

To distinguish between cases *A* and *B* the following experiment was performed. The crystal was aligned to measure the primary reflection with the counter set at the proper angle to monitor the primary intensity. The idea is then that if the situation conforms to case *B* (Bragg–Bragg) the secondary reflection could be measured on the same side of the crystal as the incident beam, while if it is in case *A* (Bragg–Laue) the secondary reflection would be eventually detected on the other side of the crystal.

In a given experiment, the intensity of the primary reflection around the azimuth  $28.212^\circ$ , corresponding to the secondary reflection  $\bar{1}\bar{1}1$  or 133 depending on whether case *A* or *B* was being produced, was measured. In order to distinguish between the two cases the detector was moved to that position on the same side of the crystal where reflection

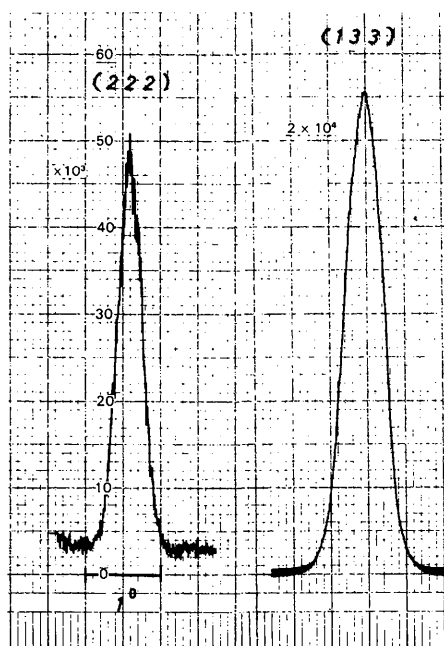


Fig. 2. The recorded intensities of the primary (222) reflection and of the secondary (133) reflection in the case of (000,222,133/ $\bar{1}\bar{1}1$ ) (Cu  $K\alpha_1$ ).

133 would appear in the Bragg–Bragg case (*B*). That this was actually the case is demonstrated by the intensities recorded in both measurements, shown in Fig. 2.

Once the Bragg–Bragg case has been identified the corresponding *umweg* peak in the Renninger diagram is attributed the indices 133, then the other multiple diffraction peaks can be indexed without ambiguity.

The method can be applied whenever there exist a couple of corresponding dynamical situations, involving two three-beam cases, one of the Bragg–Bragg and the other of Bragg–Laue type, where the secondary and the coupling reflections are interchanged. In the case of cubic structures we have actually proved that any pair of reflections  $60^\circ$  away in the Renninger diagram satisfy this exigence. In conclusion, we have thus been able to distinguish between two situations which are dynamically equivalent, thus producing the same intensity measurement, on the basis of diffraction geometry.

It is observed that the method makes a clear distinction between the two directions  $[1\bar{1}0]$  and  $[0\bar{1}1]$  which served to mark the origins of the Renninger diagram. Since any of them is transformed by the threefold axis into the opposite of the other, this implies that by using this method one is able to distinguish between the direction  $[1\bar{1}0]$ , and its opposite  $[\bar{1}10]$  without recourse to anomalous dispersion.

Finally, it is worth while to point out that the method just discussed does not provide a general way to distinguish among equivalent reflections. In fact, since germanium belongs to the centrosymmetric space group  $Fd\bar{3}m$ , it is impossible to distinguish between the direction  $[222]$  and its opposite  $[\bar{2}\bar{2}\bar{2}]$ ; moreover, the distinction would not make any sense from a physical point of view since the structure looks exactly alike from both directions and the X-ray diffracted intensities are exactly the same, as they would be for any centrosymmetric crystal.

However, after choosing the indices of the primary reflection, and because of the peculiarities of the diffraction geometry, some particular opposite directions in the structure can be distinguished, as has been shown above in the case of  $[1\bar{1}0]$  and  $[\bar{1}10]$ .

#### References

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*Acta Cryst.* (1978). **A34**, 826–827

**Seminvariants in space groups  $P312$ ,  $P3_112$ ,  $P3_212$ ,  $P\bar{6}$ ,  $P\bar{6}m2$  and  $P\bar{6}c2$ .** By SVEN HOVMÖLLER, *Department of Structural Chemistry, University of Stockholm, Fack, S-106 91 Stockholm, Sweden*

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Errors in the tables given by Hauptman & Karle [*Acta Cryst.* (1956), **9**, 45–55] are corrected.

The number of reflections needed to fix the origin in the space groups  $P312$ ,  $P3_112$ ,  $P3_212$ ,  $P\bar{6}$ ,  $P\bar{6}m2$  and  $P\bar{6}c2$  is 1, not 2 as stated by Hauptman & Karle (1956), Giacovazzo (1974) and by Karle (1974) in *International Tables for X-ray Crystallography*. The seminvariant vector in these space

groups is  $(2h + 4k + 3l)$  and the seminvariant modulus is 6. This is equivalent to the pair of congruences  $(h - k) \equiv 0 \pmod{3}$  and  $(l) \equiv 0 \pmod{2}$ . Since in all other space groups the number of elements in the seminvariant vector is equal to the number of reflections needed to fix the origin, it is

preferred to express the seminvariant as  $(2h + 4k + 3l)$  rather than  $(h - k, l)$ .

The 6 equivalent origins are correctly given as  $(0, 0, 0)$ ,  $(0, 0, \frac{1}{3})$ ,  $(\frac{1}{3}, \frac{2}{3}, 0)$ ,  $(\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$ ,  $(\frac{2}{3}, \frac{1}{3}, 0)$  and  $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ . It looks as if one needed to specify the origin in two directions, *i.e.* along the  $z$  axis and in the  $xy$  plane. However, it is only necessary to specify the origin in one direction, along the line passing through  $(0, 0, 0)$  and  $(\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$ . All the six permissible origins lie on this line since they are generated by the successive addition of  $(\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$  to  $(0, 0, 0)$ . The origin is uniquely specified through the fixation of the phase of one reflection which will take on different phase values in the six permissible origins, each differing by  $2\pi/6$ .

The only reflections which do not take on different values in the six permissible origins are those which have  $(2h + 4k + 3l) = n6$ . This proves the seminvariant vector to be  $(2h + 4k + 3l)$  and the seminvariant modulus to be 6.

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**A discussion of the solution for the best rotation to relate two sets of vectors.** BY W. KABSCH, *Max-Planck-Institut für Medizinische Forschung, Abteilung Biophysik, Jahnstrasse 29, 6900 Heidelberg, Federal Republic of Germany*

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A method is discussed for obtaining the best proper rotation to relate two sets of vectors.

The simple procedure for obtaining the best rotation to relate two sets of vectors described in an earlier paper (Kabsch, 1976) has been used in processing oscillation films (Kabsch, 1977), for the determination of non-crystallographic symmetry elements (Kabsch, Gast, Schulz & Leberman, 1977), and for a comparison of macromolecules. In the last application an improper rotation was sometimes obtained from the procedure (Nyburg & Yuen, 1977). The purpose of this communication is to show how a best proper rotation can always be obtained from the procedure.

Let  $\mathbf{x}_n$  and  $\mathbf{y}_n$  ( $n = 1, \dots, N$ ) be two given vector sets and  $w_n$  the weights corresponding to each pair  $\mathbf{x}_n, \mathbf{y}_n$ . All possible orthogonal matrices  $\mathbf{U}$  for which the function

$$E = \frac{1}{2} \sum_n w_n (\mathbf{U}\mathbf{x}_n - \mathbf{y}_n)^2 \quad (1)$$

has an extremal point must obey [see equation (9) of Kabsch, 1976]

$$\mathbf{U}(\mathbf{S} + \mathbf{L}) = \mathbf{R}. \quad (2)$$

Writing  $x_{nk}$  and  $y_{nk}$  for the  $k$ th components of the vectors  $\mathbf{x}_n$  and  $\mathbf{y}_n$  the matrices  $\mathbf{R}$  and  $\mathbf{S}$  are defined as

$$\mathbf{R} = (r_{ij}) = \left( \sum_n w_n y_{ni} x_{nj} \right) \quad (3)$$

$$\mathbf{S} = (s_{ij}) = \left( \sum_n w_n x_{ni} x_{nj} \right). \quad (4)$$

$\mathbf{L} = (l_{ij})$  is a symmetric matrix of Lagrange multipliers which is determined from the equation

$$(\mathbf{S} + \mathbf{L})(\mathbf{S} + \mathbf{L}) = \tilde{\mathbf{R}}\mathbf{R}. \quad (5)$$

In the tables given by Hauptman & Karle (1956) and Karle (1974) the type should be  $3P6$ , not  $3P32$ . In the notation of Giacovazzo (1974) the  $H-K$  group is  $(2h + 4k + 3l)P6$ . In all tables the seminvariant phases should be  $\Phi_{hkl}$  where  $(2h + 4k + 3l) \equiv 6$ . The permitted values for semi-independent phases are  $\|6\|$ , except for  $\|2\|$  for  $h + 2k = n3$  and  $\|3\|$  for  $l$  even. The number of phases linearly semi-independent to be specified is 1.

#### References

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KARLE, J. (1974). *International Tables for X-ray Crystallography*, Vol. IV, p. 343, Table 6.1C. Birmingham: Kynoch Press.

$\tilde{\mathbf{R}}\mathbf{R}$  is a known symmetric positive definite matrix whose positive eigenvalues  $\mu_k$  and eigenvectors  $\mathbf{a}_k$  can be determined by standard procedures. The general solution of (5) is of the form

$$(\mathbf{S} + \mathbf{L}) = (s_{ij} + l_{ij}) = \left( \sum_k a_{ki} a_{kj} \cdot \sigma_k \sqrt{\mu_k} \right), \quad (6)$$

where  $a_{ki}$  denotes the  $i$ th component of  $\mathbf{a}_k$  and the arbitrary quantities  $\sigma_k$  can only assume the values  $\pm 1$ . If an eigenvalue  $\mu_k$  is degenerate the eigenvector  $\mathbf{a}_k$  of  $\tilde{\mathbf{R}}\mathbf{R}$  cannot be determined uniquely. However,  $\mathbf{S} + \mathbf{L}$  will not be affected by this ambiguity if all its eigenvalues of the magnitude  $\sqrt{\mu_k}$  have identical signs. The final construction of all orthogonal matrices  $\mathbf{U} = (u_{ij})$  for which  $E$  assumes an extremal point is given by

$$u_{ij} = \sum_k b_{ki} a_{kj}, \quad (7)$$

where  $b_{ki}$  is the  $i$ th component of the vector

$$\mathbf{b}_k = \mathbf{U}\mathbf{a}_k = \mathbf{U}(\mathbf{S} + \mathbf{L})\mathbf{a}_k / (\sigma_k \sqrt{\mu_k}) = \mathbf{R}\mathbf{a}_k / (\sigma_k \sqrt{\mu_k}). \quad (8)$$

The residual  $E$  at each extremal point is

$$\begin{aligned} E &= \frac{1}{2} \sum_n w_n (\mathbf{U}\mathbf{x}_n - \mathbf{y}_n)^2 = \frac{1}{2} \sum_n w_n (\mathbf{x}_n^2 + \mathbf{y}_n^2) \\ &\quad - \sum_n w_n \mathbf{y}_n \cdot (\mathbf{U}\mathbf{x}_n) \\ &= \frac{1}{2} \sum_n w_n (\mathbf{x}_n^2 + \mathbf{y}_n^2) - \sum_n w_n \left[ \sum_k (\mathbf{b}_k \cdot \mathbf{y}_n) (\mathbf{x}_n \cdot \mathbf{a}_k) \right] \\ &= \frac{1}{2} \sum_n w_n (\mathbf{x}_n^2 + \mathbf{y}_n^2) - \sum_k \mathbf{b}_k \cdot (\mathbf{R}\mathbf{a}_k) \\ &= \frac{1}{2} \sum_n w_n (\mathbf{x}_n^2 + \mathbf{y}_n^2) - \sum_k \sigma_k \sqrt{\mu_k}. \end{aligned} \quad (9)$$