

relationship between the normal-tridecamer and the relaxed fragment could be found.

The marked difference between the conformations of the relaxed and the unrelaxed crystal fragments are probably entirely due to the small size of the fragments. Although it cannot easily be verified by calculation (in view of the large number of molecules involved), we anticipate that these differences will decrease, and eventually vanish, when more shells are added (a crystal may be considered as a central molecule with a large number of shells). These differences should be sufficiently small to render the comparison (i) feasible. Even so, the comparison (ii), although leading to the same result, has the advantage that the comparison of cluster conformations can be replaced by a comparison of energies, since a cluster that is *similar* to the unrelaxed fragment is *identical* to the relaxed fragment, with the same energy.

Conclusion

The considerable change in conformation of the 13-molecule crystal fragment upon relaxation supports the view that a 13-molecule cluster is too small to justify assumptions

concerning its significance in connection with crystallite formation. Williams's assumption that the normal cluster could lead to crystallite formation, whereas the iso-cluster could be broken up by thermal agitation, is based on the observation that the central molecule has a lower energy in the normal-tridecamer than in the iso-tridecamer. The difference is very small (*ca* 1%) and could easily change sign when more molecules are added. No conclusions can be drawn from the view that the energy of the central molecule should increase in a uniform manner, when molecules are added to the cluster: the figure -2.0 (Williams, 1980, Table 2) does not fit significantly better in the pattern of energy increments than would the figure -1.7 .

We conclude that it is necessary to add more molecules to the clusters in order to be able to relate their conformations to the observed crystal structure and to establish their significance in relation to crystallization.

References

- BACON, G. E., CURRY, N. A. & WILSON, S. A. (1964). *Proc. R. Soc. London Ser. A*, **279**, 98–110.
WILLIAMS, D. E. (1980). *Acta Cryst.* **A36**, 715–723.

Acta Cryst. (1981). **A37**, 764–765

Estimates of the standard deviations of ring-puckering coordinates. By R. NORRESTAM, *Structural Chemistry Group, Chemistry Department B, The Technical University of Denmark, DK-2800 Lyngby, Denmark*

(Received 9 February 1981; accepted 19 March 1981)

Abstract

Expressions are derived for estimating the standard deviations of Cremer–Pople ring-puckering coordinates, with the assumption that the e.s.d.'s of the atomic positions are approximately isotropic.

The puckering of an N -membered monocyclic ring may be described by the amplitude and phase coordinates introduced by Cremer & Pople (1975). Expressions for calculating the e.s.d.'s of puckering coordinates, assuming independent atomic positions with nonisotropic e.s.d.'s, become rather complicated (Taylor, 1980). As shown in the present paper, considerably simpler expressions for calculating these e.s.d.'s are obtained if isotropic e.s.d.'s of independent positions can be assumed, *viz* $\sigma'_j \sim [(\sigma_x^2 + \sigma_y^2 + \sigma_z^2)/3]^{1/2} \text{ \AA}$ for $j = 1, 2, \dots, N$. Such an assumption is frequently a good approximation, when deriving the structural parameters from three-dimensional single-crystal diffraction data.

Cremer & Pople define the ring-puckering coordinates $q_m \geq 0$ and $\varphi_m < 2\pi$ by

$$c_m \equiv q_m \cos \varphi_m = (2/N)^{1/2} \sum Z_j \cos [2\pi m(j-1)/N] \quad (1)$$

$$s_m \equiv q_m \sin \varphi_m = -(2/N)^{1/2} \sum Z_j \sin [2\pi m(j-1)/N]$$

0567-7394/81/050764-02\$01.00

for $m = 2, 3, \dots, (N-1)/2$, and an additional coordinate

$$q_{N/2} = N^{-1/2} \sum (-1)^{j-1} Z_j \quad (2)$$

if N is even. The sums are all over $j = 1, 2, \dots, N$. The Z_j values occurring in (1) and (2) denote the perpendicular displacement of the j th atom from a uniquely defined mean plane (*cf.* Cremer & Pople, 1975) passing through the geometrical center of the ring. Since this center has an e.s.d. $\sigma_0 = (1/N)(\sum \sigma_j^2)^{1/2}$ and as the coordinate transformation involved to obtain the Z_j values is unitary, the e.s.d.'s of the Z_j values can be approximated by $\sigma_j \simeq [(\sigma'_j)^2 + \sigma_0^2]^{1/2}$. By deriving the e.s.d.'s of c_m and s_m as $\sigma^2(c_m) = \sum (\sigma_j \times \partial c_m / \partial Z_j)^2$ and $\sigma^2(s_m) = \sum (\sigma_j \times \partial s_m / \partial Z_j)^2$, we obtain from (1)

$$\begin{aligned} \sigma^2(c_m) &= (2/N) \sum \{\sigma_j \cos [2\pi m(j-1)/N]\}^2 \\ \sigma^2(s_m) &= (2/N) \sum \{\sigma_j \sin [2\pi m(j-1)/N]\}^2 \\ &= [(2/N) \sum \sigma_j^2] - \sigma^2(c_m). \end{aligned} \quad (3)$$

From $q_m^2 = c_m^2 + s_m^2$ and $\tan \varphi_m = s_m/c_m$ we obtain in a similar way

$$\begin{aligned} \sigma^2(q_m) &= \sigma^2(c_m) \cos^2 \varphi_m + \sigma^2(s_m) \sin^2 \varphi_m \\ \sigma^2(\varphi_m) &= [\sigma^2(c_m) \sin^2 \varphi_m + \sigma^2(s_m) \cos^2 \varphi_m] / q_m^2. \end{aligned} \quad (4)$$

For the additional coordinate $q_{N/2}$ (N even), we obtain

$$\sigma^2(q_{N/2}) = (1/N) \sum \sigma_j^2. \quad (5)$$

© 1981 International Union of Crystallography

Thus, $\sigma(q_{N/2})$ is simply the root-mean-square (r.m.s.) value of the positional e.s.d.'s.

If the positional e.s.d.'s are roughly the same, we can as a further approximation assume that all σ_j can be replaced by $\sigma = [(1/N) \sum \sigma_j^2]^{1/2}$, i.e. replaced by the r.m.s. value σ . Since $\sum \cos^2 [2\pi m(j-1)/N] = \sum \sin^2 [2\pi m(j-1)/N] = N/2$, it follows from (3)–(5) that for this case

$$\sigma(c_m) = \sigma(s_m) = \sigma(q_m) = \sigma(q_{N/2}) = \sigma \quad (6)$$

and $\sigma(\varphi_m) = \sigma/q_m$.

For the spherical polar set (Q, θ, Φ) introduced by Cremer & Pople (1975) to describe the puckering of six-membered rings [*viz* $Q = (q_2^2 + q_3^2)^{1/2}$, $\theta = \arctan(q_2/q_3)$ and $\Phi = \varphi_2$], the expressions for the e.s.d.'s of Q and θ are (*cf.* Taylor, 1980) analogous to those for $\sigma(q_m)$ and $\sigma(\varphi_m)$. Thus,

$$\begin{aligned} \sigma^2(Q) &= \sigma^2(q_3) \cos^2 \theta + \sigma^2(q_2) \sin^2 \theta \\ \sigma^2(\theta) &= [\sigma^2(q_3) \sin^2 \theta + \sigma^2(q_2) \cos^2 \theta] / Q^2. \end{aligned} \quad (7)$$

For the case when all σ_j can be replaced by their r.m.s. value, σ , the e.s.d.'s of Q and θ become

$$\sigma(Q) = \sigma \quad \text{and} \quad \sigma(\theta) = \sigma/Q. \quad (8)$$

Taylor (1980) has given two examples of calculations of puckering-parameter e.s.d.'s, with his expressions for non-isotropic e.s.d.'s of independent atomic positions. For the

pyranose rings observed in the crystal structures of β -DL-arabinopyranose (Takagi, Nordenson & Jeffrey, 1979) and β -L-arabinopyranose (Takagi & Jeffrey, 1977) he obtained for the spherical polar set Q, θ, Φ : 0.584 (1) Å, 2.1 (1)°, 140 (3)° and 0.573 (2) Å, 1.5 (2)°, 116 (7)°, respectively. Calculating the e.s.d.'s from individual isotropic positional e.s.d.'s, as suggested in the present paper [formulas (3)–(5) and (7)], yields the same rounded-off e.s.d.'s (*viz* 0.00098 Å, 0.096°, 2.7° and 0.0018 Å, 0.18°, 6.7°, respectively). These e.s.d. values are furthermore obtained even if the individual positional e.s.d.'s are replaced by their r.m.s. value, σ [formulas (6) and (8)]. The two examples thus illustrate the validity of the different approximations utilized in the present study.

References

- CREMER, D. & POPLE, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
 TAKAGI, S. & JEFFREY, G. A. (1977). *Acta Cryst.* **B33**, 3033–3040.
 TAKAGI, S., NORDENSON, S. & JEFFREY, G. A. (1979). *Acta Cryst.* **B35**, 991–993.
 TAYLOR, R. (1980). *Acta Cryst.* **A36**, 828–829.

Acta Cryst. (1981). **A37**, 765–766

A table of maxima and minima of the Bessel functions $J_n(z)$ for $n = 0$ to $n = 30$. By K. W. ANDREWS, *Department of Metallurgy, University of Sheffield, Sheffield S1 3JD, England*

(Received 2 March 1981; accepted 13 April 1981)

Abstract

Maxima and minima are tabulated for the Bessel functions $J_n(x)$ for values of n from 0 to 30 [*i.e.* zeros of $J'_n(x)$]. The first six points are recorded for each function. The table considerably extends the range of earlier tables available in the literature. It should have applications in the interpretation of diffraction patterns from helical or wave-form structures or features, and has been used in connection with some electron microscope images.

Bessel functions of the first kind of order n , where n is a positive integer, have come into the calculations and interpretation of diffraction patterns from helical (or wave-form) structures. Particular applications include the interpretation of X-ray diffraction patterns from large biological molecules based upon helices (Cochran, Crick & Vand, 1952; Klug, Crick & Wyckoff, 1958; Sherwood, 1976). The same principles have been successfully applied to the interpretation of electron microscope images of such molecules and their associated growth forms in biological or bio-medical sections (Misell, 1978). More recently, images of metal structures containing dislocations or other features

have been interpreted in the same way (Andrews & Keown, 1981).

Standard tables are available in two volumes of functions (Abramowitz & Stegun, 1965; Jahnke & Emde, 1945). Generally, numerical values of the Bessel functions are given and their zeros. Maxima and minima are also provided in Table 9.5 of Cochran, Crick & Vand (1952) for values of n up to and including 8. Table 1 may be regarded as an extension of this table and also one provided by Spiegel (1974). A formula given by Gray & Matthews (1922) and Gray & Macrobert (1966) does not appear to be entirely reliable and the calculations have been based upon a computer program used in the Medical Research Council Laboratory of Molecular Biology (Cambridge).

For some practical purposes values to one or two decimal places are sufficiently accurate. Graphical interpolation is also accurate for some applications, and reference may also be made to the recurrence relation

$$J'_n(z) = J_{n-1}(z) - J_{n+1}(z)$$

so that the maxima and minima are at values of (z) where J_{n-1} and J_{n+1} intersect. Evidently the present tabulation is more accurate and should be available as an addition to the tables for these functions and for use when required by