

$G_{sh}^2$  will form a constant  $C_{sh}$  for an infinitesimal spherical shell in reciprocal space. Then (6) becomes

$$M_{st}^r \approx Z_r^2 \int_{sphere} C_{sh} \int_{shell} V_s V_t . \quad (7)$$

$|S|$  is constant for a given shell, and we can write  $S_t = |S| \cos \varphi$ ,  $S_k = |S| \sin \varphi$  for an orthogonal coordinate system. Now integration of the various products  $V_s V_t$  over the shell leads to the integrals

$$\int_0^{2\pi} \cos^p \varphi \sin^q \varphi d\varphi$$

with  $p, q = 0, 1, 2, 3, 4$ , and  $p + q = 4$ , and to the integral with  $p = q = 1$ . (The integrals are known in terms of  $\Gamma$ -functions.) These integrals are the same for each shell considered and are denoted by  $q_{st}$ . Then (7) becomes

$$M_{st}^r \approx CZ_r^2 q_{st} .$$

$C$  represents the integral over all shells in reciprocal space and includes all constant factors which arise on integration over the shell. For an infinite number of data  $C$  approaches infinity, and so does  $M_{st}^r$ . For establishing the weighting matrix, however, only the ratio  $M_{st}^r/C$  will be needed. If we now consider all atoms ( $r = 1 \dots n$ ), the approximate matrix  $\mathbf{Q}$  becomes a block-diagonal matrix because of non-squared geometrical terms. With the introduction of the factor of 4 the  $r$ th block is then

$$\mathbf{Q}^r = Z_r^2 \begin{pmatrix} 3 & 1 & 1 & & & \\ 1 & 3 & 1 & & & \\ 1 & 1 & 3 & & & \\ & & & 4 & & \\ & & & & 4 & \\ & & & & & 4 \end{pmatrix} . \quad (8)$$

We now eliminate the initial restriction that the coordinate system of the molecule coincides with the crystal system, but still retain orthogonality. Then the reference system in the spherical shell is rotated, but as integration is carried out over the whole shell, the integrals remain unchanged. Hence (8) holds for any orthogonal system to which the

$U^r$ -tensors are referred. Thus  $\mathbf{Q}^r$  should be used as weighting matrix for the  $r$ th atom.

Equation (8) no longer holds when the  $U^r$ -tensors refer to oblique crystal axes. We can derive (8) for this case by making use of the requirement that, with a non-orthogonal transformation w.r.t. unit axes  $\mathbf{Q}$  and  $\mathbf{M}$  have to be equally transformed. Let this transformation be

$$\mathbf{X}_C = \mathbf{A}\mathbf{X}_S$$

for the components of  $\mathbf{X}$  in  $\text{\AA}$  ( $C$  denotes the oblique,  $S$  the orthogonal (standard) crystal system); then  $\mathbf{M}$  is transformed according to

$$\mathbf{M}_C = \bar{\mathbf{L}}^{-1} \mathbf{M}_S \mathbf{L}^{-1} , \quad (9)$$

where  $\mathbf{L}$  is a  $6 \times 6$  matrix derived from the  $9 \times 9$  Kronecker-product  $\mathbf{A} \times \mathbf{A}$ . The elements of  $\mathbf{L}$  are

$$L_{uv} = A_{il} A_{kl} \quad \text{for } u = u(i, k), v = v(l, l)$$

and

$$L_{uv} = A_{il} A_{km} + A_{im} A_{kl} \quad \text{for } v = v(l, m)$$

with  $u, v = 1 \dots 6$ .  $\mathbf{Q}_C$  is obtained from  $\mathbf{Q}_S$  by substituting  $\mathbf{Q}$  for  $\mathbf{M}$  in (9).

If the appropriate weights are used in CK's method, CK's and PA's approaches are equivalent with respect to the use of diffraction data, and thus with respect to minimizing standard deviations. From the computational point of view PA's approach is certainly advantageous: the number of parameters to be refined and thus the number of normal equations to be set up is reduced to the minimum possible (see also Pawley, 1965). CK's approach, however, allows a number of tests to be made with the use of the atomic vibration tensors, of which PA's approach is inherently incapable.

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**Unit-cell parameters and space group of molybdenyl(VI) acetylacetonate.** By D. GRDENIĆ and E. TKALČEĆ\*,  
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The yellow crystals of molybdenyl(VI) acetylacetonate (Fernelius, Terada & Bryant, 1960) suitable for crystallographic measurements were obtained from an acetylacetonone solution to which petroleum spirit had been added without mixing and left over several days at room temperature. The prism-shaped crystals have a great number of faces which are found by goniometric measurements to be related through a centre of symmetry. The smallest unit cell, found from oscillation and Weissenberg photographs taken with nickel-filtered Cu K radiation, has the dimensions

$$a = 8.19 \pm 0.02, \quad b = 12.50 \pm 0.02, \quad c = 12.76 \pm 0.02 \text{ \AA};$$

$$\alpha = 104.2 \pm 0.2^\circ \quad \beta = 82.3 \pm 0.2^\circ \quad \gamma = 92.4 \pm 0.2^\circ$$

and contains four formula units of  $\text{MoO}_2(\text{C}_5\text{H}_7\text{O}_2)_2$  ( $\rho_{\text{calc}} = 1.71 \text{ g.cm}^{-3}$ ,  $\rho_{\text{obs}} = 1.79 \text{ g.cm}^{-3}$ ). No conditions limit-

ing possible reflexions were found. The goniometric measurements strongly indicated the pinacoidal class; the space group is  $P\bar{1}$  ( $C_1^1$ , No. 2).

We do not intend to proceed with the crystal-structure analysis of this compound. We are indebted to the Rudjer Bošković Institute, Zagreb for experimental facilities.

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