is much the same for all **TLS** components, we have only listed the principal components L_i of the libration tensor, and their standard deviations. Also, the maximum deviations found between any two respective components in different systems are listed under the heading Δ_{max}. Although these maximum deviations attain values up to 30% of the largest principal component L_i of a given molecule, only once do they exceed two standard deviations. As can be seen from Table 1 the trend of the values of $\Delta_{max}(L_i)$ and $\sigma(L_i)$ is much the same. The $\sigma(L_i)$ are computed from standard statistical formulae, but they do, of course, not only contain statistical errors of the observed components U_r^{ik}, but also systematic experimental errors and insufficiencies of the rigid-body model. That insufficiencies of the rigid-body model do indeed influence the standard deviations $\sigma(L_i)$ can be seen from the fact that in those cases where a negative value of L_i was computed, $\sigma(L_i)$ is fairly large.

To sum up:

(1) There is a definite influence of the choice of the (Cartesian) coordinate system – or, equally, of the choice of the weighting system – upon the values obtained for the components of **TLS**, but the variation of the results will rarely exceed two standard deviations. Thus in most cases this impact does not seem to cause much trouble. In this sense we can confirm Hirshfeld & Shmueli's (1972) conclusion.

(2) The variation of the results obtained in different (Cartesian) coordinate systems is more or less proportional to the magnitude of the calculated standard deviation, no matter what the reason for a possible large value of the standard deviation may be. Hence not only the choice of the coordinate system – or the choice of the weighting matrix – but also the standard of the **TLS** refinement has an effect on the scattering of the final values of the parameters **TLS**.

(3) In order to obtain (and publish) unique results the use of a covariance (weighting) matrix, which remains invariant under changes of the coordinate system, is recommended. Simple covariance matrices in a Cartesian system are obtained either with $\eta=0$, which is diagonal, or with $\eta=-\frac{1}{4}$, which is not diagonal but can be better defended on physical grounds.

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To find the largest sphere which can be inscribed between four others.

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An algorithm is given for determining the radius of a sphere inscribed in the cavity between four different spheres arbitrarily separated.

When considering the packing of atoms and molecules in a crystal it is often necessary to calculate the sizes of the cavities remaining in the structure. This question can be paraphrased as: find the radius of the sphere inscribed in the cavity between four tangent spheres.

If the four spheres are also mutually tangent, then the problem has an elegant solution in terms of the curvatures α, β, γ and δ (the reciprocals of the radii) of the four known spheres and the curvature ε of the inscribed (or circumscribed) sphere. These are related by $(\alpha+\beta+\gamma+\delta+\varepsilon)^2=3(\alpha^2+\beta^2+\gamma^2+\delta^2+\varepsilon^2)$. In N dimensions the general relationship $N(\sum\alpha^2)=(\sum\alpha)^2$ has been proved by Coxeter (1952).

If, however, the four spheres 1, 2, 3 and 4 are not mutually tangential but have radii r_1, r_2, r_3, and r_4 and their centres at distances d_{12}, d_{13}, *etc.* apart, no formula has been found in the literature and recourse to a computational procedure was necessary.

Five points, the centres of the five spheres, define four vectors, **12**, **13**, **14** and **15**. These four vectors involve 10 distances between the five points which would be sufficient to define a simplex (generalized tetrahedron) in four dimensions. The four-dimensional volume V of this simplex is given by a determinantal equation:

$$-(96)^2V^2=\begin{vmatrix} 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & d_{15}^2 & 1 \\ d_{12}^2 & 0 & d_{23}^2 & d_{24}^2 & d_{25}^2 & 1 \\ d_{13}^2 & d_{23}^2 & 0 & d_{34}^2 & d_{35}^2 & 1 \\ d_{14}^2 & d_{24}^2 & d_{34}^2 & 0 & d_{45}^2 & 1 \\ d_{15}^2 & d_{25}^2 & d_{35}^2 & d_{45}^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix}.$$

If our figure is not four-dimensional, but is degenerate and three-dimensional, as real configurations of atoms of course are, then this determinant will be zero. This relationship then enables us to find (from a quadratic equation) any one of the ten distances d_{ij} in terms of the others.

This can be used for at least two purposes. The first is: given the three distances of a point P from three fixed points A, B and C (at given distances from each other) and also the corresponding three distances of a point Q from the same three points, find the distance PQ. The two solu-

tions of the quadratic correspond to having P and Q on the same, or on opposite, sides of the reference triangle ABC. This application is convenient for triangulation in three dimensions using only distances and is independent of coordinate axes.

The second use is for solving the problem propounded above. Suppose the radius of the fifth sphere, inscribed between spheres 1, 2, 3 and 4, is R, then the determinant relating the ten distances becomes:

$$D(R) = \begin{vmatrix} 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & (r_1+R)^2 & 1 \\ d_{12}^2 & 0 & d_{23}^2 & d_{24}^2 & (r_2+R)^2 & 1 \\ d_{13}^2 & d_{23}^2 & 0 & d_{34}^2 & (r_3+R)^2 & 1 \\ d_{14}^2 & d_{24}^2 & d_{34}^2 & 0 & (r_4+R)^2 & 1 \\ (r_1+R)^2 & (r_2+R)^2 & (r_3+R)^2 & (r_4+R)^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0.$$

The problem thus reduces to one of finding the appropriate zero of $D(R)$. This is readily computed with a subroutine for the evaluation of a determinant by pivotal condensation. R is increased by small steps from zero. When $D(R)$ changes sign we take one step back and advance by smaller steps and so on until R is known to the required accuracy. The negative root corresponds to the circumscribing sphere.

The basic formula used above for the volume of a simplex can be proved by reducing the determinant of order 6 (rank 4) to one of order 4 by subtracting the first row from each of the other rows and doing similarly with the first column. If the four vectors corresponding to d_{12}, d_{13}, d_{14} and d_{15} are written **a**, **b**, **c** and **d** then, since $(\mathbf{a}-\mathbf{b})^2-\mathbf{a}^2-\mathbf{b}^2 = -2\,\mathbf{a}\,.\,\mathbf{b}$, the determinant becomes

$$-(-2)^4 = \begin{vmatrix} \mathbf{a}^2 & \mathbf{a}\,.\,\mathbf{b} & \mathbf{a}\,.\,\mathbf{c} & \mathbf{a}\,.\,\mathbf{d} \\ \mathbf{a}\,.\,\mathbf{b} & \mathbf{b}^2 & \mathbf{b}\,.\,\mathbf{c} & \mathbf{b}\,.\,\mathbf{d} \\ \mathbf{a}\,.\,\mathbf{c} & \mathbf{b}\,.\,\mathbf{c} & \mathbf{c}^2 & \mathbf{c}\,.\,\mathbf{d} \\ \mathbf{a}\,.\,\mathbf{d} & \mathbf{b}\,.\,\mathbf{d} & \mathbf{c}\,.\,\mathbf{d} & \mathbf{d}^2 \end{vmatrix}.$$

This is the determinant of the metric matrix and gives the square of the four-dimensional volume of the parallelepiped (measure polytope) outlined by the vectors **a**, **b**, **c** and **d**. The volume of the simplex is found from that of the parallelepiped by dividing by 4!.

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Corrections to the Tables in Chapter 5.1, *Reduced Cells*, given in the 1969 edition of Volume I of *International Tables.*

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Corrections are given to Table 5.1.2.2 of *International Tables for X-ray Crystallography*, Vol. I (1969), Birmingham: Kynoch Press)

Certain errors have been found in *International Tables for X-ray Crystallography* (1969) in addition to those already pointed out by Mighell, Santoro & Donnay (1971) and the corrections are given below.

Table 5.1.2.2 on page 532

Fourth matrix row from top of table:

Replace matrix S′ $\begin{pmatrix} \mathbf{a}\,.\,\mathbf{a} & \mathbf{b}\,.\,\mathbf{b} & \mathbf{c}\,.\,\mathbf{c} \\ \mathbf{a}\,.\,\mathbf{b}-\mathbf{a}\,.\,\mathbf{c} & \dfrac{\mathbf{a}\,.\,\mathbf{a}}{2} & \mathbf{a}\,.\,\mathbf{b} \end{pmatrix}$

by: $\begin{pmatrix} \mathbf{a}\,.\,\mathbf{a} & \mathbf{b}\,.\,\mathbf{b} & \mathbf{c}\,.\,\mathbf{c} \\ \mathbf{a}\,.\,\mathbf{b}-\mathbf{b}\,.\,\mathbf{c} & \dfrac{\mathbf{a}\,.\,\mathbf{a}}{2} & \mathbf{a}\,.\,\mathbf{b} \end{pmatrix}$

Bottom matrix row of table:

Replace matrix S $\begin{pmatrix} \mathbf{a}\,.\,\mathbf{a} & \mathbf{b}\,.\,\mathbf{b} & \mathbf{c}\,.\,\mathbf{c} \\ \mathrm{X} & \mathbf{a}\,.\,\mathbf{c} & \mathbf{a}\,.\,\mathbf{b} \end{pmatrix}$

by: $\begin{pmatrix} \mathbf{a}\,.\,\mathbf{a} & \mathbf{b}\,.\,\mathbf{b} & \mathbf{c}\,.\,\mathbf{c} \\ -\mathrm{X} & \mathbf{a}\,.\,\mathbf{c} & \mathbf{a}\,.\,\mathbf{b} \end{pmatrix}$

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