Water molecules and the incoherent nuclei within the crystal will change their distribution during a period of three to four years as a result of seasonal changes embodying a temperature variation of about 30°C. The argument advanced by Agrawal (1974) that paracrystallinity is shown only by fibrous crystals is incorrect in view of the fact that non-fibrous crystals have also been found to exhibit paracrystalline distortions (Urban & Hosemann, 1972). It can also be added that based on paracrystalline disorder the appearance of rounded and polygonal and other arbitrarily shaped spots can be easily explained, as indicated in our paper, by taking the fluctuations of a more involved type than that described in the said paper (Tiwari, Prasad & Srivastava, 1973).

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Precision lattice constant determination: erratum. By W. L. BOND, *W. W. Hansen Laboratories of Physics, Stanford University, Stanford, California, U.S.A.*

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A corrected version is given of equation (10) in Bond [*Acta Cryst.* (1960). **13**, 814–818].

In the paper by Bond (1960), equation (10) should read

$$x=(\tfrac{1}{2}w)^2 \cot 2\theta\{(2+\sin^2 2\theta)/(2-\sin^2 2\theta)\}$$

where x and w are in radians.

This value should be added to the apparent Bragg angle. For $\theta > 45°$, $\cot 2\theta$ is negative, so the correction is to be subtracted.

Reference

BOND, W. L. (1960). *Acta Cryst.* **13**, 814–818.

Acta Cryst. (1975). A**31**, 698

Preliminary refinement of protein coordinates in real space. By R. J. FLETTERICK* and H. W. WYCKOFF, *Department of Molecular Biophysics and Biochemistry, Yale University, New Haven, Connecticut* 06520, *U.S.A.*

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A simple unconstrained steepest-descent procedure is described for the preliminary refinement of protein coordinates in real space. The method is illustrated by application to ribonuclease S.

The typical procedure used to determine the atomic coordinates of proteins from single-crystal X-ray diffraction analysis makes use of the optical comparator described by Richards (1968) to build a skeletal model of the protein into the electron density map. The positions of the component atoms are then carefully measured from this model and transformed into a suitable reference frame for comparison with the Fourier map. The atomic coordinates are thus subject to systematic errors at each stage in this procedure. These errors might, for example, arise from a misplaced reference origin, rotational shifts, shears and non-orthogonality of the reference axes. The random errors related to the difficulty in fitting the skeletal model in the poorly defined regions of the electron density map and the exact disposition of the bond angles and dihedral angles within the skeletal model are exceedingly difficult problems and will not be considered here, as they have been treated by Diamond (1971).

The systematic errors are, however, amenable to treatment by a simple unconstrained steepest-descent procedure which is outlined below. The results of this analysis are presented for ribonuclease S.

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