

Many of the crystals for which structure analyses are available are not in fact of such a high degree of purity, and from the structural point of view this is generally not important. But when one is considering some physical properties, a trace of impurity may change not merely the scale, but the very nature of the phenomenon observed. Throughout this book, therefore, the author very properly deals critically at every stage with the experimental methods used in the determination of the constants referred to, and with the sources from which data are obtained, and also draws attention to such difficulties as, for example, the tendency of some physical 'constants' to change gradually for some time after recrystallization and only to settle down to their final value after several hours, or to depend upon compactness or preferred orientation, in the case of polycrystalline specimens.

In the first section of the book, the author considers what is known about molecular size, shape and weight of organic compounds in the crystalline state, attempting, as is his aim throughout, to derive general relationships between compounds in homologous series or having common features, physical or chemical. In a succeeding chapter, which crystallographers will certainly find very unsatisfactory, he offers a résumé of what is known from X-ray and crystallographic studies of organic compounds. The criticism that may be made here is not merely that the résumé is inadequate, but that it is not always accurate, either because the author has not used the latest data available at the time of writing, or because he has not realized that some of the theory to which he gives prominence is itself based on wholly inaccurate data. This is most obvious in the table illustrating Weissenberg's symmetry theory of 1928, to which he devotes three pages, by comparison with half a page given to discussion of the hydrogen bond. Nevertheless, even here, in spite of one's irritation at the opportunities lost, one is caught up, every now and then, by an interesting new facet of some well known facts or by some hitherto unknown fact or relationship. The author is particularly in his element in discussing polymorphism and reversible and irreversible transformations, isomorphism, mixed crystallization and the relationships in and between homologous series.

The chapter discussing physical constants of organic compounds in the crystalline state, which might have been expected to occupy most of the book, is in fact limited to sixty pages. Specific heat and dielectric constant account for about forty of these; density, specific volume, coefficient of expansion and compressibility for another eight; mechanical properties for two-and-a-half; while rotatory power, piezo- and pyro-electric effects, magnetochemistry, refractive indices, dispersion, Raman and infra-red spectra are given the remaining nine pages and are then never mentioned again.

The whole of the remaining 350 pages of the book is really devoted to the phenomena of transformation, solidification and melting. Seventy-two pages are given up to a list, with references, of organic substances having melting points below -20° C. One wonders why. Very little is said about the actual process of crystallization and nothing about modern theories of crystal growth. But the author enjoys himself tremendously in pointing out all sorts of relationships, many of them previously unknown to at least one X-ray crystallographer, between

melting points of different substances and different groups of substances under different conditions; and there is a riot of curves and tables showing critical points, phase diagrams, latent heats, entropies and the connection of these with molecular constitution and shape, crystal lattice and so on. One could not help feeling that there is an absolute mine of information only a little way outside the field in which crystallographers usually wander.

Did you know that *cis*-isomers are usually yellowish and have low m.p.'s relative to *trans*-isomers, which are colourless? Did you know that the high members of normal long-chain homologous series all converge towards a m.p. of about 110° C.? Did you know that the speed of crystallization of methyl alcohol is sensitive to the presence of even 1 part in 20,000 of water? Or that CCl_4 and CBr_4 , which have two isomorphous forms at lower pressures, are apparently not isomorphous at high pressures, and why? Or that the entropy of melting is apparently directly related to the molecular 'surface area'? Well, perhaps you did; but even so, you will almost certainly find here some other interesting and suggestive data.

As in most French books there is a table of contents but no subject index. The long bibliographic index does not mention W. H. Bragg, although he is mentioned in the text. The index of compounds occupies twenty-four pages.

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Crystal Data. Classification of Substances by Space Groups and their Identification from Cell Dimensions. By J. D. H. DONNAY and WERNER NOWACKI with the collaboration of GABRIELLE DONNAY. Pp. ix + 719. The Geological Society of America; Memoir 60. 1954. Price \$5.00.

This volume undertakes to give crystallographic data, obtained by X-ray and electron diffraction, for some thousands of substances. The information concerns the symmetry and geometry of the cell.

The work consists of two parts. These were originally two separate compilations and joint publication was not considered until after Part I was finished and Part II near its completion. The intention is that this publication will be the prelude to a *Handbook of Crystallography*.

Part I (*Systematic Tables*) by Werner Nowacki (University of Berne), classifies crystalline substances by space groups. The important section of Part I, the Main Table *B* (following *A*, the Introduction) shows the distribution of 3800 different compounds among the space groups. These are arranged under the seven crystal systems and are subdivided according to their chemical composition into seven categories. The subdivision according to chemical composition is arbitrary but may have its uses.

Following the Main Table *B*, are six tables under *C* which give statistical information as follows: distribution of crystalline substances among the 219 distinguishable space groups; among the seven crystal systems (lattice symmetries); among the 32 crystal classes; among the translation groups; into symmorphic, hemisymmorphic and asymmorphic and among the most frequent space groups.

Under *D* we find abbreviations of the names of scien-

tific journals used in Table *E*, and under *E* are given the full references to literature indicated by a number only in the Main Table *B*.

In a paper in 1942, Nowacki described the result of a statistical survey of the space-group determinations that had been published up to that date. The work now under review includes in addition about 800 new space-group determinations, thus bringing this information up to the year 1948. The purpose of this statistical survey, as the author points out, is to collect empirical data and not to draw conclusions.

J. D. H. Donnay (The Johns Hopkins University, Baltimore), with the collaboration of Gabrielle Donnay, is responsible for Part II (*Determinative Tables*), which forms the larger part of *Crystal Data* (pp. 137-719). This contains tables for the identification of some 5000 crystalline substances from cell dimensions, space groups, specific gravity and other properties.

In the Introduction *A*, Donnay advocates M. J. Buerger's precession method (1944), showing that it is easy and fast to obtain cell dimensions and space group, especially when precession and Weissenberg methods are

| <i>a/b</i> | <i>c/b</i> | beta | <i>a</i> | <i>b</i> | <i>c</i> | Space group | <i>Z</i> | Struct. type | Spec. grav. | |
|------------|------------|---------|----------------|--------------|--------------|-------------|----------|--------------|------------------|----------------|
| | | | | | | | | | meas. | calc. |
| 0.774 | 0.364 | 93° 19' | 7.51 ± 0.04 | 9.70 0.04 | 3.53 0.03 | $P2_1/n$ | 4 | GO_{12} | 2.221 or 2.20 | 2.16 ± 0.04 |

Sodium acid carbonate, $NaHCO_3$ (SB III, 86, 804)A. (*a* : *b* : *c*)_{lit.} = 0.7645 : 1 : 0.3582. beta_{lit.} = 93° 19'.

used together. The work involved, in a favourable case, is not greater than that required for measuring the many interplanar spacings from a powder pattern and in estimating the relative intensities of the lines. He says 'Since identification by powder diffraction data cannot, in all rigor, be considered reliable until all the lines have been indexed, or matched with those of a previously indexed standard, the knowledge of the cell dimensions and diffraction aspect actually is a prerequisite to a safe application of the powder method. Although single-crystal data obtained by X-rays are given in several compendia, they are not listed in such a manner as to be useful for determinative purposes.'

Donnay describes his *Determinative Tables* as based on cell constants such that the absolute dimensions of the cell edges are known. The cell chosen to define the lattice must obey a set of rules applied in a given sequence. For example, the cell chosen for a triclinic crystal, after other rules have been satisfied, is that whose cell edges are the shortest lattice translations that render all inter-edge angles non-acute. Its edges will then be labelled so that $c < a < b$. Axial ratios have been chosen nevertheless as determinative numbers so that the tables may also be used where relative dimensions obtained by measurement with the goniometer are the only ones

available. These axial ratios are arranged in order of increasing magnitude. It may seem surprising when absolute measurements of cell dimensions are available that axial ratios should be used, but the ratios are not limited as they are in practice when based on angles between developed faces. Thus in the monoclinic system, *a* : *b* varies from 0.167 to 19.45. Also the accuracy with which some cell dimensions are known makes possible 3 or 4 significant figures in the axial ratio, and thus leaves room for a very large number of substances distinguishable from the numerical tables alone.

Still under the heading *A* (Introduction) are notes concerning the sources from which the data have been drawn; concordance of space-group notation, on the indexes of chemical formulae and chemical names, method of citing references, tables of transformations and finally notes on symbols and abbreviations used in Part II.

B (*Determinative Tables*), covering 423 pages, form the most important part of the volume and these are arranged under the crystal systems. A specimen is given below:

These tables are followed by *C* (Appendix). Tables of space group criteria, the formula index and name index bring this volume to an end.

In order to avoid misprints the main portion of this book is produced by 'off-set printing' and an electric typewriter was used. Although the latter imposed certain minor restrictions, the reader welcomes the clarity and sharpness of the reproduction of the tables. This has been achieved in spite of the smallness of the type. The book lies open easily in spite of its bulk.

A certain overlapping between Parts I and II has resulted from the circumstances in which these originally independent parts have been brought together. The disarming modesty of the authors in their Preface makes criticism difficult and it is obvious to the user of the book that great and painstaking labour has gone into its making. The many transformations of axial ratios necessary is in itself a formidable task of calculation.

The authors are much to be congratulated on the production of this work which should find its place in every laboratory concerned with crystallography.

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