

the relationship  $a^3 = V = 3n\lambda^3/(32\pi)$  (or  $a^2 = A = n\lambda^2/(4\pi)$  in the two-dimensional case). This method then gives a theoretical value for the curvature of a particular atom with a known scattering factor, which may differ from the experimental value because the crystal unit-cell volume may not satisfy  $V = 3n\lambda^3/(32\pi)$ . The difference will be largest for a point atom, in which case  $\Sigma h^2 \cdot f_{\sin\theta} = Z\Sigma h^2$ , which is constant for constant  $n$ , while the coefficient  $4\pi^2/(a^2V)$  will vary with  $V$ . The error thus depends on how much  $V = a^3$  differs from  $3n\lambda^3/(32\pi)$ , and will be  $[(3n\lambda^3/32\pi V)^{5/3} - 1] \times 100\%$  (or  $[(n\lambda^2/4\pi A)^2 - 1] \times 100\%$  in two dimensions). With more diffuse atoms  $\Sigma h^2 \cdot f_{\sin\theta}$  will vary with  $V$  and partly compensate for this error. Thus the expressions above give the maximum error. Table 2 gives the values of  $-\partial^2\rho/\partial x^2$  as calculated from two values of  $a$  for which  $n = 81$ .  $a = 2.07 \text{ \AA}$  is the optimum value.

Hence using Cu  $K\alpha$  radiation the curvature may be calculated from the equation

$$\partial^2\rho/\partial x^2 = 9.12[f_{0.500} + 4f_{0.707} + 4f_{0.866} + 4f_{1.000}]$$

(corresponding to  $a = 1.54 \text{ \AA}$ ) for the three-dimensional case.

For diffuse atoms it is probably better to use

$$\partial^2\rho/\partial x^2 = 2.08[f_{0.372} + 4f_{0.526} + 4f_{0.645} + 4f_{0.744} + 20f_{0.832} + 24f_{0.911}]$$

(corresponding to  $a = 2.07 \text{ \AA}$ ).

The equation for two dimensions is

$$\partial^2\rho/\partial x^2 = 5.03[f_{0.386} + 2f_{0.547} + 4f_{0.774} + 10f_{0.865}]$$

(corresponding to  $a = 1.99 \text{ \AA}$ ).

This method of determining  $\partial^2\rho/\partial x^2$  is thus both rapid and reliable, and can easily be adapted for use with other wave lengths of X-radiation. By sampling the Fourier transform at such large intervals one might expect considerable errors, but it is also found that calculating  $\rho_{\max}$  using such wide meshes, remarkably good results are obtained.

### Reference

COSTAIN, W. (1941). Ph.D. Thesis, University of Birmingham.

### Erratum to Laue Obituary, *Acta Cryst.* (1960), 13, 513.

The verse from Kallimachos is, unfortunately, incorrectly quoted, and this will make it difficult to find it in

anthologies. Instead of ξφησαν (they said) it should begin with εἰπέτις (someone said).

P. P. EWALD.

## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands).*

### World Directory of Crystallographers

The second edition of this Directory appeared in August 1960. It contains short biographical data of 3557 scientists from 54 countries, arranged in alphabetical order by countries, and individuals within the countries. The biographical data include (a) full name and title; (b) year of birth; (c) information on field of study, university and year of highest degree; (d) present position, name and address of institution; (e) in some cases private address; and (f) major scientific interests. General Editor: D. W. Smits.

### Crystallographic Data for Various Polymers

For purposes of ready reference a table listing currently available crystallographic data for a variety of crystal-

lizable polymers was compiled and has been published: R. L. Miller and L. E. Nielsen, *J. Polymer Sci.* 44, 391 (1960). Copies are available from the authors who would be pleased to receive further data and/or references for inclusion in the table and to receive any comments on it. Address: Robert L. Miller, Research Department, Plastics Division, Monsanto Chemical Company, Springfield 2, Mass., U. S. A.

### The Geophysical Laboratory of the Carnegie Institution

The Geophysical Laboratory of the Carnegie Institution offers a postdoctoral fellowship in crystallography. The attention of interested people is called to their advertisement in this issue of *Acta*.