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Recensiones

Molecular Structures and Dimensions, Vol. A 1, Interatomic Distances 1960—65, Organic and Organometallic Crystal Structures; Edited by Olga Kennard, D. G. Watson, F. H. Allen, N. W. Isaacs, W. D. S. Motherwell, R. C. Pettersen, W. G. Town. Utrecht: A. Oosthock 1972, $ 45

This volume is the first in a new reference series published by the International Union of Crystallography as a continuation of the Tables of Interatomic Distances by L. E. Sutton. It makes conveniently available a wealth of X-ray and some neutron diffraction data on 86 chemical classes of solids published from 1960 to 1965. The key information consists of tables on bond lengths, bond angles and torsion angles between atoms (excluding hydrogen) for more than 1000 compounds. The molecules range in size from carbon tetrabromide (CBr_4) to Vitamin B_{12} ($C_{63}H_{88}CoN_{14}O_{14}P$); the classes include e.g. peptides, antibiotics, steroids, alkaloids and a large number of metal complexes.

The way the material is organized is impressive. An introduction outlines criteria for inclusion and ordering of entries, describes the setup of standard, partial, multiple and amalgamated entries and finally elaborates on the evaluation procedures. Then a list of the 86 classes follows. The actual information is contained in the entries. Each entry consists of the name of the compound, molecular formula, bibliographic reference, chemical diagram and stereographic diagram (most helpful!), text and data. The text can contain seven categories of information: editorial comments, space group symbol, number of formula units per unit cell, the realiability factor R of the structure determination, supplementary references, code for computer usage and Landholt-Börnstein number. Most important is that the published data were screened for errors before inclusion. Summary tables are given for C–C, C–N and C–O bonds. All other interatomic distances between element-pairs are listed with their particular references. Finally, a molecular formula index, an author index and a multiple entry compound name index provide efficient access to the data.

What impresses the non-specialist, i.e. non-crystallographer most, is that a concerted effort has been made to organize, screen and present material in a useful way for a large group of potential users. The editors have set an example for researchers in other fields: particularly quantum chemistry could and should afford a systematic survey and critical presentation of its molecular data beyond the scope presently envisioned.

It is almost needless to add that the setup is lavish. Computerized printing has contributed to keep the cost of this valuable volume down so that even individuals can afford it. For libraries the acquisition of this volume is a must.

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