parison of Figs. 3*a* and 3*b* shows that this is so, and that whereas in the untwinned structure $(H_2O)_2$ formed hydrogen bonds with O_1 and O_3, in the twinned structure it can form hydrogen bonds of approximately the same length with ${}_tO_1$ and ${}_tO_2$. Similarly $(H_2O)_1$ can form bonds with ${}_tO_2$ and ${}_tO_3$ and $(H_2O)_3$ with ${}_tO_1$ and ${}_tO_3$.

The explanation can be summarized by saying that the operation of a diad axis with a mirror plane perpendicular to it is equivalent to a centre of symmetry, and since in this structure β is nearly 90° and the plane (001) is almost a plane of symmetry the twinning operation, or rotation of the structure through 180° about the z axis, is nearly equivalent to the operation of a centre of symmetry in the actual structure.

We wish to thank Sir Lawrence Bragg and Dr W. H. Taylor for facilities and constant encouragement, and Dr Rodd of Imperial Chemical Industries Ltd., Dyestuffs Division, for suggesting this problem and providing material. One of us (J. M. B.) is indebted to the Department of Scientific and Industrial Research for a maintenance grant.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

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The accuracy of electron-density maps in X-ray structure analysis.

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With the increasing application of X-ray crystallography to the study of details of molecular structure, considerable attention is now being given to the accuracy of the electron-density maps obtained in X-ray crystallography. To obtain the maximum value from the results of structure analysis, as of any scientific investigation, it is necessary to eliminate systematic errors, and, having estimated the random errors, to subject any metrical interpretation of the results to standard statistical tests of significance. The systematic errors of electron-density maps are due to the use of finite Fourier series; Booth (1945, 1946*a*, 1947) has shown how these may be corrected by evaluating syntheses in which the coefficients are structure factors calculated from the 'final' atomic co-ordinates. These syntheses have their peaks slightly displaced due to the finite series; corrected co-ordinates are then obtained by applying these displacements with reversed signs to the 'final' co-ordinates.

The random errors are due to the method of correction for finite series, experimental errors, and rounding-off errors in computation. In the case of three-dimensional syntheses it can be shown that the experimental and finite-series-correction errors lead to a standard deviation (S.D.) of the error in the slope of the electron density in the x-direction (at any point in the unit cell) given by

$$\sigma\,(A_x)=\frac{2\pi}{aV}\left[\sum_3 mh^2\overline{\Delta F}^2\right]^{\frac{1}{2}}, \qquad (1)$$

and to similar expressions for $\sigma\,(A_y)$ and $\sigma\,(A_z)$. In this and following expressions ΔF is the difference between observed and calculated structure factors; $\sigma\,(U)$ or σ_u is a S.D.; A_p and A_{pq} are first and second differentials respectively of the electron-density ρ; h, k and l are Miller indices (for brevity the subscripts in ΔF_{hkl} are omitted); a, b and c are cell dimensions; and V is the volume of the unit cell ($=abc\sin\beta$ in the monoclinic case). In (1) each independent ΔF appears once only and m is the multiplicity of the F concerned; alternatively, the contents of the bracket may be written $\sum_3 h^2\overline{\Delta F}^2$, the summation then being over every plane in the synthesis. The S.D.'s of the errors in the density and second differentials are

$$\sigma\,(\rho)=\frac{1}{V}\left[\sum_3 m\overline{\Delta F}^2\right]^{\frac{1}{2}}, \quad \sigma\,(A_{xy})=\frac{4\pi^2}{abV}\left[\sum_3 mh^2k^2\overline{\Delta F}^2\right]^{\frac{1}{2}}.$$

The corresponding formulae for plane projections are exactly analogous. The above results are for centrosymmetric structures; for non-centrosymmetric structures they must be multiplied by $\sqrt{2}$.

The S.D.'s of a peak position are obtained, after substituting $\sigma\,(A_x)$, $\sigma\,(A_y)$ and $\sigma\,(A_z)$, by statistical solutions of Booth's (1946*b*) differential equations for peak positions. For spherically symmetrical peaks in a monoclinic cell this gives

$$\sigma_y=\sigma\,(A_y)/A_{yy}$$

and

$$\sigma_x=[\overline{\sigma\,(A_x)}^2-\cos^2\beta\,\overline{\sigma\,(A_z)}^2]^{\frac{1}{2}}/A_{xx}\sin^2\beta,$$

with a similar expression for σ_z, where A_{pq}, the second differential at the peak, is obtained either from the electron-density map or by differential synthesis (Booth, 1946*b*). For orthorhombic cells (or monoclinic with β nearly 90°),

$$\sigma_x = \sigma\ (A_x)/A_{xx}.$$

To these errors the random errors of computational rounding-off must be added. With three-figure computing methods these will be negligible. An analysis, unfortunately not reducible to a simple formula, shows that using two-figure Beevers-Lipson strips the computing error for dibenzyl (Jeffrey, 1945, 1947) is $\sigma_x = 0{\cdot}004$ A., roughly half the other random error.

As the number of ΔF's involved is large, the probability distribution for the random errors is Gaussian, so that significance levels are easily obtained from error functions. Suppose that a bond length A is found to be a, with S.D. σ_a, and that another bond length B (in the same or a different structure) is b ($<a$), with S.D. σ_b, and that it is wished to test whether A is significantly longer than B. If A has the same actual bond length as B the probability that its observed length should, on account of random errors, exceed that of B by $(a-b)$ or more is

$$P = \tfrac{1}{2} - \frac{1}{\sqrt{\pi}} \int_0^x \exp\,[-t^2]\,dt = \tfrac{1}{2} - \tfrac{1}{2}\,\mathrm{erf}\,x,$$

where

$$\sqrt{2}\,x = (b-a)/(\sigma_a^2 + \sigma_b^2)^{\frac{1}{2}}.$$

Values of $P \leqslant 0{\cdot}01$ are commonly taken as indicating a significant difference between a and b, and $0{\cdot}01 < P < 0{\cdot}05$ as 'possibly significant'.

We illustrate the method by examining the central C–C bonds in dibenzyl. Using punched card methods, similar to those described by Cox, Gross & Jeffrey (1947), but adapted for differential syntheses, the bond lengths after correction for finite series are found to be C_1'–$C_1 = 1{\cdot}510$ A. (across the centre of symmetry), and C_1–$C_2 = 1{\cdot}523$ A. The problem is, are these lengths significantly less than the C–C single bond as found in diamond (1·5445 A. with an error which is negligible for our present purpose (Lonsdale, 1947))? The random error was found to be $\sigma_x = 0{\cdot}0074$ A.; hence the S.D.'s of the bond lengths are respectively $2 \times 0{\cdot}0074$ A. (since the peaks are symmetrically dependent), and $\sqrt{2} \times 0{\cdot}0074$ A. Applying significance tests we find $P = 0{\cdot}010$ and $0{\cdot}020$ respectively. For the difference of the angle C_1'–C_1–C_2 from the normal tetrahedral angle we find $P = 0{\cdot}00024$. Statistical analysis thus gives confirmation to the conclusion (Jeffrey, 1945, 1947) that these bonds are different from C–C single bonds.

The assumptions made in the treatment of errors outlined above may not be universally valid; this and other points will be discussed in a detailed account of accuracy problems now being prepared.

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Notes and News

International Union of Crystallography

Statutes and By-Laws

The Statutes and By-Laws of the International Union of Crystallography, as adopted on 31 March 1947, are printed below. Copies of these Statutes and By-Laws may be obtained from the General Secretary (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

STATUTES

I. *Objects of the Union*

1. The objects of the Union are:
   - (i) To promote international co-operation in crystallography.
   - (ii) To promote international publication of crystallographic research and of crystallographic works.
   - (iii) To facilitate standardization of methods and of units in crystallography.
   - (iv) To form a focus for the relations of crystallography to other sciences.
2. The Union is a member of the International Council of Scientific Unions.

II. *Membership*

3. A country adheres to the Union through a National Committee duly recognized by the General Assembly. Each National Committee represents Crystallography in its own country.
4. The term 'country' shall be understood to include Dominions, Colonies, Protectorates and any dependencies which budget independently for scientific purposes.
5. Each country may adhere to the Union in any one of eight Groups I–VIII with corresponding voting powers and contributions as set out in paragraphs 8 and 10.
6. A country may select different Groups for general purposes and for individual special projects. The National Committee of each country shall inform the General Secretary at the beginning of each General Assembly of the Group, or Groups, adopted for the period to the next General Assembly.

III. *Administration*

7. The work of the Union shall be directed by the General Assembly of delegates appointed by the National Committees.
8. Voting at General Assemblies shall be by countries,