shells
ISP's **5**(L) **6**(T) for the first shell
ISP's **7**(L) **8**(T) for the second shell
ISP's **9**(L) **10**(T) for the third shell

If all Born-von Kármán interactions are specified a **blank** input card indicates the end of input for interactions of type 1.

b)   Born-Mayer potential between atoms 3 and 6 up to the second neighbouring shell and between atoms 4 and 7 for nearest neighbours only. (Suppose you have 4 different types of atoms in the crystal):
Interaction type **2**
Born-Mayer radii σ as ASP's: **11 12 13 14**
Prefactor V_o as GP: **15**
Applied to pair **3 6** considering **2** shells
No ISP's
Applied to pair **4 7** considering **1** shell
No ISP's

If all Born-Mayer interactions are specified a **blank** input card indicates the end of input for interaction type 2. (The short-range interactions 3 (Lennard-Jones potential) and 4 (van der Waals potential) are treated similarly.)

c)   Coulomb potential assuming 4 different atom types:

For the Coulomb potential an extra input card specifying the maximal radius for the summation in direct space has to be given. A proper choice is 5 ... 10Å.

Interaction type **5**

Maximal radius: **7.5**

Charges as ASP's: **16 16 17 18**

and nothing else, since the Coulomb potential applies to the whole crystal. Note, in this example the same charge, given by parameter 16, is assigned to atoms of type 1 and 2.

d)   Shell model:

(If the shell model is required the Coulomb potential has to be specified as well.)

Nearest neighbour atoms 5 and 8 are coupled by the shell model interactions:

Interaction type **6**

ASP's: shell charges **19 19 19 20** and polarizabilities **21 21 21 22**

Pair **5 8** considering **1** shell

ISP's: **23**(L^{c-s}) **24**(T^{c-s}) **23**(L^{s-c}) **24**(T^{s-c}) **25**(L^{s-s}) **26**(T^{s-s})

Again, a **blank** input card indicates the end of input for interaction type 6. Note, in this example the same charges and polarizabilities are assigned to atoms of type 1, 2 and 3 (given by parameters 19 and 21) and the core-shell and the shell-core coupling between atoms 5 and 8 are identical (given by parameters 23 and 24).

If no other interaction types are needed a further **blank** input card indicates the end of model specification.

Finally, the values for all the parameters (1...26) are given in the corresponding units listed in table 1 on page 29.

It should be noticed again that the specification of a model is to be confined to the independent interactions listed by program **IND**.

The input for program **MODEL1** is completed by a card with output-control parameters and by one or more cards containing the masses of the different types of atoms.

The input is interpreted by the subroutine GETPAR which automatically transfers the specification of a particular interaction to all the symmetrical equivalent ones.

4.4.5 Mode of Parameter-Storage

All parameter numbers used within a particular model set-up are stored one behind the other, just as they are read in, in the integer vector IP. In order to find the correct parameter numbers for one specific interaction during the model calculation there are two pointers to elements of IP:

LOCM(N)   points to the location containing the number of the first atom-specific parameter (ASP) of interaction type N.

LOC(I,J,N)   points to the location containing the number of neighbouring shells (multiplied by 1000) which are to be considered for the interaction between atom I and J according to interaction type N.

A special subroutine NPM determines the number of ASP's and ISP's for a given interaction type N returning the variables:

NPAR(1,N) = total number of ASP's + total number of GP's
NPAR(2,N) = total number of ISP's per neighbouring shell[7] .

Obviously, the total number of ASP's depends on the number of different atom types determined by program **IND**. The numbers of the NPAR(1,N) atom-specific and general parameters are stored one behind the other on the vector IP starting at location LOCM(N)+1. Similarly, the numbers of the NPAR(2,N) ISP's for the different neighbouring shells are stored starting at location LOC(I,J,N)+1.

A schematical representation of the vector IP is given in Fig. 5 on page 45.

Note, that the implementation of new interaction types requires the modification of subroutine NPM.

If the interaction between atoms I and J is specified by input and the interaction between IT and JT is symmetrical equivalent it is sufficient to assign.

LOC(IT,JT,N) = LOC(I,J,N)

in order to obtain a proper model set-up. The relation

LOC(J,I,N) = LOC(I,J,N) ,

however, is not always true: In the shell model, the core-shell coupling and the shell-core coupling might be different. In this case, the parameters for the interaction between J and I as deduced from those for the I-J interaction are transferred to an unused location on the vector IP.

---

[7]   A value NPAR(2,N)=-1 indicates that there are no ISP's but the particles to which the interaction type N is applied must be specified.

Location	Content of IP
	· · ·
LOCM(N) ————————▶	Number of the first ASP for atom type 1
LOCM(N) + 1 ————————▶	Number of the first ASP for atom type 2
	· · ·
LOCM(N) + MAXTYP-1 ———▶	Number of the first ASP for atom type MAXTYP
	· · ·
LOCM(N) + NPAR(1,N)-1 ——▶	Number of the last GP
	· · ·
LOC(I,J,N) ————————▶	Number of neighbouring shells (×1000) to be considered for interaction I-J
LOC(I,J,N) + 1 ————————▶	Number of the first ISP for the first shell
	· · ·
LOC(I,J,N) + NPAR(2,N) ——▶	Number of the last ISP for the first shell
	· · ·
LOC(I,J,N) + NPAR(2,N)×NS ▶	Number of the last ISP for shell no. NS
	· · ·

Fig. 5. Parameter storage for interaction N within the vector IP

The actual value of a parameter entering in the calculation is stored in the real vector P: P(I) is the value of the parameter number I.

The total interaction (as a superposition of different model potentials) between atoms I and J is coded in the array NMOD(I,J) which is defined by

$$NMOD(I,J) = \sum_m w_m 2^{m-1} \tag{4.6}$$

where the summation runs over all interaction types and $w_m = 1$ (0) if interaction m is (not) included in the model set-up for the I-J coupling.

4.4.6 Calculation of the Dynamical Matrix

As can be seen from Fig. 4 on page 39 the calculation of the Dynamical Matrix is performed in subroutine DYN2. DYN2 itself represents a network of relatively small subroutines each of which dealing with a very specific job. Fig. 6 on page 47 displays the overall structure of DYN2. Within the loop over all pairs of particles I,J the (3×3) submatrices corresponding to the I-J interaction are calculated. In a first step, the interaction types are determined in subroutine MODX. The main job is then done by subroutine DIJ which returns the Fourier transformed force constant matrix $F(IJ|q)$ ($=DD$)[8], the matrix of Coulomb coefficients multiplied by the charges $F^c(IJ|q)$ ($=CEM$) (if the Coulomb potential is invoked) and, in case of the shell model, the matrices $F^T(IJ|q)$ ($=TT$), $F^{T'}(IJ|q)$ ($=TT1$) and $F^s(IJ|q)$ ($=SS$). Furthermore, the corresponding matrices for $q=0$ (resp. $q=\delta q$ for Coulomb interaction) which enter in the self terms (PP, MST, PTT, PTT1 and PSS) are calculated in DIJ as well. The difference vectors between atoms I and J for the various neighbouring shells are read from the disk-dataset **XNN** (logical unit 4) and the different interaction types are considered in a do-loop. Decoding the information contained in the vector IP (see section 4.4.5) subroutine GETPM gets the specific parameter values determining the interaction according to one single model potential.

Subroutine MODELX serves as a switch to the different routines performing the calculation for a particular interaction type. Obviously, new model potentials can easily be included just by supplying additional short subroutines at this stage.

Leaving the subroutine DIJ the matrix elements are rounded; *i.e.* all numbers with moduli smaller than 10^{-20} are set zero. Subroutine CTOD changes the matrices to the D-definition corresponding to equation (2.13) (c.f. footnote [1] on page 5).

The resulting matrices are inserted into the full (3N×3N) matrices $F(q)$ ($=D$), $F^c(q)$ ($=C$), $F^{T'}(q)$ ($=T$) and $F^s(q)$ ($=S$) by subroutine CINS. The same is done for the real $q=0$-matrices by subroutine MINS (yielding PH, MC, PT and PS). The symmetrical equivalent interactions are considered in subroutines CTRNSF and MTRNSF according to equation (2.82).

All interactions for which the matrix elements are determined either by direct calculation or by symmetry considerations are labelled by $ID(I,J)=1$. Thus, a multiple treatment of the same submatrix is avoided.

For the matrices **F** ($=D$) and, if the shell model is used, $F^{T'}$ ($=T$) and F^s ($=S$) the self term is calculated from the condition of translational invariance (equation (2.6)) in subroutine SELF. If needed, the polarization part of the Dynamical Matrix, *i.e.* the third term on the right hand side of equation (2.67), is calculated and added to the rest of the Fourier transformed force constant matrix in subroutine SHELL2. Here, for the inversion of the matrix F^{ss} + **YCY** the IMSL routine LINCG is used which may be replaced if desired.

---

8 In brackets, the names used in the program listing are given.

Loop over Particles   I,J

Have the
(I,J)-submatrices already
been determined
?   — yes

no

Which model-potentials are used
for the (I,J)-interaction ?   SR MODX

Determine the 3×3 Submatrices
F(IJIq), F^C(IJIq), F^T(IJIq), F^T(JIIq), F^S(IJIq)

SR DIJ

Read the Difference-Vectors
between Particles I and J

Loop over Interaction-Types

Get Actual Parameter Values   SR GETPM

Switch to Subroutines
for Model-Potentials   SR MODELX

| Force Const Model FCM | Bern-Mayer BMP | Lennard-Jones LJP | van der Waals VDWP | Coulomb CP | Shell Model SHELL1 |

Rounding of Matrixelements   SR ROUND

Change to D-Definition   SR CTOD

Insert into full 3N×3N Matrices   SR CINS
                                   SR MINS

Calculate the Symmetrical   SR CTRNSF
Equivalent Submatrices   SR MTRNSF

Calculate the Self Term   SR SELF

Is the shell
model required
?   — yes

no

Calculate the Polarization Part
of the Dynamical Matrix   SR SHELL2

Multiply by the Mass Tensor   SR MOM

The Dynamical Matrix

Fig. 6.   The structure of subroutine DYN2

As the final operation in DYN2, the multiplication with the mass-tensor (in subroutine MDM) yields the complete Dynamical Matrix **D**.

4.4.7 Input

The idea of the input procedure has already been described in section 4.4.4. Here, we give the specification of the input cards required. A comprehensive list without comment is given in appendix B.3.

Card 1 **(IDIR(I), I = 1,10)**   **[10I5]**

Control parameters:

IDIR(1) = 1(0): (no) printout of symmetry coordinates

IDIR(2) = 1(0): (no) printout of the Dynamical Matrix

IDIR(3) = 1(0): (no) printout the block-diagonalized
              Dynamical Matrix

IDIR(4) = 1(0): (no) printout the block matrices

IDIR(5) = 1(0): (no) check of diagonalization

IDIR(6) = 1(0): (no) printout of eigenvectors

IDIR(7) = 1(0): (no) printout of parameters for Ewald-summation

IDIR(8) = 1(0): (no) check of translational invariance

IDIR(9) = 1(0): (not) all matrix elements will be calculated
              independently. Symmetry relations will not be
              (will be) considered.

IDIR(10) = 1(0): (no) storage of results on disk

Card 2 **(MASS(I), I = 1,MAXTYP)**   **[8F10.5]**

MASS(I) = mass of atom I in atomic mass units

MAXTYP= number of different atom types as
        determined by program **IND**

Card 3 **N**   **[I5]**

N   = Number of interaction type which has to be
        considered:

N = 1: longitudinal and transverse springs

N = 2: Born-Mayer potential

N = 3: Lennard-Jones potential

N = 4: van der Waals potential

N = 5: Coulomb potential

N = 6: shell model

For Coulomb interaction only:

Card 4 **DMAX**   **[F10.5]**

DMAX   = maximal radius in Å for summation
        in direct space

Only for interaction types containing atom-specific
or general parameters (see Tab. 1 on page 40):

Card 5	((IASP(I,J), J = 1,MAXTYP), I = 1,NASP) (IGP(K), K = 1,NGP)	[16I5]
	MAXTYP= number of different atom types (see program **IND**)	
	NASP = number of ASP's of interaction N	
	NGP = number of GP's of interaction N	
	IASP(I,J)= number of the I-th ASP for atom J	
	IGP (K) = number of the K-th GP	

Not for Coulomb interaction:

Card 6	**I J NS**	[3I5]
	I, J = number of the atoms between which this interaction N is acting	
	NS = number of neighbouring shells to be considered	

If interaction N contains interaction-specific parameters (see Tab. 1)
for each of the NS shells a card of the following type must be given:

Card 7	(IISP(I), I = 1,NISP)	[16I5]
	NISP = number of ISP's of interaction N	
	IISP(I) = number of the I-th ISP of interaction N	

Further cards of type 6 and 7.
The end of input for the interaction N (N≠5)
is indicated by a card of type 6 with I = 0.

Further interactions may be specified by repeating the input 3.-7.
The end of the model set-up is indicated by a card of type 3 with N = 0.

Card 8	(P(I), I = 1,NP)	[8F10.5]
	NP = largest parameter number used in model set-up (cards 3-7)	
	P(I) = value of parameter number I.	

4.4.8 Output

The output is controlled by the vector IDIR (see section 4.4.7). Generally, a list of all interactions within the model set-up is printed by subroutine PRINT1 along with the corresponding parameter numbers and values. By a careful inspection of this list the model can be checked and possible input errors can be detected.

For each value of the wavevector, phonon frequencies $v_{qj} = \omega_{qj}/2\pi$ and, if desired, phonon eigenvectors $e(\kappa|qj)$ in cartesian coordinates are listed according to their symmetry (subroutine PRINT2). The wavevectors are printed in cartesian coordinates (in Å^{-1}) as well as in units of the reciprocal lattice vectors. An example is given in appendix A.4, page 82.

If needed, the data may be stored on the disk-dataset **RESULT** (logical unit 4) by the subroutines STORE1 and STORE2.

4.5 HIST

4.5.1 General Purpose

The program **HIST** produces a histogram plot of phonon dispersion curves calculated by **MODEL1**. The different branches may be displayed according to their symmetries (irreducible multiplier representations). Obviously, this program can be used in a meaningful way only if the model calculation is performed for a whole sequence of q-values. It is, however, not necessary to restrict the wavevectors to a straight line in reciprocal space. Rather, the program recognizes if the sequence corresponds to a zig-zag line. This is especially useful for hexagonal structures, e.g., where normally the phonon dispersion within the hexagonal plane is displayed according to a closed loop of wavevectors: Leaving the Γ-point in direction [100] the zone-boundary is reached at the M-point. On the zone-boundary one can travel from the M- to the K-point from which the Γ-point is approached again in direction [110]. Thus, if the semigraphical representation of phonon frequencies is desired the q-values should be carefully selected in program **GROUP**. It should be noticed that the q-values need not be of equal distance. The program automatically displays the results according to an absolute scale (except for rounding errors due to the discrete nature of the histogram plot).

There is another criterion for an adequate display of the phonon branches: Suppose, you have more than one irreducible multiplier representation (IMR) of the group of the wavevector for a particular symmetry direction. Then two of them may degenerate at the Γ-point or at the zone-boundary (Z.B.). In this case, it is very illustrative to plot the corresponding branches in an extended zone scheme as may be seen from the following example.

Example In the space group P6$_3$ the main symmetry direction is the hexagonal c-axis. Here, one has six different representations (1 to 6). At the Γ-point IMR 2 is degenerate with IMR 6 and IMR 3 is degenerate with IMR 5, while at the zone-boundary, the A-point, IMR 1 is degenerate with IMR 4, IMR 2 with IMR 3 and IMR 5 with IMR 6. These relations may be checked immediately by inspection of the character tables printed by program **GROUP**. In order to account for the degeneracies it is convenient to plot the dispersion curves according to Fig. 7 on page 52.

Fig. 7. Schematical illustration of a phonon dispersion: For the hexagonal direction of the cyclic space group P6₃ the dispersion is displayed conveniently according to the different symmetries taking into account the degeneracies at special points within the Brillouin zone.
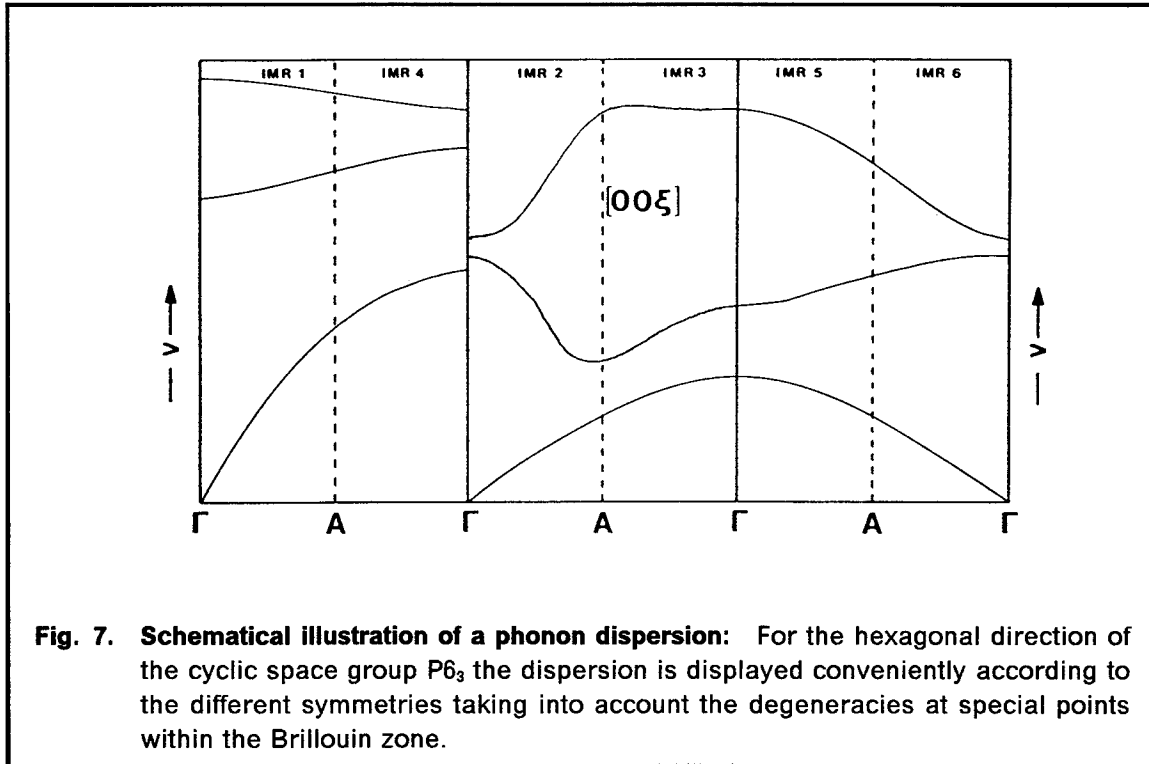
In fact, the program **HIST** allows to arrange the plot in a very specific way: The sequence of the various irreducible representations can be chosen arbitrarily. The plot direction ($\Gamma \rightarrow$ Z.B. or Z.B. $\rightarrow \Gamma$) can be selected by giving the number of the corresponding representation with a positive or a negative sign. In the above example a plot according to Fig. 7 is obtained by specifying the following sequence of irreducible representations:

1 -4 2 -3 5 -6

If this sequence starts with 0, all phonon branches are plotted in one picture and different symbols are used to distinguish between the irreducible multiplier representations.

The program **HIST** needs the output results of **GROUP, IND** and **MODEL1** which are read from the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **RESULT** (logical unit 2), respectively.

4.5.2 Input

Card 1	**NYMAX**	**[F10.6]**
	NYMAX = maximum frequency in THz	
Card 2	**(IDIR(I), I = 1,20)**	**[16I5]**
	This is a double card !	
	IDIR(1),IDIR(2)... is the sequence of irreducible	
	representations to be displayed	
	If IDIR(I)> 0: the corresponding dispersion	
	curves are plotted from Γ-point	
	towards the zone boundary.	
	If IDIR(I)< 0: the corresponding dispersion	
	curves are plotted from the zone	
	boundary towards Γ-point.	
	If IDIR(1)= 0: plot without consideration of symmetry	

Card 3	**NMARK**	**[I5]**
	selects the symbol used for phonons	
	NMARK = 1 : *	
	2 : +	
	3 : 0	
	4 : #	
	5 : @	
	6 : .	
	7 : &	
	8 : $	
	9 :	
	10 : X	

4.5.3 Output

An example for an output is given in appendix A.5, page 92. It should be noticed again that the quality of the plot obtained by **HIST** depends on a proper choice of the q-values and of the sequence of representations. The display according to the different symmetries has the advantage that the calculated points can immediately be joined by lines corresponding to the different phonon branches since there is no intersection of branches (except at points of higher symmetry).

4.6 SF

4.6.1 General Purpose

The experimental determination of phonon dispersion curves by neutron scattering can effectively be supported by model calculations. The phonon intensities are given by the dynamical structure factor as discussed in section 2.8. Model calculations do not only yield the eigenfrequencies but also the eigenvectors of lattice vibrations and, hence, the intensity for any particular phonon can be predicted.

The program **SF** calculates the dynamical structure factors on the basis of the lattice-dynamical model considered in program **MODEL1**. According to equation (2.95) the expression

$$F \left| \sum_{\kappa} \frac{b_{\kappa}}{\sqrt{m_{\kappa}}} \ e^{-W_{\kappa}} (g + q) e(\kappa | qj) \ e^{-iQr^{\circ}_{\kappa}} \right|^2 \tag{4.7}$$

is listed for any phonon mode j and for a specified range of Brillouin zones **g**. F is a normalizing factor which can be chosen arbitrarily in order to get reliable numbers on output. If desired, the $1/\omega_{qj}$-factor or the Bose-occupation factor n_{qj} are included. The Debye-Waller factor $e^{-W_{\kappa}}$ is calculated as:

$$e^{-W_{\kappa}} = e^{-\frac{1}{2}(g+q)B_{\kappa}(g+q)} , \tag{4.8}$$

where B_{κ} is the symmetrical matrix of anisotropic temperature factors:

$$B_{\kappa} = \begin{pmatrix} TF_{\kappa}(1) & TF_{\kappa}(2) & TF_{\kappa}(3) \\ TF_{\kappa}(2) & TF_{\kappa}(4) & TF_{\kappa}(5) \\ TF_{\kappa}(3) & TF_{\kappa}(5) & TF_{\kappa}(6) \end{pmatrix} . \tag{4.9}$$

This matrix has to be given as input as well as the coherent scattering lengths b_{κ}. It is, however, sufficient to specify B_{κ} and b_{κ} for only one atom of each type. The temperature factors of all other atoms of the same type are obtained by a simple matrix transformation.

The output list can be arranged according to irreducible multiplier representations or according to increasing frequencies. The most convenient choice depends on the specific crystal system under consideration.

On the zone boundary or at the zone center, the eigenvectors of two degenerate phonon modes may be calculated to be complex conjugate quantities. Any linear combination of both is again an eigenvector. Thus, the real and imaginary parts, in particular, provide the physically meaningful eigenvectors in this case. As an option, the calculation of dynamic structure factors may therefore be performed on the basis of these real eigenvectors rather than on the basis of the complex ones as calculated in **MODEL1**.

The results obtained by programs **GROUP**, **IND** and **MODEL1** are used via the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **RESULT** (logical unit 2), respectively.

4.6.2 Input

The range of Brillouin zones for which the dynamical structure factors are calculated is determined by the lower and upper limits for the Miller indices (HMIN, HMAX, KMIN, KMAX, LMIN, LMAX) as well as by a limiting radius QMAX which is to be given in Å^{-1}. In particular, the following cards are required for the program **SF**:

Card 1	**HMIN, HMAX, KMIN, KMAX, LMIN, LMAX**	[6I5]
	define the range of Brillouin-zones for which phonon intensities are calculated:	
	HMIN $\leq$ h $\leq$ HMAX	
	KMIN $\leq$ k $\leq$ KMAX	
	LMIN $\leq$ l $\leq$ LMAX	

Card 2	**QMAX**	[F10.6]
	QMAX = maximum value for **q** in Å^{-1}	
	limiting the range of Brillouin zones	

Card 3	**(B(I), I = 1,MAXTYP)**	[8F10.6]
	B(I) = coherent scattering length in 10^{-14} m	
	for atoms of type I	
	MAXTYP= number of different particle types	
	as determined by program **IND**	

For each of the MAXTYP types of particles a card of the following type must be given:

Card 4	**I, (TF(K), K = 1,6)**	[I5,6F10.6]
	I = number of atom (representing the	
	class of corresponding type)	
	TF(K) = components of the tensor B of anisotropic	
	temperature factors in Å^{-2} (see equation (4.9))	

Card 5	**T**	[F10.6]
	T = temperature in K	

Card 6	**FNORM**	[F10.6]
	FNORM = normalizing factor.	

```
Card 7   (IDIR(I), I = 1,10)                                    [10I5]
         Control parameters:
         IDIR(1)  = 1: output arranged according to
                       irreducible representations
         IDIR(1)  = 2: output arranged according to frequency scale
         IDIR(2)  = 0: complex eigenvectors are used
                  = 1: real parts of eigenvectors are used
                  = 2: imaginary parts of eigenvectors are used
         IDIR(4)  = 1(0): calculations (do not) take into
                       account 1/v-factor
         IDIR(5)  = 1(0): calculations (do not) take into
                       account Bose-factor
```

4.6.3 Output

An output example is given in appendix A.6, page 94. The list may serve as a guide for neutron scattering experiments: For a particular phonon, a Brillouin zone is picked out where its intensity is large and, simultaneously, the intensities of neighbouring phonons (on the frequency scale) are sufficiently small. If the lattice-dynamical model is adequate the phonon under consideration should be very well detected in this particular Brillouin zone.

4.7 PARDER

4.7.1 General Purpose

The program **PARDER** calculates the partial derivatives of phonon frequencies with respect to each of the model parameters. It can thus be used for the optimization of a particular lattice-dynamical model.

If **p** denotes the parameter vector determining the Dynamical Matrix the squares of phonon frequencies are represented by:

$$\begin{pmatrix} \omega_1^2 & & \\ & \ddots & \\ & & \omega_{3N}^2 \end{pmatrix} = \mathbf{E^+ D(p) E} , \tag{4.10}$$

where **E** is the matrix of the eigenvectors. All matrices appearing in equation (4.10) are determined by program **MODEL1**. If the parameter vector is altered by $\Delta \mathbf{p}$ a new Dynamical Matrix $\mathbf{D(p + \Delta p)}$ is obtained and, to first approximation, the new phonon frequencies are given by:

$$\begin{pmatrix} \tilde{\omega}_1^2 & & \\ & \ddots & \\ & & \tilde{\omega}_{3N}^2 \end{pmatrix} = \mathbf{E^+ D(p + \Delta p) E} . \tag{4.11}$$

The variations in ω^2 are:

$$\begin{pmatrix} \Delta\omega_1^2 & & \\ & \ddots & \\ & & \Delta\omega_{3N}^2 \end{pmatrix} = \mathbf{E^+ [D(p + \Delta p) - D(p)] E} . \tag{4.12}$$

The corresponding shifts of the frequencies ω_i are calculated as:

$$\Delta\omega_i = \frac{\Delta\omega_i^2}{2\omega_i} \qquad \text{if} \quad \omega_i > 0 \tag{4.13}$$

and

$$\Delta\omega_i = \sqrt{\Delta\omega_i^2} \qquad \text{if} \quad \omega_i = 0 . \tag{4.14}$$

The values $\Delta v_i = \Delta\omega_i/2\pi$ are listed for all phonons calculated by **MODEL1** and for variations of all model parameters. Note, that a negative squared frequency ω_i^2 or v_i^2 obtained by program **MODEL1** is treated as being zero. If, however, the frequency is less or equal zero and, simultaneously, the shift of its square, Δv^2, is calculated to be negative, Δv cannot be obtained. In this case, Δv^2 itself is listed and a corresponding message is printed.

The individual variations of the different model parameters for which the frequency shifts are calculated are given as input.

As can be seen from equation (4.12) the main task within **PARDER** is to compute a new Dynamical Matrix with slightly modified parameter values. Remembering the modular set-up of the program **MODEL1**, it is obvious that the subroutine DYN2 can be used within **PARDER** as well. Therefore, **PARDER** itself turns out to be a rather simple program constructed around the general subroutine DYN2.

The output list illustrates the effect of each of the model parameters on each phonon frequency. It may serve as a guide if the model has to be modified in order to reproduce the experimental results.

The results of the programs **GROUP**, **IND**, **NN** and **MODEL1** are used via the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3), **XNN** (logical unit 4) and **RESULT** (logical unit 2), respectively.

4.7.2 Input

In analogy with program **MODEL1** a control card is used to select the mode of computing the Dynamical Matrix:

Card 1	**(IDIR(I), I = 1,10)**	[10I5]
	IDIR(1) = 1(0): (no) compressed output restricted to those parameters with non-zero variations DP(I)	
	IDIR(7) = 1(0): (no) printout of parameters for Ewald-summation	
	IDIR(9) = 1(0): (not) all of the matrix elements of **D** will be calculated independently. Symmetry relations will not be (will be) considered.	

Card 2	**(DP(I), I = 1,NP)**	[8F10.6]
	Variation of parameter values for which the frequency shifts are calculated NP is the total number of parameters for the model specified in program **MODEL1**.	

4.7.3 Output

An example for an output list is given in appendix A.7, page 96. Note that all frequencies calculated in **MODEL1** as being imaginary $(v^2 < 0)$ are denoted by $v = 0.0$ THz.. If the frequency is imaginary or zero and the shift of v^2 is negative, Δv^2 is listed instead of Δv. A corresponding message is printed on the previous output page.

4.8 ROTINV

4.8.1 General Purpose

The program **ROTINV** provides a test of the rotational invariance condition as discussed in section 2.6.2. For a particular lattice-dynamical model the net forces are calculated which act upon the different atoms if the crystal as a whole is rotated around the x-, y- or z-axis. These forces should be zero for a proper model set-up. They can be calculated from the Dynamical Matrix taken at wavevectors δq along different directions near the Γ-point as expressed by equations (2.76)-(2.78). For numerical calculations the modulus δq of the wavevectors has to be chosen carefully: If it is too large the approximation of equation (2.72) may become invalid and, consequently, the results are incorrect. If, on the other hand, δq is too small rounding errors may come into play. The following two conditions can be used as criteria for a proper choice of δq:

1. The component of the force along the direction of rotation $f_\alpha^\alpha(\kappa)$ vanishes for every atom κ in the case of central forces. Thus, the calculated numerical values for f_α^α can be regarded as a monitor of rounding errors.

2. The two components f_α^β and $-f_\beta^\alpha$ of the force tensor have to be identical, irrespective of the special model. The force tensor is antisymmetrical. Again, numerical differences show the influence of rounding errors.

The model to be tested by **ROTINV** is defined in just the same manner as in program **MODEL1**. Thus, the same subroutines are used for the interpretation of input (GETPAR) as well as for the calculation of the Dynamical Matrix (DYN2) (cf. section 4.4). Having these routines available, **ROTINV** is a rather simple and straightforward program.

Obviously, **ROTINV** uses all results of the programs **GROUP**, **IND** and **NN** just as **MODEL1** does.

Within one run of **ROTINV**, a particular model set-up can be analyzed for different sets of parameter values. Thus, it can be used to select a proper parameter set (leading to a rotational invariant model) prior to the actual model calculation.

4.8.2 Input

The following input card are required:

Card 1	QL		[F10.6]
	QL	= modulus of the wavevector δq used for the calculation. It should be small enough to be sure that the approximation (2.72) is valid. On the other hand, QL should not be too small because of rounding errors.	

Card 2-9	are the same as *Cards 1-8* for program **MODEL1** The control variable IDIR(1), however, has a different meaning: IDIR(1) = 1(0) : (no) printout of model specifications

Other parameter sets may be considered by supplying additional cards of type 9 (*i.e.* type 8 of **MODEL1**).

4.8.3 Output

An example for the output of program **ROTINV** is given in appendix A.8, page 98. The net forces are given in units of 10^{-10} N. A particular model can be regarded as being nearly rotational invariant if the moduli of all force components are smaller than 0.01×10^{-10} N. Rounding errors may be detected by checking the conditions $f_\alpha^\alpha = 0$ and $f_\alpha^\beta = -f_\beta^\alpha$.

4.9 EFG

4.9.1 General Purpose

The program **EFG** calculates local static electrical fields and field gradients for a given structure according to equations (2.103) and (2.104), section 2.10. The lattice sum is evaluated by Ewald's method in just the same way as for the dynamical model calculations. In fact, the electrical field gradients are proportional to a sum over Coulomb coefficients which are calculated by subroutine CP dealing with the Coulomb potential (see Fig. 6 on page 47). The same subroutine is therefore used in **EFG** as well. Note, however, that the self-potential has to be excluded. Obviously, the calculations have to be performed for zero wavevector since we are dealing with static properties. In practice, however, **q** is a small but non zero vector in order to overcome the difficulties in numerical calculations mentioned earlier (see footnote [2] on page 8).

Concerning the components of the electrical field, equation (2.104), the method of summation is the same as for the determination of the Coulomb coefficients, except the $g = 0$ term is excluded. This term comes into play for dynamical calculations only, since lattice vibrations carry a macroscopic electrical field if they are polarized in longitudinal direction.

If desired, the contributions of the different sublattices (containing all atoms of the same type) to the Coulomb force acting upon any particular ion can be listed individually. Thus, partial Madelung constants are obtained if unit charges are considered.

The structural parameters used for the calculations in **EFG** are read from the disk-datasets **COORD** (logical unit 1), **INDDAT** (logical unit 3) and **XNN** (logical unit 4). Thus the programs **GROUP, IND** and **NN** have to be run first. As in program **MODEL1** the ordered arrangements of atoms in neighbouring shells provided by program **NN** are used to simplify the summation in direct space. The maximal radius is given as input and is automatically modified by the program, if necessary (*cf.* section 4.4.1). The final parameters for the Ewald-summation may be printed.

4.9.2 Input

The following input cards are required for program **EFG**:

Card 1	**(IDIR(I), I = 1,10)**	**[10I5]**
	Control parameters:	
	IDIR(1) = 1(0): (no) printout of the contributions of the different sublattices to the total Coulomb force	
	IDIR(7) = 1(0): (no) printout of parameters for Ewald summation	

Card 2	**(Z(I), I = 1,MAXTYP)**	**[8F10.6]**
	Z(I) = charge of ions of type I in units of the elementary charge	
	MAXTYP= number of different atom types as determined by program **IND**	

Card 3	**DMAX**	**[F10.6]**
	DMAX = maximal distance for summation in direct space in Å	

4.9.3 Output

An example for the output of the program **EFG** is given in appendix A.9, page 100. The components of the local electrical field are given in units of $V\text{Å}^{-1}$, those of the field gradient tensor are given in units of $V\text{Å}^{-2}$.

5.0 Computer Requirements

UNISOFT is originally written in the FORTRAN IV programming language supported by the most computers. Where necessary, it is adapted to FORTRAN 77. Special features which might be specific to a particular computer system are avoided. Three subroutines are used from the IMSL-library:

1. the random number generator GGUBS used within **GROUP**

2. the diagonalization routine E2CHF for a complex hermitian matrix called by subroutine EIGEN within **MODEL1**

3. the routine LINCG for the inversion of a hermitian matrix called by subroutine SHELL2 within **MODEL1, ROTINV** and **PARDER**.

If UNISOFT is to be installed at a computer which does not support the IMSL-routines, these subroutines have to be replaced.

The data transfer between the different programs is achieved via the four disk-datasets **COORD, INDDAT, XNN** and **RESULT** by formatted sequential input and output. Before UNISOFT can be used, these files must be installed. The required sizes of the datasets depend on the crystal structure to be considered. It can be estimated as follows: Suppose, you have a crystal structure with N particles per primitive cell and the calculations are to be performed for M values of the phonon wavevector. Then, the following storage capacities are needed:

COORD	$145 + N + M(9 + 2.25N^2)$ records
INDDAT	28 records
XNN	$100(N^2 + N)$ records
RESULT	$484 + M(4 + 0.6N + 13.5N^2) \simeq 500 + 14MN^2$ records.

The logical record length is 80 bytes.

It should be mentioned that UNISOFT is not optimized with respect to storage capacity or with respect to computing time. The main attention has been paid to an easy mode of operation.

6.0 Possible Extensions of UNISOFT

Discussing possible extensions of UNISOFT, one has to distinguish between extensions concerning the lattice-dynamical model on the one hand, and extensions concerning other physical implications of a given model on the other hand.

As already mentioned in section 4, it is rather simple to implement new types of pair interactions. In principle, also tensor forces should be feasible.

The consideration of anharmonic effects obviously requires a more complex treatment. On the basis of the perturbation theory it should, however, be possible to calculate frequency shifts and phonon line widths. In general, this procedure leads to a summation over a large number of phonon states within the whole Brillouin zone. Thus, the computing time for those calculations will become large, especially if the crystal structure under consideration is not a simple one.

The introduction of the concept of molecular groups can also provide a useful extension of the present system: In many crystalline solids there are molecular groups which, from the lattice-dynamical point of view, can be considered as nearly rigid bodies. Thus, not all atoms have to be treated individually. Rather, the dynamics of an entire molecular group, such as SO_4, CH_4, NH_4 etc. can be described by three translational and three rotational degrees of freedom. This approach is justified, if the frequencies of the internal vibrations of a molecular group are much larger than the frequencies of the lattice modes. By the introduction of this concept of molecular crystals obviously the dimension of the Dynamical Matrix and, hence, the computing time can be reduced.

On the basis of a given lattice-dynamical model, other physical properties of a crystal may be calculated by adding new programs: Phonon densities of state, e.g., can be calculated if the phonon frequencies have been determined by **MODEL1** for a large number of q-values distributed all over the Brillouin zone. In a next step, the contribution of lattice vibrations to the specific heat can be deduced from the phonon density of states. Lattice energies can be calculated. And there are certainly more possible extensions of UNISOFT.

In principle, it is also possible to use **MODEL1** within a least-squares fit program which adjusts the calculated phonon frequencies to measured ones. Often, however, the experimental assignment of phonon peaks to phonon branches is rather difficult. A wrong labelling of a phonon might have fatal consequences: The fitting procedure can lead to definitely wrong results, especially if more complicated crystal structures are considered.

Plot programs for the pair-correlation or for the dispersion curves are not provided within the program package, because usually the graphics software depends on the particular computer system in a crucial way. Hence, for the sake of generality, we restrict ourselves to represent the data by histograms. The user may replace the corresponding routines (PCF, HIST) by his own graphics software.

7.0 References

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Appendix A. Example for the Application of UNISOFT

As an example all programs of UNISOFT are applied to the room temperature phase of $KLiSO_4$ which belongs to the space group $P6_3$. In fact, the crystal structure is disordered which can, however, be neglected for lattice-dynamical considerations.

The input data are given along with an excerpt of the resulting output list for each of the individual programs. The complete listings are too voluminous in order to be presented here.

A.1 GROUP

INPUT

```
GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
   14    1    0    3    0
K1  K2  LI1 LI2 S1  S2  O1  O5  O2  O6  O3  O7  O4  O8
   UNIT 1 = K1;        UNIT 2 = K2 ;       UNIT 3 = LI1 ;     UNIT 4 = LI2;
   UNIT 5 = S1;        UNIT 6 = S2 ;
   UNIT 7 = O1;        UNIT 8 = O5;        UNIT 9 = O2;       UNIT 10 = O6;
   UNIT 11 = O3;       UNIT 12 = O7;
   UNIT 13 = O4;       UNIT 14 = O8;

5.142      .000    0.000   -2.571  4.453   0.000   0.000   0.000   8.624
       1  0.          0.         0.         0
       1  0.          0.         4.312      0
       2  0.          2.96874    5.882      0
       2  2.571       1.48437    1.570      0
       3  0.          2.96874    2.535      0
       3  2.571       1.48437    6.847      0
       4  0.          2.9687     3.9670     0
       4  2.5710      1.4844     8.2790     0
       5  1.3909      2.9257     2.0611     0
       5  1.1801      1.5274     6.3731     0
       5  4.4838      4.1948     2.0611     0
       5  3.2292      0.2583     6.3731     0
       5  4.4093      1.7857     2.0611     0
       5  3.3037      2.6674     6.3731     0

       1    0
   Gamma-Point
   0.000       0.00000      0.00010
       0    0
   0 0 1 -DIRECTION
   0.000       0.00000    0.20000
       1    0
   0 0 1 -DIRECTION
   0.0000      0.000000   0.400
       1    0
   0 0 1 -DIRECTION
   0.000       0.00000    0.60000
       1    0
   0 0 1 -DIRECTION
   0.0000      0.000000   0.800
       1    0
   0 0 1 -DIRECTION
   0.000       0.00000    1.00000
       0    0
```

GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
UNIT 1 = K1;   UNIT 2 = K2 ;   UNIT 3 = LI1 ;   UNIT 4 = LI2; UNIT 5 = S1;   UNIT 6 = S2 ;
UNIT 7 = O1;   UNIT 8 = O5;   UNIT 9 = O2;   UNIT 10 = O6 UNIT 11 = O3;   UNIT 12 = O7;
UNIT 13 = O4;   UNIT 14 = O8;

```
            RECIPROCAL SPACE LATTICE VECTORS                         POSITION VECTOR SPACE LATTICE VECTORS
                   A1(I)*A(J)=DELTA(I,J)                                   A1             A2             A3
          A|1= (  0.19448,  0.11228,  0.00000)                   (  5.14200 ) ( -2.57100 )  (  0.00000 )
          A|2= (  0.00000,  0.22457,  0.00000)                   (  0.00000 ) (  4.45300 )  (  0.00000 )
          A|3= (  0.00000,  0.00000,  0.11596)                   (  0.00000 ) (  0.00000 )  (  8.62400 )
```

THE CRYSTAL SYSTEM IS HEXAGONAL   WITH OPERATIONS: 1 2 3 4 5 6

THE SPACE GROUP IS NON-SYMMORPHIC OR ELSE A NON STANDARD ORIGIN OF COORDINATES WAS USED.

```
                                                  ATOM TRANSFORMATION TABLE
                                     OPERATION NUMBER      1  2  3  4  5  6
MOVES ATOM  1 TYPE  1 AT (  0.0000,  0.0000,  0.0000) TO ATOM    1  2  1  2  1  2
MOVES ATOM  2 TYPE  1 AT (  0.0000,  0.0000,  4.3120) TO ATOM    2  1  2  1  2  1
MOVES ATOM  3 TYPE  2 AT (  0.0000,  2.9687,  5.8820) TO ATOM    3  4  3  4  3  4
MOVES ATOM  4 TYPE  2 AT (  2.5710,  1.4844,  1.5700) TO ATOM    4  3  4  3  4  3
MOVES ATOM  5 TYPE  3 AT (  0.0000,  2.9687,  2.5350) TO ATOM    5  6  5  6  5  6
MOVES ATOM  6 TYPE  3 AT (  2.5710,  1.4844,  6.8470) TO ATOM    6  5  6  5  6  5
MOVES ATOM  7 TYPE  4 AT (  0.0000,  2.9687,  3.9670) TO ATOM    7  8  7  8  7  8
MOVES ATOM  8 TYPE  4 AT (  2.5710,  1.4844,  8.2790) TO ATOM    8  7  8  7  8  7
MOVES ATOM  9 TYPE  5 AT (  1.3909,  2.9257,  2.0611) TO ATOM    9 14 11 10 13 12
MOVES ATOM 10 TYPE  5 AT (  1.1801,  1.5274,  6.3731) TO ATOM   10 13 12  9 14 11
MOVES ATOM 11 TYPE  5 AT (  4.4838,  4.1948,  2.0611) TO ATOM   11 10 13 12  9 14
MOVES ATOM 12 TYPE  5 AT (  3.2292,  0.2583,  6.3731) TO ATOM   12  9 14 11 10 13
MOVES ATOM 13 TYPE  5 AT (  4.4093,  1.7857,  2.0611) TO ATOM   13 12  9 14 11 10
MOVES ATOM 14 TYPE  5 AT (  3.3037,  2.6674,  6.3731) TO ATOM   14 11 10 13 12  9
```

MULTIPLICATION TABLE,30X,23HFRACTIONAL TRANSLATIONS

```
        1  2  3  4  5  6                                                          V(1)      V(2)      V(3)
   1    1  2  3  4  5  6                                                         0.0000    0.0000    0.0000
   2    2  3  4  5  6  1                                                         0.0000    0.0000    0.5000
   3    3  4  5  6  1  2                                                         0.0000    0.0000    0.0000
   4    4  5  6  1  2  3                                                         0.0000    0.0000    0.5000
   5    5  6  1  2  3  4                                                         0.0000    0.0000    0.0000
   6    6  1  2  3  4  5                                                         0.0000    0.0000    0.5000
```
THE INPUT WAVE-VECTORS WILL BE SCALED BY THE DISTANCE TO THE BRILLOUIN ZONE BOUNDARIES ALONG THE CARTESIAN AXES
THE CARTESIAN AXES INTERSECT THE BRILLOUIN ZONE BOUNDARIES AT (0.81463, 0.70550, 0.36428)

****

GROUP THEORETICAL ANALYSIS OF THE K LI SO4-STRUCTURE
Gamma-Point   K/KMAX = 0.00000 0.00000 0.00010

****

K IS ONE HALF OF A WAVE VECTOR SPACE LATTICE VECTOR, THEREFORE THE DYNAMICAL MATRIX MUST BE REAL.

                                              CHARACTER TABLE

```
OP    IR( 1)     IR( 2)     IR( 3)     IR( 4)     IR( 5)     IR( 6)
 1   1.0  0.0   1.0  0.0   1.0  0.0   1.0  0.0   1.0  0.0   1.0  0.0
 2   1.0  0.0   0.5 -0.9  -0.5 -0.9  -1.0  0.0  -0.5  0.9   0.5  0.9
 3   1.0  0.0  -0.5 -0.9  -0.5  0.9   1.0  0.0  -0.5 -0.9  -0.5  0.9
 4   1.0  0.0  -1.0  0.0   1.0  0.0  -1.0  0.0   1.0  0.0  -1.0  0.0
 5   1.0  0.0  -0.5  0.9   0.5 -0.9   1.0  0.0  -0.5  0.9  -0.5 -0.9
 6   1.0  0.0   0.5  0.9  -0.5  0.9  -1.0  0.0  -0.5 -0.9   0.5 -0.9
```
IMR NUMBER 6 IS TIME REVERSAL DEGENERATE WITH IMRNUMBER 2. IN THE DECOMPOSITION IMR 6 WILL BE DROPPED
AND IMR 2 WILL HAVE TWICE THE DIMENSION IT HAD.
IMR NUMBER 5 IS TIME REVERSAL DEGENERATE WITH IMRNUMBER 3. IN THE DECOMPOSITION IMR 5 WILL BE DROPPED
AND IMR 3 WILL HAVE TWICE THE DIMENSION IT HAD.

    THE DECOMPOSITION IS 7 IR(1) + 7 IR(2) + 7 IR(3) + 7 IR(4)

AMPLITUDES

	1 2 3	4 5 6	7 8 9	10 11 12	13 14 15	16 17 18	19 20 21	22 23 24	25 26 27	28 29 30
1	AA	AB	AC AD ..	AE AF ..	AG AH ..	AI AJ ..	AK AL ..	AM AN ..	AO AP AQ	AR AS AT
2	.. AA ..	.. AB ..	AD AC ..	AF AE ..	AH AG ..	AJ AI ..	AL AK ..	AN AM ..	BG BH BI	BJ BK BL
3	.. .. BY	.. .. BZ	.. .. CA	.. .. CB	 CC	.. .. CD	.. .. CE	.. .. CF	CG CH CI	CJ CK CL
4	AB	AA	AE AF ..	AC AD ..	AI AJ ..	AG AH ..	AM AN ..	AK AL ..	AR AS AT	AO AP AQ
5	.. AB ..	.. AA ..	AF AE ..	AD AC ..	AJ AI ..	AH AG ..	AN AM ..	AL AK ..	BJ BK BL	BG BH BI
6	.. .. BZ	.. .. BY	.. .. CB	.. .. CA	.. .. CD	 CC	.. .. CF	.. .. CE	CJ CK CL	CG CH CI
7	AC AD ..	AE AF ..	CU	CV	CW CX ..	CY CZ ..	DA DB ..	DC DD ..	DE DF DG	DH DI DJ
8	AD AC ..	AF AE ..	.. CU ..	.. CV ..	CX CW ..	CZ CY ..	DB DA ..	DD DC ..	DW DX DY	DZ EA EB
9	.. .. CA	.. .. CB	.. .. EO	.. .. EP	.. .. EQ	.. .. ER	.. .. ES	.. .. ET	EU EV EW	EX EY EZ
10	AE AF ..	AC AD ..	CV	CU	CY CZ ..	CW CX ..	DC DD ..	DA DB ..	DH DI DJ	DE DF DG
11	AF AE ..	AD AC ..	.. CV ..	.. CU ..	CZ CY ..	CX CW ..	DD DC ..	DB DA ..	DZ EA EB	DW DX DY
12	.. .. CB	.. .. CA	.. .. EP	.. .. EO	.. .. ER	.. .. EQ	.. .. ET	.. .. ES	EX EY EZ	EU EV EW
13	AG AH ..	AI AJ ..	CW CX ..	CY CZ ..	FI	FJ	FK FL ..	FM FN ..	FO FP FQ	FR FS FT
14	AH AG ..	AJ AI ..	CX CW ..	CZ CY ..	.. FI ..	.. FJ ..	FL FK ..	FN FM ..	GG GH GI	GJ GK GL
15	 CC	.. .. CD	.. .. EQ	.. .. ER	.. .. GY	.. .. GZ	.. .. HA	.. .. HB	HC HD HE	HF HG HH
16	AI AJ ..	AG AH ..	CY CZ ..	CW CX ..	FJ	FI	FM FN ..	FK FL ..	FR FS FT	FO FP FQ
17	AJ AI ..	AH AG ..	CZ CY ..	CX CW ..	.. FJ ..	.. FI ..	FN FM ..	FL FK ..	GJ GK GL	GG GH GI
18	.. .. CD	 CC	.. .. ER	.. .. EQ	.. .. GZ	.. .. GY	.. .. HB	.. .. HA	HF HG HH	HC HD HE
19	AK AL ..	AM AN ..	DA DB ..	DC DD ..	FK FL ..	FM FN ..	HQ	HR	HS HT HU	HV HW HX
20	AL AK ..	AN AM ..	DB DA ..	DD DC ..	FL FK ..	FN FM ..	.. HQ ..	.. HR ..	IK IL IM	IN IO IP
21	.. .. CE	.. .. CF	.. .. ES	.. .. ET	.. .. HA	.. .. HB	.. .. JC	.. .. JD	JE JF JG	JH JI JJ
22	AM AN ..	AK AL ..	DC DD ..	DA DB ..	FM FN ..	FK FL ..	HR	HQ	HV HW HX	HS HT HU
23	AN AM ..	AL AK ..	DD DC ..	DB DA ..	FN FM ..	FL FK ..	.. HR ..	.. HQ ..	IN IO IP	IK IL IM
24	.. .. CF	.. .. CE	.. .. ET	.. .. ES	.. .. HB	.. .. HA	.. .. JD	.. .. JC	JH JI JJ	JE JF JG
25	AO BG CG	AR BJ CJ	DE DW EU	DH DZ EX	FO GG HC	FR GJ HF	HS IK JE	HV IN JH	JS JT JU	JV JW JX
26	AP BH CH	AS BK CK	DF DX EV	DI EA EY	FP GH HD	FS GK HG	HT IL JF	HW IO JI	JT KK KL	JW KM KN
27	AQ BI CI	AT BL CL	DG DY EW	DJ EB EZ	FQ GI HE	FT GL HH	HU IM JG	HX IP JJ	JU KL LA	JX KN LB
28	AR BJ CJ	AO BG CG	DH DZ EX	DE DW EU	FR GJ HF	FO GG HC	HV IN JH	HS IK JE	JV JW JX	JS JT JU
29	AS BK CK	AP BH CH	DI EA EY	DF DX EV	FS GK HG	FP GH HD	HW IO JI	HT IL JF	JW KM KN	JT KK KL
30	AT BL CL	AQ BI CI	DJ EB EZ	DG DY EW	FT GL HH	FQ GI HE	HX IP JJ	HU IM JG	JX KN LB	JU KL LA
31	AU BM CM	AX BP CO	DK EC FA	DN EF FC	FU GM HI	FX GP HK	HY IQ JK	IB IT JM	JY KO LC	KB KR LF
32	AV BN CN	AY BQ CP	DL ED FB	DO EG FD	FV GN HJ	FY GQ HL	HZ IR JL	IC IU JN	JZ KP LD	KC KS LG
33	AW BO CI	AZ BR CL	DM EE EW	DP EH EZ	FW GO HE	FZ GR HH	IA IS JG	ID IV JJ	KA KQ LE	KD KT LH
34	AX BP CO	AU BM CM	DN EF FC	DK EC FA	FX GP HK	FU GM HI	HY IQ JK	IB IT JM	KB KR LF	JY KO LC
35	AY BQ CP	AV BN CN	DO EG FD	DL ED FB	FY GQ HL	FV GN HJ	HZ IR JL	IC IU JN	KC KS LG	JZ KP LD
36	AZ BR CL	AW BO CI	DP EH EZ	DM EE EW	FZ GR HH	FW GO HE	IA IS JG	ID IV JJ	KD KT LH	KA KQ LE
37	BA BS CQ	BD BV CS	DQ EI FE	DT EL FG	GA GS HM	GD GV HO	IE IW JO	IH IZ JQ	KE KU LI	KH KX LK
38	BB BT CR	BE BW CT	DR EJ FF	DU EM FH	GB GT HN	GE GW HP	IF IX JP	II JA JR	KF KV LJ	KI KY LL
39	BC BU CI	BF BX CL	DS EK EW	DV EN EZ	GC GU HE	GF GX HH	IG IY JG	IJ JB JJ	KG KW LE	KJ KZ LH
40	BD BV CS	BA BS CQ	DT EL FG	DQ EI FE	GD GV HO	GA GS HM	IH IZ JQ	IE IW JO	KH KX LK	KE KU LI
41	BE BW CT	BB BT CR	DU EM FH	DR EJ FF	GE GW HP	GB GT HN	II JA JR	IF IX JP	KI KY LL	KF KV LJ
42	BF BX CL	BC BU CI	DV EN EZ	DS EK EW	GF GX HH	GC GU HE	IJ JB JJ	IG IY JG	KJ KZ LH	KG KW LE

PHASE ANGLE MATRIX

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	0	0	0	180	0	0	180	0	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	0	0	0	0	180	180	180
2	0	0	0	0	180	0	180	180	0	180	0	0	180	0	0	0	0	0	180	0	0	180	0	0	180	180	0	0	0	0
3	0	0	180	0	0	180	0	0	180	0	0	0	0	0	180	0	0	180	0	0	180	0	0	0	0	0	0	0	180	180
4	180	0	0	0	0	0	0	0	0	180	0	0	0	180	0	0	0	0	0	0	0	0	0	0	180	180	0	0	0	0
5	0	180	0	0	0	0	180	0	0	180	180	0	0	0	0	180	0	0	180	0	0	180	0	0	0	0	180	180	180	180
6	0	0	180	0	0	180	0	0	0	0	0	180	0	0	0	0	0	180	0	0	180	0	0	180	180	0	180	180	180	0
7	180	180	0	0	180	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	180	180	0	0	0	0	180	180	0
8	0	180	0	0	0	0	0	0	0	0	180	0	0	180	180	0	180	180	0	180	180	0	0	0	0	180	180	0	0	180
9	0	0	180	0	0	0	0	0	180	0	0	0	0	0	0	0	0	180	0	0	0	0	0	180	180	180	0	0	180	180
10	0	180	0	180	180	0	180	0	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	180	180	0	180	180	180
11	0	0	0	0	180	0	0	180	0	0	0	0	180	180	0	180	180	0	0	180	0	180	180	0	0	0	0	0	180	0
12	0	0	0	0	0	180	0	0	0	0	0	180	0	0	180	0	0	180	0	0	0	0	0	180	0	180	0	0	0	0
13	0	180	0	0	0	0	180	180	0	180	180	0	180	0	0	180	0	0	180	180	0	0	0	0	180	180	180	0	0	0
14	0	0	180	0	0	0	180	0	0	0	180	0	0	180	0	0	180	0	180	0	0	180	0	0	180	180	0	180	180	180
15	0	0	180	0	0	0	0	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	180	0	180	0	0	180	0
16	0	0	0	0	180	0	180	180	0	180	180	0	180	0	0	180	0	0	0	0	0	180	180	0	180	0	180	180	180	0
17	180	0	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	0	180	0	0	180	0	180	0	180	180	180	180
18	0	0	0	0	180	0	0	0	180	0	0	0	0	0	180	0	0	0	0	0	180	0	180	0	180	0	180	180	0	0
19	0	180	0	0	180	0	180	180	0	180	0	0	180	0	0	180	0	0	0	0	0	0	0	0	180	180	180	180	180	0
20	0	0	0	0	180	0	0	180	0	180	180	0	180	180	0	0	0	0	0	0	0	0	0	0	180	180	0	180	180	0
21	0	0	180	0	0	0	0	0	180	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	180	180	0	0	0	180
22	0	180	0	0	180	0	180	0	0	180	180	0	0	180	0	180	0	0	0	0	0	0	0	0	180	180	180	180	180	0
23	0	0	0	0	0	0	180	0	0	180	0	0	180	0	0	180	0	0	0	0	0	0	0	0	180	180	180	180	180	180
24	0	0	0	0	0	180	0	0	0	0	0	0	0	0	180	0	0	0	0	0	0	0	0	0	180	180	0	180	180	180
25	0	180	0	180	0	180	0	0	180	180	0	180	180	0	180	180	180	180	180	180	180	180	180	180	180	180	180	0	0	180
26	0	180	0	180	0	0	0	0	180	180	180	0	180	180	180	0	180	0	180	180	180	0	180	180	180	180	180	0	0	180
27	180	0	0	0	180	180	0	180	0	180	0	180	180	0	180	0	180	0	180	0	180	180	180	180	180	180	0	0	0	180
28	180	0	0	0	180	180	180	0	180	0	0	0	180	180	0	180	180	0	180	180	0	180	180	180	0	180	0	180	180	0
29	180	0	180	0	180	180	180	0	180	0	180	0	0	180	0	180	180	180	180	0	180	180	0	180	0	0	0	180	180	0
30	180	0	180	0	180	0	0	180	0	180	180	180	0	0	180	0	180	0	180	0	180	0	0	180	180	180	180	0	0	0
31	0	180	180	180	0	0	180	0	180	0	0	0	180	180	180	180	180	180	180	180	0	180	0	0	0	180	180	0	0	0
32	0	0	0	180	180	180	180	0	180	180	180	0	0	0	0	0	180	0	0	180	0	180	0	0	0	0	0	180	180	0
33	0	180	0	180	0	180	0	180	0	180	0	180	0	180	180	0	180	0	180	180	0	0	0	180	0	0	0	180	180	0
34	180	0	180	0	0	0	0	0	0	180	180	180	0	180	180	180	0	180	180	0	180	0	0	180	180	180	0	180	0	180
35	180	0	180	0	0	0	180	180	180	180	0	180	0	180	0	0	180	0	0	180	0	0	0	180	180	0	0	180	0	0
36	0	180	180	180	0	0	0	0	180	0	180	0	180	0	180	0	180	180	0	180	180	0	0	0	0	180	0	180	180	0
37	180	0	180	0	180	0	0	180	0	0	180	0	180	180	0	180	180	180	0	180	0	180	0	0	180	0	0	180	180	180
38	0	0	180	180	180	0	0	0	0	180	0	180	0	180	180	0	180	180	0	180	0	180	0	0	180	0	0	180	180	180
39	0	0	180	180	180	0	180	180	180	0	0	0	0	180	0	0	180	0	180	0	0	180	0	0	180	0	0	0	180	180
40	0	0	180	180	180	180	180	0	180	0	0	0	180	180	180	180	180	0	0	180	0	180	0	180	0	180	0	180	180	180
41	180	180	180	0	0	180	0	0	0	0	180	0	180	0	180	0	180	0	0	180	180	0	180	180	180	180	0	180	0	0
42	0	0	180	180	180	0	180	180	180	0	0	0	180	180	180	180	180	0	0	180	180	180	180	0	180	180	0	0	180	0

AMPLITUDES

	31 32 33	34 35 36	37 38 39	40 41 42
1	AU AV AW	AX AY AZ	BA BB BC	BD BE BF
2	BM BN BO	BP BQ BR	BS BT BU	BV BW BX
3	CM CN CI	CO CP CL	CQ CR CI	CS CT CL
4	AX AY AZ	AU AV AW	BD BE BF	BA BB BC
5	BP BQ BR	BM BN BO	BV BW BX	BS BT BU
6	CO CP CL	CM CN CI	CS CT CL	CQ CR CI
7	DK DL DM	DN DO DP	DQ DR DS	DT DU DV
8	EC ED EE	EF EG EH	EI EJ EK	EL EM EN
9	FA FB EW	FC FD EZ	FE FF EW	FG FH EZ
10	DN DO DP	DK DL DM	DT DU DV	DQ DR DS
11	EF EG EH	EC ED EE	EL EM EN	EI EJ EK
12	FC FD EZ	FA FB EW	FG FH EZ	FE FF EW
13	FU FV FW	FX FY FZ	GA GB GC	GD GE GF
14	GM GN GO	GP GQ GR	GS GT GU	GV GW GX
15	HI HJ HE	HK HL HH	HM HN HE	HO HP HH
16	FX FY FZ	FU FV FW	GD GE GF	GA GB GC
17	GP GQ GR	GM GN GO	GV GW GX	GS GT GU
18	HK HL HH	HI HJ HE	HO HP HH	HM HN HE
19	HY HZ IA	IB IC ID	IE IF IG	IH II IJ
20	IQ IR IS	IT IU IV	IW IX IY	IZ JA JB
21	JK JL JG	JM JN JJ	JO JP JG	JQ JR JJ
22	IB IC ID	HY HZ IA	IH II IJ	IE IF IG
23	IT IU IV	IQ IR IS	IZ JA JB	IW IX IY
24	JM JN JJ	JK JL JG	JQ JR JJ	JO JP JG
25	JY JZ KA	KB KC KD	KE KF KG	KH KI KJ
26	KO KP KQ	KR KS KT	KU KV KW	KX KY KZ
27	LC LD LE	LF LG LH	LI LJ LE	LK LL LH
28	KB KC KD	JY JZ KA	KH KI KJ	KE KF KG
29	KR KS KT	KO KP KQ	KX KY KZ	KU KV KW
30	LF LG LH	LC LD LE	LK LL LH	LI LJ LE
31	LM LN LO	LP LQ LR	LS LT LU	LV LW LX
32	LN LY LZ	LQ MA MB	MC MD ME	MF MG MH
33	LO LZ LA	LR MB LB	MI MJ LE	MK ML LH
34	LP LQ LR	LM LN LO	LV LW LX	LS LT LU
35	LQ MA MB	LN LY LZ	MF MG MH	MC MD ME
36	LR MB LB	LO LZ LA	MK ML LH	MI MJ LE
37	LS MC MI	LV MF MK	MM MN MO	MP MQ MR
38	LT MD MJ	LW MG ML	MN MS MT	MQ MU MV
39	LU ME LE	LX MH LH	MO MT LA	MR MV LB
40	LV MF MK	LS MC MI	MP MQ MR	MM MN MO
41	LW MG ML	LT MD MJ	MQ MU MV	MN MS MT
42	LX MH LH	LU ME LE	MR MV LB	MO MT LA

PHASE ANGLE MATRIX

	31	32	33	34	35	36	37	38	39	40	41	42
1	0	0	0	180	180	0	180	0	0	0	180	0
2	180	0	180	0	180	180	180	0	0	0	180	0
3	180	0	0	180	0	180	0	180	0	180	180	180
4	180	180	180	0	0	180	0	180	180	180	0	180
5	0	180	0	180	0	0	0	180	180	180	0	180
6	0	180	180	0	180	0	0	0	180	180	0	0
7	0	180	180	0	180	0	180	0	180	180	180	180
8	180	180	0	0	180	0	0	0	180	0	0	180
9	0	180	0	0	180	180	0	0	0	180	0	180
10	0	180	180	0	180	0	180	180	0	180	0	0
11	0	180	180	180	180	180	0	0	0	0	0	0
12	180	0	180	180	0	0	0	180	180	180	180	0
13	180	0	0	180	0	180	180	0	0	180	0	180
14	180	0	180	180	180	0	0	180	0	180	180	180
15	180	0	0	0	0	180	180	180	0	180	0	180
16	180	0	0	180	0	180	180	0	0	180	0	180
17	180	180	180	180	0	0	180	180	0	0	180	180
18	180	180	180	0	180	0	0	180	180	0	0	0
19	180	0	0	180	180	180	180	0	0	180	0	0
20	180	0	180	0	0	180	0	180	0	0	180	180
21	0	180	0	180	180	180	0	0	0	0	180	180
22	180	180	0	180	0	180	180	0	180	180	0	180
23	0	0	0	180	0	0	0	180	0	0	180	180
24	0	0	180	180	0	0	180	0	180	180	180	0
25	0	0	0	180	180	0	180	180	180	0	180	180
26	0	0	0	0	0	180	180	0	0	180	180	180
27	0	180	0	180	0	0	0	180	0	0	0	0
28	180	180	180	0	0	180	0	180	0	180	180	0
29	0	0	0	0	0	180	180	180	0	180	0	180
30	0	180	0	180	0	0	180	180	0	180	0	0
31	180	0	0	0	0	0	0	180	180	0	0	180
32	0	0	180	0	180	0	180	180	0	0	180	0
33	0	180	0	180	180	180	0	0	0	0	180	0
34	0	0	180	180	0	180	0	0	0	0	180	0
35	0	180	180	0	0	0	0	180	180	180	180	180
36	0	0	180	180	0	0	180	0	0	180	180	0
37	0	180	0	0	0	180	0	0	180	180	180	180
38	180	180	0	0	180	0	0	180	0	180	0	0
39	180	0	0	0	180	0	180	0	0	0	180	180
40	0	0	0	0	180	180	180	180	0	0	0	0
41	0	180	180	180	180	180	0	0	180	0	180	180
42	180	0	0	0	180	0	180	0	180	0	180	0

Top block group — IR D M = (1 1 1), (1 1 2), (1 1 3), (1 1 4), (1 1 5), (1 1 6)

#	111 a	111 b	112 a	112 b	113 a	113 b	114 a	114 b	115 a	115 b	116 a	116 b
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
14	0.00000	0.00000	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
15	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
16	0.00000	0.00000	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
18	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
19	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000
20	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
21	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
22	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.70711	0.00000	0.00000	0.00000	0.00000	0.00000
23	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000
24	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000
25	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
26	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.40825	0.00000	-0.40825	0.00000
27	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
28	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	-0.35355	0.00000
30	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.35355	0.00000	-0.20412	0.00000
31	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
32	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20412	0.00000	0.35355	0.00000
33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.35355	0.00000	0.20412	0.00000
34	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
35	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	0.35355	0.00000
36	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.35355	0.00000	-0.20412	0.00000
37	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
38	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20412	0.00000	-0.35355	0.00000
39	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.35355	0.00000	0.20412	0.00000
40	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
41	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
42	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
43	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
44	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Middle block group — IR D M = (1 1 7), (2 1 1), (2 1 2), (2 1 3), (2 1 4), (2 1 5)

#	117 a	117 b	211 a	211 b	212 a	212 b	213 a	213 b	214 a	214 b	215 a	215 b
1	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.50000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000
14	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
15	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
16	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000
17	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000
18	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000
19	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000
20	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
21	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
22	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
23	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000
24	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
25	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000
26	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
27	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
28	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
29	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10206	-0.17678
30	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.17678	0.30619
31	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
32	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10206	-0.17678
33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.17678	0.30619
34	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
35	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10206	0.17678
36	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.17678	0.30619
37	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
38	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10206	0.17678
39	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.17678	0.30619
40	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
41	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Bottom block group — IR D M = (2 1 6), (2 1 7), (2 2 1), (2 2 2), (2 2 3), (2 2 4)

#	216 a	216 b	217 a	217 b	221 a	221 b	222 a	222 b	223 a	223 b	224 a	224 b
1	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000

```
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.50000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000   -0.50000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.50000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000   -0.50000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.50000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000   -0.50000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.50000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000   -0.50000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.40825    0.00000     0.40825    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.40825    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000    -0.40825    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.17678   -0.30619     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.10206   -0.17678     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000    -0.20412    0.35355     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.17678   -0.30619     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.10206   -0.17678     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.20413   -0.35355     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
-0.17678  -0.30619     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.10206    0.17678     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000    -0.20412   -0.35355     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
-0.17678  -0.30619     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.10206    0.17678     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
0.00000    0.00000     0.20412    0.35355     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000     0.00000    0.00000
```

```
  IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M
   2  2  5           2  2  6           2  2  7           3  1  1           3  1  2           3  1  3
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.40825   0.00000   0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000  -0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.10206   0.17678   0.10206   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
-0.17678 -0.30619   0.10206   0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000  -0.20412  -0.35355   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.10206   0.17678   0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
-0.17678 -0.30619   0.10206   0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.20412   0.35355   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.10206  -0.17678  -0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.17678  -0.30619   0.10206  -0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000  -0.20412   0.35355   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.10206  -0.17678  -0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.17678  -0.30619   0.10206  -0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.20412  -0.35355   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
```

```
  IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M          IR  D  M
   3  1  4           3  1  5           3  1  6           3  1  7           3  2  1           3  2  2
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.50000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.50000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.50000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000  -0.50000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
-0.50000  0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.50000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.40825   0.00000   0.00000   0.00000   0.40825   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.40825   0.00000   0.00000   0.00000   0.40825   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000  -0.40825   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.10206   0.17678   0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.17678  -0.30619   0.10206   0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.20412  -0.35355   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.10206  -0.17678  -0.17678  -0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.17678   0.30619  -0.10206  -0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.20412  -0.35355   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.10206  -0.17678  -0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.17678  -0.30619   0.10206  -0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.20413   0.35355   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.10206   0.17678  -0.17678   0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.17678   0.30619   0.10206  -0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.20413   0.35355   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.10206   0.17678  -0.17678  -0.30619   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000  -0.17678   0.30619  -0.10206   0.17678   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  -0.20412   0.35355   0.00000   0.00000   0.00000   0.00000
```

Elements of the block-diagonalized dynamical matrix (real and imaginary parts listed in pairs under each IR / D / M label).

3 2 3		3 2 4		3 2 5		3 2 6		3 2 7		4 1 1	
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.70711	0.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.70711	-0.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-0.50000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	-0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	-0.50000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000	0.40825	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.40825	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.40825	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.17678	-0.17678	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10206	-0.17678	-0.20412	0.35355	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.10206	-0.17678	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.17678	0.30619	-0.17678	0.30619	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.10206	0.17678	-0.20412	0.35355	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.10206	0.17678	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.17678	-0.30619	-0.17678	0.17678	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	-0.35355	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.10206	0.17678	-0.17678	-0.30619	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.17678	0.30619	0.10206	0.17678	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	-0.35355	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.10206	-0.17678	0.17678	0.30619	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.17678	-0.30619	-0.10206	-0.17678	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	-0.35355	0.00000	0.00000

4 1 2		4 1 3		4 1 4		4 1 5		4 1 6		4 1 7	
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.70711	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-0.70711	-0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.70711	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	-0.70711	-0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.70711	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	-0.70711	-0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00001	0.40825	0.00001	0.40825	0.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000	0.40825	0.00000	0.40825	0.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	-0.35355	0.00000	-0.40825	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.35355	0.00000	-0.20412	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40825	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	-0.35355	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.35355	0.00000	-0.20412	0.00000	-0.40825	-0.00001
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	0.35355	0.00000	0.40825	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.35355	0.00000	-0.20412	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.20412	0.00000	0.35355	0.00000	0.40825	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.35355	0.00000	-0.20412	0.00000	0.00000	0.00000
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	-0.40825	0.00000

ELEMENTS OF THE BLOCK-DIAGONALIZED DYNAMICAL MATRIX

```
IR NUMBER  1  IS  INFRARED ACTIVE.
IR NUMBER  1  IS  RAMAN ACTIVE.
IR NUMBER  2  IS  INFRARED ACTIVE.
IR NUMBER  2  IS  RAMAN ACTIVE.
IR NUMBER  3  IS  RAMAN ACTIVE.
```

⋮

A.2 IND

OUTPUT

```
THERE ARE  5 DIFFERENT UNIT TYPES
       NAMELY :
                 UNIT   1 = K1
                 UNIT   3 = LI1
                 UNIT   5 = S1
                 UNIT   7 = O1
                 UNIT   9 = O2

A MAXIMUM OF  32 INTERACTIONS CAN BE SPECIFIED
       NAMELY :
                 INTERACTION    1 BETWEEN  K1    AND K1
                 INTERACTION    2 BETWEEN  K1    AND K2
                 INTERACTION    3 BETWEEN  K1    AND LI1
                 INTERACTION    4 BETWEEN  K1    AND LI2
                 INTERACTION    5 BETWEEN  K1    AND S1
                 INTERACTION    6 BETWEEN  K1    AND S2
                 INTERACTION    7 BETWEEN  K1    AND O1
                 INTERACTION    8 BETWEEN  K1    AND O5
                 INTERACTION    9 BETWEEN  K1    AND O2
                 INTERACTION   10 BETWEEN  K1    AND O6
                 INTERACTION   11 BETWEEN  LI1   AND LI1
                 INTERACTION   12 BETWEEN  LI1   AND LI2
                 INTERACTION   13 BETWEEN  LI1   AND S1
                 INTERACTION   14 BETWEEN  LI1   AND S2
                 INTERACTION   15 BETWEEN  LI1   AND O1
                 INTERACTION   16 BETWEEN  LI1   AND O5
                 INTERACTION   17 BETWEEN  LI1   AND O2
                 INTERACTION   18 BETWEEN  LI1   AND O6
                 INTERACTION   19 BETWEEN  S1    AND S1
                 INTERACTION   20 BETWEEN  S1    AND S2
                 INTERACTION   21 BETWEEN  S1    AND O1
                 INTERACTION   22 BETWEEN  S1    AND O5
                 INTERACTION   23 BETWEEN  S1    AND O2
                 INTERACTION   24 BETWEEN  S1    AND O6
                 INTERACTION   25 BETWEEN  O1    AND O1
                 INTERACTION   26 BETWEEN  O1    AND O5
                 INTERACTION   27 BETWEEN  O1    AND O2
                 INTERACTION   28 BETWEEN  O1    AND O6
                 INTERACTION   29 BETWEEN  O2    AND O2
                 INTERACTION   30 BETWEEN  O2    AND O6
                 INTERACTION   31 BETWEEN  O2    AND O3
                 INTERACTION   32 BETWEEN  O2    AND O7
```

A.3 NN

INPUT

```
        1    2    0
       10
      .005   15.
```

OUTPUT

```
K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE  5.14 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        (-1 -1  0)                    ( -2.571 -4.453  0.000)
                                                                        (-1  0  0)                    ( -5.142  0.000  0.000)
                                                                        ( 0 -1  0)                    (  2.571 -4.453  0.000)
                                                                        ( 0  1  0)                    ( -2.571  4.453  0.000)
                                                                        ( 1  0  0)                    (  5.142  0.000  0.000)
                                                                        ( 1  1  0)                    (  2.571  4.453  0.000)


K1   HAS  2 NEIGHBORS OF TYPE K1   AT THE DISTANCE  8.62 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        ( 0  0 -1)                    (  0.000  0.000 -8.624)
                                                                        ( 0  0  1)                    (  0.000  0.000  8.624)


K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE  8.91 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        (-2 -1  0)                    ( -7.713 -4.453  0.000)
                                                                        (-1 -2  0)                    (  0.000 -8.906  0.000)
                                                                        (-1  1  0)                    ( -7.713  4.453  0.000)
                                                                        ( 1 -1  0)                    (  7.713 -4.453  0.000)
                                                                        ( 1  2  0)                    (  0.000  8.906  0.000)
                                                                        ( 2  1  0)                    (  7.713  4.453  0.000)


K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 10.04 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        (-1 -1 -1)                    ( -2.571 -4.453 -8.624)
                                                                        (-1 -1  1)                    ( -2.571 -4.453  8.624)
                                                                        (-1  0 -1)                    ( -5.142  0.000 -8.624)
                                                                        (-1  0  1)                    ( -5.142  0.000  8.624)
                                                                        ( 0 -1 -1)                    (  2.571 -4.453 -8.624)
                                                                        ( 0 -1  1)                    (  2.571 -4.453  8.624)
                                                                        ( 0  1 -1)                    ( -2.571  4.453 -8.624)
                                                                        ( 0  1  1)                    ( -2.571  4.453  8.624)
                                                                        ( 1  0 -1)                    (  5.142  0.000 -8.624)
                                                                        ( 1  0  1)                    (  5.142  0.000  8.624)
                                                                        ( 1  1 -1)                    (  2.571  4.453 -8.624)
                                                                        ( 1  1  1)                    (  2.571  4.453  8.624)


K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE 10.28 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        (-2 -2  0)                    ( -5.142 -8.906  0.000)
                                                                        (-2  0  0)                    (-10.284  0.000  0.000)
                                                                        ( 0 -2  0)                    (  5.142 -8.906  0.000)
                                                                        ( 0  2  0)                    ( -5.142  8.906  0.000)
                                                                        ( 2  0  0)                    ( 10.284  0.000  0.000)
                                                                        ( 2  2  0)                    (  5.142  8.906  0.000)


K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 12.40 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                                        (-2 -1 -1)                    ( -7.713 -4.453 -8.624)
                                                                        (-2 -1  1)                    ( -7.713 -4.453  8.624)
                                                                        (-1 -2 -1)                    (  0.000 -8.906 -8.624)
                                                                        (-1 -2  1)                    (  0.000 -8.906  8.624)
                                                                        (-1  1 -1)                    ( -7.713  4.453 -8.624)
                                                                        (-1  1  1)                    ( -7.713  4.453  8.624)
                                                                        ( 1 -1 -1)                    (  7.713 -4.453 -8.624)
                                                                        ( 1 -1  1)                    (  7.713 -4.453  8.624)
                                                                        ( 1  2 -1)                    (  0.000  8.906 -8.624)
                                                                        ( 1  2  1)                    (  0.000  8.906  8.624)
                                                                        ( 2  1 -1)                    (  7.713  4.453 -8.624)
                                                                        ( 2  1  1)                    (  7.713  4.453  8.624)
```
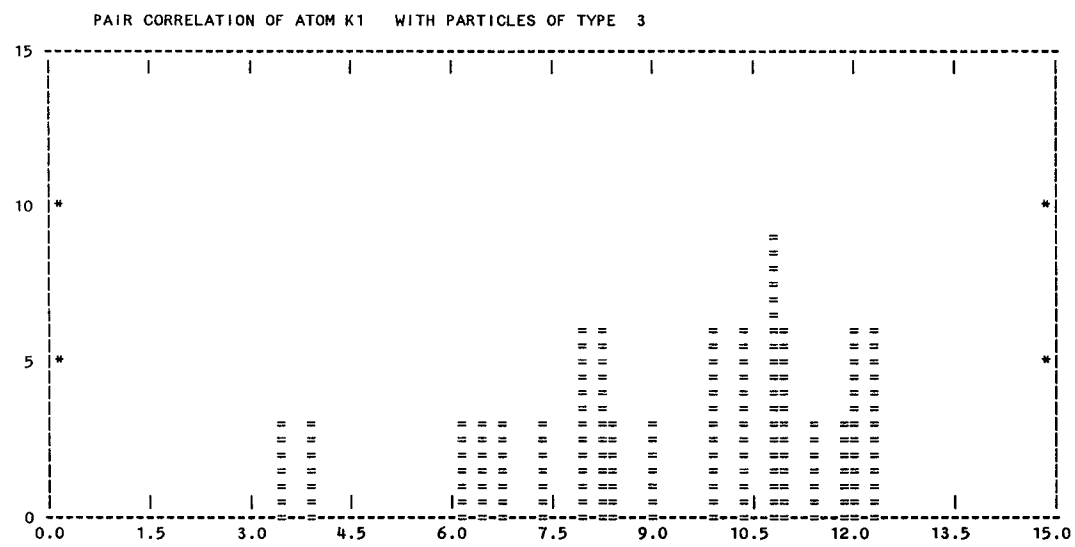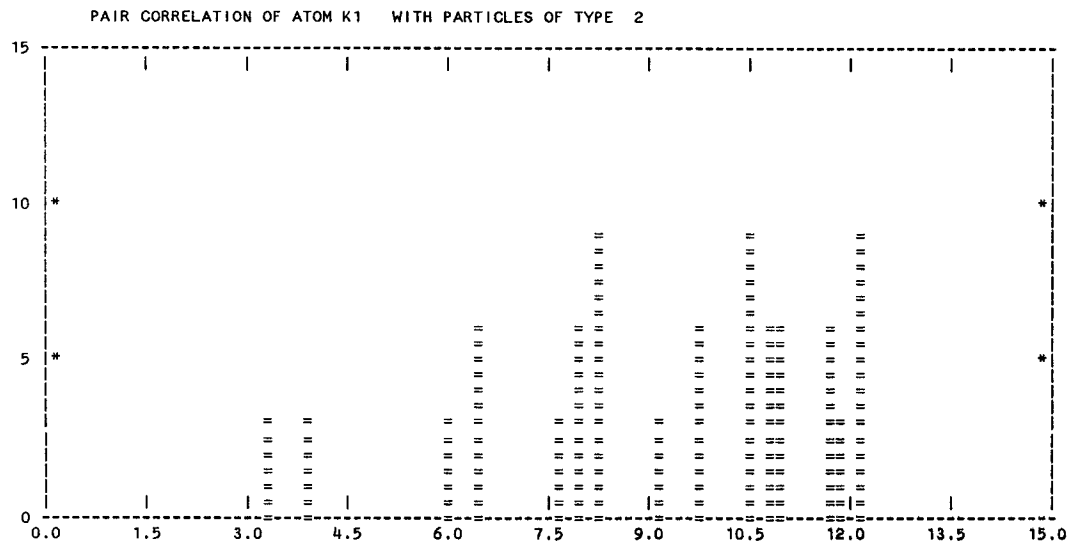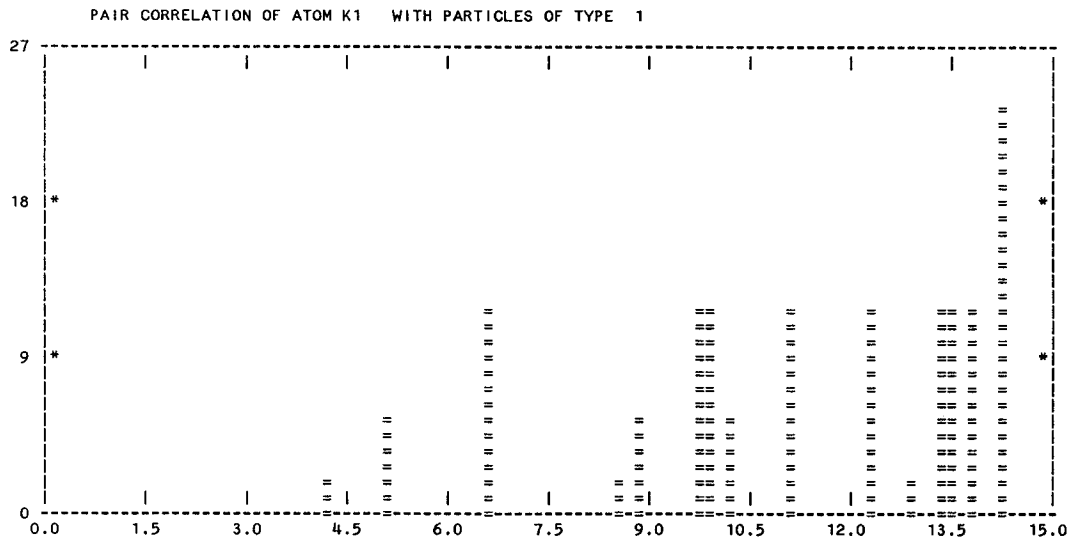
```
K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 13.42 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-2 -2 -1)                      ( -5.142 -8.906 -8.624)
                                                          (-2 -2  1)                      ( -5.142 -8.906  8.624)
                                                          (-2  0 -1)                      (-10.284  0.000 -8.624)
                                                          (-2  0  1)                      (-10.284  0.000  8.624)
                                                          ( 0 -2 -1)                      (  5.142 -8.906 -8.624)
                                                          ( 0 -2  1)                      (  5.142 -8.906  8.624)
                                                          ( 0  2 -1)                      ( -5.142  8.906 -8.624)
                                                          ( 0  2  1)                      ( -5.142  8.906  8.624)
                                                          ( 2  0 -1)                      ( 10.284  0.000 -8.624)
                                                          ( 2  0  1)                      ( 10.284  0.000  8.624)
                                                          ( 2  2 -1)                      (  5.142  8.906 -8.624)
                                                          ( 2  2  1)                      (  5.142  8.906  8.624)


K1   HAS 12 NEIGHBORS OF TYPE K1   AT THE DISTANCE 13.60 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-3 -2  0)                      (-10.284 -8.906  0.000)
                                                          (-3 -1  0)                      (-12.855 -4.453  0.000)
                                                          (-2 -3  0)                      ( -2.571-13.359  0.000)
                                                          (-2  1  0)                      (-12.855  4.453  0.000)
                                                          (-1 -3  0)                      (  2.571-13.359  0.000)
                                                          (-1  2  0)                      (-10.284  8.906  0.000)
                                                          ( 1 -2  0)                      ( 10.284 -8.906  0.000)
                                                          ( 1  3  0)                      ( -2.571 13.359  0.000)
                                                          ( 2 -1  0)                      ( 12.855 -4.453  0.000)
                                                          ( 2  3  0)                      (  2.571 13.359  0.000)
                                                          ( 3  1  0)                      ( 12.855  4.453  0.000)
                                                          ( 3  2  0)                      ( 10.284  8.906  0.000)


K1   HAS  6 NEIGHBORS OF TYPE K1   AT THE DISTANCE 15.43 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-3 -3  0)                      ( -7.713-13.359  0.000)
                                                          (-3  0  0)                      (-15.426  0.000  0.000)
                                                          ( 0 -3  0)                      (  7.713-13.359  0.000)
                                                          ( 0  3  0)                      ( -7.713 13.359  0.000)
                                                          ( 3  0  0)                      ( 15.426  0.000  0.000)
                                                          ( 3  3  0)                      (  7.713 13.359  0.000)


K1   HAS 24 NEIGHBORS OF TYPE K1   AT THE DISTANCE 16.11 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-3 -2 -1)                      (-10.284 -8.906 -8.624)
                                                          (-3 -2  1)                      (-10.284 -8.906  8.624)
                                                          (-3 -1 -1)                      (-12.855 -4.453 -8.624)
                                                          (-3 -1  1)                      (-12.855 -4.453  8.624)
                                                          (-2 -3 -1)                      ( -2.571-13.359 -8.624)
                                                          (-2 -3  1)                      ( -2.571-13.359  8.624)
                                                          (-2  1 -1)                      (-12.855  4.453 -8.624)
                                                          (-2  1  1)                      (-12.855  4.453  8.624)
                                                          (-1 -3 -1)                      (  2.571-13.359 -8.624)
                                                          (-1 -3  1)                      (  2.571-13.359  8.624)
                                                          (-1  2 -1)                      (-10.284  8.906 -8.624)
                                                          (-1  2  1)                      (-10.284  8.906  8.624)
                                                          ( 1 -2 -1)                      ( 10.284 -8.906 -8.624)
                                                          ( 1 -2  1)                      ( 10.284 -8.906  8.624)
                                                          ( 1  3 -1)                      ( -2.571 13.359 -8.624)
                                                          ( 1  3  1)                      ( -2.571 13.359  8.624)
                                                          ( 2 -1 -1)                      ( 12.855 -4.453 -8.624)
                                                          ( 2 -1  1)                      ( 12.855 -4.453  8.624)
                                                          ( 2  3 -1)                      (  2.571 13.359 -8.624)
                                                          ( 2  3  1)                      (  2.571 13.359  8.624)
                                                          ( 3  1 -1)                      ( 12.855  4.453 -8.624)
                                                          ( 3  1  1)                      ( 12.855  4.453  8.624)
                                                          ( 3  2 -1)                      ( 10.284  8.906 -8.624)
                                                          ( 3  2  1)                      ( 10.284  8.906  8.624)


K1   HAS  2 NEIGHBORS OF TYPE K2   AT THE DISTANCE  4.31 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          ( 0  0  0)                      (  0.000  0.000 -4.312)
                                                          ( 0  0  1)                      (  0.000  0.000  4.312)


K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE  6.71 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-1 -1  0)                      ( -2.571 -4.453 -4.312)
                                                          (-1 -1  1)                      ( -2.571 -4.453  4.312)
                                                          (-1  0  0)                      ( -5.142  0.000 -4.312)
                                                          (-1  0  1)                      ( -5.142  0.000  4.312)
                                                          ( 0 -1  0)                      (  2.571 -4.453 -4.312)
                                                          ( 0 -1  1)                      (  2.571 -4.453  4.312)
                                                          ( 0  1  0)                      ( -2.571  4.453 -4.312)
                                                          ( 0  1  1)                      ( -2.571  4.453  4.312)
                                                          ( 1  0  0)                      (  5.142  0.000 -4.312)
                                                          ( 1  0  1)                      (  5.142  0.000  4.312)
                                                          ( 1  1  0)                      (  2.571  4.453 -4.312)
                                                          ( 1  1  1)                      (  2.571  4.453  4.312)


K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE  9.90 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-2 -1  0)                      ( -7.713 -4.453 -4.312)
                                                          (-2 -1  1)                      ( -7.713 -4.453  4.312)
                                                          (-1 -2  0)                      (  0.000 -8.906 -4.312)
                                                          (-1 -2  1)                      (  0.000 -8.906  4.312)
                                                          (-1  1  0)                      ( -7.713  4.453 -4.312)
                                                          (-1  1  1)                      ( -7.713  4.453  4.312)
                                                          ( 1 -1  0)                      (  7.713 -4.453 -4.312)
                                                          ( 1 -1  1)                      (  7.713 -4.453  4.312)
                                                          ( 1  2  0)                      (  0.000  8.906 -4.312)
                                                          ( 1  2  1)                      (  0.000  8.906  4.312)
                                                          ( 2  1  0)                      (  7.713  4.453 -4.312)
                                                          ( 2  1  1)                      (  7.713  4.453  4.312)


K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 11.15 A IN THE CELLS :        WITH RADIUS VECTOR :
                                                          (-2 -2  0)                      ( -5.142 -8.906 -4.312)
                                                          (-2 -2  1)                      ( -5.142 -8.906  4.312)
                                                          (-2  0  0)                      (-10.284  0.000 -4.312)
                                                          (-2  0  1)                      (-10.284  0.000  4.312)
                                                          ( 0 -2  0)                      (  5.142 -8.906 -4.312)
                                                          ( 0 -2  1)                      (  5.142 -8.906  4.312)
                                                          ( 0  2  0)                      ( -5.142  8.906 -4.312)
                                                          ( 0  2  1)                      ( -5.142  8.906  4.312)
                                                          ( 2  0  0)                      ( 10.284  0.000 -4.312)
                                                          ( 2  0  1)                      ( 10.284  0.000  4.312)
                                                          ( 2  2  0)                      (  5.142  8.906 -4.312)
                                                          ( 2  2  1)                      (  5.142  8.906  4.312)
```
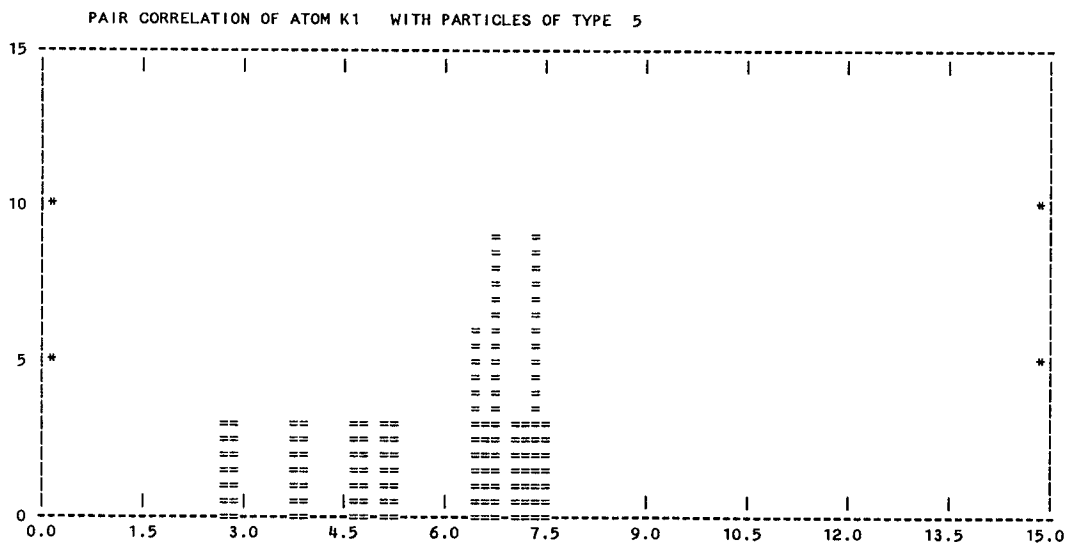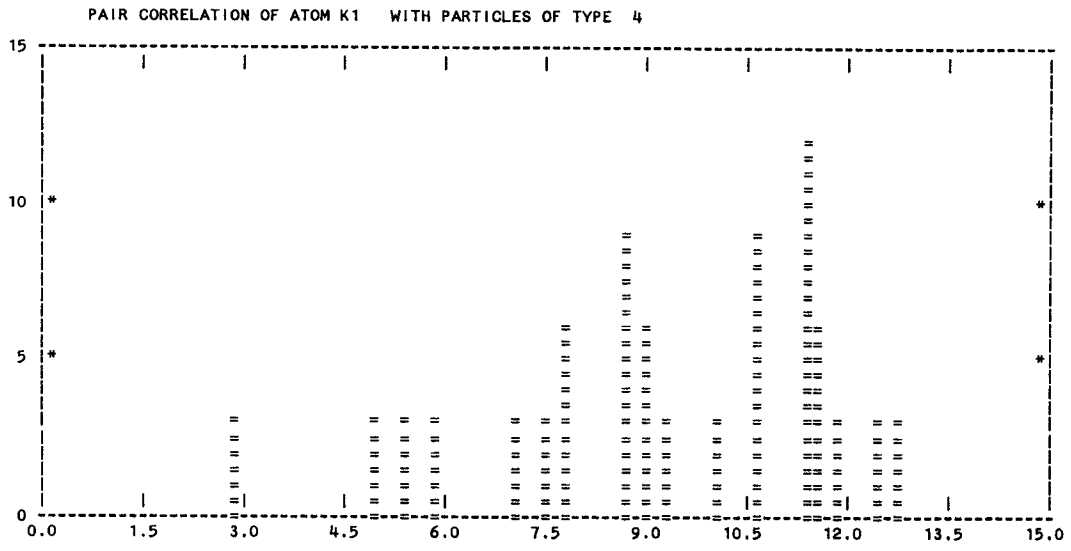
K1   HAS 2 NEIGHBORS OF TYPE K2   AT THE DISTANCE 12.94 A IN THE CELLS :   WITH RADIUS VECTOR :

```
( 0  0 -1)                              ( 0.000  0.000-12.936)
( 0  0  2)                              ( 0.000  0.000 12.936)
```

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 13.92 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-1 -1 -1)                              ( -2.571 -4.453-12.936)
(-1 -1  2)                              ( -2.571 -4.453 12.936)
(-1  0 -1)                              ( -5.142  0.000-12.936)
(-1  0  2)                              ( -5.142  0.000 12.936)
( 0 -1 -1)                              (  2.571 -4.453-12.936)
( 0 -1  2)                              (  2.571 -4.453 12.936)
( 0  1 -1)                              ( -2.571  4.453-12.936)
( 0  1  2)                              ( -2.571  4.453 12.936)
( 1  0 -1)                              (  5.142  0.000-12.936)
( 1  0  2)                              (  5.142  0.000 12.936)
( 1  1 -1)                              (  2.571  4.453-12.936)
( 1  1  2)                              (  2.571  4.453 12.936)
```

K1   HAS 24 NEIGHBORS OF TYPE K2   AT THE DISTANCE 14.27 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-3 -2  0)                              (-10.284 -8.906 -4.312)
(-3 -2  1)                              (-10.284 -8.906  4.312)
(-3 -1  0)                              (-12.855 -4.453 -4.312)
(-3 -1  1)                              (-12.855 -4.453  4.312)
(-2 -3  0)                              ( -2.571-13.359 -4.312)
(-2 -3  1)                              ( -2.571-13.359  4.312)
(-2  1  0)                              (-12.855  4.453 -4.312)
(-2  1  1)                              (-12.855  4.453  4.312)
(-1 -3  0)                              (  2.571-13.359 -4.312)
(-1 -3  1)                              (  2.571-13.359  4.312)
(-1  2  0)                              (-10.284  8.906 -4.312)
(-1  2  1)                              (-10.284  8.906  4.312)
( 1 -2  0)                              ( 10.284 -8.906 -4.312)
( 1 -2  1)                              ( 10.284 -8.906  4.312)
( 1  3  0)                              ( -2.571 13.359 -4.312)
( 1  3  1)                              ( -2.571 13.359  4.312)
( 2 -1  0)                              ( 12.855 -4.453 -4.312)
( 2 -1  1)                              ( 12.855 -4.453  4.312)
( 2  3  0)                              (  2.571 13.359 -4.312)
( 2  3  1)                              (  2.571 13.359  4.312)
( 3  1  0)                              ( 12.855  4.453 -4.312)
( 3  1  1)                              ( 12.855  4.453  4.312)
( 3  2  0)                              ( 10.284  8.906 -4.312)
( 3  2  1)                              ( 10.284  8.906  4.312)
```

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 15.71 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-2 -1 -1)                              ( -7.713 -4.453-12.936)
(-2 -1  2)                              ( -7.713 -4.453 12.936)
(-1 -2 -1)                              (  0.000 -8.906-12.936)
(-1 -2  2)                              (  0.000 -8.906 12.936)
(-1  1 -1)                              ( -7.713  4.453-12.936)
(-1  1  2)                              ( -7.713  4.453 12.936)
( 1 -1 -1)                              (  7.713 -4.453-12.936)
( 1 -1  2)                              (  7.713 -4.453 12.936)
( 1  2 -1)                              (  0.000  8.906-12.936)
( 1  2  2)                              (  0.000  8.906 12.936)
( 2  1 -1)                              (  7.713  4.453-12.936)
( 2  1  2)                              (  7.713  4.453 12.936)
```

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 16.02 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-3 -3  0)                              ( -7.713-13.359 -4.312)
(-3 -3  1)                              ( -7.713-13.359  4.312)
(-3  0  0)                              (-15.426  0.000 -4.312)
(-3  0  1)                              (-15.426  0.000  4.312)
( 0 -3  0)                              (  7.713-13.359 -4.312)
( 0 -3  1)                              (  7.713-13.359  4.312)
( 0  3  0)                              ( -7.713 13.359 -4.312)
( 0  3  1)                              ( -7.713 13.359  4.312)
( 3  0  0)                              ( 15.426  0.000 -4.312)
( 3  0  1)                              ( 15.426  0.000  4.312)
( 3  3  0)                              (  7.713 13.359 -4.312)
( 3  3  1)                              (  7.713 13.359  4.312)
```

K1   HAS 12 NEIGHBORS OF TYPE K2   AT THE DISTANCE 16.53 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-2 -2 -1)                              ( -5.142 -8.906-12.936)
(-2 -2  2)                              ( -5.142 -8.906 12.936)
(-2  0 -1)                              (-10.284  0.000-12.936)
(-2  0  2)                              (-10.284  0.000 12.936)
( 0 -2 -1)                              (  5.142 -8.906-12.936)
( 0 -2  2)                              (  5.142 -8.906 12.936)
( 0  2 -1)                              ( -5.142  8.906-12.936)
( 0  2  2)                              ( -5.142  8.906 12.936)
( 2  0 -1)                              ( 10.284  0.000-12.936)
( 2  0  2)                              ( 10.284  0.000 12.936)
( 2  2 -1)                              (  5.142  8.906-12.936)
( 2  2  2)                              (  5.142  8.906 12.936)
```

K1   HAS 3 NEIGHBORS OF TYPE LI1 AT THE DISTANCE 4.04 A IN THE CELLS :   WITH RADIUS VECTOR :

```
( 0  0  1)                              (  0.000 -2.969  2.742)
( 0  1  1)                              ( -2.571  1.484  2.742)
( 1  1  1)                              (  2.571  1.484  2.742)
```

K1   HAS 3 NEIGHBORS OF TYPE LI1 AT THE DISTANCE 6.54 A IN THE CELLS :   WITH RADIUS VECTOR :

```
(-1  0  1)                              ( -5.142 -2.969  2.742)
( 1  0  1)                              (  5.142 -2.969  2.742)
( 1  2  1)                              (  0.000  5.937  2.742)
```

K1   HAS 3 NEIGHBORS OF TYPE LI1 AT THE DISTANCE 6.59 A IN THE CELLS :   WITH RADIUS VECTOR :

```
( 0  0  0)                              (  0.000 -2.969 -5.882)
( 0  1  0)                              ( -2.571  1.484 -5.882)
( 1  1  0)                              (  2.571  1.484 -5.882)
```

PAIR CORRELATION OF ATOM K1   WITH PARTICLES OF TYPE 1

PAIR CORRELATION OF ATOM K1   WITH PARTICLES OF TYPE 2

PAIR CORRELATION OF ATOM K1   WITH PARTICLES OF TYPE 3

PAIR CORRELATION OF ATOM K1   WITH PARTICLES OF TYPE 4

```
15 |-----------------------------------------------------------------------------|
   |      I       I       I       I       I       I       I       I       I      |
   |                                                                             |
   |                                                         =                   |
   |                                                         =                   |
10 |*                                                        =                  *|
   |                                               =         =                   |
   |                                               =         =                   |
   |                                               =    = =  =                   |
   |                                       =       =    = =  ==                  |
 5 |*                                      =       =    = =  ==                 *|
   |                                       =       =    = =  ==                  |
   |                                       =       =    = =  ==                  |
   |                 =             = = =    =    = =    = =   ==                  |
   |                 =             = = =    =  = =    =   =   == =    = =          |
   |                 =             = = =    =  = =    =   =   == =    = =          |
   |                 =             = = =    =  = =    =   =   === =   = =          |
 0 |-----I-------=I----I--=-=-=I--=--=-=----=-=-=--=-I=---==-=I--=-=--I----I-------|
   0.0     1.5     3.0     4.5     6.0     7.5     9.0    10.5    12.0    13.5    15.0
```

PAIR CORRELATION OF ATOM K1   WITH PARTICLES OF TYPE 5

```
15 |-----------------------------------------------------------------------------|
   |      I       I       I       I       I       I       I       I       I      |
   |                                                                             |
   |                                                                             |
   |                                                                             |
10 |*                                                                           *|
   |                                           =    =                            |
   |                                           =    =                            |
   |                                           =    =                            |
   |                                           =    =                            |
   |                                         = =    =                            |
 5 |*                                        = =    =                           *|
   |                                         = =    =                            |
   |                                         = =    =                            |
   |                  ==      ==     == ==    === ====                           |
   |                  ==      ==     == ==    === ====                           |
   |                  ==      ==     == ==    === ====                           |
   |                  ==      ==     == ==    === ====                           |
 0 |------I------==I----==----|==--==----I----===--====--------I-------I----I-----|
   0.0     1.5     3.0     4.5     6.0     7.5     9.0    10.5    12.0    13.5    15.0
```

.
.
.

A.4 MODEL1

INPUT

```
    0     0     0     0    .0     1     0     0     0     1
  39.10      6.940-     32.06     16.00     16.00
    1
    5     7     1
   15    16
    5     9     1
   17    18
    7     9     1
   11    12
    9    11     1
   13    14
    0
    2
    6     7     7     8     9    10
    1     8     1
    1     9     1
    1    10     1
    3     7     1
    3    10     1
    0
    5
     7.
    1     2     3     4     5
    0
  1.20      0.400     1.35     -0.850    -0.700    0.1970    0.086     0.106
  0.100     2000.     130.0    -0.50      130.     -0.30     800.0     -53.80
  800.     -38.60
```

OUTPUT

```
--------------------------------------------------------------------------------------------------------
LATTICE DYNAMICAL MODEL-CALCULATION FOR THE FOLLOWING STRUCTURE:

   POSITION VECTOR SPACE LATTICE VECTORS
 A 1 = (   5.14200,   0.00000,   0.00000)
 A 2 = (  -2.57100,   4.45300,   0.00000)
 A 3 = (   0.00000,   0.00000,   8.62400)

   RECIPROCAL SPACE LATTICE VECTORS
AI 1 = (   0.19448,   0.11228,   0.00000)
AI 2 = (   0.00000,   0.22457,   0.00000)
AI 3 = (   0.00000,   0.00000,   0.11595)

      14 PARTICLES PER UNIT CELL :

                        POSITION                    MASS

       K1       (   0.00000,   0.00000,   0.00000)    39.10
       K2       (   0.00000,   0.00000,   4.31200)    39.10
       LI1      (   0.00000,   2.96874,   5.88200)     6.94
       LI2      (   2.57100,   1.48437,   1.57000)     6.94
       S1       (   0.00000,   2.96874,   2.53500)    32.06
       S2       (   2.57100,   1.48437,   6.84700)    32.06
       O1       (   0.00000,   2.96870,   3.96700)    16.00
       O5       (   2.57100,   1.48440,   8.27900)    16.00
       O2       (   1.39090,   2.92570,   2.06110)    16.00
       O6       (   1.18010,   1.52740,   6.37310)    16.00
       O3       (   4.48380,   4.19480,   2.06110)    16.00
       O7       (   3.22920,   0.25830,   6.37310)    16.00
       O4       (   4.40930,   1.78570,   2.06110)    16.00
       O8       (   3.30370,   2.66740,   6.37310)    16.00
```

MODEL SPECIFICATIONS :

INTERACTION	TYPE	NEIGHBOUR	PARAMETER-NO.S							
K1 - K1	COULOMB (M-M)	**	Z1	=	1	Z2	=	1		
K1 - K2	COULOMB (M-M)	**	Z1	=	1	Z2	=	1		
K1 - LI1	COULOMB (M-M)	**	Z1	=	1	Z2	=	2		
K1 - LI2	COULOMB (M-M)	**	Z1	=	1	Z2	=	2		
K1 - S1	COULOMB (M-M)	**	Z1	=	1	Z2	=	3		
K1 - S2	COULOMB (M-M)	**	Z1	=	1	Z2	=	3		
K1 - 01	COULOMB (M-M)	**	Z1	=	1	Z2	=	4		
K1 - 05	BORN-MAYER	1	R1	=	6	R2	=	8	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	4		
K1 - 02	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K1 - 06	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K1 - 03	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K1 - 07	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K1 - 04	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K1 - 08	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - K2	COULOMB (M-M)	**	Z1	=	1	Z2	=	1		
K2 - LI1	COULOMB (M-M)	**	Z1	=	1	Z2	=	2		
K2 - LI2	COULOMB (M-M)	**	Z1	=	1	Z2	=	2		
K2 - S1	COULOMB (M-M)	**	Z1	=	1	Z2	=	3		
K2 - S2	COULOMB (M-M)	**	Z1	=	1	Z2	=	3		
K2 - 01	BORN-MAYER	1	R1	=	6	R2	=	8	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	4		
K2 - 05	COULOMB (M-M)	**	Z1	=	1	Z2	=	4		
K2 - 02	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - 06	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - 03	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - 07	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - 04	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
K2 - 08	BORN-MAYER	1	R1	=	6	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	1	Z2	=	5		
LI1 - LI1	COULOMB (M-M)	**	Z1	=	2	Z2	=	2		
LI1 - LI2	COULOMB (M-M)	**	Z1	=	2	Z2	=	2		
LI1 - S1	COULOMB (M-M)	**	Z1	=	2	Z2	=	3		
LI1 - S2	COULOMB (M-M)	**	Z1	=	2	Z2	=	3		
LI1 - 01	BORN-MAYER	1	R1	=	7	R2	=	8	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	4		
LI1 - 05	COULOMB (M-M)	**	Z1	=	2	Z2	=	4		
LI1 - 02	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI1 - 06	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI1 - 03	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI1 - 07	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI1 - 04	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI1 - 08	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - LI2	COULOMB (M-M)	**	Z1	=	2	Z2	=	2		
LI2 - S1	COULOMB (M-M)	**	Z1	=	2	Z2	=	3		
LI2 - S2	COULOMB (M-M)	**	Z1	=	2	Z2	=	3		
LI2 - 01	COULOMB (M-M)	**	Z1	=	2	Z2	=	4		
LI2 - 05	BORN-MAYER	1	R1	=	7	R2	=	8	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	4		
LI2 - 02	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - 06	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - 03	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - 07	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - 04	BORN-MAYER	1	R1	=	7	R2	=	9	V0 = 10	
	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
LI2 - 08	COULOMB (M-M)	**	Z1	=	2	Z2	=	5		
S1 - S1	COULOMB (M-M)	**	Z1	=	3	Z2	=	3		
S1 - S2	COULOMB (M-M)	**	Z1	=	3	Z2	=	3		
S1 - 01	SPRINGS	1	LONG	=	15	TRANS	=	16		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	4		
S1 - 05	COULOMB (M-M)	**	Z1	=	3	Z2	=	4		
S1 - 02	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S1 - 06	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S1 - 03	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S1 - 07	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S1 - 04	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S1 - 08	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - S2	COULOMB (M-M)	**	Z1	=	3	Z2	=	3		
S2 - 01	COULOMB (M-M)	**	Z1	=	3	Z2	=	4		
S2 - 05	SPRINGS	1	LONG	=	15	TRANS	=	16		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	4		
S2 - 02	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - 06	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - 03	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - 07	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - 04	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		
S2 - 08	SPRINGS	1	LONG	=	17	TRANS	=	18		
	COULOMB (M-M)	**	Z1	=	3	Z2	=	5		

01	-	01	COULOMB (M-M)	**	Z1 =	4	Z2 =	4
01	-	05	COULOMB (M-M)	**	Z1 =	4	Z2 =	4
01	-	02	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
01	-	06	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
01	-	03	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
01	-	07	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
01	-	04	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
01	-	08	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	05	COULOMB (M-M)	**	Z1 =	4	Z2 =	4
05	-	02	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	06	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	03	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	07	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	04	COULOMB (M-M)	**	Z1 =	4	Z2 =	5
05	-	08	SPRINGS	1	LONG =	11	TRANS =	12
			COULOMB (M-M)	**	Z1 =	4	Z2 =	5
02	-	02	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
02	-	06	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
02	-	03	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
02	-	07	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
02	-	04	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
02	-	08	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
06	-	06	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
06	-	03	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
06	-	07	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
06	-	04	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
06	-	08	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
03	-	03	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
03	-	07	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
03	-	04	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
03	-	08	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
07	-	07	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
07	-	04	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
07	-	08	SPRINGS	1	LONG =	13	TRANS =	14
			COULOMB (M-M)	**	Z1 =	5	Z2 =	5
04	-	04	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
04	-	08	COULOMB (M-M)	**	Z1 =	5	Z2 =	5
08	-	08	COULOMB (M-M)	**	Z1 =	5	Z2 =	5

PARAMETER-VALUES :

PAR.-NO.	VALUE	
1	1.200	E
2	0.400	E
3	1.350	E
4	-0.850	E
5	-0.700	E
6	0.197	A
7	0.086	A
8	0.106	A
9	0.100	A
10	2000.000	EV
11	130.000	N/M
12	-0.500	N/M
13	130.000	N/M
14	-0.300	N/M
15	800.000	N/M
16	-53.800	N/M
17	800.000	N/M
18	-38.600	N/M

EIGENVALUES AND EIGENVECTORS FOR IRM 1

```
NY**2 =  -0.0015 THZ**2    NEGATIV !!!
   K1       0.000000 0.000000    0.000000 0.000000    0.638167 0.000002
   K2       0.000000 0.000000    0.000000 0.000000    0.638167 0.000002
   LI1      0.000000 0.000000    0.000000 0.000000    0.268865 0.000001
   LI2      0.000000 0.000000    0.000000 0.000000    0.268865 0.000001
   S1       0.000000 0.000000    0.000000 0.000000    0.577899 0.000002
   S2       0.000000 0.000000    0.000000 0.000000    0.577899 0.000002
   O1       0.000000 0.000000    0.000000 0.000000    0.408250 0.000001
   O5       0.000000 0.000000    0.000000 0.000000    0.408250 0.000001
   O2       0.000000 0.000000   -0.000009 0.000000    0.408249 0.000001
   O6       0.000000 0.000000    0.000009 0.000000    0.408249 0.000001
   O3       0.000008 0.000000    0.000004 0.000000    0.408249 0.000001
   O7      -0.000008 0.000000   -0.000004 0.000000    0.408249 0.000001
   O4      -0.000008 0.000000    0.000005 0.000000    0.408249 0.000001
   O8       0.000008 0.000000   -0.000005 0.000000    0.408249 0.000001
NY =  4.59 THZ

   K1       0.000000 0.000000    0.000000 0.000000   -0.177698-0.000001
   K2       0.000000 0.000000    0.000000 0.000000   -0.177698-0.000001
   LI1      0.000000 0.000000    0.000000 0.000000    0.103683 0.000000
   LI2      0.000000 0.000000    0.000000 0.000000    0.103683 0.000000
   S1       0.000000 0.000000    0.000000 0.000000    0.059540 0.000000
   S2       0.000000 0.000000    0.000000 0.000000    0.059540 0.000000
   O1       0.000000 0.000000    0.000000 0.000000    0.040881 0.000000
   O5       0.000000 0.000000    0.000000 0.000000    0.040881 0.000000
   O2       0.011527 0.000000    0.408249 0.000001    0.028118 0.000000
   O6      -0.011527 0.000000   -0.408249-0.000001    0.028118 0.000000
   O3      -0.359318-0.000001   -0.194141 0.000000    0.028118 0.000000
   O7       0.359318 0.000001    0.194141 0.000001    0.028118 0.000000
   O4       0.347790 0.000001   -0.214107 0.000000    0.028118 0.000000
   O8      -0.347790-0.000001    0.214107 0.000000    0.028118 0.000000
NY =  6.14 THZ

   K1       0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   K2       0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   LI1      0.000000 0.000000    0.000000 0.000000   -0.306284-0.000001
   LI2      0.000000 0.000000    0.000000 0.000000   -0.306284-0.000001
   S1       0.000000 0.000000    0.000000 0.000000   -0.273536-0.000001
   S2       0.000000 0.000000    0.000000 0.000000   -0.273536-0.000001
   O1       0.000000 0.000000    0.000000 0.000000   -0.166013 0.000000
   O5       0.000000 0.000000    0.000000 0.000000   -0.166013 0.000000
   O2       0.022360 0.000000    0.154775 0.000000   -0.116798 0.000000
   O6      -0.022360 0.000000   -0.154775 0.000000   -0.116798 0.000000
   O3      -0.145219 0.000000   -0.058024 0.000000   -0.116798 0.000000
   O7       0.145219 0.000000    0.058024 0.000000   -0.116798 0.000000
   O4       0.122860 0.000000   -0.096751 0.000000   -0.116798 0.000000
   O8      -0.122860 0.000000    0.096751 0.000000   -0.116798 0.000000
NY =  9.76 THZ

   K1       0.000000 0.000000    0.000000 0.000000    0.149269 0.000000
   K2       0.000000 0.000000    0.000000 0.000000    0.149269 0.000000
   LI1      0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   LI2      0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   S1       0.000000 0.000000    0.000000 0.000000   -0.267678-0.000001
   S2       0.000000 0.000000    0.000000 0.000000   -0.267678-0.000001
   O1       0.000000 0.000000    0.000000 0.000000   -0.132925 0.000000
   O5       0.000000 0.000000    0.000000 0.000000   -0.132925 0.000000
   O2       0.028143 0.000000   -0.017251 0.000000   -0.062394 0.000000
   O6      -0.028143 0.000000    0.017251 0.000000   -0.062394 0.000000
   O3       0.000869 0.000000    0.032998 0.000000   -0.062394 0.000000
   O7      -0.000869 0.000000   -0.032998 0.000000   -0.062394 0.000000
   O4      -0.029011 0.000000   -0.015747 0.000000   -0.062394 0.000000
   O8       0.029011 0.000000    0.015747 0.000000   -0.062394 0.000000
NY = 15.30 THZ

   K1       0.000000 0.000000    0.000000 0.000000   -0.120437 0.000000
   K2       0.000000 0.000000    0.000000 0.000000   -0.120437 0.000000
   LI1      0.000000 0.000000    0.000000 0.000000   -0.129428 0.000000
   LI2      0.000000 0.000000    0.000000 0.000000   -0.129428 0.000000
   S1       0.000000 0.000000    0.000000 0.000000   -0.491661-0.000001
   S2       0.000000 0.000000    0.000000 0.000000   -0.491661-0.000001
   O1       0.000000 0.000000    0.000000 0.000000   -0.255259-0.000001
   O5       0.000000 0.000000    0.000000 0.000000   -0.255259-0.000001
   O2       0.235903 0.000001   -0.008874 0.000000    0.408249 0.000001
   O6      -0.235903-0.000001    0.008874 0.000000    0.408249 0.000001
   O3      -0.110266 0.000000    0.208734 0.000001    0.408249 0.000001
   O7       0.110266 0.000001   -0.208734-0.000001    0.408249 0.000001
   O4      -0.125636 0.000000   -0.199861-0.000001    0.408249 0.000001
   O8       0.125636 0.000000    0.199861 0.000001    0.408249 0.000001
NY = 34.15 THZ

   K1       0.000000 0.000000    0.000000 0.000000   -0.020773 0.000000
   K2       0.000000 0.000000    0.000000 0.000000   -0.020773 0.000000
   LI1      0.000000 0.000000    0.000000 0.000000   -0.030688 0.000000
   LI2      0.000000 0.000000    0.000000 0.000000   -0.030688 0.000000
   S1       0.000000 0.000000    0.000000 0.000000   -0.491466-0.000001
   S2       0.000000 0.000000    0.000000 0.000000   -0.491466-0.000001
   O1       0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   O5       0.000000 0.000000    0.000000 0.000000    0.707107 0.000002
   O2      -0.119257 0.000000    0.002294 0.000000    0.013757 0.000000
   O6       0.119257 0.000000   -0.002294 0.000000    0.013757 0.000000
   O3       0.057642 0.000000   -0.104426 0.000000    0.013757 0.000000
   O7      -0.057642 0.000000    0.104426 0.000000    0.013757 0.000000
   O4       0.061615 0.000000    0.102133 0.000000    0.013757 0.000000
   O8      -0.061615 0.000000   -0.102133 0.000000    0.013757 0.000000
```

NY = 34.74 THZ

K1	0.000000 0.000000	0.000000 0.000000	0.004149 0.000000
K2	0.000000 0.000000	0.000000 0.000000	0.004149 0.000000
LI1	0.000000 0.000000	0.000000 0.000000	0.000367 0.000000
LI2	0.000000 0.000000	0.000000 0.000000	0.000367 0.000000
S1	0.000000 0.000000	0.000000 0.000000	0.093664 0.000000
S2	0.000000 0.000000	0.000000 0.000000	0.093664 0.000000
01	0.000000 0.000000	0.000000 0.000000	0.280104 0.000001
05	0.000000 0.000000	0.000000 0.000000	0.280104 0.000001
02	0.408249 0.000001	-0.015231 0.000000	-0.139808 0.000000
06	-0.408249-0.000001	0.015231 0.000000	-0.139808 0.000000
03	-0.190934 0.000000	0.361168 0.000001	-0.139808 0.000000
07	0.190934 0.000001	-0.361168-0.000001	-0.139808 0.000000
04	-0.217314 0.000000	-0.345938-0.000001	-0.139808 0.000000
08	0.217314 0.000000	0.345938 0.000001	-0.139808 0.000000

EIGENVALUES AND EIGENVECTORS FOR IRM 2

(2-FOLD DEGENERATE)
NY = 0.00 THZ

K1	0.500000 0.000003	-0.000002 0.500000	0.000000 0.000000
K2	0.500001 0.000001	-0.000002 0.499999	0.000000 0.000000
LI1	0.210673-0.000015	0.000015 0.210673	0.000000 0.000000
LI2	0.210673-0.000015	0.000015 0.210673	0.000000 0.000000
S1	0.452801-0.000016	0.000017 0.452801	0.000000 0.000000
S2	0.452802-0.000018	0.000017 0.452800	0.000000 0.000000
01	0.319774-0.000010	0.000011 0.319774	0.000000 0.000000
05	0.319775-0.000011	0.000011 0.319773	0.000000 0.000000
02	0.319921-0.000012	0.000015 0.319916	0.000109-0.000007
06	0.319921-0.000014	0.000017 0.319916	-0.000109 0.000007
03	0.319918-0.000019	0.000013 0.319917	-0.000048 0.000098
07	0.319918-0.000017	0.000013 0.319917	0.000048-0.000098
04	0.319915-0.000013	0.000016 0.319920	-0.000061-0.000091
08	0.319915-0.000014	0.000017 0.319921	0.000061 0.000091

NY = 2.06 THZ

K1	-0.111861 0.091120	-0.091120-0.111861	0.000000 0.000000
K2	-0.111861 0.091120	-0.091120-0.111861	0.000000 0.000000
LI1	0.012639-0.026167	0.026167 0.012639	0.000000 0.000000
LI2	0.012639-0.026167	0.026167 0.012639	0.000000 0.000000
S1	0.034156-0.021282	0.021282 0.034156	0.000000 0.000000
S2	0.034156-0.021282	0.021282 0.034156	0.000000 0.000000
01	-0.383366-0.045575	0.045574-0.383366	0.000000 0.000000
05	-0.383367-0.045574	0.045574-0.383365	0.000000 0.000000
02	0.167669-0.011185	0.021835 0.166424	0.408248 0.000003
06	0.167669-0.011186	0.021836 0.166424	-0.408248-0.000001
03	0.171346-0.019713	0.013310 0.162746	-0.204125 0.353553
07	0.171346-0.019712	0.013309 0.162746	0.204126-0.353552
04	0.162123-0.018634	0.014387 0.171969	-0.204123-0.353554
08	0.162123-0.018634	0.014388 0.171969	0.204124 0.353554

NY = 4.23 THZ

K1	0.500000 0.000003	-0.000002 0.500000	0.000000 0.000000
K2	0.500001 0.000001	-0.000002 0.499999	0.000000 0.000000
LI1	-0.041377-0.002106	0.002106-0.041377	0.000000 0.000000
LI2	-0.041377-0.002106	0.002106-0.041376	0.000000 0.000000
S1	-0.170981 0.001739	-0.001740-0.170981	0.000000 0.000000
S2	-0.170982 0.001740	-0.001740-0.170981	0.000000 0.000000
01	-0.194520-0.062346	0.062346-0.194520	0.000000 0.000000
05	-0.194520-0.062346	0.062346-0.194519	0.000000 0.000000
02	-0.102050 0.019048	-0.021783-0.109815	0.063643 0.049469
06	-0.102049 0.019049	-0.021783-0.109815	-0.063644-0.049469
03	-0.109057 0.017737	-0.023095-0.102806	-0.074663 0.030383
07	-0.109057 0.017737	-0.023095-0.102807	0.074663-0.030382
04	-0.106689 0.024462	-0.016369-0.105175	0.011019-0.079851
08	-0.106689 0.024462	-0.016370-0.105175	-0.011019 0.079851

NY = 8.60 THZ

K1	-0.027525 0.000728	-0.000728-0.027525	0.000000 0.000000
K2	-0.027526 0.000728	-0.000728-0.027525	0.000000 0.000000
LI1	0.500000 0.000003	-0.000002 0.500000	0.000000 0.000000
LI2	0.500001 0.000001	-0.000002 0.499999	0.000000 0.000000
S1	-0.070309-0.007083	0.007083-0.070309	0.000000 0.000000
S2	-0.070309-0.007083	0.007083-0.070309	0.000000 0.000000
01	-0.052377 0.010192	-0.010192-0.052377	0.000000 0.000000
05	-0.052377 0.010192	-0.010192-0.052377	0.000000 0.000000
02	-0.050103-0.007651	-0.006778-0.039478	-0.006988-0.008347
06	-0.050103-0.007651	-0.006778-0.039478	0.006988 0.008347
03	-0.048382 0.007772	0.008644-0.041199	0.010723-0.001878
07	-0.048382 0.007772	0.008645-0.041199	-0.010723 0.001878
04	-0.035886-0.001430	-0.000557-0.053695	-0.003735 0.010225
08	-0.035886-0.001430	-0.000557-0.053695	0.003735-0.010225

NY = 12.63 THZ

K1	0.006700-0.002799	0.002799 0.006700	0.000000 0.000000
K2	0.006700-0.002799	0.002799 0.006700	0.000000 0.000000
LI1	0.010730 0.019610	-0.019610 0.010730	0.000000 0.000000
LI2	0.010730 0.019610	-0.019610 0.010730	0.000000 0.000000
S1	0.016550 0.037426	-0.037426 0.016550	0.000000 0.000000
S2	0.016550 0.037426	-0.037426 0.016550	0.000000 0.000000
01	-0.058894 0.351172	-0.351172-0.058893	0.000000 0.000000
05	-0.058892 0.351173	-0.351171-0.058893	0.000000 0.000000
02	0.011948 0.133115	0.408249 0.000003	-0.031197 0.332615
06	0.011949 0.133115	0.408249 0.000001	0.031196-0.332615
03	0.237405-0.278081	-0.002948-0.225456	-0.272456-0.193324
07	0.237405-0.278080	-0.002947-0.225455	0.272455 0.193325
04	-0.231428-0.267734	0.007398 0.243379	0.303652-0.139291
08	-0.231429-0.267733	0.007399 0.243379	-0.303652 0.139292

```
NY = 14.38 THZ

K1      -0.016388 0.003803   -0.003803-0.016388    0.000000 0.000000
K2      -0.016388 0.003803   -0.003803-0.016388    0.000000 0.000000
LI1      0.004207-0.021296    0.021296 0.004207    0.000000 0.000000
LI2      0.004207-0.021296    0.021296 0.004207    0.000000 0.000000
S1       0.500000 0.000003   -0.000002 0.500000    0.000000 0.000000
S2       0.500001 0.000001   -0.000002 0.499999    0.000000 0.000000
O1      -0.416354-0.032177    0.032177-0.416354    0.000000 0.000000
O5      -0.416355-0.032176    0.032176-0.416353    0.000000 0.000000
O2       0.159627-0.018717   -0.045553-0.338671   -0.221068-0.005162
O6       0.159627-0.018718   -0.045555-0.338671    0.221068 0.005161
O3      -0.241928-0.186282   -0.213119 0.062884    0.115004-0.188870
O7      -0.241926-0.186283   -0.213119 0.062883   -0.115004 0.188870
O4      -0.186266 0.245255    0.218418 0.007222    0.106064 0.194031
O8      -0.186264 0.245255    0.218419 0.007221   -0.106065-0.194031

NY = 34.43 THZ

K1       0.001002 0.000388   -0.000388 0.001002    0.000000 0.000000
K2       0.001002 0.000388   -0.000388 0.001002    0.000000 0.000000
LI1     -0.002156-0.002126    0.002126-0.002156    0.000000 0.000000
LI2     -0.002156-0.002126    0.002126-0.002156    0.000000 0.000000
S1      -0.368082-0.011963    0.011962-0.368082    0.000000 0.000000
S2      -0.368083-0.011961    0.011962-0.368081    0.000000 0.000000
O1      -0.036535-0.003417    0.003417-0.036535    0.000000 0.000000
O5      -0.036535-0.003417    0.003417-0.036534    0.000000 0.000000
O2       0.408249 0.000003   -0.014094-0.036636   -0.154912-0.000578
O6       0.408249 0.000001   -0.014094-0.036636    0.154912 0.000577
O3       0.068482-0.182070   -0.196164 0.303130    0.077956-0.133870
O7       0.068483-0.182069   -0.196165 0.303129   -0.077957 0.133869
O4       0.080687 0.203211    0.189115 0.290925    0.076956 0.134447
O8       0.080688 0.203211    0.189116 0.290925   -0.076956-0.134447

NY = 0.00 THZ

K1       0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
K2       0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
LI1      0.210673 0.000019    0.000019-0.210673    0.000000 0.000000
LI2      0.210673 0.000019    0.000019-0.210673    0.000000 0.000000
S1       0.452798 0.000030    0.000030-0.452798    0.000000 0.000000
S2       0.452798 0.000030    0.000030-0.452798    0.000000 0.000000
O1       0.319774-0.000002   -0.000002-0.319774    0.000000 0.000000
O5       0.319774-0.000002   -0.000002-0.319774    0.000000 0.000000
O2       0.319916 0.000032    0.000034-0.319909    0.000103 0.000034
O6       0.319916 0.000032    0.000034-0.319909   -0.000103-0.000034
O3       0.319911 0.000036    0.000029-0.319913   -0.000023-0.000106
O7       0.319911 0.000037    0.000030-0.319913    0.000023 0.000106
O4       0.319909 0.000030    0.000036-0.319914   -0.000081 0.000073
O8       0.319909 0.000030    0.000036-0.319914    0.000081-0.000073

NY = 2.06 THZ

K1      -0.111839-0.091109   -0.091109 0.111839    0.000000 0.000000
K2      -0.111839-0.091109   -0.091109 0.111839    0.000000 0.000000
LI1      0.012641 0.026174    0.026174-0.012641    0.000000 0.000000
LI2      0.012641 0.026174    0.026174-0.012641    0.000000 0.000000
S1       0.034153 0.021300    0.021300-0.034153    0.000000 0.000000
S2       0.034153 0.021300    0.021300-0.034153    0.000000 0.000000
O1      -0.383371 0.045581    0.045581 0.383371    0.000000 0.000000
O5      -0.383371 0.045581    0.045581 0.383371    0.000000 0.000000
O2       0.167666 0.011199    0.021851-0.166423    0.408248 0.000000
O6       0.167666 0.011199    0.021851-0.166423   -0.408248 0.000000
O3       0.171345 0.019726    0.013323-0.162743   -0.204124-0.353554
O7       0.171345 0.019727    0.013324-0.162743    0.204124 0.353554
O4       0.162121 0.018649    0.014401-0.171967   -0.204124 0.353553
O8       0.162121 0.018649    0.014401-0.171967    0.204124-0.353553

NY = 4.23 THZ

K1       0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
K2       0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
LI1     -0.041378 0.002104    0.002104 0.041378    0.000000 0.000000
LI2     -0.041378 0.002104    0.002104 0.041378    0.000000 0.000000
S1      -0.170981-0.001741   -0.001741 0.170981    0.000000 0.000000
S2      -0.170981-0.001741   -0.001741 0.170981    0.000000 0.000000
O1      -0.194508 0.062345    0.062345 0.194508    0.000000 0.000000
O5      -0.194508 0.062345    0.062345 0.194508    0.000000 0.000000
O2      -0.102053-0.019051   -0.021786 0.109816    0.063633-0.049471
O6      -0.102053-0.019051   -0.021786 0.109816   -0.063633 0.049471
O3      -0.109059-0.017740   -0.023096 0.102809   -0.074660-0.030373
O7      -0.109059-0.017741   -0.023096 0.102809    0.074660 0.030373
O4      -0.106691-0.024463   -0.016373 0.105178    0.011027 0.079844
O8      -0.106691-0.024463   -0.016373 0.105178   -0.011027-0.079844

NY = 8.60 THZ

K1      -0.027525-0.000728   -0.000728 0.027525    0.000000 0.000000
K2      -0.027525-0.000728   -0.000728 0.027525    0.000000 0.000000
LI1      0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
LI2      0.500000 0.000000    0.000000-0.500000    0.000000 0.000000
S1      -0.070311 0.007083    0.007083 0.070311    0.000000 0.000000
S2      -0.070311 0.007083    0.007083 0.070311    0.000000 0.000000
O1      -0.052377-0.010193   -0.010193 0.052377    0.000000 0.000000
O5      -0.052377-0.010193   -0.010193 0.052377    0.000000 0.000000
O2      -0.050105 0.007650   -0.006778 0.039478   -0.006988 0.008346
O6      -0.050105 0.007650   -0.006778 0.039478    0.006988-0.008346
O3      -0.048382-0.007773    0.008645 0.041200    0.010722 0.001879
O7      -0.048382-0.007773    0.008644 0.041200   -0.010722-0.001879
O4      -0.035887 0.001430   -0.000559 0.053696   -0.003734-0.010225
O8      -0.035887 0.001430   -0.000559 0.053696    0.003734 0.010225
```

NY = 12.63 THZ

K1	0.006701 0.002798	0.002798-0.006701	0.000000 0.000000
K2	0.006701 0.002798	0.002798-0.006701	0.000000 0.000000
L I 1	0.010729-0.019610	-0.019610-0.010729	0.000000 0.000000
L I 2	0.010729-0.019610	-0.019610-0.010729	0.000000 0.000000
S1	0.016554-0.037429	-0.037429-0.016554	0.000000 0.000000
S2	0.016554-0.037429	-0.037429-0.016554	0.000000 0.000000
O1	-0.058892-0.351164	-0.351164 0.058892	0.000000 0.000000
O5	-0.058892-0.351164	-0.351164 0.058892	0.000000 0.000000
O2	0.011949-0.133116	0.408249 0.000000	-0.031200-0.332612
O6	0.011949-0.133116	0.408249 0.000000	0.031200 0.332612
O3	0.237405 0.278081	-0.002949 0.225456	-0.272451 0.193326
O7	0.237404 0.278081	-0.002949 0.225456	0.272451-0.193326
O4	-0.231431 0.267733	0.007399-0.243379	0.303651 0.139286
O8	-0.231431 0.267733	0.007399-0.243379	-0.303651-0.139286

NY = 14.38 THZ

K1	-0.016387-0.003803	-0.003803 0.016387	0.000000 0.000000
K2	-0.016387-0.003803	-0.003803 0.016387	0.000000 0.000000
L I 1	0.004209 0.021296	0.021296-0.004209	0.000000 0.000000
L I 2	0.004209 0.021296	0.021296-0.004209	0.000000 0.000000
S1	0.500000 0.000000	0.000000-0.500000	0.000000 0.000000
S2	0.500000 0.000000	0.000000-0.500000	0.000000 0.000000
O1	-0.416362 0.032176	0.032176 0.416362	0.000000 0.000000
O5	-0.416362 0.032176	0.032176 0.416362	0.000000 0.000000
O2	0.159624 0.018719	-0.045560 0.338669	-0.221071 0.005164
O6	0.159624 0.018719	-0.045560 0.338669	0.221071-0.005164
O3	-0.241929 0.186277	-0.213117-0.062885	0.115008 0.188871
O7	-0.241929 0.186276	-0.213117-0.062884	-0.115008-0.188871
O4	-0.186261-0.245257	0.218416-0.007217	0.106063-0.194035
O8	-0.186261-0.245257	0.218416-0.007217	-0.106063 0.194035

NY = 34.43 THZ

K1	0.001002-0.000388	-0.000388-0.001002	0.000000 0.000000
K2	0.001002-0.000388	-0.000388-0.001002	0.000000 0.000000
L I 1	-0.002156 0.002126	0.002126 0.002156	0.000000 0.000000
L I 2	-0.002156 0.002126	0.002126 0.002156	0.000000 0.000000
S1	-0.368082 0.011961	0.011961 0.368082	0.000000 0.000000
S2	-0.368082 0.011961	0.011961 0.368082	0.000000 0.000000
O1	-0.036535 0.003417	0.003417 0.036535	0.000000 0.000000
O5	-0.036535 0.003417	0.003417 0.036535	0.000000 0.000000
O2	0.408249 0.000000	-0.014094 0.036636	-0.154912 0.000577
O6	0.408249 0.000000	-0.014094 0.036636	0.154912-0.000577
O3	0.068482 0.182070	-0.196164-0.303130	0.077956 0.133870
O7	0.068482 0.182070	-0.196163-0.303130	-0.077956-0.133870
O4	0.080688-0.203211	0.189117-0.290924	0.076956-0.134447
O8	0.080688-0.203211	0.189117-0.290924	-0.076956 0.134447

EIGENVALUES AND EIGENVECTORS FOR IRM 3

(2-FOLD DEGENERATE)
NY = 1.62 THZ

K1	0.312416-0.116089	-0.116089-0.312416	0.000000 0.000000
K2	-0.312416 0.116089	0.116089 0.312416	0.000000 0.000000
L I 1	0.007918-0.181654	-0.181654-0.007918	0.000000 0.000000
L I 2	-0.007918 0.181654	0.181654 0.007918	0.000000 0.000000
S1	0.001357 0.374416	0.374416-0.001357	0.000000 0.000000
S2	-0.001357-0.374416	-0.374416 0.001357	0.000000 0.000000
O1	0.012836-0.117710	-0.117710-0.012835	0.000000 0.000000
O5	-0.012835 0.117710	0.117710 0.012835	0.000000 0.000000
O2	0.001894 0.404087	0.408248 0.000002	-0.014655 0.393976
O6	-0.001895-0.404088	-0.408249-0.000001	-0.014654 0.393976
O3	0.002275 0.408030	0.404307 0.000381	0.348521-0.184298
O7	-0.002274-0.408029	-0.404306-0.000382	0.348521-0.184297
O4	-0.001330 0.406387	0.405949-0.003222	-0.333866-0.209679
O8	0.001328-0.406386	-0.405948 0.003224	-0.333866-0.209678

NY = 2.92 THZ

K1	0.500000 0.000002	0.000001-0.500000	0.000000 0.000000
K2	-0.500000-0.000001	-0.000001 0.500000	0.000000 0.000000
L I 1	-0.019950 0.046996	0.046996 0.019950	0.000000 0.000000
L I 2	0.019950-0.046996	-0.046996-0.019950	0.000000 0.000000
S1	-0.073480-0.270016	-0.270016 0.073481	0.000000 0.000000
S2	0.073481 0.270016	0.270016-0.073481	0.000000 0.000000
O1	-0.166618-0.331411	-0.331411 0.166618	0.000000 0.000000
O5	0.166618 0.331411	0.331411-0.166618	0.000000 0.000000
O2	-0.013525-0.139626	-0.137902-0.006582	0.099101 0.149095
O6	0.013525 0.139627	0.137902 0.006582	0.099101 0.149095
O3	0.002302-0.147040	-0.130489 0.009245	0.079569-0.160372
O7	-0.002302 0.147040	0.130489-0.009245	0.079569-0.160371
O4	0.000809-0.129627	-0.147902 0.007751	-0.178670 0.011277
O8	-0.000808 0.129626	0.147902-0.007752	-0.178670 0.011277

NY = 3.87 THZ

K1	0.500000 0.000002	0.000001-0.500000	0.000000 0.000000
K2	-0.500000-0.000001	-0.000001 0.500000	0.000000 0.000000
L I 1	-0.068980 0.027313	0.027313 0.068980	0.000000 0.000000
L I 2	0.068980-0.027313	-0.027313-0.068980	0.000000 0.000000
S1	0.112219 0.128720	0.128720-0.112219	0.000000 0.000000
S2	-0.112219-0.128720	-0.128720 0.112219	0.000000 0.000000
O1	0.118825 0.371142	0.371142-0.118826	0.000000 0.000000
O5	-0.118826-0.371142	-0.371142 0.118826	0.000000 0.000000
O2	0.054116-0.001647	-0.006149-0.056078	-0.065637-0.260113
O6	-0.054116 0.001647	0.006149 0.056078	-0.065637-0.260113
O3	0.053638-0.005873	-0.001923-0.056556	-0.192446 0.186901
O7	-0.053638 0.005873	0.001923 0.056556	-0.192446 0.186900
O4	0.057537-0.004174	-0.003622-0.052657	0.258084 0.073213
O8	-0.057537 0.004174	0.003622 0.052657	0.258083 0.073213

NY = 8.49 THZ

```
K1        0.031930 0.006998     0.006998-0.031930     0.000000 0.000000
K2       -0.031930-0.006998    -0.006998 0.031930     0.000000 0.000000
L11       0.500000 0.000002     0.000001-0.500000     0.000000 0.000000
L12      -0.500000-0.000001    -0.000001 0.500000     0.000000 0.000000
S1        0.031846-0.005456    -0.005456-0.031846     0.000000 0.000000
S2       -0.031846 0.005456     0.005456 0.031846     0.000000 0.000000
O1        0.041671 0.016380     0.016380-0.041671     0.000000 0.000000
O5       -0.041671-0.016380    -0.016380 0.041671     0.000000 0.000000
O2        0.049434-0.008624     0.006697-0.031731     0.068961-0.012228
O6       -0.049435 0.008624    -0.006697 0.031731     0.068961-0.012228
O3        0.042791 0.010532    -0.012460-0.038375    -0.045071-0.053608
O7       -0.042791-0.010532     0.012460 0.038375    -0.045071-0.053608
O4        0.029523-0.004799     0.002872-0.051643    -0.023890 0.065836
O8       -0.029523 0.004800    -0.002872 0.051643    -0.023890 0.065836
```

NY = 12.45 THZ

```
K1        0.010330-0.022191    -0.022191-0.010330     0.000000 0.000000
K2       -0.010330 0.022191     0.022191 0.010330     0.000000 0.000000
L11      -0.011151 0.083513     0.083513 0.011151     0.000000 0.000000
L12       0.011151-0.083513    -0.083513-0.011151     0.000000 0.000000
S1       -0.016283-0.013643    -0.013643 0.016283     0.000000 0.000000
S2        0.016283 0.013643     0.013643-0.016283     0.000000 0.000000
O1       -0.005459-0.364821    -0.364821 0.005459     0.000000 0.000000
O5        0.005459 0.364821     0.364821-0.005459     0.000000 0.000000
O2        0.003723-0.123515     0.408248 0.000002    -0.002341-0.344324
O6       -0.003723 0.123516    -0.408249-0.000001    -0.002342-0.344324
O3        0.231190 0.276920     0.007813 0.227469    -0.297023 0.174191
O7       -0.231189-0.276920    -0.007812-0.227469    -0.297023 0.174190
O4       -0.229331 0.273695     0.011038-0.233052     0.299365 0.170134
O8        0.229330-0.273695    -0.011037 0.233053     0.299365 0.170133
```

NY = 14.46 THZ

```
K1       -0.001355-0.011669    -0.011669 0.001355     0.000000 0.000000
K2        0.001355 0.011669     0.011669-0.001355     0.000000 0.000000
L11       0.052981-0.017850    -0.017850-0.052981     0.000000 0.000000
L12      -0.052981 0.017850     0.017850 0.052981     0.000000 0.000000
S1        0.500000 0.000002     0.000001-0.500000     0.000000 0.000000
S2       -0.500000-0.000001    -0.000001 0.500000     0.000000 0.000000
O1       -0.410661-0.030819    -0.030818 0.410661     0.000000 0.000000
O5        0.410661 0.030818     0.030818-0.410661     0.000000 0.000000
O2        0.170757 0.015282    -0.015506 0.354514    -0.196832-0.013891
O6       -0.170757-0.015281     0.015505-0.354515    -0.196832-0.013891
O3       -0.236527 0.219641    -0.219864-0.052770     0.086386 0.177407
O7        0.236528-0.219640     0.219864 0.052771     0.086386 0.177407
O4       -0.209866-0.235258     0.235034-0.026108     0.110446-0.163516
O8        0.209866 0.235257    -0.235034 0.026109     0.110445-0.163516
```

NY = 34.43 THZ

```
K1       -0.001865-0.001400    -0.001400 0.001865     0.000000 0.000000
K2        0.001865 0.001400     0.001400-0.001865     0.000000 0.000000
L11       0.001926-0.002103    -0.002103-0.001926     0.000000 0.000000
L12      -0.001926 0.002103     0.002103 0.001926     0.000000 0.000000
S1       -0.368655 0.013119     0.013120 0.368655     0.000000 0.000000
S2        0.368655-0.013120    -0.013120-0.368655     0.000000 0.000000
O1       -0.034465-0.001089    -0.001089 0.034465     0.000000 0.000000
O5        0.034465 0.001089     0.001089-0.034465     0.000000 0.000000
O2        0.408248 0.000002    -0.014463 0.036449    -0.154802 0.000368
O6       -0.408249-0.000001     0.014463-0.036449    -0.154802 0.000369
O3        0.068463 0.181713    -0.196174-0.303337     0.077721 0.133878
O7       -0.068462-0.181712     0.196173 0.303337     0.077720 0.133878
O4        0.080989-0.203406     0.188945-0.290811     0.077082-0.134247
O8       -0.080988 0.203407    -0.188944 0.290811     0.077081-0.134247
```

NY = 1.62 THZ

```
K1        0.312381 0.115996    -0.115996 0.312381     0.000000 0.000000
K2       -0.312381-0.115996     0.115996-0.312381     0.000000 0.000000
L11       0.007921 0.181660    -0.181660 0.007921     0.000000 0.000000
L12      -0.007921-0.181660     0.181660-0.007921     0.000000 0.000000
S1        0.001378-0.374402     0.374402 0.001378     0.000000 0.000000
S2       -0.001378 0.374402    -0.374402-0.001377     0.000000 0.000000
O1        0.012885 0.117746    -0.117746 0.012885     0.000000 0.000000
O5       -0.012885-0.117746     0.117746-0.012886     0.000000 0.000000
O2        0.001898-0.404085     0.408249 0.000001    -0.014687-0.393994
O6       -0.001898 0.404085    -0.408249-0.000001    -0.014687-0.393994
O3        0.002277-0.408028     0.404303-0.000380     0.348552 0.184277
O7       -0.002277 0.408028    -0.404303 0.000380     0.348552 0.184278
O4       -0.001328-0.406385     0.405947 0.003227    -0.333865 0.209717
O8        0.001329 0.406385    -0.405946-0.003226    -0.333865 0.209717
```

NY = 2.92 THZ

```
K1        0.500000 0.000001    -0.000001 0.500000     0.000000 0.000000
K2       -0.500000-0.000001     0.000000-0.500000     0.000000 0.000000
L11      -0.019927-0.046996     0.046996-0.019927     0.000000 0.000000
L12       0.019927 0.046996    -0.046996 0.019927     0.000000 0.000000
S1       -0.073561 0.270015    -0.270015-0.073561     0.000000 0.000000
S2        0.073561-0.270015     0.270016 0.073560     0.000000 0.000000
O1       -0.166678 0.331422    -0.331422-0.166678     0.000000 0.000000
O5        0.166678-0.331422     0.331423 0.166678     0.000000 0.000000
O2       -0.013578 0.139622    -0.137898 0.006528     0.099109-0.149105
O6        0.013578-0.139622     0.137898-0.006528     0.099109-0.149105
O3        0.002248 0.147035    -0.130485-0.009298     0.079575 0.160384
O7       -0.002248-0.147035     0.130485 0.009298     0.079574 0.160384
O4        0.000755 0.129623    -0.147898-0.007805    -0.178684-0.011278
O8       -0.000755-0.129623     0.147897 0.007805    -0.178684-0.011278
```

NY = 3.87 THZ

K1	0.500000 0.000001	-0.000001 0.500000	0.000000 0.000000
K2	-0.500000-0.000001	0.000000-0.500000	0.000000 0.000000
LI1	-0.068976-0.027311	0.027311-0.068976	0.000000 0.000000
LI2	0.068976 0.027311	-0.027310 0.068976	0.000000 0.000000
S1	0.112227-0.128693	0.128693 0.112227	0.000000 0.000000
S2	-0.112227 0.128693	-0.128693-0.112226	0.000000 0.000000
O1	0.118845-0.371075	0.371075 0.118845	0.000000 0.000000
O5	-0.118845 0.371075	-0.371075-0.118844	0.000000 0.000000
O2	0.054116 0.001647	-0.006151 0.056080	-0.065653 0.260062
O6	-0.054116-0.001647	0.006151-0.056080	-0.065653 0.260062
O3	0.053639 0.005875	-0.001922 0.056557	-0.192394-0.186887
O7	-0.053639-0.005875	0.001922-0.056557	-0.192394-0.186888
O4	0.057539 0.004174	-0.003623 0.052657	0.258047-0.073174
O8	-0.057539-0.004174	0.003623-0.052657	0.258047-0.073174

NY = 8.49 THZ

K1	0.031930-0.006999	0.006999 0.031930	0.000000 0.000000
K2	-0.031930 0.006999	-0.006999-0.031930	0.000000 0.000000
LI1	0.500000 0.000001	-0.000001 0.500000	0.000000 0.000000
LI2	-0.500000-0.000001	0.000000-0.500000	0.000000 0.000000
S1	0.031848 0.005456	-0.005456 0.031848	0.000000 0.000000
S2	-0.031848-0.005456	0.005456-0.031848	0.000000 0.000000
O1	0.041673-0.016378	0.016378 0.041673	0.000000 0.000000
O5	-0.041673 0.016378	-0.016378-0.041673	0.000000 0.000000
O2	0.049436 0.008624	0.006696 0.031731	0.068962 0.012229
O6	-0.049436-0.008624	-0.006696-0.031731	0.068962 0.012229
O3	0.042791-0.010533	-0.012460 0.038376	-0.045071 0.053608
O7	-0.042791 0.010533	0.012460-0.038376	-0.045072 0.053608
O4	0.029523 0.004800	0.002872 0.051643	-0.023890-0.065837
O8	-0.029523-0.004800	-0.002873-0.051643	-0.023890-0.065837

NY = 12.45 THZ

K1	0.010331 0.022190	-0.022190 0.010331	0.000000 0.000000
K2	-0.010331-0.022190	0.022190-0.010331	0.000000 0.000000
LI1	-0.011151-0.083516	0.083516-0.011151	0.000000 0.000000
LI2	0.011151 0.083516	-0.083516 0.011151	0.000000 0.000000
S1	-0.016278 0.013643	-0.013643-0.016278	0.000000 0.000000
S2	0.016278-0.013643	0.013643 0.016278	0.000000 0.000000
O1	-0.005462 0.364818	-0.364818-0.005462	0.000000 0.000000
O5	0.005462-0.364818	0.364819 0.005461	0.000000 0.000000
O2	0.003723 0.123516	0.408249 0.000001	-0.002349 0.344324
O6	-0.003723-0.123516	-0.408249-0.000001	-0.002349 0.344324
O3	0.231192-0.276919	0.007813-0.227469	-0.297020-0.174195
O7	-0.231192 0.276919	-0.007813 0.227469	-0.297020-0.174196
O4	-0.229329-0.273695	0.011037 0.233053	0.299368-0.170129
O8	0.229330 0.273695	-0.011037-0.233053	0.299368-0.170129

NY = 14.46 THZ

K1	-0.001354 0.011668	-0.011668-0.001354	0.000000 0.000000
K2	0.001354-0.011668	0.011668 0.001354	0.000000 0.000000
LI1	0.052981 0.017848	-0.017848 0.052981	0.000000 0.000000
LI2	-0.052981-0.017848	0.017848-0.052981	0.000000 0.000000
S1	0.500000 0.000001	-0.000001 0.500000	0.000000 0.000000
S2	-0.500000-0.000001	0.000000-0.500000	0.000000 0.000000
O1	-0.410664 0.030815	-0.030815-0.410664	0.000000 0.000000
O5	0.410664-0.030815	0.030816 0.410663	0.000000 0.000000
O2	0.170756-0.015282	-0.015507-0.354515	-0.196832 0.013886
O6	-0.170756 0.015282	0.015507 0.354515	-0.196832 0.013886
O3	-0.236529-0.219639	-0.219864 0.052771	0.086390-0.177405
O7	0.236529 0.219639	0.219864-0.052771	0.086390-0.177405
O4	-0.209864 0.235258	0.235033 0.026106	0.110442 0.163519
O8	0.209864-0.235259	-0.235034-0.026105	0.110442 0.163519

NY = 34.43 THZ

K1	-0.001865 0.001400	-0.001400-0.001865	0.000000 0.000000
K2	0.001865-0.001400	0.001400 0.001865	0.000000 0.000000
LI1	0.001926 0.002102	-0.002102 0.001926	0.000000 0.000000
LI2	-0.001926-0.002102	0.002102-0.001926	0.000000 0.000000
S1	-0.368654-0.013122	0.013122-0.368654	0.000000 0.000000
S2	0.368654 0.013122	-0.013121 0.368654	0.000000 0.000000
O1	-0.034465 0.001089	-0.001089-0.034465	0.000000 0.000000
O5	0.034465-0.001089	0.001089 0.034465	0.000000 0.000000
O2	0.408249 0.000001	-0.014463-0.036449	-0.154802-0.000370
O6	-0.408249-0.000001	0.014463 0.036449	-0.154802-0.000370
O3	0.068463-0.181713	-0.196175 0.303336	0.077721-0.133878
O7	-0.068463 0.181713	0.196175-0.303336	0.077721-0.133878
O4	0.080988 0.203407	0.188943 0.290812	0.077081 0.134248
O8	-0.080988-0.203407	-0.188944-0.290811	0.077081 0.134248

EIGENVALUES AND EIGENVECTORS FOR IRM 4

NY = 4.06 THZ

K1	0.000000 0.000000	0.000000 0.000000	-0.324204-0.000004
K2	0.000000 0.000000	0.000000 0.000000	0.324204 0.000003
LI1	0.000000 0.000000	0.000000 0.000000	-0.090890-0.000001
LI2	0.000000 0.000000	0.000000 0.000000	0.090890 0.000001
S1	0.000000 0.000000	0.000000 0.000000	-0.273393-0.000003
S2	0.000000 0.000000	0.000000 0.000000	0.273393 0.000003
O1	0.000000 0.000000	0.000000 0.000000	-0.175521-0.000002
O5	0.000000 0.000000	0.000000 0.000000	0.175521 0.000002
O2	0.024063 0.000000	0.408249 0.000006	-0.151388-0.000002
O6	0.024063 0.000000	0.408249 0.000004	0.151388 0.000000
O3	-0.365586-0.000003	-0.183284-0.000002	-0.151388-0.000001
O7	-0.365586-0.000005	-0.183284-0.000003	0.151388 0.000002
O4	0.341522 0.000004	-0.224963-0.000002	-0.151388-0.000002
O8	0.341522 0.000003	-0.224963-0.000002	0.151388 0.000001

NY = 4.61 THZ

K1	0.000000 0.000000	0.000000 0.000000	-0.351115-0.000004
K2	0.000000 0.000000	0.000000 0.000000	0.351115 0.000003
LI1	0.000000 0.000000	0.000000 0.000000	-0.019781 0.000000
LI2	0.000000 0.000000	0.000000 0.000000	0.019781 0.000000
S1	0.000000 0.000000	0.000000 0.000000	0.669500 0.000009
S2	0.000000 0.000000	0.000000 0.000000	-0.669500-0.000007
01	0.000000 0.000000	0.000000 0.000000	0.442958 0.000006
05	0.000000 0.000000	0.000000 0.000000	-0.442958-0.000004
02	0.000103 0.000000	0.269900 0.000004	0.408248 0.000006
06	0.000103 0.000000	0.269900 0.000003	-0.408248-0.000004
03	-0.233792-0.000002	-0.134861-0.000001	0.408248 0.000004
07	-0.233792-0.000003	-0.134861-0.000002	-0.408248-0.000006
04	0.233689 0.000003	-0.135039-0.000001	0.408248 0.000005
08	0.233689 0.000002	-0.135039-0.000001	-0.408248-0.000003

NY = 6.18 THZ

K1	0.000000 0.000000	0.000000 0.000000	0.707106 0.000009
K2	0.000000 0.000000	0.000000 0.000000	-0.707106-0.000007
LI1	0.000000 0.000000	0.000000 0.000000	0.041870 0.000001
LI2	0.000000 0.000000	0.000000 0.000000	-0.041870 0.000000
S1	0.000000 0.000000	0.000000 0.000000	0.044655 0.000001
S2	0.000000 0.000000	0.000000 0.000000	-0.044655 0.000000
01	0.000000 0.000000	0.000000 0.000000	0.014211 0.000000
05	0.000000 0.000000	0.000000 0.000000	-0.014211 0.000000
02	0.007610 0.000000	0.213874 0.000003	0.032444 0.000000
06	0.007610 0.000000	0.213874 0.000002	-0.032444 0.000000
03	-0.189025-0.000002	-0.100346-0.000001	0.032444 0.000000
07	-0.189025-0.000003	-0.100346-0.000001	-0.032444 0.000000
04	0.181415 0.000002	-0.113527-0.000001	0.032444 0.000000
08	0.181415 0.000002	-0.113527-0.000001	-0.032444 0.000000

NY = 8.73 THZ

K1	0.000000 0.000000	0.000000 0.000000	-0.062247-0.000001
K2	0.000000 0.000000	0.000000 0.000000	0.062247 0.000001
LI1	0.000000 0.000000	0.000000 0.000000	0.707107 0.000009
LI2	0.000000 0.000000	0.000000 0.000000	-0.707107-0.000007
S1	0.000000 0.000000	0.000000 0.000000	0.071661 0.000001
S2	0.000000 0.000000	0.000000 0.000000	-0.071661-0.000001
01	0.000000 0.000000	0.000000 0.000000	0.045779 0.000001
05	0.000000 0.000000	0.000000 0.000000	-0.045779 0.000000
02	-0.032222 0.000000	0.030044 0.000000	-0.082009-0.000001
06	-0.032222 0.000000	0.030044 0.000000	0.082009 0.000001
03	-0.009908 0.000000	-0.042927 0.000000	-0.082009-0.000001
07	-0.009908 0.000000	-0.042927-0.000001	0.082009 0.000001
04	0.042129 0.000000	0.012883 0.000000	-0.082009-0.000001
08	0.042129 0.000000	0.012883 0.000000	0.082009 0.000001

NY = 15.57 THZ

K1	0.000000 0.000000	0.000000 0.000000	-0.025268 0.000000
K2	0.000000 0.000000	0.000000 0.000000	0.025268 0.000000
LI1	0.000000 0.000000	0.000000 0.000000	0.249578 0.000003
LI2	0.000000 0.000000	0.000000 0.000000	-0.249578-0.000002
S1	0.000000 0.000000	0.000000 0.000000	-0.558659-0.000007
S2	0.000000 0.000000	0.000000 0.000000	0.558659 0.000006
01	0.000000 0.000000	0.000000 0.000000	-0.267080-0.000003
05	0.000000 0.000000	0.000000 0.000000	0.267080 0.000003
02	0.248794 0.000004	-0.014426 0.000000	0.408248 0.000006
06	0.248794 0.000002	-0.014426 0.000000	-0.408248-0.000004
03	-0.111903-0.000001	0.222675 0.000002	0.408248 0.000004
07	-0.111903-0.000002	0.222675 0.000003	-0.408248-0.000006
04	-0.136890-0.000001	-0.208249-0.000002	0.408248 0.000005
08	-0.136890-0.000001	-0.208249-0.000002	-0.408248-0.000003

NY = 34.07 THZ

K1	0.000000 0.000000	0.000000 0.000000	0.014242 0.000000
K2	0.000000 0.000000	0.000000 0.000000	-0.014242 0.000000
LI1	0.000000 0.000000	0.000000 0.000000	-0.011563 0.000000
LI2	0.000000 0.000000	0.000000 0.000000	0.011563 0.000000
S1	0.000000 0.000000	0.000000 0.000000	-0.446730-0.000006
S2	0.000000 0.000000	0.000000 0.000000	0.446730 0.000004
01	0.000000 0.000000	0.000000 0.000000	0.707107 0.000009
05	0.000000 0.000000	0.000000 0.000000	-0.707107-0.000007
02	-0.059695-0.000001	0.004190 0.000000	-0.010398 0.000000
06	-0.059695-0.000001	0.004190 0.000000	0.010398 0.000000
03	0.026218 0.000000	-0.053792 0.000000	-0.010398 0.000000
07	0.026218 0.000000	-0.053792-0.000001	0.010398 0.000000
04	0.033476 0.000000	0.049602 0.000001	-0.010398 0.000000
08	0.033476 0.000000	0.049602 0.000000	0.010398 0.000000

NY = 34.72 THZ

K1	0.000000 0.000000	0.000000 0.000000	0.006885 0.000000
K2	0.000000 0.000000	0.000000 0.000000	-0.006885 0.000000
LI1	0.000000 0.000000	0.000000 0.000000	-0.016717 0.000000
LI2	0.000000 0.000000	0.000000 0.000000	0.016717 0.000000
S1	0.000000 0.000000	0.000000 0.000000	0.146562 0.000002
S2	0.000000 0.000000	0.000000 0.000000	-0.146562-0.000001
01	0.000000 0.000000	0.000000 0.000000	0.189770 0.000002
05	0.000000 0.000000	0.000000 0.000000	-0.189770-0.000002
02	0.408249 0.000006	-0.014565 0.000000	-0.137523-0.000002
06	0.408249 0.000004	-0.014565 0.000000	0.137523 0.000001
03	-0.191510-0.000002	0.360836 0.000003	-0.137523-0.000001
07	-0.191510-0.000003	0.360836 0.000005	0.137523 0.000002
04	-0.216738-0.000002	-0.346271-0.000004	-0.137523-0.000002
08	-0.216738-0.000002	-0.346271-0.000003	0.137523 0.000001

A.5   HIST

INPUT

```
6.5
  1   -4    2   -3    5   -6    0
  0
  3
```

OUTPUT

The heading is the same as for **MODEL1**.

```
FREQUENCY (THZ)
                    0.0    0.8    1.6    2.4    3.2    4.0    4.8    5.6    6.4    7.2    8.0
( 0.00 0.00 0.00)

( 0.00 0.00 0.10)

( 0.00 0.00 0.20)
IMR  1
( 0.00 0.00 0.30)

( 0.00 0.00 0.40)

( 0.00 0.00 0.50)

( 0.00 0.00 0.40)

( 0.00 0.00 0.30)
IMR  4
( 0.00 0.00 0.20)

( 0.00 0.00 0.10)

( 0.00 0.00 0.00)

( 0.00 0.00 0.10)

( 0.00 0.00 0.20)
IMR  2
( 0.00 0.00 0.30)

( 0.00 0.00 0.40)

( 0.00 0.00 0.50)

( 0.00 0.00 0.40)

( 0.00 0.00 0.30)
IMR  3
( 0.00 0.00 0.20)

( 0.00 0.00 0.10)

( 0.00 0.00 0.00)

( 0.00 0.00 0.10)

( 0.00 0.00 0.20)
IMR  5
( 0.00 0.00 0.30)

( 0.00 0.00 0.40)

( 0.00 0.00 0.50)

( 0.00 0.00 0.40)

( 0.00 0.00 0.30)
IMR  6
( 0.00 0.00 0.20)

( 0.00 0.00 0.10)

( 0.00 0.00 0.00)
                    0.0    0.8    1.6    2.4    3.2    4.0    4.8    5.6    6.4    7.2    8.0
                                        FREQUENCY (THZ)
```

Appendix A. Example for the Application of UNISOFT 93

A.6 SF

INPUT

```
        0    3    0    3    0    3
   5.0
   0.35       -0.18     0.31      0.577     0.577
          1   0.0174    0.000     0.000     0.0174    0.000     0.0174
          3   0.0201    0.000     0.000     0.0201    0.000     0.0201
          5   0.0084    0.000     0.000     0.0084    0.000     0.0084
          7   0.0218    0.000     0.000     0.0218    0.000     0.0218
          9   0.00142   0.00101   0.00097   0.00205  -0.0022    0.00507
   298.
   1000.
          1   0    0    0    0    0    0    0    0    0
```

OUTPUT

```
------------------------------------------------------------------------------------------------------
LATTICE DYNAMICAL MODEL-CALCULATION FOR THE FOLLOWING STRUCTURE:

POSITION VECTOR SPACE LATTICE VECTORS
A 1 = (   5.14200,   0.00000,   0.00000)
A 2 = (  -2.57100,   4.45300,   0.00000)
A 3 = (   0.00000,   0.00000,   8.62400)

RECIPROCAL SPACE LATTICE VECTORS
AI 1 = (  0.19448,   0.11228,   0.00000)
AI 2 = (  0.00000,   0.22457,   0.00000)
AI 3 = (  0.00000,   0.00000,   0.11595)
```

14 PARTICLES PER UNIT CELL	POSITION			MASS	SCATT. LENGTH	TENSOR OF TEMP.FACTORS		
K1	(0.00000,	2.96874,	0.00000)	39.10	0.35	0.01740	0.00000	0.00000
						0.00000	0.01740	0.00000
						0.00000	0.00000	0.01740
K2	(0.00000,	0.00000,	4.31200)	39.10	0.35	0.01740	0.00000	0.00000
						0.00000	0.01740	0.00000
						0.00000	0.00000	0.01740
LI1	(0.00000,	2.96874,	5.88200)	6.94	-0.18	0.02010	0.00000	0.00000
						0.00000	0.02010	0.00000
						0.00000	0.00000	0.02010
LI2	(2.57100,	1.48437,	1.57000)	6.94	-0.18	0.02010	0.00000	0.00000
						0.00000	0.02010	0.00000
						0.00000	0.00000	0.02010
S1	(0.00000,	2.96874,	2.53500)	32.06	0.31	0.00840	0.00000	0.00000
						0.00000	0.00840	0.00000
						0.00000	0.00000	0.00840
S2	(2.57100,	1.48437,	6.84700)	32.06	0.31	0.00840	0.00000	0.00000
						0.00000	0.00840	0.00000
						0.00000	0.00000	0.00840
O1	(0.00000,	2.96870,	3.96700)	16.00	0.58	0.02180	0.00000	0.00000
						0.00000	0.02180	0.00000
						0.00000	0.00000	0.02180
O5	(2.57100,	1.48440,	8.27900)	16.00	0.58	0.02180	0.00000	0.00000
						0.00000	0.02180	0.00000
						0.00000	0.00000	0.02180
O2	(1.39090,	2.92570,	2.06110)	16.00	0.58	0.00142	0.00101	0.00097
						0.00101	0.00205	-0.00220
						0.00097	-0.00220	0.00507
O6	(1.18010,	1.52740,	6.37310)	16.00	0.58	0.00142	0.00101	-0.00097
						0.00101	0.00205	0.00220
						-0.00097	0.00220	0.00507
O3	(4.48380,	4.19480,	2.06110)	16.00	0.58	0.00102	-0.00078	-0.00239
						-0.00078	0.00245	0.00026
						-0.00239	0.00026	0.00507
O7	(3.22920,	0.25830,	6.37310)	16.00	0.58	0.00102	-0.00078	0.00239
						-0.00078	0.00245	-0.00026
						0.00239	-0.00026	0.00507
O4	(4.40930,	1.78570,	2.06110)	16.00	0.58	0.00277	-0.00023	0.00142
						-0.00023	0.00070	0.00194
						0.00142	0.00194	0.00507
O8	(3.30370,	2.66740,	6.37310)	16.00	0.58	0.00277	-0.00023	-0.00142
						-0.00023	0.00070	-0.00194
						-0.00142	-0.00194	0.00507

```
----------------------------------------------------------------------------------------------------
MODEL SPECIFICATIONS :
      INTERACTION          TYPE        NEIGHBOR    PARAMETER-NO.S

        K1  - K1      COULOMB (M-M)      **        Z1   =   1   Z2   =   1
                                           •
                                           •
                                           •
```

```
********* Q  = ( 0.00, 0.00, 0.00) 1/A  ********** QHKL  = ( 0.00, 0.00, 0.00)  **********
```

```
H  K  L  IMR          STRUCTURE-FACTORS FOR THE MODES
                  (                                                    )
          1  0.00  4.59   6.14   9.76  15.30  34.15  34.74
          2  0.00  2.06   4.23   8.60  12.63  14.38  34.43
          2  0.00  2.06   4.23   8.60  12.63  14.38  34.43
          3  1.62  2.92   3.87   8.49  12.45  14.46  34.43
          3  1.62  2.92   3.87   8.49  12.45  14.46  34.43
          4  4.06  4.61   6.18   8.73  15.57  34.07  34.72
```

```
0  0  1      0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
            18.  122.    4.    0.   58.   18.    7.

0  0  2    100.    2.   45.   37.  356.   96.   77.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.

0  0  3      0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
             0.    0.    0.    0.    0.    0.    0.
            67.  546.   25.   44.  665.  286.   94.

0  1  0      0.   26.    4.    0.    6.    1.   17.
             3.    1.   21.    5.   24.   41.   22.
             3.    1.   21.    5.   24.   41.   22.
            19.   39.   26.    4.    8.   51.   16.
            19.   39.   26.    4.    8.   51.   16.
             8.    4.    2.    1.   25.    1.   65.

0  1  1     21.    8.    6.    2.    9.    2.   93.
            49.    4.    8.    6.   18.   91.   35.
            49.    0.    8.    6.  128.   10.    4.
            14.   10.   16.    5.    1.   78.   39.
             4.    1.   29.    2.  112.    3.    9.
            15.   22.   20.    1.    2.    2.   23.

0  1  2     21.   30.   17.    2.    7.   26.   28.
            12.   15.    5.    2.  185.   10.    4.
            12.   80.   11.    2.    2.   53.   53.
            70.    5.    9.   19.  225.   11.    4.
           150.   14.   47.   11.   50.   44.   54.
            20.    3.    1.   17.   20.   77.   89.

0  1  3     37.   15.    8.   18.   64.  265.   35.
             9.  322.   11.    5.   19.   24.   77.
             9.  245.   19.    7.  188.   10.   10.
           216.   45.   50.    4.    7.   44.   68.
           107.   27.   57.    0.  188.   33.    4.
            72.   25.    8.    6.   22.   77.   12.

0  2  0      0.  327.   49.    0.    1.    0.    4.
            30.   40.   35.    7.    2.   54.  119.
            30.   40.   35.    7.    2.   54.  119.
            22.   58.   79.   25.    4.  223.  285.
            22.   58.   79.   25.    4.  223.  285.
            89.   41.   25.    1.    7.    0.   17.

0  2  1      5.   94.    8.    6.   27.   20.    8.
            49.  120.   19.   37.   94.  116.  239.
            49.   83.   22.   29.  118.   74.  285.
           199.   54.   26.    3.   57.   35.   80.
             5.   47.   67.    6.   40.   28.  145.
           381.  125.   60.    4.   10.    5.    2.

0  2  2     12.  317.   90.    2.   20.   27.    1.
            29.  108.   85.    4.    8.   17.  169.
            29.   78.   51.    4.  248.   45.   42.
            17.  114.  121.   31.  132.   11.  272.
            37.   47.   38.   51.  374.   11.  173.
            66.  128.   28.   18.   34.   70.   10.

0  2  3     50.   73.   37.   36.   32.  161.   53.
            51.   42.   12.   28.  478.   81.  132.
            51.   72.   20.   26.   69.  274.  284.
           283.    5.  132.   20.  370.   55.   21.
            26.   44.  226.   20.   38.  137.  209.
           225.  160.  205.   17.   25.   57.    9.

0  3  0      0.   17.    7.    2.  204.   52.  611.
          1645.    8.   73.  180.   24.  335.    4.
          1645.    8.   73.  180.   24.  335.    4.
             2.    0.    0.    0.  269.  262.  186.
             2.    0.    0.    0.  269.  262.  186.
            91.   39.   25.    0.    1.    0.    3.

0  3  1      0.   89.   14.    0.    1.    0.    3.
             1.    2.    0.    0.  275.  249.  190.
             1.    4.    0.    0.  284.  231.  182.
           975.  232.  430.  119.  325.   99.    7.
           656.  829.   97.  101.  222.  166.   13.
            35.   44.   15.    3.  305.   49.  556.

0  3  2     25.   12.   44.   20.  413.  139.  570.
           132.  688.  200.   68.  594.   25.   20.
           132.  730.   64.   70.  685.  122.   25.
            21.    2.    4.    1.  274.  253.  178.
             4.    2.    6.    1.  274.  271.  193.
            90.   39.   24.    0.    1.    0.    3.
```

                                    .
                                    .
                                    .
                                    ▲

A.7   PARDER

INPUT

```
     0     0    0     0    0     0    0     0    0     0
    .01        .01        .01        .01        .01        .001       .001       .001
    .001       50.        5.0        1.0        5.0        1.0        10.0       1.0
   10.0        1.0
```

OUTPUT

The heading is the same as for **MODEL1**.

```
MESSAGE FOR Q = ( 0.00, 0.00, 0.00) 1/A :

***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO.  1 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO.  1 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO.  2 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO.  2 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  1 WITH RESPECT TO PARAMETER NO.  3 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO.  3 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO.  3 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO.  4 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO.  4 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO.  8 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO.  8 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 10 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 10 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 11 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 11 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 12 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 12 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 13 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 13 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 14 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 14 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 15 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 15 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 16 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 16 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 17 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 17 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO.  8 WITH RESPECT TO PARAMETER NO. 18 IS DERIVATIVE OF NY**2
***   PARTIAL-DERIVATIVE OF FREQUENCY NO. 15 WITH RESPECT TO PARAMETER NO. 18 IS DERIVATIVE OF NY**2
```

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------------------------------------------------------------------------------------------------
********* Q = ( 0.00, 0.00, 0.00) 1/A *********  QHKL = ( 0.00, 0.00, 0.00) **********
------------------------------------------------------------------------------------------------
```

THE FREQUENCY-SHIFTS ARE CALCULATED WITH RESPECT TO THE FOLLOWING PARAMETER-VARIATIONS:

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0.010	0.010	0.010	0.010	0.010	0.001	0.001	0.001	0.001	50.000	5.000	1.000	5.000	1.000	10.000

16	17	18
1.000	10.000	1.000

PARTIAL DERIVATIVES IN THZ/DP FOR IRM 1

NY =	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0.00 THz	0.014 0.011 0.014 0.013		0.018	0.016	0.017	0.015	0.013	0.015	0.014	0.015	0.008	0.012	0.014	0.014	0.009
4.59 THz	-0.007	-0.018	0.044 0.104	0.005	-0.072	0.024	0.053	0.004	0.073	0.053		0.103		0.310	
6.14 THz		-0.032	-0.010 0.014	-0.024	-0.035	0.090	0.039	0.015	0.113	0.112		0.012		0.033	
9.76 THz	-0.008	-0.007	-0.013 0.005	0.024	-0.076	0.003	0.231	0.241	-0.006	0.144	0.002		0.004		0.003
15.30 THz	0.003	0.026	0.071 0.116	0.010	-0.168	0.022	-0.011		0.011	0.016	0.146	0.063	0.155		0.005
34.15 THz	0.004	-0.007 0.044	-0.036 0.008	0.056			0.028	0.025		0.015	0.100	0.021	0.018		0.309
34.74 THz		-0.003 0.168	-0.019	-0.004	0.004	0.002	0.012	0.003	0.011	0.009	0.138		0.205		0.012

PARTIAL DERIVATIVES IN THZ/DP FOR IRM 2

(2-FOLD DEGENERATE)

NY =	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0.00 THz				0.013		0.006		0.005							
2.06 THz	0.154	0.118	0.266 0.287	-0.017	0.141	0.190	-0.054	0.033	0.103	0.156		1.070		0.691	
4.23 THz	-0.014 0.004	0.012	0.016 0.005	0.026	0.019	0.122		0.073	0.048	0.120		0.024		0.013	
8.60 THz	0.006		0.007	-0.013	0.039		0.202	-0.028	0.230	0.113					
12.63 THz	-0.004 0.017	0.003	0.046 0.070	-0.011	-0.052	0.034	0.021	0.009	0.047	0.046	0.182	0.131	0.248	0.125	
14.38 THz	-0.002 0.078	0.024	0.097 0.110	-0.083	-0.108	0.025	0.024	0.009	0.040	0.038	0.267	0.024	0.187	0.066	
34.43 THz	0.003	0.385	-0.037 0.005	-0.006	0.070	0.003	0.009		0.012	0.008	0.062	0.006	0.061	0.018	

PARTIAL DERIVATIVES IN THZ/DP FOR IRM 3
(2-FOLD DEGENERATE)

NY =	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1.62 THz	0.036 0.172	0.124	0.325 0.344	-0.011	0.127	0.114	-0.034	0.054	0.026	0.103		1.240		0.821	
2.92 THz	-0.008 0.021	0.041	0.045 0.041		0.018	0.093	-0.015	0.031	0.047	0.086		0.155		0.094	
3.87 THz	-0.029 0.039	0.039	0.070 0.067	0.011	0.045	0.200	-0.018	0.085	0.096	0.184	0.002	0.265		0.159	
8.49 THz	0.006	-0.003	0.008	-0.010	0.038	0.002	0.200	-0.022	0.224	0.114	0.004			0.005	
12.45 THz	-0.004 0.019		0.048 0.070	-0.010	-0.037	0.038	0.038	0.006	0.069	0.058	0.202	0.137	0.242	0.130	
14.46 THz	-0.003 0.077	0.005 0.023	0.098 0.111	-0.084	-0.111	0.026	0.018	0.008	0.036	0.036	0.249	0.026	0.204	0.064	
34.43 THz	0.003	0.386	-0.037 0.005	-0.006	0.070	0.003	0.009		0.012	0.008	0.062	0.006	0.061	0.018	

PARTIAL DERIVATIVES IN THZ/DP FOR IRM 4

NY =	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
4.06 THz	0.008		0.045 0.118		-0.107	-0.005	0.024	-0.004	0.023	0.013		0.117		0.351	
4.61 THz	0.010	-0.029	0.011 0.047	-0.004	-0.073	0.043	0.141	0.077	0.107	0.125		0.045		0.135	
6.18 THz		-0.016	0.021	-0.014	-0.009	0.098	0.019	-0.004	0.121	0.105		0.021		0.063	
8.73 THz	-0.011	-0.021	-0.009 0.006	0.020	-0.066		0.191	0.196	-0.003	0.117	0.011	0.004	0.005		
15.57 THz		0.033	0.078 0.129	0.011	-0.196	0.014	0.026	0.043	-0.003	0.031	0.145	0.066	0.170		0.010
34.07 THz	0.004	-0.007 0.020	-0.034 0.006	0.053	-0.004		0.025	0.023		0.013	0.124	0.019	0.005		0.291
34.72 THz		-0.003 0.177	-0.018	-0.004	0.007	0.002	0.011	0.002	0.011	0.009	0.105		0.205		0.002

```
------------------------------------------------------------------------------------------------
                                            .
                                            .
                                            .
```

A.8   ROTINV

INPUT

```
.02
     0     0     0     0     0     1     0     0     0     1
  39.10      6.940      32.06      16.00      16.00
     1
     5     7     1
    15    16
     5     9     1
    17    18
     7     9     1
    11    12
     9    11     1
    13    14
     0
     2
     6     7     7     8     9    10
     1     8     1
     1     9     1
     1    10     1
     3     7     1
     3    10     1
     0
     5
     7.
     1     2     3     4     5
     0
  1.20       0.400      1.35      -0.850     -0.700     0.1970     0.086      0.106
  0.100      2000.      125.0     -0.50      125.      -0.30      800.0     -53.80
  870.       -38.60
  1.10       0.500      1.35      -0.850     -0.700     0.1970     0.086      0.106
  0.100      2000.      125.0     -0.50      125.      -0.30      800.0     -53.80
  870.       -38.60
```

OUTPUT

NEW PARAMETERVECTOR :

```
      1.200       0.400       1.350      -0.850      -0.700       0.197       0.086
      0.106       0.100    2000.000     125.000      -0.500     125.000      -0.300
    800.000     -53.800     870.000     -38.600
```

ATOM	AXIS OF ROTATION	FORCE IN 10**-10 N		
K1	1	(0.000	-0.072	0.002)
	2	(0.069	0.000	0.001)
	3	(-0.007	-0.001	0.000)
K2	1	(0.000	-0.072	-0.003)
	2	(0.069	-0.001	0.000)
	3	(0.006	0.000	0.000)
LI1	1	(0.002	-0.101	0.001)
	2	(0.100	-0.002	-0.001)
	3	(0.003	0.004	0.000)
LI2	1	(-0.001	-0.101	-0.002)
	2	(0.102	0.001	0.001)
	3	(-0.002	-0.004	0.000)
S1	1	(0.001	0.177	0.006)
	2	(-0.176	-0.003	0.008)
	3	(0.006	-0.046	0.002)
S2	1	(-0.005	0.180	-0.005)
	2	(-0.175	0.004	-0.012)
	3	(-0.007	0.042	0.002)
O1	1	(-0.003	0.195	0.001)
	2	(-0.193	0.001	0.011)
	3	(-0.007	-0.005	0.002)
O5	1	(0.001	0.194	-0.001)
	2	(-0.194	-0.003	-0.012)
	3	(0.005	0.005	0.002)

```
O2    1    ( -0.001  -0.061   0.032)
      2    (  0.082   0.000  -0.084)
      3    ( -0.020   0.117   0.002)

O6    1    ( -0.001  -0.066  -0.028)
      2    (  0.088   0.000   0.083)
      3    (  0.020  -0.117   0.001)

O3    1    (  0.003  -0.074   0.038)
      2    (  0.062   0.009   0.057)
      3    ( -0.047  -0.059  -0.012)

O7    1    (  0.007  -0.064  -0.041)
      2    (  0.055   0.006  -0.055)
      3    (  0.050   0.062  -0.013)

O4    1    ( -0.004  -0.065  -0.072)
      2    (  0.052  -0.004   0.002)
      3    (  0.073  -0.003   0.008)

O8    1    (  0.001  -0.069   0.072)
      2    (  0.059  -0.009   0.001)
      3    ( -0.072   0.004   0.008)
```

NEW PARAMETERVECTOR :

```
1.100     0.500     1.350    -0.850    -0.700    0.197     0.086
0.106     0.100   2000.000   125.000   -0.500  125.000    -0.300
800.000  -53.800   870.000   -38.600
```

ATOM	AXIS OF ROTATION	FORCE IN 10**-10 N		

```
K1    1    (  0.000   0.886   0.002)
      2    ( -0.889   0.000   0.001)
      3    ( -0.008  -0.001   0.000)

K2    1    (  0.000   0.885  -0.002)
      2    ( -0.888   0.000   0.000)
      3    (  0.006   0.000   0.000)

LI1   1    (  0.002   1.041   0.001)
      2    ( -1.043  -0.002  -0.001)
      3    (  0.003   0.005   0.000)

LI2   1    ( -0.001   1.042  -0.002)
      2    ( -1.040   0.001   0.002)
      3    ( -0.002  -0.004   0.000)

S1    1    (  0.001  -0.663   0.006)
      2    (  0.663  -0.002   0.009)
      3    (  0.006  -0.046   0.001)

S2    1    ( -0.005  -0.660  -0.004)
      2    (  0.664   0.003  -0.012)
      3    ( -0.008   0.043   0.001)

O1    1    ( -0.003  -3.246   0.002)
      2    (  3.249   0.001   0.011)
      3    ( -0.007  -0.005   0.002)

O5    1    (  0.001  -3.247  -0.001)
      2    (  3.248  -0.003  -0.013)
      3    (  0.005   0.005   0.002)

O2    1    ( -0.001   0.666  -2.898)
      2    ( -0.645   0.000  -1.238)
      3    (  2.909   1.271   0.001)

O6    1    ( -0.001   0.661   2.901)
      2    ( -0.639   0.000   1.237)
      3    ( -2.908  -1.270   0.001)

O3    1    (  0.003   0.653   2.503)
      2    ( -0.666   0.008  -1.903)
      3    ( -2.510   1.901  -0.012)

O7    1    (  0.007   0.662  -2.506)
      2    ( -0.672   0.006   1.905)
      3    (  2.513  -1.898  -0.013)

O4    1    ( -0.004   0.662   0.392)
      2    ( -0.674  -0.004   3.115)
      3    ( -0.393  -3.116   0.008)

O8    1    (  0.000   0.658  -0.393)
      2    ( -0.667  -0.008  -3.113)
      3    (  0.394   3.117   0.008)
```

A.9 EFG

INPUT

```
        1    0    0    0    0    0    0    0    0    0
      1.2       0.4       1.35      -0.85      -0.70
      7.0
```

OUTPUT

```
FORCES DUE TO INTERACTION BETWEEN EACH OF THE SUBLATTICES OF UNIT CHARGES IN 10**-10 N

      *  K1      LI1     S1      O1      O2
*********************************************************************************************************
K1    *
      *  0.000   0.000   0.000   0.000   0.000
      *  0.000   0.001   0.000   0.001   0.001
      *  0.000  -5.396   3.729   3.654  -5.547
LI1   *
      *  0.000   0.000   0.000   0.000  -0.004
      *  0.000   0.000  -0.001   0.001  -0.006
      *  5.396   0.000  -2.498  44.150 -36.713
S1    *
      *  0.000   0.000   0.000   0.000   0.000
      *  0.000  -0.001   0.000   0.003   0.002
      * -3.728   2.498   0.000 -98.427  91.254
O1    *
      *  0.000   0.000   0.000   0.000  -0.001
      *  0.001  -0.001  -0.003   0.000   0.000
      * -3.653 -44.150  98.427   0.000  39.957
O2    *
      * -8.810 -25.291  86.817  11.635  28.099
      *-10.616  31.232  -2.033   3.580   0.676
      *  1.849  12.237 -30.418 -13.319  -0.001
```

		ELECTRICAL FIELD IN V/A	ELECTRICAL FIELD GRADIENT IN V/A**2
K1	CHARGE = 1.20 AT (0.000 0.000 0.000) :	(0.00000 -0.00003 0.22821)	-0.06105 0.00003 0.00000 0.00003 -0.06120 0.00003 0.00000 0.00003 0.12231
K2	CHARGE = 1.20 AT (0.000 0.000 4.312) :	(0.00000 0.00000 0.22824)	-0.06097 0.00002 0.00000 0.00002 -0.06112 -0.00005 0.00000 -0.00005 0.12228
LI1	CHARGE = 0.40 AT (0.000 2.969 5.882) :	(0.00016 0.00017 -0.54537)	-0.15979 0.00024 0.00012 0.00024 -0.15942 0.00028 0.00012 0.00028 0.31925
LI2	CHARGE = 0.40 AT (2.571 1.484 1.570) :	(-0.00016 -0.00020 -0.54534)	-0.15953 0.00018 -0.00012 0.00018 -0.15938 -0.00022 -0.00012 -0.00022 0.31929
S1	CHARGE = 1.35 AT (0.000 2.969 2.535) :	(-0.00002 -0.00025 1.01937)	-0.92635 -0.00013 0.00004 -0.00013 -0.92633 -0.00026 0.00004 -0.00026 1.85302
S2	CHARGE = 1.35 AT (2.571 1.484 6.847) :	(0.00001 0.00021 1.01936)	-0.92629 0.00009 -0.00004 0.00009 -0.92648 0.00007 -0.00004 0.00007 1.85296
O1	CHARGE = -0.85 AT (0.000 2.969 3.967) :	(0.00002 -0.00023 5.17892)	5.39009 0.00001 0.00002 0.00001 5.39005 0.00055 0.00002 0.00055 -10.78013
O5	CHARGE = -0.85 AT (2.571 1.484 8.279) :	(-0.00002 0.00012 5.17882)	5.39027 0.00001 -0.00002 0.00001 5.39005 -0.00042 -0.00002 -0.00042 -10.78019
O2	CHARGE = -0.70 AT (1.391 2.926 2.061) :	(4.18469 -0.40673 -1.41435)	-8.10557 0.36394 4.58665 0.36394 4.72201 -0.18960 4.58665 -0.18960 3.38340
O6	CHARGE = -0.70 AT (1.180 1.527 6.373) :	(-4.18484 0.40661 -1.41439)	-8.10560 0.36382 -4.58665 0.36382 4.72192 0.18955 -4.58665 0.18955 3.38347
O3	CHARGE = -0.70 AT (4.484 4.195 2.061) :	(-1.74039 3.82740 -1.41438)	1.82993 5.37240 -2.12923 5.37240 -5.21347 4.06701 -2.12923 4.06701 3.38352
O7	CHARGE = -0.70 AT (3.229 0.258 6.373) :	(1.74036 -3.82724 -1.41434)	1.82997 5.37231 2.12916 5.37231 -5.21347 -4.06691 2.12916 -4.06691 3.38345
O4	CHARGE = -0.70 AT (4.409 1.786 2.061) :	(-2.44442 -3.42094 -1.41433)	1.20012 -5.73625 -2.45744 -5.73625 -4.58377 -3.87746 -2.45744 -3.87746 3.38360
O8	CHARGE = -0.70 AT (3.304 2.667 6.373) :	(2.44458 3.42092 -1.41438)	1.20016 -5.73640 2.45750 -5.73640 -4.58372 3.87760 2.45750 3.87760 3.38345

Appendix B. Comprehensive List of Input Cards

B.1   Input for Program GROUP

Card 1	Comment	[18A4]
Card 2	NA, IPM, IDC, NCC, NX	[5I5]
Card 3	(NAME(I), I = 1,NA)	[18A4]
Card 4	Comment	[33A4]
Card 5	((A(I,J), I = 1,3), J = 1,3)	[9F8.5]

For each of the NA + NX atoms one card of the following type must be given:

Card 6	TY, (X(I), I = 1,3), JM	[I5,3F10.5,I5]
Card 7	(QS(I), I = 1,3)	[3F10.5]
Card 8	NIR, IT	[2I5]
Card 9	Comment	[18A4]
Card 10	(Q(I), I = 1,3)	[3F10.5]

B.2   Input for Program NN

Card 1	(IDIR(I), I = 1,3)	[3I5]
Card 2	NNS	[I5]
Card 3	DELTA, DMAX	[2F10.6]

B.3 Input for Program MODEL1

Card 1 **(IDIR(I), I = 1,10)** [10I5]

Card 2 **(MASS(I), I = 1,MAXTYP)** [8F10.5]

Card 3 **N** [I5]

For Coulomb interaction only:
Card 4 **DMAX** [F10.5]

Only for interaction types containing atom-specific
or general parameters (see table 1)
Card 5 **((IASP(I,J), J = 1,MAXTYP), I = 1,NASP)**
   (IGP(K), K = 1,NGP) [16I5]

Not for Coulomb interaction:
Card 6 **I J NS** [3I5]

If interaction N contains interaction-specific parameters
(see the table 1) for each of the NS shells a card of the
following type must be given:
Card 7 **(IISP(I), I = 1,NISP)** [16I5]

Further cards of type 6 and 7.
The end of input for the interaction N (N≠5)
is indicated by a card of type 6 with I = 0.

Further interactions may be specified by repeating
the input 3.-7. The end of the model set-up
is indicated by a card of type 3 with N = 0.

Card 8 **(P(I), I = 1,NP)** [8F10.5]

B.4 Input for Program HIST

Card 1	**NYMAX**	[F10.6]
Card 2	**(IDIR(I), I = 1,20)**	[16I5]
Card 3	**NMARK**	[I5]

B.5 Input for Program SF

Card 1	**HMIN, HMAX, KMIN, KMAX, LMIN, LMAX**	[6I5]
Card 2	**QMAX**	[F10.6]
Card 3	**(B(I), I = 1,MAXTYP)**	[8F10.6]

For each of the MAXTYP types of particles a card
of the following type must be given:

Card 4	**I, (TF(K), K = 1,6)**	[I5,6F10.6]
Card 5	**T**	[F10.6]
Card 6	**FNORM**	[F10.6]
Card 7	**(IDIR(I), I = 1,10)**	[10I5]

B.6 Input for Program PARDER

Card 1	**(IDIR(I), I = 1,10)**	[10I5]
Card 2	**(DP(I), I = 1,NP)**	[8F10.6]

B.7 Input for Program ROTINV

Card 1 **QL**   [F10.6]

Card 2 **(IDIR(I), I = 1,10)**   [10I5]

Card 3 **(MASS(I), I = 1,MAXTYP)**   [8F10.5]

Card 4 **N**   [I5]

For Coulomb interaction only:
Card 5 **DMAX**   [F10.5]

Only for interaction types containing atom-specific
or general parameters (see table 1)
Card 6 **((IASP(I,J), J = 1,MAXTYP), I = 1,NASP)**
(IGP(K), K = 1,NGP)   [16I5]

Not for Coulomb interaction:
Card 7 **I J NS**   [3I5]

If interaction N contains interaction-specific parameters
(see the table 1) for each of the NS shells a card of the
following type must be given:
Card 8 **(IISP(I), I = 1,NISP)**   [16I5]

Further cards of type 7 and 8.
The end of input for the interaction N (N≠5)
is indicated by a card of type 7 with I = 0.
Further interactions may be specified by repeating
the input 4-8. The end of the model set-up
is indicated by a card of type 4 with N = 0.

Card 9 **(P(I), I = 1,NP)**   [8F10.5]

Other parameter sets may be considered by supplying
additional cards of type 9.

B.8 Input for Program EFG

Card 1 (IDIR(I), I = 1,10)   [10I5]

Card 2 (Z(I), I = 1,MAXTYP)   [8F10.6]

Card 3 DMAX   [F10.6]

Appendix C. Alphabetical List of Subroutines

The subroutines used in **GROUP**, developed by *WARREN* and *WORLTON*, are not included.

BL	stores the elements of the block diagonalized Dynamical Matrix into individual matrices.
BMP	calculates the force constants according to the Born-Mayer potential.
BOSE	calculates the Bose-factor n_{qj}.
CCF	calculates the (3×3) submatrices of Coulomb coefficients.
CHECKT	checks the translational invariance of the force constant matrix.
CINS	inserts complex (3×3) submatrices into a full (3N×3N) matrix.
CMLIST	lists a complex matrix.
CMMULT	calculates the complex matrix product **A** = **B C**.
CMQ	equates two complex matrices.
CMZ	complex matrix zeroing routine
CP	calculates the Coulomb contribution to a (3×3) submatrix of the Dynamical Matrix.
CTOD	changes the Dynamical Matrix and related matrices from C- to D-definition.
CTRNSF	calculates the symmetrical equivalent submatrices of the Dynamical Matrix.
DIJ	calculates the complete (3×3) submatrices of the Dynamical Matrix.
DSF	calculates the dynamical structure factor for a particular phonon in a given Brillouin zone.
DWF	calculates Debye-Waller factors.
DYN2	constructs the entire Dynamical Matrix of dimension (3N×3N).
E2CHF	diagonalizes a complex hermitian matrix (IMSL library routine).
EIGEN	calculates eigenvalues and eigenvectors of the Dynamical Matrix.
EMPTY	collects a string of characters which is needed for a histogram of dispersion curves.

EXTIP	extends the vector IP of parameter numbers in case of the shell model in order to account for the non-hermiticity of the matrix for the core-shell coupling.
FCCF	calculates the local electrical field.
FCM	calculates the (3×3) submatrix of the Dynamical Matrix on the basis of given longitudinal and transverse force constants.
FCP	calculates the local electrical field.
FREQ	transforms the eigenvalues of the Dynamical Matrix to frequency scale.
GETDT	reads the symmetry coordinates from file **COORD**.
GETPAR	interprets the user input for the model specification.
GETPM	gets the actual parameter values for a particular interaction by decoding the information contained in the vector IP.
GETTF	reads the temperature factors for one representative atom per atom type and calculates the temperature factors of symmetrical equivalent atoms.
GETXX	reads the atomic positions from file **COORD**.
HTRANS	calculates the hermitian matrix transformation $A = B^+ C B$.
IMZ	integer matrix zeroing routine
INDINT	determines the total number of independent interactions.
IREP	determines the irreducible representation of modes which have been re-arranged by subroutine SORT.
LENGTH	is a function and calculates the length of a N-dimensional vector.
LINCG	calculates the inverse of a complex matrix (IMSL library routine).
LINE	is a function and determines the print-line corresponding to a particular phonon wavevector within a histrogram plot.
LJP	computes force constants according to the Lennard-Jones potential.
MDM	multiplies the Dynamical Matrix by the mass-tensor.
MINS	inserts real (3×3) submatrices into the full force constant matrix.
MODELX	is called by SR DIJ and serves as a switch to a model potential number M.
MODX	represents an integer by a bit-pattern. MODX is used to determine which interaction types are superimposed for modelling a particular pair inter-action.

MTRNSF	calculates symmetrical equivalent submatrices of the force constant matrix.
MZ	real matrix zeroing routine
NBR	analyzes the neighbourhood of a particular atom.
NPM	determines the number of atom-specific and interaction-specific parameters for a given model potential.
PCF	displays the pair correlation function as a histogram plot.
PDRV	calculates the partial derivates of phonon frequencies with respect to each of the model parameters.
PHASE	converts the Dynamical Matrix from D- to C-definition.
PRINT1	prints the model specification as the heading for an output list.
PRINT2	prints the results of model calculations.
PRINT3	prints the results of structure factor calculations.
PRINT4	prints the headings for structure factor output.
PRINT5	prints the headings for the results of structure factor calculations including the temperature factors and the scattering lengths.
PRINT6	prints the partial derivates of phonon frequencies.
RINV	checks the rotational invariance of a given lattice-dynamical model.
ROUND	zeroes those matrix elements whose moduli are smaller than a given amount.
RSTOR1	restores the parameters of model calculations from file **RESULT**.
RSTOR2	restores the results of model calculations from file **RESULT**.
SELF	calculates the self-term for the Dynamical Matrix and related matrices.
SHELL1	calculates the (3×3) submatrices for a particular pair interaction according to the shell model.
SHELL2	calculates the polarization part of the Dynamical Matrix according to the shell model.
SORT	rearranges the elements of a real vector according to their moduli.
STOEIG	stores eigenvalues and eigenvectors.
STORE1	stores the parameters of model calculations on file **RESULT**.
STORE2	stores the results of model calculations on file **RESULT**.

TYPE   determines the number of different unit types of the given structure.

VDWP   computes the force constants according to the van der Waals potential.

VPROD   calculates the vector product $c = a \times b$.

Appendix D. Subroutine Reference List

In the following, for each program of UNISOFT (except **GROUP**) the required subroutines are listed.

IND	GETXX, INDINT, TYPE
NN	EMPTY, GETXX, LENGTH, NBR, PCF
MODEL1	BL, BMP, CCF, CHECKT, CINS, CMLIST, CMMULT, CMQ, CMZ, CP,CTOD, CTRNSF, DIJ, DYN2, E2CHF, EIGEN, EXTIP, FCM, GETDT, GETPAR, GETPM, GETXX, IMZ, HTRANS, LENGTH, LINCG, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, NPM, PRINT1, PRINT2, ROUND, SELF, SHELL1, SHELL2, STOEIG, STORE1, STORE2, VDWP
HIST	EMPTY, GETXX, LENGTH, LINE, MODX, PRINT1, RSTOR1 RSTOR2, VPROD
SF	BOSE, DSF, DWF, FREQ, GETTF, GETXX, IREP, LENGTH, MODX, PRINT3, PRINT4, PRINT5, RSTOR1, RSTOR2, SORT
PARDER	BMP, CCF, CINS, CMZ, CP, CTOD, CTRNSF, DIJ, DYN2, FCM, FREQ, GETDT, GETPM, GETXX, HTRANS,IMZ LENGTH, LINCG, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, PDRV, PRINT1, PRINT6, ROUND, SELF, SHELL1, SHELL2, RSTOR1, RSTOR2, VDWP
ROTINV	BMP, CCF, CINS, CMLIST, CMZ, CP, CTOD, CTRNSF, DIJ, DYN2, EXTIP, FCM, GETPAR, GETPM, GETXX, IMZ, HTRANS, LENGTH, LINCG, LJP, MDM, MINS, MODELX, MODX, MTRNSF, MZ, NPM, PHASE, PRINT1, RINV, ROUND, SELF, SHELL1, SHELL2, VDWP
EFG	CCF, CMZ, CP, FCCF, FCP, GETXX, MZ

Appendix E. List of Symbols

As a general convention, bold printed capital letters are used to denote matrices, while bold printed lower case letters represent vectors.

a_{qj}	annihilation operator for a phonon state qj
a_{qj}^+	creation operator for a phonon state qj
$\mathbf{B}_\kappa$	matrix of temperature factors of atom κ
b_κ	scattering length of atom κ
$\mathbf{C}(q)$	matrix of Coulomb coefficients at wavevector q
$\mathbf{C}(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{C}(q)$
$\mathbf{D}(q)$	Dynamical Matrix at wavevector q
$\mathbf{D}^x$	block diagonalized Dynamical Matrix
$\mathbf{D}(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{D}(q)$
$\mathbf{D}^{(m)}(\kappa\kappa'\|q)$	contribution of interaction type m to $\mathbf{D}(\kappa\kappa'\|q)$
d_n	radius of the n-th neighbouring shell
$\mathbf{E}$	matrix of eigenvectors
$\mathbf{e}(qj)$	eigenvector of the Dynamical Matrix corresponding to the phonon state qj
$\mathbf{e}_i^x$	eigenvector of the block diagonalized Dynamical Matrix
$\mathbf{e}(\kappa\|qj)$	eigenvector of atom κ corresponding to the phonon state qj
erf	error function
e^{-W_κ}	Debye-Waller factor of atom κ
$\mathbf{F}(q)$	Fourier transformed force constant matrix at wavevector q
$\mathbf{F}(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{F}(q)$
$\mathbf{F}^c(q)$	Coulomb part of $\mathbf{F}(q)$
$\mathbf{F}^c(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{F}^c(q)$
$\mathbf{F}^{cc}(q)$	Fourier transformed force constant matrix for the *effective* core-core coupling
$\mathbf{F}^{cs}(q)$	Fourier transformed force constant matrix for the *effective* core-shell coupling
$\mathbf{F}^s(q)$	Fourier transformed force constant matrix for the shell-shell coupling
$\mathbf{F}^s(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{F}^s(q)$
$\mathbf{F}^{sc}(q)$	Fourier transformed force constant matrix for the *effective* shell-core coupling
$\mathbf{F}^{ss}(q)$	Fourier transformed force constant matrix for the *effective* shell-shell coupling
$\mathbf{F}^T(q)$	Fourier transformed force constant matrix for the core-shell coupling
$\mathbf{F}_0^T$	matrix of the self terms of $\mathbf{F}^T(q)$
$\mathbf{F}^T(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{F}^T(q)$
$\mathbf{F}^{T'}(q)$	Fourier transformed force constant matrix for the shell-core coupling
$\mathbf{F}_0^{T'}$	matrix of the self terms of $\mathbf{F}^{T'}(q)$
$\mathbf{F}^{T'}(\kappa\kappa'\|q)$	(3×3) submatrix of $\mathbf{F}^{T'}(q)$
$\mathbf{F}^{(m)}(\kappa\kappa'\|q)$	contribution of interaction type m to $\mathbf{F}(\kappa\kappa'\|q)$

$f^\beta_\alpha(\kappa l)$	α-component of the force acting upon an atom (κl) during a rigid rotation of the whole crystal around the β-axis
g	reciprocal lattice vector
G	order of a symmetry group
g	element of a symmetry group
G_q	symmetry group of the wavevector **q**
H	tensor of electrical field gradients
h	local electrical field
h	Planck constant $(6.626 \times 10^{-34}\,Js)$
$\hbar$	$h/2\pi$ $(1.055 \times 10^{-34}\,Js)$
H	Hamiltonian
H_{qj}	Hamiltonian for one particular phonon state **qj**
$\hbar\omega$	energy transfer in neutron scattering experiments
I	unit matrix
K	diagonal matrix of intraatomic core-shell force constants
K_κ	core-shell force constant within the same atom κ
k_B	Boltzmann constant $(1.381 \times 10^{-23}\,JK^{-1})$
$\mathbf{k}_i$, $\mathbf{k}_j$	neutron wavevectors
L	longitudinal force constant
l,l',m,m'	label different primitive cells
M	mass-tensor
m_κ	mass of atom κ
m_n	neutron mass
N	number of atoms per primitive cell
n_{qj}	Bose-factor corresponding to the phonon state **qj**
p	parameter vector corresponding to a particular model
$\Delta\mathbf{p}$	variation of **p**
$\mathbf{p}_{\kappa l}$	momentum of atom (κl)
$\mathbf{p}^e_{\kappa l}$	electric dipole moment of atom (κl)
p	parameter for the Ewald-summation
Q	scattering *vector* (the only exception from the above convention)
q	phonon wavevector
$\delta\mathbf{q}$	small increment of **q**
δq	modulus of $\delta\mathbf{q}$
qj	phonon state
Q_{qj}	normal coordinate corresponding to the phonon state **qj**
r	vector in real space
r	modulus of vector **r**
$\mathbf{r}_{\kappa l}$	position vector of atom (κl)
$\mathbf{r}^0_{\kappa l}$	equilibrium position of atom (κl)
S	rotational matrix corresponding to a symmetry operation
(**S**|**v**)	symmetry operation
$S_{coh}(\mathbf{Q}, \omega)$	coherent scattering function
$S^{(qj)}_{coh}(\mathbf{Q}, \omega)$	coherent scattering function due to the interaction of a neutron with a single phonon state **qj**
T	transverse force constant
T	temperature
t	time variable

$TF_\kappa(i)$	component of the tensor of temperature factors B_κ
$u_{\kappa l}$	displacement vector of atom (κl)
$V(\kappa l, \kappa' l')$	force constant matrix for the interaction between atoms (κl) and $(\kappa' l')$
$V^s(\kappa l, \kappa' l')$	force constant matrix for the shell-shell interaction between atoms (κl) and $(\kappa' l')$
$V^{SR}(\kappa l, \kappa' l')$	force constant matrix for the short-range core-core interaction between atoms (κl) and $(\kappa' l')$
$V^T(\kappa l, \kappa' l')$	force constant matrix for the core-shell interaction between atoms (κl) and $(\kappa' l')$
$V^{T'}(\kappa l, \kappa' l')$	force constant matrix for the shell-core interaction between atoms (κl) and $(\kappa' l')$
v	fractional translation of a symmetry operation
$V(\kappa l, \kappa' l')$	potential energy due to the interaction between atoms (κl) and $(\kappa' l')$
V_o	prefactor for model potentials
v	volume of the primitive cell
$w_{\kappa l}$	displacement vector of the electron shell of atom (κl) with respect to its equilibrium position
$\overline{w}_{\kappa l}$	relative displacement vector of the electron shell of atom (κl) with respect to corresponding core-position
X	matrix of symmetry coordinates
X_κ	charge of the ionic core of atom κ
Y	matrix of shell charges
Y_κ	charge of the electron shell of atom κ
Z	matrix of ionic charges
Z_κ	charge of ion κ
α_κ	polarizability of the free ion κ
Γ_{3N}	3N-dimensional representation of a symmetry group
γ_i	irreducible multiplier representation no. i
$\delta_{\alpha,\beta}$	Kronecker-symbol
ε_o	vacuum permittivity $(8.854 \times 10^{-12} \, As(Vm)^{-1})$
$\kappa, \kappa', \lambda, \lambda'$	label atoms within a primitive cell
v_{qj}	$= \omega_{qj}/2\pi$, frequency of the phonon state qj
Δv	variation of frequency v
δv^2	variation of squared frequency v^2
ρ_κ	charge distribution representing the ion κ
$\sum$	sum
σ_κ	short range repulsion parameter of atom κ
χ	character of a representation
ω_{qj}	frequency of the phonon state qj
$\Delta\omega$	variation of the frequency ω
$\delta\omega^2$	variation of the squared frequency ω^2
$*$	complex conjugate
$+$	hermitian conjugate