Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1972). A**28**, 213

Comments on Gruber's algorithm.

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Gruber's algorithm [Gruber, B. (1970) *Acta Cryst.* A**26**, 622] for determining the symmetry and stacking properties of Bravais-lattice planes can be applied to problems in reciprocal space.

Gruber (1970) has published an interesting algorithm for determining the symmetry and stacking properties of Bravais-lattice planes.

It would seem that the algorithm can be applied to problems in reciprocal space as well, with useful results as follows. The normal to the direct lattice plane (*hkl*) is the reciprocal axis [*hkl*]*. From reciprocity, it follows that the normal to the reciprocal lattice plane (*uvw*)* is the direct space zone axis [*uvw*]. Thus, by supplying *uvw* instead of *hkl*, and reciprocal lattice parameters instead of direct ones the algorithm will determine the size and shape of reciprocal lattice planes as seen on precession photographs or on thin-crystal electron diffraction patterns.

The second of the worked-out examples in Gruber's paper contains a misprint. In the value for t_3, the ratio $\frac{21}{42}$ should read $\frac{1}{42}$.

The author has programmed the algorithm in Fortran. Copies of the program may be obtained upon request.

Reference

GRUBER, B. (1970). *Acta Cryst.* A**26**, 622.

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The standard deviation of the torsion angle.

By R. H. STANFORD JR and JÜRG WASER, *Gates and Crellin Laboratories of Chemistry,* California Institute of Technology, Pasadena, California* 91109, *U.S.A.*

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Formulas are derived for calculating a torsion angle and its standard deviation. The positions of the four atoms defining the torsion angle are assumed to be uncorrelated and the positional standard deviations are assumed to be isotropic.

Given a sequence of four (usually bonded) atoms, 1, 2, 3, and 4, whose positions are uncorrelated, and the isotropic standard deviations of their positions, formulas are derived for the torsion angle about the line between atoms 2 and 3 and its standard deviation.

The position of each atom can be represented by:

$$\mathbf{r}_n = x_n\mathbf{i} + y_n\mathbf{j} + z_n\mathbf{k} \quad (n = 1, 2, 3 \text{ or } 4), \tag{1}$$

where x_n, y_n, z_n are the orthogonalized coordinates of atom n, and **i**, **j**, and **k** are the usual Cartesian unit vectors. The variances of the atomic positions are assumed to be isotropic, that is

$$\sigma^2(x_n) = \sigma^2(y_n) = \sigma^2(z_n) = \sigma_n^2. \tag{2}$$

Define the interatomic vectors:

$$\mathbf{r}_{mn} = \mathbf{r}_n - \mathbf{r}_m . \tag{3}$$

Then, a vector normal to the plane defined by atoms 1, 2, and 3 is:

$$\mathbf{t}_1 = \mathbf{r}_{21} \times \mathbf{r}_{23}; \tag{4}$$

and a vector normal to the plane defined by atoms 2, 3, and 4 is:

$$\mathbf{t}_2 = \mathbf{r}_{32} \times \mathbf{r}_{34} . \tag{5}$$

The angle between these normals is the torsion angle, τ, about the line between atoms 2 and 3, and

$$\cos\tau = \mathbf{t}_1 \cdot \mathbf{t}_2 / t_1 t_2 . \tag{6}$$

(The conventional sign of τ is discussed later.)

Substitution of (1) and (3) into (4) and (5) yields:

$$\mathbf{t}_l = a_l\mathbf{i} + b_l\mathbf{j} + c_l\mathbf{k} \quad (l = 1 \text{ or } 2), \tag{7}$$

where the coefficients a_l, b_l, c_l are given under 'general coordinates' in Table 1,

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