Table 5 it can be seen that the strongest 50 reflexions of the test structure contain 296 reliable SQR's with $E_4^* > 10$, their mean value being 14·9. This means that the 50 phases are correlated by a highly overdetermined system of relations so that a reliable starting set can easily be constructed. The SQR's cannot be used for extending the set of phases to say 200 or 300, because the new phases are linked by a small number of rather weak SQR's to the starting set.

Thus the properties of triplet-relations and SQR's are complementary. By using the two types of relations at the same time the advantages of both can be combined.

### Practical procedure for structure determinations

We have adopted the following procedure in our computer programs:

1. Calculating triplet relations and SQR's.
2. Convergence mapping (Germain, Main & Woolfson, 1970) applied to the *n* strongest reflexions only with the following modifications:
    *a*. The reliability of a phase is estimated by

$$R_H=\sum_{\substack{K\\ \text{triplets}}} E_4^2+\sum_{K}\sum_{\substack{L\\ \text{SQR's}}} E_4^{*2}.$$

    *b*. If all $E_4^*$ and $E_4$ values contributing to an $R_H$ are below a limit value (approximately 30% of the maximum $E_4$) this $R_H$ is set equal to zero.
    *c*. No prior choice of origin-defining reflexions is made.
3. The output reflexions of the convergence mapping form the starting group of phases. Some of them are used for the definition of the origin and other are given symbolic phases.
4. Extension of the group of symbolically phased reflexions.
5. Finding the most reliable solution on the basis of the appropriate criterion (Schenk, 1972*c*).

The method was applied to a structure in $P2_1/c$, for which previously only after two failures a proper starting set could be found. By the new method this starting set was obtained automatically. In another structure determination, for which our former phasing process failed several times, a new starting set, found by means of the above procedure, lead to the correct solution.

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# The Dependence of the Debye–Waller Temperature Factors on the Atomic Masses

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The question of how the Debye–Waller temperature factors depend on the atomic masses is discussed in terms of lattice dynamics.

## 1. Introduction

Recently Huiszoon & Groenewegen (1972) investigated whether or not the Debye–Waller factors depend on the atomic masses. We quote their result: '... a theorem will be derived which states that Debye–Waller *B* values of individual atoms in a crystal lattice do not depend on the atomic masses when the temperature of the crystal is above its Debye temperature'. The equations derived by Huiszoon & Groenewegen are correct; we believe, however, that their equations should be interpreted in another manner.

Huiszoon & Groenewegen (1972) base their interpretation on their equations (15) and (18). We quote equation (18) for reference as

$$\langle u_i(\begin{smallmatrix}l\\r\end{smallmatrix})u_k(\begin{smallmatrix}l\\r\end{smallmatrix})\rangle = U_r^{ik}= \frac{k_BT}{N}\sum_{\mathbf{q}}(L^{-1})_{ik}(\begin{smallmatrix}\mathbf{q}\\rr\end{smallmatrix}) + \frac{\hbar^2\delta_{ik}}{12k_BTm_r} - \frac{\hbar^4}{720k_B^3T^3m_r^2N}\sum_{\mathbf{q}}L_{ik}(\begin{smallmatrix}\mathbf{q}\\rr\end{smallmatrix})+\ldots,\ T>\Theta_D/2\,. \quad (1)$$

The symbols have the following meanings:

$U_r^{ik}$ = component $ik$ of the vibration tensor $\mathbf{U}_r$ of the atom $r$; $i,k=1,2,3$.
$k_B$ = Boltzmann's constant.
$T$ = absolute temperature
$\Theta_D$ = Debye temperature
$N$ = number of cells in the crystal
$\mathbf{q}$ = wave vector
$\hbar$ = Planck's constant divided by $2\pi$
$m_r$ = mass of atom $r$
$\delta_{ik}$ = Kronecker symbol.

The elements of the dynamical matrix $\mathbf{L}(\mathbf{q})$, which occur in equation (1), are

$$L_{ik}\binom{\mathbf{q}}{rr'} = \sum_{l-l'} \varphi_{ik}\binom{ll'}{rr'} \exp\left\{-i\mathbf{q} \cdot \left[\mathbf{X}\binom{l}{r} - \mathbf{X}\binom{l'}{r'}\right]\right\}, \qquad (2)$$

where the indices $l,l'$ denote the cells in the crystal and $\mathbf{X}\binom{l}{r}$ is the vector to the atom $\binom{l}{r}$ in the crystal. The important point about equations (1) and (2) is that the components $U_r^{ik}$ of the vibration tensor of the atom $r$ are expressed in terms of the dynamical matrices of the crystal, $\mathbf{L}(\mathbf{q})$, and thus in terms of the interatomic force constants $\varphi_{ik}\binom{ll'}{rr'}$. In treating the question of the coupling of the thermal motions of the atoms we derived corresponding equations, *cf.* Scheringer (1972*a*), equations (10) and (15).

For high temperatures, $T \rightarrow \infty$, all terms on the right-hand side of equation (1) vanish except for the first. Thus the first term is the most important one. Since the atomic mass $m_r$ does not explicitly occur either in this term or in equation (2) Huiszoon & Groenewegen (1972) conclude that the components $U_r^{ik}$ are largely independent of the atomic masses. Only with low temperatures do the higher terms in the series expansion in equation (1) become important and thus – according to Huiszoon & Groenewegen – establish a certain dependence of the components $U_r^{ik}$ on the atomic masses.

Our criticism of this interpretation refers to the fact that Huiszoon & Groenewegen (1972) do not take into account constraints among the force constants, which are necessary for limiting the motions of the atoms to the internal vibrations of the crystal. As a consequence of the constraints a mass dependence of the atomic vibration tensors $\mathbf{U}_r$ arises.

## 2. The constraints on the force constants

In the lattice-dynamical treatment of the motions of the atoms in a crystal all quantities are usually referred to a Cartesian reference system. Therefore the vibration coordinates $u_i\binom{l}{r}$ of the atoms initially refer to external and internal vibrations of the crystal. Hence it is necessary to introduce constraints which provide for the exclusion of the external motions of the crystal. The constraints, which are important for our problem of mass dependency, arise from the fact that the interatomic forces remain invariant when the crystal undergoes a rigid translation. The constraints are

$$\sum_{r'} \sum_{l'} \varphi_{ik}\binom{ll'}{rr'} = 0; \quad i,k=1,2,3; \qquad (3)$$

*cf.* Maradudin, Montroll & Weiss (1963), equation (2.1.12*b*). Thus, in the following we have to investigate the impact of the constraints (3) on the elements of the dynamical matrix (2). Here the phase factors

$$\exp\left\{-i\mathbf{q} \cdot \left[\mathbf{X}\binom{l}{r} - \mathbf{X}\binom{l'}{r'}\right]\right\}, \qquad (4)$$

which occur in the elements of the dynamical matrix, play an important part. These factors, on the one hand, take into account the coordinations of the atoms in the crystal and, on the other, the magnitudes of the various wave vectors, $|\mathbf{q}|=q$, which occur in the crystal. For sufficiently small values of $q$ the phase factors are nearly unity. Then a consequence of the constraints (3) is that, for the optic modes, the centre of gravity of each cell in the crystal remains nearly at rest. As a consequence of this behaviour a mass dependence of the atomic mean-square amplitudes arises. For large values of $q$ the phase factors (4) deviate from unity and the constraints (3), which only refer to force constants, do not represent rigorous conditions on the elements of the dynamical matrix (2). Hence, for the optic modes, the centre of gravity of the unit cell does not remain at rest. Thus the strength of the mass dependence is dependent on how the constraints (3) cooperate with the phase factors (4) in the elements of the dynamical matrix (2), and is essentially independent of the temperature. Since the mass dependence of the atomic mean-square amplitudes varies with the different values of $q$ we consider the three cases

(1) $q$ is zero,
(2) $q$ is small but non-zero,
(3) $q$ is large

in succession.

## 3. $q$ is zero

The phase factors (4) are unity, and hence the dynamical matrix contains force constants only. The constraints (3) render the dynamical matrix $\mathbf{L}$ singular and give rise to 3 frequencies $\omega_j=0$, which represent the limiting values of the 3 acoustic branches. The remaining $3n-3$ frequencies, which belong to the optic branches, are non-zero. Therefore the constraints (3), applied to the secular equation of the crystal, yield

$$\sum_{r=1}^{n} m_r u_i\binom{l}{r} = 0; \quad i=1,2,3; \qquad (5)$$

for the optic modes, $\omega_j>0$; *cf.* the calculation given by von Laue (1948), equations (21.21) to (21.29). The result (5) holds for each cell $l$ of the crystal. Equation (5) means that, for the optic modes, the centre of gravity of the atoms in the unit cell remains at rest (for $q=0$). We may picture the situation as follows. There are no acoustic modes with an infinitely large wavelength but only $3n-3$ optic modes. Thus three coordinates of vibration are redundant. For the $3n-3$ optic modes all cells of the crystal vibrate in the same manner. Since the crystal as a whole remains at rest, the centre of gravity of each cell also remains at rest. Thus we can use equation (5) in order to eliminate the three redundant coordinates of vibration.

For this purpose we define a $3n-3$ column matrix $\mathbf{u}_{\rm opt}$ which represents the coordinates of the internal vibrations of the unit cell (coordinates of the optic modes). (The index $l$, referring to the cell in the crystal, can be dropped.) By using the conditions (5) we then determine a $3n \times 3n-3$ matrix $\mathbf{G}_{\rm opt}$ which performs the transformation of the internal coordinates to the coordinates $\mathbf{u}$ of the Cartesian reference system so that

$$\mathbf{u}=\mathbf{G}_{\rm opt}\mathbf{u}_{\rm opt}\,. \tag{6}$$

Since $\mathbf{G}_{\rm opt}$ was gained with the aid of the conditions (5), the elements of $\mathbf{G}_{\rm opt}$ contain the atomic masses. With equation (6) we obtain for the $3n-3 \times 3n-3$ dynamical matrix of the internal vibrations of the unit cell

$$\mathbf{L}_{\rm opt}=\mathbf{G}^{\rm T}_{\rm opt}\mathbf{L}\mathbf{G}_{\rm opt}\,. \tag{7}$$

$\mathbf{L}_{\rm opt}$ is essentially independent of the atomic masses since it contains force constants only. With equations (6) and (7) we now obtain for the $3n \times 3n$ mean-square amplitude matrix, referred to the Cartesian reference system,

$$\mathbf{U}=k_BT\mathbf{G}_{\rm opt}\mathbf{L}^{-1}_{\rm opt}\mathbf{G}^{\rm T}_{\rm opt}\,, \tag{8}$$

in the high-temperature approximation. $\mathbf{U}$ is dependent on the atomic masses since $\mathbf{G}_{\rm opt}$ depends on the masses and $\mathbf{L}^{-1}_{\rm opt}$ does not.

The simplest example of the equations (5) to (8) is given by a crystal with two atoms in the unit cell. Here we already have three optic branches. Calculation shows that, for $q=0$, the mean-square amplitudes are inversely proportional to the squares of the atomic masses, *i.e.* there is a strong mass dependence of the mean-square amplitudes, *cf.* von Laue (1948), p. 219.

Furthermore, the equations (5), (6), (7) and (8), modified for all temperatures, can be applied to the internal modes of molecules. For free molecules there are no wave vectors, *i.e.* we can assume $q=0$. But the force-constant matrix for the internal modes of a molecule is only of order $3n-6$ since, as well as the degrees of rigid translation, the degrees of rigid rotation must be subtracted. However, this does not touch the principle of our consideration. For a diatomic molecule we have the result that the mean-square amplitudes are inversely proportional to the squares of the atomic masses, *cf.* Herzberg (1957), pp. 73–76, in agreement with the result for the diatomic lattice.

For some molecules the force constants are well known from spectroscopic investigations and the atomic mean-square amplitudes have been calculated. We have studied the mass dependence for several of these molecules. In order to define a measure for the strength of the mass dependence we use the equation

$$m_r^p\langle\text{trace}\,(\mathbf{U}_r)^{\rm int}\rangle=m_s^p\langle\text{trace}\,(\mathbf{U}_s)^{\rm int}\rangle, \tag{9}$$

from which we can calculate the power $p$. We consider $p$ as such a measure. (The superscript 'int' means that we regard internal modes only.) We use the trace in equation (9) in order to average over the three directions of space, and the brackets $\langle\;\rangle$ to average over all atoms of the same type in the molecule. The results of our calculation are listed in Table 1. In each row the compound, the number $n$ of the atoms in the molecule, $\langle\text{trace}\,(\mathbf{U}_r)^{\rm int}\rangle$ and $\langle\text{trace}\,(\mathbf{U}_s)^{\rm int}\rangle$ together with the chemical symbols of the considered atoms $r$ and $s$, the power $p$, and the authors who calculated the mean-square amplitudes are listed. $0<p\le 2$ is found. The largest value, $p=2$, only occurs for diatomic molecules since here the condition (5) attains its highest efficiency. For the molecules in Table 1, the value of $p$ is approximately unity, the smallest value is 0·91. This corresponds to the 'product rule' ($p=1$) which we have used in a preceding paper (Scheringer, 1972*b*). Thus there is a distinct dependence of the mean-square amplitudes on the atomic masses. Probably $p$ will become smaller with a growing number of atoms in the molecule because the effect of the conditions (5) on the individual atom will then decrease. Unfortunately we have no experimental data for molecules larger than those of Table 1 at our disposal. It is possible that the value of $p=1{\cdot}89$ is not correct (too large) for the $P_4O_{10}$ molecule. The mass ratio $m(\text{P})/m(\text{O})=1{\cdot}94$ is relatively close to unity which may give rise to errors in the value of $p$, calculated with the aid of equation (9). For, errors in the experimentally determined force constants are carried over to the ratio $\langle\text{trace}\,(\mathbf{U}_s)^{\rm int}\rangle/\langle\text{trace}\,(\mathbf{U}_r)^{\rm int}\rangle$ which may have a strong effect on the calculated value of $p$ if the ratio $m_r/m_s$ comes close to unity.

## 4. Small values of $q$

With $q>0$ the singularity of the dynamical matrix $\mathbf{L}$ vanishes, and the question arises if, with the transition $q=0 \rightarrow q>0$, the condition (5) loses its validity abruptly or continuously. Formally, the transition to $q>0$ means that the phase factors (4) begin to deviate from unity. Therefore the constraints (3) no longer impact rigorously on the elements of the dynamical matrix (2) and $\mathbf{L}$ becomes ill-conditioned but no longer singular. When $\mathbf{L}$ has been mass-normalized it yields three eigenvalues $\omega^2_j(\mathbf{q})$ which are small and belong to the three acoustic branches. In order to picture the situation we may say: with small values of $q$ we have long acoustic waves in the crystal which move the cells almost like undisturbed units. Thus we can consider these motions of the cells, to a very good approximation, as external modes of the cells. With the transition to $q>0$ the amplitude of the acoustic modes is introduced abruptly and with it the motion of the centre of gravity of the cells in the crystal. The internal vibrations (optic modes) of the cells, however, remain nearly unaltered by this transition. Hence the condition (5) remains valid for the internal modes of the cells to a very good approximation. In contrast to the case $q=0$, we now have to take into account that there are three acoustic modes which behave to a very good approximation like external modes of the cells.

Thus it is expedient to transform the vibration coordinates $\mathbf{u}$ of the Cartesian reference system so that they are resolved into internal and external coordinates of the motions of a unit cell. For this purpose we introduce a $3n \times 3$ matrix $\mathbf{G}_{\rm ac}$ and form the $3n \times 3n$ compound matrix $\mathbf{G} \equiv (\mathbf{G}_{\rm opt} \mid \mathbf{G}_{\rm ac})$. $\mathbf{G}_{\rm ac}$ refers to the external motions of the cell (acoustic modes) and does not depend on the atomic masses. By analogy with equation (6) we obtain

$$\mathbf{u} = \mathbf{G}\mathbf{u}_{\rm opt,\,ac}\,. \tag{10}$$

In the column matrix $\mathbf{u}_{\rm opt,\,ac}$ the coordinates are resolved into $3n-3$ internal and 3 external vibration coordinates. By analogy with equation (7) we now obtain

$$\left(\begin{array}{c|c} \mathbf{L}_{\rm opt} & 0 \\ \hline 0 & \mathbf{L}_{\rm ac} \end{array}\right) \equiv \mathbf{L}_{\rm opt,\,ac} = \mathbf{G}^T\mathbf{L}\mathbf{G}\,. \tag{11}$$

For small values of $q$ the off-diagonal blocks of $\mathbf{L}_{\rm opt,\,ac}$ are zero, to a very good approximation. Thus the constraints (3) have the effect that, to a very good approximation, a reduced number of elements in the dynamical matrix is now sufficient to describe the vibrational problem, $\mathbf{L}_{\rm opt}$ and $\mathbf{L}_{\rm ac}$, and these refer to internal and external motions of the cells respectively. Using equations (10) and (11) we finally obtain

$$\mathbf{L}^{-1} = \mathbf{G}_{\rm opt}\mathbf{L}_{\rm opt}^{-1}\mathbf{G}_{\rm opt}^{\rm T} + \mathbf{G}_{\rm ac}\mathbf{L}_{\rm ac}^{-1}\mathbf{G}_{\rm ac}^{\rm T}\,. \tag{12}$$

The second term in (12), referring to the long acoustic waves, does not depend on the atomic masses whereas the first term does (as in the case $q=0$). Hence, even in the high temperature approximation, the mean-square amplitude matrix $\mathbf{U} = k_BT\mathbf{L}^{-1}$, which is referred to the Cartesian reference system, is dependent on the atomic masses. Although the temperature constitutes a slight mass dependence of the mean-square amplitude matrix, *cf.* equation (1), it is obvious from our discussion that the temperature does not play a prominent part in our problem.

## 5. Large values of *q*

For large values of $q$ the previously made assumptions no longer hold. The phase factors (4) are complex and deviate considerably from unity. Thus, they diminish the effect of the constraints (3) on the elements of the dynamical matrix. The acoustic modes can no longer be interpreted as external motions of the cells but rather represent internal motions of the cells. Hence

Table 1. *Mass dependency of the average atomic mean-square amplitudes in terms of p for several molecules*

The values of $\langle \text{trace}\,(\mathbf{U}_r)^{\rm int}\rangle$ are in Å², multiplied by $10^5$.

| Compound | $n$ | $\langle \text{trace}(\mathbf{U}_r)^{\rm int}\rangle$ | | $\langle \text{trace}(\mathbf{U}_s)^{\rm int}\rangle$ | | $p$ | Reference |
|---|---|---|---|---|---|---|---|
| Cyclopropene | 7 | C | 181 | H | 3906 | 1·24 | Cyvin & Hagen (1970) |
| Cyclopropene-$d_4$ | 7 | C | 245 | D | 2609 | 1·32 | |
| 1,2,5-Oxadiazole | 7 | O | 205 | H | 4053 | 1·08 | Cyvin, Cyvin, Hagen & Markov (1969) |
| | | N | 250 | H | 4053 | 1·06 | |
| | | C | 281 | H | 4053 | 1·07 | |
| 1,2,5-Thiadiazole | 7 | S | 94 | H | 4389 | 1·11 | |
| | | N | 286 | H | 4389 | 1·03 | |
| | | C | 310 | H | 4389 | 1·06 | |
| 1,2,5-Selendiazole | 7 | Se | 4 | H | 4457 | 1·63 | |
| | | N | 402 | H | 4457 | 0·91 | |
| | | C | 363 | H | 4457 | 1·01 | |
| Furan | 9 | O | 200 | H | 4111 | 1·09 | |
| | | C | 295 | H | 4111 | 1·06 | |
| Furan-$d_4$ | 9 | O | 229 | D | 2814 | 1·21 | |
| | | C | 325 | D | 2814 | 1·20 | |
| Thiophene | 9 | S | 97 | H | 4333 | 1·10 | |
| | | C | 372 | H | 4333 | 0·99 | |
| Thiophene-$d_4$ | 9 | S | 112 | D | 3038 | 1·19 | |
| | | C | 347 | D | 3038 | 1·21 | |
| Cyclopropane | 9 | C | 206 | H | 3560 | 1·15 | Cyvin & Hagen (1970) |
| Cyclopropane-$d_6$ | 9 | C | 262 | D | 2426 | 1·24 | |
| $P_4O_6$ | 10 | P | 360 | O | 830 | 1·26 | Cyvin & Cyvin (1971) |
| Propane | 11 | C | 336 | H | 6336 | 1·18 | Cyvin & Vizi (1970) |
| Propane-$d_8$ | 11 | C | 404 | D | 5200 | 1·42 | |
| Cyclobutane | 12 | C | 414 | H | 4970 | 1·00 | Johnson (1970) |
| Benzene | 12 | C | 382 | H | 4190 | 0·96 | |
| $P_4O_{10}$ | 14 | P | 270 | O | 940 | 1·89 | Cyvin & Cyvin (1971) |
| Naphthalene | 18 | C | 665 | H | 6560 | 0·92 | Cyvin, Cyvin, Hagen, Cruickshank & Pawley (1972) |
| Naphthalene-$d_8$ | 18 | C | 672 | D | 5343 | 1·16 | |
| Hexamethylenetetramine | 22 | N | 390 | H | 493 | 0·96 | Elvebredd & Cyvin (1972) |
| | | C | 500 | H | 493 | 0·92 | |
| Hexamethylenetetramine-$d_{12}$ | 22 | N | 420 | D | 381 | 1·13 | |
| | | C | 500 | D | 381 | 1·13 | |

for these motions the centre of gravity of the atoms in the unit cell is not at rest and a matrix **G** which resolves the vibration coordinates into internal and external ones, cannot be constructed. Therefore the mass dependency of the matrices **L**, $\mathbf{L}^{-1}$ and **U** vanishes.

## 6. Discussion

To sum up: it is the long-wave optic modes of a crystal which cause a strong mass dependence of the atomic mean-square amplitudes. The smaller the value of $q$ the more pronounced the mass dependence will be. According to equation (1) the vibration tensors $\mathbf{U}_r$ are calculated from the inverse dynamical matrices of all wave vectors $\mathbf{q}$ of the crystal. Since the long waves with small $q$ are less frequent than the short waves with large $q$, the long waves do not govern the vibration tensors $\mathbf{U}_r$ but still have an impact upon them. Thus the mass dependency, which is expressed by equation (9) for $q=0$, is greatly weakened but not fully eliminated in the vibration tensors $\mathbf{U}_r$. This result is in full agreement with the observations made on actual structures. Generally, for a given structure, we find the smaller amplitudes for the heavy atoms and the larger amplitudes for the light atoms. Exceptions to this behaviour were observed; however, they remain the rare cases. A detailed statistics, gained from many structures, would certainly be interesting.

Two predictions can be made from the treatment given in this paper:

(1) Given a fixed mass ratio of two atoms in the unit cell then, the fewer the atoms in the unit cell the greater the tendency for the heavy (light) atom to have the smaller (larger) amplitude. Thus, one will primarily observe that a heavy (light) atom has a relatively large (small) amplitude when the unit cell is large.

(2) Given a fixed number of atoms in the unit cell the bigger the difference between the masses the greater the tendency for the heavy (light) atom to have the smaller (larger) amplitude.

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# A Simplified Procedure for Orientation of Single Crystals of Any Structure

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Single crystals with any type of crystal structure can be set up in any desired orientation by a simple and time-saving method of comparing the Laue pattern of the single crystal with a computed and plotted Laue pattern. For this orientation procedure a special goniometer polishing jig has been developed. As examples, both the determination of an unknown direction and the preparation of a specified crystal plane of a hexagonal structure are demonstrated.

## Introduction

In the field of solid-state and surface physics many physical properties depend on the orientation of single crystals (see *e.g.* Butz, Erley & Wagner, 1971; Krahl-Urban & Wagner, 1972). As long as such investigations are restricted to the main directions (*e.g.* [100], [110], and [111]) of cubic crystals, it will be easy to recognize