

display the level symmetry of trigonal systems as shown schematically in Fig. 2. This is to be expected if the heavy atoms occupy special positions in the hexagonal lattice. For instance, reflexions on planes (110), ( $\bar{1}20$ ), and ( $2\bar{1}0$ ), of the trigonal system give rise to strong intensities. The indices of these planes transform to (120), ( $\bar{1}30$ ) and ( $\bar{2}10$ ) respectively in the intermediate monoclinic system and are seen to be among the strongest reflexions in the triclinic system. They form with the equivalent  $h\bar{k}0$  reflexions, a group which has

very nearly  $C_6$  symmetry (Fig. 2). Furthermore the three strongest reflexions form an approximately trigonal arrangement in the first reciprocal layer, reminiscent of the upper-layer symmetry of the  $C_3$  point group.

#### Reference

WANG, S. N. & LU, C. S. (1944). *J. Amer. Chem. Soc.* **66**, 1113–1114.

### Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (M.M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.*

**Critical evaluation of chemical and physical structural information.** Edited by D. R. LIDE JR and M. A. PAUL. Pp. xii + 628, Figs. 108, Tables 85. Washington: National Academy of Sciences, 1974. Price \$26.25.

The rather uninspiring title of this book hides the fact that it is really a record of substantial progress in a variety of methods of structure determination. Or, to anyone who makes a rather superficial use of the methods concerned, it is a record of how to do better.

The book contains the proceedings of the Conference on Critical Evaluation of Chemical and Physical Structural Information held in the U.S.A. in June 1973. It could be called a high-powered conference, and certainly the list of contributors is most distinguished, but the book is a mine of information (even simple advice) on how to get the best from one's measurements.

The word 'structure' is interpreted in its widest molecular sense to include the following types of information: the geometric arrangement of atoms in a free molecule or crystal (symmetry, interatomic distances, bond angles); the description of the forces between these atoms (bond-stretching and bending-force constants, barriers to internal rotation, and other large amplitude motions); molecular parameters related to the electronic charge distribution (electric and magnetic moments, chemical shifts, coupling constants, charge-density maps).

Experimental methods whose data-processing techniques are discussed include gas-phase electron diffraction, rotational, vibrational and optical spectroscopies, liquid-crystal n.m.r., crystallography, and protein crystallography. Emphasis is given to consideration of the accuracy and reliability of the structural information obtained, and stress is made of the pitfalls which can occur when results from separate determinations, by similar as well as different methods, are compared. Other topics considered include the methods of deriving harmonic and anharmonic force fields and data on large-amplitude motions, and there are sections on the determination of electronic charge distributions and the *ab initio* method of calculating structural information.

In his preface to the book, which could be regarded as a reliable review in itself, D. R. Lide Jr makes some general observations about the views expressed by contributors: 'in most of the fields discussed, the statistical treatment of experimental data cannot be regarded as completely satisfactory . . . least-squares fitting techniques now in use

are not necessarily the best way of handling large data sets . . . no fitting technique can be expected to replace completely the judgement of the experimentalist in distinguishing random errors from systematic errors or model deficiencies'.

Some may shudder when confronted with this book and its implications on the need for time-consuming statistical analysis (and for time-consuming *thinking*) but if reliability is required, then the requisite care must be taken: 'fools rush in where angels fear to tread' is a suitable proverbial warning for the unwary! This is not just another book of conference proceedings, but a major milestone in its field.

BRIAN BEAGLEY

*Department of Chemistry*  
*UMIST*  
*Sackville Street*  
*Manchester M60 1QD*  
*England*

**Landolt-Börnstein. Numerical data and functional relationships in science and technology. Group III. Crystal and solid state physics. Vol. 7. Crystal structure data of inorganic compounds.** Edited by K. -H. HELLWEGE and A. M. HELLWEGE. Part *a*: by W. PIES and A. WEISS. Pp. xxxii + 647. Berlin: Springer, 1973. Price (cloth) DM 436, U. S. \$178.80. Part *g*: by W. PIES and A. WEISS. Pp. 463. Berlin: Springer, 1974. Price (cloth) DM 220, U. S. \$90.20.

The Landolt-Börnstein New Series Group III Volumes *5a* and *5b*, giving crystal data on organic crystals, and volume *6* giving data on elements and intermetallic phases have already been published [for reviews see *Acta Cryst.* (1972). **B28**, 1317–1318; *J. Appl. Cryst.* (1972). **5**, 384]. Volume 7 Parts *a* to *h* are to give data on inorganic crystals (some 18000 compounds). Fig. 1, taken from the inside cover of Volume 7, shows the arrangement of compounds by key elements in Parts *a* to *f*. Thus Part *a*, under review here, gives data on halides. Part *g*, also under review, lists the literature references for Parts *a* to *f* and Part *h* will be a comprehensive index for Volume 7.

The tables of crystal data give the formula of the compound, the space group and lattice parameters,  $Z$  (the number of formula units in the unit cell),  $D_m$  and  $D_x$  (in parentheses), the crystal structure type, whether the atomic positions were determined, how the crystal data were obtained and other incidental information such as colour of