CRYSTAL DATA

DETERMINATIVE TABLES

Third Edition

Volume II: INORGANIC COMPOUNDS

General Editors: J. D. H. Donnay
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Committee for the Joint ACA–NBS Crystal Data Project

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ABSTRACT

This edition, which will comprise two volumes, is a thoroughly revised and updated work, containing over 24,000 entries. Some 7,500 carbon-containing crystalline compounds are given in Volume I. They are listed, within each crystal system, according to increasing values of a determinative number: a/b ratio in trimetric systems, c/a ratio in dimetric systems, cubic cell edge a in the isometric system. Conventional rules insure the uniqueness of crystal setting.

For each crystalline species the following properties are listed on the first line: axial ratio(s) and interaxial angles not fixed by symmetry, cell dimensions, space group or diffraction aspect, number of formula units per cell, crystal structure (whether determined), measured density, x-ray calculated density. Then come: name of the compound, synonym(s), chemical formula, literature reference, transformation matrix (when the original data had to be recast to conventional cell and setting). Additional information includes some or all of the following: crystal-structure type (if any), goniometric axial ratio(s), crystal habit, cleavages, twinning, color, optical properties, indices of refraction, optical orientation (except in the anorthic system), melting point, transition point.

Nearly all the data were obtained from original sources. "Limits of error" on numerical values are quoted from the reference. The data have been tested for self-consistency by means of computer programs. Any erratum found either in the reference or in an abstracting journal (e.g., *Structure Reports*) is specifically mentioned: erroneous values are thus identified. Editorial critical remarks point out possible errors in the literature.

Formula and name indexes enable one to learn if crystallographic information is available on any given compound, thereby providing a starting point for bibliographic searches.

Key words: Cleavage; compilation; crystal; crystal habit; crystal space group; crystal structure types; density; determination; identification; minerals; optical properties; twinning; unit-cell dimensions.

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FOREWORD

The National Standard Reference Data System provides effective access to the quantitative data of physical science, critically evaluated and compiled for convenience, and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, with responsibility to administer it assigned to the National Bureau of Standards.

The System now comprises a complex of data centers and other activities, carried on in academic institutions and other laboratories both in and out of government. The independent operational status of existing critical data projects is maintained and encouraged. Data centers that are components of the NSRDS produce compilations of critically evaluated data, critical reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. In addition, the centers and projects establish criteria for evaluation and compilation of data and make recommendations on needed improvements in experimental techniques. They are normally closely associated with active research in the relevant field.

The technical scope of the NSRDS is indicated by the principal categories of data compilation projects now active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

The NSRDS receives advice and planning assistance from the National Research Council of the National Academy of Sciences-National Academy of Engineering. An overall Review Committee considers the program as a whole and makes recommendations on policy, long-term planning, and international collaboration. Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The NSRDS–NBS series of publications is intended primarily to include evaluated reference data and critical reviews of long-term interest to the scientific and technical community.

LEWIS M. BRANSCOMB, *Director*

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The preparation of the third edition of *Crystal Data (Determinative Tables)* has been supported by the Office of Standard Reference Data, National Bureau of Standards, since 1963. Our thanks go to Dr. Edward L. Brady, Associate Director for Information Programs, formerly Chief of the Office, who has endorsed our efforts, given encouragement, and obtained the necessary funds to carry on the work. We are grateful to Dr. David R. Lide, Jr., the present Chief of the Office, who has continued this support and taken a personal interest in the success of our publication. The project was established in the Crystallography Section of the Institute for Materials Research of the National Bureau of Standards when it was under the direction of Mr. Howard F. McMurdie and it is now being continued under Dr. Stanley Block, present Chief of the Section. These two gentlemen deserve our thanks for the support they gave us, both as administrators and as crystallographers. In addition the Institute of Physics (Great Britain), through its X-ray Analysis Group, has provided financial help to the Cambridge editorial center, during the period 1962–63, in support of the work on organic compounds.

Moral support and active cooperation were obtained from the International Union of Crystallography and its Commission on Crystallographic Data.

Responsibility for data published in Russian was assumed by a group of crystallographers organized by Dr. N. L. Smirnova (MGU) in the U.S.S.R. Their names are: Z. P. Burmistrova (MGU), T. L. Khotsyanova (INEOS), P. I. Kripyakevich (L'vov State University), A. E. Miskinyan (MGU), Z. V. Pudovkina (IMGRE), and M. L. Vongaz (MGU). Help with Japanese data was given by Professor Ryoichi Sadanaga (University of Tokyo) and Professor Nobuo Morimoto (Osaka University) and with Italian publications by Professor Alessandro Vaciago (University of Rome). We would like to place on record this valuable international cooperation.

In this country the American Crystallographic Association demonstrated its interest in the work by establishing a permanent committee, known as the Committee for the Joint ACA–NBS Crystal Data Project. Its members are the various editors of Crystal Data. Our thanks are also due to the Director of the U.S. Geological Survey who authorized the participation of Miss Mary E. Mrose as Mineral Editor. We are very grateful for the special bibliographic facilities extended to us by Professor Jean Wyart, Director of the Centre de Documentation du C.N.R.S., Paris, France.

The updating of organic data was begun at the National Institute for Medical Research and at Birkbeck College, London, England. In 1962 the project was transferred to Cambridge, England. The Section Editor wishes to thank the Medical Research Council for allowing her to carry out this work and Professor Lord Todd for taking an interest in its development and providing space and facilities in the University Chemical Laboratory. The data compilation for the post-1959 period was begun by Mr. R. C. Cave and continued, from 1963, by Mrs. Stella Weeds, joined in 1966 by Dr. W. Tundak. Mrs. Weeds has done particularly valuable work in correcting entries of the first and second editions, amalgamating multiple entries, and checking the indexes. The Editors were also helped over the years by a number of part-time documentalists, including Dr. B. Rimmer, Mrs. L. Seward, and Mrs. J. Wheeler.

In 1965 the Office for Scientific and Technical Information undertook the support of new crystallographic data activities in Great Britain and established the nucleus of a Crystallographic Data Center in Cambridge. Members of this organization helped with the abstracting and checking of data sheets, and gave advice on a variety of problems. We are very indebted to the following colleagues: Dr. J. C. Goppola, Dr. J. K. Fawcett, Dr. K. Ann Kerr, and Dr. A. C. Larson. Our thanks are due to the Office for Scientific and Technical Informa-

tion for their generous support. We would like to thank Professor J. D. Bernal for his active interest and the inspiration he provided at various up-hill stages in the preparation of volume I.

A large number of crystallographers have kindly sent corrections to the second edition. Some have also contributed unpublished data. Several colleagues have helped with little-known languages. To all of them we tender our best thanks. The following names deserve special mention: L. G. Berry (Queen's University, Kingston, Ontario), Philip Coppens (Brookhaven National Laboratory), Eloise H. Evans (NBS), G. Gottardi (University of Modena, Italy), David J. Haas (U.S. Naval Research Laboratory, Washington, D.C.), David Harker (Roswell Park Memorial Institute, Buffalo, N.Y.), Sukeaki Hosoya (University of Tokyo), Jun Ito (NBS), G. Katz (Israel Mining Industries, Haifa), C. P. Kempter (Los Alamos Scientific Laboratory), F. H. Kruse (Los Alamos Scientific Laboratory), G. Kullerud (Geophysical Laboratory, Carnegie Institution of Washington), F. Liebau (University of Kiel, Germany), Caroline H. MacGillavry (University of Amsterdam), H. F. McMurdie (NBS), Rose Mooney-Slater (Massachusetts Institute of Technology), Marlene C. Morris (NBS), Dorita A. Norton (then at Roswell Park Memorial Institute, Buffalo, N.Y.), Y. Okaya (IBM Research Center, Yorktown Heights, N.Y.), Adolf Pabst (University of California, Berkeley), Jonathan Parsons (Henry Ford Hospital, Detroit, Michigan), Hans Ringertz (Karolinska Institutet, Stockholm), D. Rogers (Imperial College of Science and Technology, London), A. Rosenzweig (University of New Mexico), I. W. Ruderman (Isomet, Palisades Park, N.J.), A. Santoro (NBS), G. Strahs (New York Medical College, New York, N.Y.), H. E. Swanson (NBS), H. Takeda (University of Tokyo), David H. Templeton (University of California, Berkeley), M. Zocchi (NBS).

Library work has been materially facilitated by the cooperation of the staffs of the National Bureau of Standards Library, the Johns Hopkins University Library, the Geophysical Laboratory of the Carnegie Institution of Washington, the library of the U.S. Geological Survey, the New York Public Library, the library of the University Chemical Laboratory in Cambridge, England, and the library of the University of Marburg-on-Lahn, Germany.

Assistance, guidance, and encouragement were given by the staff of the NBS Office of Technical Information and Publications under the direction of W. R. Tilley. Particular thanks are given to John Carpenter and Betty Oberholtzer of the Publication Section, and to Rubin Wagner of the Computer Assisted Printing Section who served as liaison with the Government Printing Office. The exacting manipulation of the paper tapes, proof copy, and magnetic tapes, and the operation of the Linofilm and Linotron phototypesetting machines was performed by the Electronic Photocomposition Unit of the Government Printing Office under the direction of John Boyle and Elmo Wood. Advice and facilities were generously provided in the early stages by the Phototypographic Division of the National Geographic Society.

The following persons helped in the checking of data against the original references: Randolph Barton, Jr. (The Johns Hopkins University), Barry Castleman (JHU), Lawrence B. Coleman (JHU), Gregory Glass (Yale University), Joyce Grimes (NBS), Marie E. Hallam (JHU), Julia Hohl (Crystal Data), Zora Kipel (New York Public Library), Vitaut Kipel (NYPL), Harold Marr (University of Maryland), Sylvia Naldrett (Crystal Data), Milan Rieder (JHU), Karen Smith (NBS).

Computer programs for transformation of co-ordinate axes, space-group symbols, etc., and for checking the compatibility of data were first written by Hiroshi Takeda (University of Tokyo, pro tem. JHU). Consulting help was obtained from James Stewart (University of Maryland), who rewrote some of the original programs. These programs were used in code-checking the similar programs, compatible with the *Crystal Data* input, written at NBS. L. Taylor (Pennsylvania State University), Richard Yockman (Service Bureau Corporation), Marilyn J. Verdier (NBS), E. J. Howard (NBS), and George P. Hill (NBS) assisted with

various phases of computer programming. J. Hilsenrath (NBS), Carla Messina (NBS), and Rubin Wagner (NBS) converted the output tape from Linofilm to Linotron.

Proof-reading of the input copy was done by Sylvia Naldrett, Ellen Bailey Runk (NBS), and Virginia Boone Cullison (NBS). The paper tapes used as computer input were processed and prepared by James Thompson (Howard University), Karen Smith, Marie Krum (NBS), Virginia Boone Cullison (NBS), and Kay V. Sadtler (Crystal Data).

Alvin Perloff deserves special recognition for his meticulous scanning of computer output and page proof, leading to the detection of many errors which he was able to trace to the abstractor or the author himself. Boris Paretzkin and Carl R. Robbins provided invaluable help in checking data, particularly in the anorthic and monoclinic systems, where cell transformations are required.

Many helpers have given part-time assistance in various capacities. Their names follow: B. Rosine Bonanno (NBS), Simon J. Carmel (NBS), Martin Engelmann (Crystal Data), M. S. Monmonier (JHU), Frederic and Winifred E. Sykes (Morgan State College, Baltimore), Irene Munoz (Crystal Data), Colin C. McAneny (JHU), Sabine Stoss (Crystal Data), Betty L. Weigand (Crystal Data).

Mrs. Eula Lawson (NBS) performed, with infinite patience and unfailing accuracy, the monumental task of typing all our hand-written data on the intricate keyboard that produced the Linofilm paper tape. It is hard to find words that will adequately express our appreciation of her work.

PREFACE

The first edition of *Crystal Data*, published as Memoir 60 of the Geological Society of America (1954) comprised two parts: Systematic Tables, by Werner Nowacki, and Determinative Tables, by J. D. H. Donnay.

The two parts appeared separately in the second edition, as Monographs 5 and 6 of the American Crystallographic Association*: Determinative Tables, by J. D. H. Donnay, Gabrielle Donnay, E. G. Cox, Olga Kennard, and Murray Vernon King (1963); and Systematic Tables, by Werner Nowacki, A. Edenharter, and T. Matsumoto (1967).

This, the third edition of the Determinative Tables, has become so extensive that it is no longer feasible to publish it in a single volume. Volume I deals with organic compounds, a term here used to designate all carbon-containing compounds, for which Olga Kennard (Cambridge, England) is the section editor. It includes an updated revision of the appendix on protein crystal data, by Murray Vernon King (Massachusetts General Hospital), assisted by Krishna Venkatasubramanian, who helped with calculations. Volume II covers the elements and all compounds that contain no carbon. Data on some carbon-containing compounds, such as some carbides, carbonates, cyanides, and cyanates are listed in both volumes. The data on intermetallic compounds, which had been largely omitted from the previous edition, have now been completely recast by a group of specialists, M. H. Mueller (assisted by Harold W. Knott), Q. Johnson, E. R. Ryba, and D. A. Hansen, under the section editorship of Sten Samson (California Institute of Technology). Minerals have been the responsibility of Mary E. Mrose (U.S. Geological Survey); for this section we also received help from Rudolf Allmann (University of Marburg, Germany) and, for pyroxenes and amphiboles, from Michael Bown (University of Chicago). The remaining inorganic compounds have been processed by Helen M. Ondik (U.S. National Bureau of Standards) with the collaboration of Gerard M. Wolten (Aerospace Corporation, Los Angeles). Cellulose compounds, fibers, rubbers, other polymers, and compounds of high molecular weight have been omitted, as in previous editions.

The first edition covered the literature to 1950 inclusive. The second edition attempted to cover it to the end of 1960, but many entries were found to have been omitted. The cut-off date for inclusion in the third edition is January 1, 1967. The number of entries, which was about 6,000 in the first edition and about 13,000 in the second, now exceeds 24,000, despite a large-scale elimination of solid solution data and many amalgamations of entries.

Almost all the entries are based on original references. A few secondary references, mainly to *Strukturbericht* or *Structure Reports*, could not be eliminated. The 1961 *Chemical Abstracts* system of abbreviations of journal names has been adopted.

Computer data processing has been used extensively in the preparation of the present edition. All of the data for this edition were keyboarded manually on a keyboard designed for typesetting. This keyboard was chosen because it had available the special typographic symbols that we needed, e.g., Greek letters, subscripts, overscored numbers, accented letters, etc.

After the paper tape was prepared, it was run through a phototypesetting machine, which produced galleys for proofreading. The paper tape was read onto a magnetic tape for use by the computer. Corrections were keyboarded and put on magnetic tape. This correction tape and the master tape were merged by the computer, then these corrected tapes were assembled for each crystal system and sorted by determinative numbers.

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Computer programs were written to check the compatibility of certain numerical values and to prepare magnetic tapes for operating phototypesetting machines, which produced camera-copy for offset printing. The application of computers to printing has been described by W. R. Bozman (1966, 1968).

Having all the data on magnetic tape has several advantages. Systematic searches can be made by computer. For example, if someone wants a list of all the entries with cell dimensions and angles between specified limits, a density greater than a given value and a chemical formula containing certain elements, the computer can make the search and print out the desired list. Corrections and updating are facilitated so that subsequent editions will be easier to prepare and, let us hope, can be published sooner after their cutoff dates.

INTRODUCTION

THE IDENTIFICATION OF CRYSTALLINE SUBSTANCES FROM CELL DIMENSIONS

a. SCOPE AND RELIABILITY OF DATA

The idea of identifying crystalline substances by ratios of cell edges and by inter-edge angles did intrigue pre-x-ray crystallographers. The chief stumbling block was the lack of agreement on conventional rules to insure uniqueness of crystal setting. We are indebted to crystal morphologists for such determinative schemes as Federov's *Krystallreich* (1920) and Barker's *Index* (Porter and Spiller, 1951–56; Porter and Codd, 1964). For more than thirty years, the determinative method based on x-ray diffraction powder data (Hanawalt *et al.*, 1938) has ruled supreme, to the extent that some crystallographers, in order to obtain powder data, have not hesitated to smash good crystals to smithereens, while others, refusing to turn crystalloclasts, have invented ingenious devices to rock the single crystal in the x-ray beam (Mathews and McIntosh, 1948).

Progress in single-crystal techniques and x-ray instrumentation, particularly Buerger's *precession method* (1944) and the commercial availability of his *precession camera*, makes it easy and fast to obtain cell dimensions and systematic omissions, especially when precession and Weissenberg methods are used jointly. In favorable cases the total amount of work required is not any greater than that involved in measuring the many interplanar spacings from a powder pattern and estimating the relative intensities of the lines, to say nothing of their indexing. 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, which otherwise could lead to a pseudo-cell. Although single-crystal data obtained by x-rays are given in several compendia, the way in which they are listed is not adequate for determinative purposes.

The present work provides determinative tables based on cell constants. The data used in their preparation have been obtained by x-ray, electron, or neutron diffraction, so that the actual lengths of the cell edges are known. Axial ratios have nevertheless been chosen as determinative numbers, so that the Tables may also be used when relative dimensions obtained by goniometry are the only ones available. The actual lengths of the cell edges are given, together with space group, density, and other auxiliary determinative criteria. A set of rules is needed for choosing and orienting the cell. They are explained in the next section. These rules must, of course, be adhered to if the determination is to succeed.

At the risk of hindering the determinative process, we have, in many cases, included several sets of data for the same compound. We have followed this policy for two reasons: (1) so that our tables will represent as complete a survey as possible of all available references, and (2) so that the reliability of the data may be appraised from the juxtaposition of results coming from different sources. We must admit that we have made no systematic attempt to present the best data on the first line of the entry or to follow rigid rules in deciding on amalgamation of entries. We have, however, made an effort to cross-reference the entries so as to facilitate comparisons and critical appraisal of conflicting data.

Computer programs were written to check the self-consistency of the data. The chemical formula, cell dimensions, and number of formula units per cell were checked by computing the density *Dx* and comparing it with the measured value *Dm*, if available. In order to check the empirical chemical formulae of organic compounds, the molecular weight was calculated both from the expanded formula given in the entry and from the empirical one given in the index. The space-group symbol has been checked, in each case, against a table of all space-group and aspect symbols used in the appropriate crystal system. The abbreviations of names of the more frequent periodicals were checked against a master list to insure uniformity of spelling. The name and formula indexes were compiled and alphabetized according to special rules. A large number of errors were detected, either copying mistakes or author's errors. The latter were corrected when they could be explained; if the conflict could not be resolved, the error was pointed out.

b. CHOICE AND ORIENTATION OF THE CELL

General Rules.—The cell chosen to define the lattice should obey the following rules (Donnay, 1943*a*), to be applied in the sequence given.

(1) Whenever possible the cell edges should coincide with symmetry directions[1] of the lattice and the cell should have the same symmetry as the lattice.

(2) Symmetry-equivalent edges should be chosen, if possible.

(3) The cell should be the smallest possible cell that obeys conditions (1) and (2).

(4) Cell edges that cannot be symmetry directions should be the shortest possible lattice translations.

(5) A cell edge parallel to a single 2-fold axis of the lattice is called b. A cell edge parallel to a principal singular axis ($n \geq 3$) is called c. Cell edges, the naming of which is not governed by the lattice symmetry, should obey the inequalities $c < a < b$.

(6) The axes of co-ordinates should be directed, along the cell edges, so as to form a right-handed system with non-acute inter-edge angles α and β. (Angle γ can vary from 60° to 120°, both values included; angles α and β cannot exceed 120°.)

These rules hold for all crystal systems, whenever applicable. Note that the requirement for the system of co-ordinates to be right-handed is superfluous for determinative purposes since it does not affect the cell dimensions: a left-handed system can always be converted into a right-handed one by reversing the senses of all three axes, a transformation that leaves the interaxial angles unchanged.

In the **anorthic** (triclinic) system, as symmetry directions do not exist, Rule 1 does not apply. The point-group symmetry of the lattice is $\bar{1}$; every cell is centrosymmetric. Rule 2 does not apply. The cell chosen should be primitive (P) in order to comply with Rule 3. Its edges must be the shortest three non-coplanar lattice translations (Rule 4) that define the Niggli reduced cell.[2] The cell edges are labeled so as to have $c < a < b$ (Rule 5) and oriented so that the angles α and β are non-acute (Rule 6).

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[1] By difinition a *symmetry direction* is either a symmetry axis, or the normal to a symmetry plane ($1/m = \bar{2}$), or both. This concept is used in dealing with point-group symmetries, either of polyhedra or of lattices. In lattices the possible symmetry directions are: $2/m$, $4/m$, $6/m$, $\bar{3}$. Note that we use the word *lattice* in the sense given to it by Bravais, *viz.* a spatial assemblage of points that are the termini of the vectors $\mathbf{L}(uvw) = u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$, where u, v, w are integers (positive, negative, or zero).

[2] The Niggli reduced cell (1928) is the one that satisfies the conditions derived from the reduction theory of quadratic forms. It is primitive since it is built on the shortest three non-coplanar lattice translations. The reduction procedure given by Buerger (1957, 1960) and extended by Davis (1961) has been used to transform any primitive cell into one based on the shortest three non-coplanar translations. If the end point of this procedure was not Niggli's cell, the reduction was completed by the transformations given by Santoro and Mighell (1970). Further discussion of the determination of reduced cells and their relationships to the Bravais lattices is given by Mighell, Santoro and Donnay (1969) in the *International tables for x-ray crystallography*. The cell setting used in the present classification (Rules 5 and 6) was obtained from the setting of Niggli's reduced cell by means of the following transformations

Type I (triacute) cell: $0\bar{1}0/00\bar{1}/100$
Type II (trinonacute) cell: 010/001/100.

The cell thus defined may differ from the *Delaunay cell*, used in the first edition of this book. Delaunay (1933) chooses the shortest three translations that enable all three inter-edge angles to be non-acute; they are not necessarily the shortest three non-coplanar translations, but they are among the shortest four. For discussions of the Delaunay algorithm see Ito (1950), Henry and Lonsdale (1952), Donnay and Nowacki (1954), Balashov (1956), Patterson and Love (1957), Allmann (1968).

The point-group symmetry of a **monoclinic** lattice is $2/m$. There is one symmetry direction, which (Rule 1) fixes one cell edge, conventionally labeled b. **Rule 2 does not apply.** The shortest two translations in the net perpendicular to b, together with b, define a cell that obeys Rule 3. Take angle β non-acute[3] (Rule 4) and $c < a$ (Rule 5). The resulting cell may be primitive or centered (C, A, or I).

The point-group symmetry of an **orthorhombic** lattice is $2/m\ 2/m\ 2/m$. The three symmetry directions fix the three cell edges (Rule 1). Rule 2 does not apply.[4] The cell, in accordance with Rule 3 is the smallest possible one that obeys the first rule. All inter-edge angles are 90°, fixed by symmetry, so that Rule 4 does not apply. Take $c < a < b$ (Rule 5). The resulting cell may be primitive (P), one-face centered (A, B, or C), body-centered (I), or all-face-centered (F). Note also that point group $mm2$ may have to be oriented as $2mm$ or as $m2m$.

The point-group symmetry of a **tetragonal** lattice is $4/m\ 2/m\ 2/m$. Of the five symmetry directions, one is perpendicular to a plane containing the other four. This singular direction must be taken as a cell edge (Rule 1): it is conventionally labeled c. The remaining cell edges must (Rules 1 and 2) coincide with two equivalent 2-fold axes, either those of the first or those of the second kind, so that all angles are right angles by symmetry. The axes of the first kind must be chosen, as they lead to the smaller cell (Rule 3). Rules 4 and 5 do not apply. The resulting cell may be primitive (P) or body-centered (I).

The point-group symmetry of the **hexagonal** lattice is $6/m\ 2/m\ 2/m$. Of the seven symmetry directions, one is perpendicular to a plane containing the other six. This singular direction must be taken as a cell edge (Rule 1); it is conventionally labeled c. The remaining cell edges must (Rules 1 and 2) coincide with two equivalent 2-fold axes, of either the first or the second kind. Two 2-fold axes of the first kind are chosen, as they give the smaller cell (Rule 3). Angles α and β, fixed by symmetry, are equal to 90°; angle γ is taken equal to 120° in preference to 60°. Rules 4 and 5 do not apply. The resulting cell is primitive (P, formerly designated C).

The **rhombohedral** lattice, which has point-group symmetry $\bar{3}\ 2/m$, is here described by a cell referred to hexagonal axes (Bravais axes).[5] Of the four symmetry directions, one is perpendicular to a plane containing the other three. This singular direction must be taken as a cell edge (Rule 1); it is conventionally labeled c. The remaining cell edges must (Rules 1 and 2) coincide with two of the three 2-fold axes, so that all angles are fixed by symmetry ($\gamma = 120°$, $\alpha = \beta = 90°$). The resulting cell satisfies Rule 3. Rules 4 and 5 do not apply. The R cell is a triple cell; the additional nodes are chosen at $\frac{1}{3}\ \frac{2}{3}\ \frac{2}{3}$ and $\frac{2}{3}\ \frac{1}{3}\ \frac{1}{3}$.

The point-group symmetry of a **cubic** lattice is $4/m\ \bar{3}\ 2/m$. The three 4-fold axes are the symmetry directions to be taken as edges of the cubic cell (Rule 1). This cell obeys Rules 2 and 3. Rules 4 and 5 do not apply. The resulting cell may be primitive (P), body-centered (I), or face-centered (F).

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[3] If β happens to be equal to 90° within the limits of experimental error, two cells satisfy the rules, namely $a\ b\ c$ and $\bar{a}\ \bar{b}\ c$. Although it changes the values of the atomic co-ordinates, this ambiguity does not affect the determinative procedure: the cell dimensions remain the same and the space group retains the same symbol after transformation.

[4] Rule 2 was obeyed in the old Lévy cell, in which two edges were taken along the diagonals of a face; *e.g.*, along $[1\bar{1}0]$ and $[110]$ of our conventional Miller cell. Such rows are equivalent under lattice symmetry. Note that the Lévy cell violates Rule 1.

[5] It can also be described by a cell referred to rhombohedral axes (Miller axes) in which three rows equally inclined on the singular direction are used as cell edges. Rule 2 is obeyed, at the expense of Rule 1. The cell is primitive and should be designated P by those who wish to use it.

Additional nodes at $\frac{1}{3}\ \frac{1}{3}\ \frac{1}{3}$ and $\frac{2}{3}\ \frac{2}{3}\ \frac{2}{3}$ would make the lattice hexagonal. A triple cell, rhombohedral in shape, could thus be used to describe a hexagonal lattice. Its use has never been advocated, and no symbolic letter has ever been assigned to it.

Most crystallographers agree that the choice of Bravais axes simplifies calculations; herein lies the justification of our conventional rules. The use of Bravais axes does not obliterate the fact that the rhombohedral lattice is less symmetrical than the hexagonal lattice and is no argument for abandoning the point symmetry of the lattice as the basis of the classification into 7 crystal systems: the rhombohedral system can be called the hexagonal-R system; the hexagonal one then becomes the hexagonal-P system. In this book entries of both systems are collected in a single section.

c. THE DATA

Substances included

All truly crystalline substances for which cell data were available have been included. All carbon-containing compounds appear in Volume I. Volume II covers all elements, intermetallic, and inorganic compounds, including minerals. Note that some carbides, carbonates, cyanides, and cyanates appear in both volumes.

Proteins will be found as an appendix to Volume I. Other compounds of high molecular weight have been excluded, such as rubbers, polymers, cellulose compounds, and fibers.

Sources of data

The data that appeared in our first two editions (Donnay and Nowacki, 1954; Donnay *et al.*, 1963) have been scrutinized for omissions, misprints, and errors. To this end they have been compared with the data in *Structure Reports* (vols. I to XVIII). Practically all entries have been checked against the original references, and only a few secondary references had to be retained. Strunz's *Mineralogische Tabellen* (4th ed. 1967) and Winchell and Winchell's *Mineralogy* (1951) again proved of great help in comparing conflicting data and tracking down misprints. For papers not yet abstracted in *Structure Reports*, *viz.* data published in 1959–66, our coverage of the literature should be at least as complete as that of the *Bulletin signalétique* of the French Documentation Center (C.N.R.S.), on which we have relied heavily as our chief source of references.

Unit of length

All cubic cell edges are given in Å (ångström) units.[6] Data published up to and including 1948 were originally expressed in kX units (erroneously called ångströms at the time); they have been converted according to the factor 1 kX = 1.00202 Å (*Acta Cryst. 1*, 46, 1948).[7] Most post-1948 data were published in Å; some, still in kX, were converted and are marked "Å from kX".

For all non-cubic substances, the date of the reference indicates whether the unit is kX (pre-1949) or Å (post-1948). The post-1948 data that were still expressed in kX in the original paper have been converted and are marked "Å from kX". In all such cases, the numerical data that follow the reference in the parenthesis are the converted original values.

Elements have received special treatment. Where accuracy is claimed, the original data are quoted in the original unit and, whenever possible, the x-ray wavelength used is also quoted, in the same original unit. The converted values (in Å from kX) are based on the factor Λ 1.00202 and are not to be considered the accurate values. The Editor for Metals has also rounded off some original values, when the limits of error warranted such course of action; for example, 2.64347 ± 30 has been quoted as 2.6435 ± 3.

Although we have made a genuine effort to ascertain the unit used by the author, there remain a number of cases where the uncertainty persists.

Presentation of data

We have attempted to give the following data for each substance: determinative number and other axial elements, cell dimensions, space group, number of formula units per cell, information on structure, density (measured and calculated), name, and chemical formula. Additional properties, such as melting point, crystal habit, cleavage, twinning, color, and other optical properties have been given systematically, whenever mentioned in the original reference.

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[6] To the accuracy of most crystal data, the Å ($= 10^{-10}$ m) is equal to the newly redefined Å* (Bearden, 1964), originally designated by the symbol $\overset{*}{\text{Å}}$.

[7] It is now known (Bearden, 1964) that this factor must be given different values depending on the wavelength to be converted. For instance, the 2 in the fifth place should be replaced by 5.6 ± 0.5 (for $\lambda \mathrm{CuK}\alpha_1 = 1.537400$ kX) or by 7.6 ± 0.5 (for $\lambda \mathrm{WK}\alpha_1 = 0.208577$ kX), to convert to the new standard wavelength $\lambda \mathrm{WK}\alpha_1 = 0.2090100$ Å*. In view of the limited accuracy of the data, we decided to retain the factor 1.00202, except for a few highly accurate values.

The entries are sorted in order of increasing values of the following determinative numbers: a/b, c/b, and b, in the trimetric systems: c/a and a, in the dimetric systems: a in the cubic system. If necessary the sorting is completed alphabetically by names. Some axial ratios have been calculated to more decimal places than are warranted by the accuracy of the measurements, so as to increase the usefulness of the axial ratio as a reference number for indexing purposes. In all cases the accuracy should be judged from the original data, not from the recalculated data.

The *space group*, whenever possible, is given in the oriented Hermann-Mauguin notation, the latter being used in its later, more explicit, form (Henry and Lonsdale, 1952). If the orientation of the space group is not known, the Schoenflies symbol is given as a last resort. To indicate a choice between two or more space groups, the diffraction aspect has been used: for example, the symbol $Bb{*}{*}$ means that three space groups are compatible with the diffraction data: $Bbmm$, $Bb2m$, and $Bbm2$. (The space group may not be known until the crystal structure is fully worked out.) The original aspect symbols (Donnay and Harker, 1940) express all the space groups allowed within a crystal system: later symbols (Donnay and Kennard, 1964) restrict the choice of space groups to a known Laue class. The *Tables of Space-group Criteria* of 1940 have been reprinted with some modifications: an additional column for each Laue class lists the 1964 symbols; the last column lists the 1940 aspect symbols, save that any symbol corresponding to only one space group has been omitted as superfluous. When the diffraction aspect is not known, the translation group (crystal lattice), the point group (crystal class), or the Laue class may be given in the *remarks*.

The number Z of formula units per cell is always stated as an integer on the first line of the entry. If Z is fractional it appears under *remarks*.

Under the heading *Structure* appears one of three words: quant., qual., none. A crystal structure is considered *quantitative* if all three co-ordinates for each atom (other than hydrogen atoms) have been established from intensities of diffracted beams. It is called *qualitative* if not all atomic co-ordinates have been ascertained in this way or if only the structure type is known. The designation *none* means that no structural information was obtained by diffraction methods. If the structure type is known, it may be designated by the *Strukturbericht* symbols (see appended list), the name of a compound, or both. For sterols the original symbols of Bernal and co-workers have been retained. The word *type* means that the structure of the compound described is the type itself. Most recent structures do not appear in *Strukturbericht* and no type symbols have been assigned to them.

Both measured density Dm and calculated density Dx are given (in g/cm^3) when known. The temperature of the determination and limits of error are given for Dm when recorded by the author. Whenever the reference does not give Dx, but records the non-integral value of Z (e.g., Z 3.96), we have used it to obtain Dx. In all cases where the Dx was not available, our calculated value is given between brackets. Note, however, that this Dx value is based on the formula that appears after the name, and that this formula may be idealized, as in the case of a mineral.

In cases of discrepancies, our calculated value of Dx, given between brackets, follows the author's published Dx. If, in a post-1948 entry, the bracketed value is the larger by $\sim$ 0.6 percent, the disagreement can be explained in two ways: either the author used the old value (6.06) for Avogadro's number with cell edges expressed in Å units, in which case the bracketed value is right, or we used the new value of Avogadro's number (6.02252), thinking the cell edges were in Å when they actually were in kX, in which case the author's value for Dx is correct but the numerical values of the cell edges should be converted from kX to Å. The second explanation would also hold for a cubic pre-1949 entry that we failed to convert to Å. Larger discrepancies may be due to the fact that our recalculations are based on the C^{12} unified scale of atomic weights, and the more recent values may depart considerably from the old ones, for instance, for the transuranium elements.

The *inorganic chemical name* is usually given according to the 1957 Report of the Commission on the Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry (J. Am. Chem. Soc. **82**, 5523, 1960). The name given by the author has also been retained as a synonym. For intermetallic compounds the names and formulae have been alphabetized. In the case of a mineral, a chemical name is given in addition to the mineral name, except where too complex a composition would have made the chemical name unwieldly. When more than one mineral name is in use, we have followed the recommendations of the International Mineralogical Association or those of Hey (1955, 1963). Some names found in *Structure Reports* have also been used, even though they may be unconventional. When a mineral name is used to designate a compound with the same crystal structure as the mineral, as in the expression a *cobalt "spinel"*, we place the mineral name between quotation marks. Cobalt "spinel" is not a mineral; it is compound with a spinel-type structure that contains cobalt. Likewise we write *erbium "garnet"*.

The *chemical formula* is written in one of the several accepted forms. Dual chemistry formulation has been avoided: we write $PbAs_2S_4$, not $PbS \cdot As_2S_3$. For an organic compound the condensed formula is used in the index, but a more explicit form generally appears in the tables.

Melting point and other temperatures are expressed in degrees Celsius unless otherwise stated.

Whenever the transformation of co-ordinate axes alters the numerical values of the data, the original data are also given, so that the transformation can be checked. Note that all symbols (space group, cleavage, forms, etc.) refer to the new setting. In anorthic, monoclinic, and orthorhombic entries, original data follow the literature reference, within the parenthesis.

Miscellaneous remarks are placed at the end of the entry. Axial ratios obtained by goniometry, $(a{:}b{:}c)_{gon}$, found either in the reference or in the literature, are usually given when available. When they are multiples or submultiples of the x-ray ratios, they are written in such a way as to permit easy comparison of the numerical values. The source of any numerical value quoted in the reference is given by citing the author's name and year of publication; the full reference is to be found in the paper being abstracted.

Habit is described by means of adjectives such as: acicular, long prismatic, prismatic, stout prismatic, short prismatic (followed by the direction of elongation); equant; thick tabular, tabular, thin tabular, platy (followed by plane of flattening); pyramidal; dipyramidal; lath-shaped (followed by plane of flattening and elongation direction), *e.g.*: Prismatic *b*; Tabular (010); Lath-shaped (100), elong. [011]. Note that, in this terminology, the word *prismatic* indicates a ratio of length to width and does not refer to any *prism*, in the sense of a crystal form, nor to any point-group symmetry, as in Groth's nomenclature, where $2/m$ is called the *prismatic* class of the monoclinic system. We use the word *dipyramidal* to indicate a doubly terminated habit, whether dipyramids or pyramids are involved, and whether the pyramids are complementary or not.

Under optical data, the optical orientation is given, when known, for monoclinic and orthorhombic substances. The angle of the optic axes, $2V$ or $2E$, is given only if it is a measured value. In the monoclinic system an extinction angle with c is taken as positive in the obtuse angle β. By this convention the ca plane is oriented, so that the sign of the extinction angle with a follows as a consequence. Example: $\beta = 110°$, γ to $c = +5°$, $\beta = b$, α to $a = -15°$. Other example: $\beta = 100°$, γ to $c = +20°$, $\beta = b$, α to $a = +10°$.

For most references information is given on powder data: whether they are "indexed" or simply "recorded". "Powder work" means that no single-crystal work was mentioned.

Statements between brackets are editorial comments.

Although many cross-references have been entered in the Tables, it is recommended that the Indexes be consulted to locate all entries pertaining to a given compound.

Anorthic (triclinic) System

The cell used is the reduced cell, oriented so as to obey the condition $c < a < b$, with angles α and β non-acute. The determinative number is the axial ratio a/b. It is followed by c/b, a, b, c. Space group, number Z of formula units per cell, information on structure, *D*m and *D*x complete the first line. The angles α, β, γ are given under a, b, c, respectively. The name and formula begin the third line. The literature reference follows, together with the original data, between parentheses. The "old-to-new" transformation of co-ordinate axes is represented by the three rows of its matrix, placed immediately after the reference. "Old-to-new" means "from the literature setting to the setting in the Table".

For a number of the triclinic crystals, there is more than one cell based on the shortest three vectors. Although there is only one reduced cell for a crystal, in some cases it is very difficult to determine this cell because of the experimental error. Thus for some of the triclinic crystals an alternative cell is given in the text with a second "old-to-new" transformation of coordinate axes.

Monoclinic System

The symmetry direction is chosen as b. The shortest two translations perpendicular to b obey the condition $c < a$, and β cannot be acute. The determinative number is a/b. It is followed by c/b, β, a, b, c. Whenever the transformation of co-ordinate axes made it necessary to find a new value for β, the calculated angle is given in degrees and minutes.

The literature reference is placed between parentheses, together with the original data when necessary, and is immediately followed by the matrix of the "old to new" transformation. Except when the transformation is expressed by the identity matrix, 100/010/001, the original data are given. When the acute angle β is reported in an old reference, its supplement will usually be found under *original data*, because the old convention was to call β the angle between $+c$ and $-a$ directions. If an acute β is reported in a crystal-structure paper, it is kept as such and the transformation matrix takes it into account and operates on the unconventional original axes.

Orthorhombic System

The cell edges, taken along symmetry directions, obey the conditions $c < a < b$. The determinative number is a/b. It is followed by c/b, a, b, c. Since only six transformations are possible, the transformation matrix is designated by a conventional triplet of letters, which follows the reference parenthesis. The possible matrices are the six permutations of $a\ b\ c$. The minus signs that would be required to keep the system of axes right-handed, have been omitted for the sake of convenience. The original data are not given, because the numerical values of the cell edges are not altered by the transformation, but the limits of error are stated for the original a, b, and c numerical values.

Tetragonal System

The smaller cell is used (P or I), with the singular direction taken as c. The determinative number is c/a. It is followed by a and c, each value being accompanied by its limits of error whenever available. The only transformation to be considered is $\frac{1}{2}\,\frac{1}{2}\,0/\bar{\frac{1}{2}}\,\frac{1}{2}\,0/001$, which changes the unconventional C and F cells into P and I cells respectively. The old (unconventional) c/a has, in such cases, been multiplied by $\sqrt{2}$ to give the new c/a ratio.

Hexagonal and Rhombohedral Systems

The smallest hexagonal cell[8] is used (P or R) with the singular direction taken as c. The determinative number is c/a. It is followed by a and c, each value being accompanied by its limits of error whenever available.

For substances with rhombohedral space groups, the elements a_{rh} and α of the primitive rhombohedral cell are also quoted, whenever published. To avoid any possible misunderstanding, the number Z of formula units is specified for each cell. When the original data referred to the rhombohedral cell, they had to be recast before they could be entered in the hexagonal table. The calculated hexagonal cell edges may look fallaciously accurate; the accuracy should be judged from that of original rhombohedral data.

Cubic System

The edge a of the cubic cell is used as determinative number. It is expressed in Å units (transformed from kX where necessary).

In this system the first line of an entry gives: cell edge, with limits of error (if known), space group, number Z of formula units per cell, information on crystal structure, structure type, Dm, Dx.

d. THE INDEXES

Each volume has its *Formula Index.* In the Organic Formula Index chemical formulae have been listed according to the rules followed by *Chemical Abstracts.* The symbols of the elements in the formula are listed alphabetically, except that C always comes first, and is followed by H when hydrogen is present. Organic compounds are first arranged in groups according to the number of carbon atoms in the formula: C_1, C_2, C_3, ... The formulae are then alphabetized within each group on the element symbols. Example: CCl_4 precedes CH_4, which precedes CI_4.

Only when several compounds contain the same elements are they listed according to increasing values of the subscripts, the first subscript being taken first, the second next, and so on. Examples: AsFe, $AsFe_2$, As_2Fe. Water of hydration or other solvates are not taken into account in the alphabetical listing of the formulae. Consequently an anhydrous compound is immediately followed by its various hydrates. Polymorphic forms are not identified in the Formula Indexes.

In the Inorganic Formula Index, the formulae of the intermetallic compounds only have been "alphabetized" on the element symbols prior to listing.

Three *Name Indexes* are provided. The Organic Name Index lists the names of all carbon-containing compounds. The Inorganic Name Index contains chemical names of all compounds other than minerals with complex compositions. Names of compounds appear in simplified form. For example all the sodium phosphates will be found together, the numbers of Na, P, and O atoms being given between parentheses: (3·1·4), (4·2·7), (5·3·10), and the degree of hydration being indicated: 6-hydrate, 10-hydrate, 12-hydrate. Some common names and trade names have also been used as synonyms. A special Mineral Name Index has also been prepared.

In all Indexes every reference to an entry in the Tables is made by the initial letter of the crystal system followed by the determinative number. The letter A stands for anorthic (or triclinic); the letter T, for tetragonal. The letter H refers to the section that covers both hexagonal and rhombohedral systems.

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[8] In the symbols of space groups that have a primitive hexagonal lattice, the initial letter P is used, instead of C as in the Hermann-Mauguin notation. This designation, which I had suggested for the 7th edition of the Dana *System of Mineralogy* (1944), has proven convenient and gained popularity. It has been adopted by the ***International tables for x-ray crystallography*** (1952). Carl Hermann (private communication) explained as follows why C was used rather than P in the original international symbols. C was used to indicate that symmetry planes symbolized by the letter *m* consist of mirrors interleaved by *a* glide planes; in all other P lattices, *m* stands for mirrors alternating with other mirrors. Likewise C would indicate that a sheaf of 2-fold axes consists of 2-axes and 2_1-axes, whereas in all other P lattices a sheaf of 2-fold axes contains rotation axes only.

J.D.H.D.