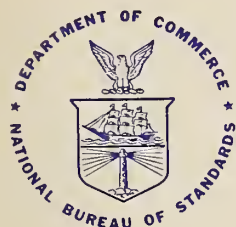


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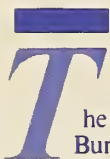
U.S. DEPARTMENT OF COMMERCE/National Bureau of Standards

Crystal Data

Version 1.0
Database Specifications

Judith K. Stalick and Alan D. Mighell

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Crystal Data

Version 1.0 Database Specifications

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FOREWORD

The National Standard Reference Data System was established in 1963 to promote the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data needed by the scientific and engineering community.

In recent years, the use of computers in data activities has become very important, both from an efficiency and from a technical viewpoint. This report is a description of one major effort in this direction and provides an in-depth overview of the NBS *Crystal Data* database. From this database, a wide variety of products, both computer-oriented and published, will be made available.

David R. Lide, Jr., *Director*
Standard Reference Data
National Bureau of Standards

PREFACE

This report describes the format and specifications of the NBS *Crystal Data* database, which contains the most comprehensive collection of crystallographic and related chemical information in the world. The data have come from the six published volumes of *Crystal Data* Determinative Tables (1972-1983), from newer data abstracted by the NBS Crystal Data Center and the Cambridge Crystallographic Data Centre, and from collaboration with the JCPDS--International Centre for Diffraction Data (Swarthmore, PA), the Metals Data Center (Ottawa, Canada), and the Inorganic Structural Data Center (Federal Republic of Germany).

The database contains many searchable parameters that do not appear in the published works. All data have been reevaluated by the Editors of the NBS Crystal Data Center with the aid of computer programs and errors or possible errors are noted. At this time the rapidly-expanding database contains information on more than 100,000 materials. Information on the availability of *Crystal Data* products may be obtained from the JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA.

The authors wish to acknowledge the numerous individuals at the National Bureau of Standards and at the collaborating data centers who have made this large collection of data possible, through over 30 years of abstracting and evaluation of data entries. We recognize that it is this dedicated work that actually results in the value of the database. In addition, we thank Dr. Camden R. Hubbard of the National Bureau of Standards for his contributions to the development of the database format and computer evaluation routines.

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CRYSTAL DATA

Version 1.0 Database Specifications

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National Bureau of Standards, Gaithersburg, MD 20899, USA*

The NBS *Crystal Data* database is a file of crystallographic and chemical data covering a broad spectrum of solid-state materials: inorganics, minerals, metals, intermetallics, organics, and organometallics. To be included in the database the unit-cell parameters of a material must be known. With the aid of computer programs, the data were evaluated by the Editors for reasonableness and self-consistency, and errors or possible errors are noted. The data items have been formatted in a standard way to permit searches. Each entry in the database contains unit-cell data (initial cell, conventional Crystal Data cell, and reduced cell), space group or diffraction aspect, formula units per cell, observed and calculated densities, literature reference, chemical or mineral name, chemical formula, empirical formula, and an indication of the extent to which the atomic positional parameters have been determined. Additional information may include structure type, locality for minerals, crystal habit, color, melting point, temperature of data collection, information on sub-, super-, or pseudocells, and an indication if cleavage, twinning, or powder data is included in the original literature reference. In addition to identification of unknowns by lattice-matching techniques, the large size of the database along with the combination of crystallographic, chemical, and physical information make this file a valuable resource for all of solid-state science. Detailed format and content specifications are given.

Key words: chemical formula; computer database; crystallographic data; identification; inorganic materials; intermetallics; minerals; NBS Crystal Data Center; organic materials; organometallics; unit-cell dimensions.

INTRODUCTION

The NBS *Crystal Data* database is a large, formatted file of evaluated crystallographic, chemical, and physical data. The data items have been

checked for legality and reasonableness, and, where necessary, transformed into standard forms to facilitate computer searches. Additional data items have been derived from the literature data, and strict adherence to specified formats has been ensured by extensive computer evaluation of the database.

THE DATA

a. Substances included and data sources

The database contains data on organic and inorganic crystalline substances for which cell parameters have been published. Also included are minerals, metals, intermetallic compounds, and organometallic compounds. Many compounds of biological interest are present, although proteins, high polymers, and solid solutions are, in general, excluded. The only requirement for inclusion of a material in the database is that the lattice has been defined by unit-cell dimensions; in over 50 percent of the cases, the data in an entry result from a full structure determination by single-crystal x-ray diffraction techniques.

The majority of information contained in this database has been abstracted from over 1000 journals and, to a lesser extent, from collected conference abstracts. A relatively small number of entries refer to Government and industrial research reports, theses, and books. The data were abstracted primarily by the NBS Crystal Data Center (inorganics, minerals, metals, and intermetallics) and by the Cambridge Crystallographic Data Centre in Cambridge, England (organics and organometallics). Other data entries have originated from collaboration with the JCPDS--International Centre for Diffraction Data (Swarthmore, PA), the Metals Data Center (Ottawa, Canada), and the Inorganic Structural Data Center (Federal Republic of Germany). All data entries have been evaluated by the NBS Crystal Data Center.

b. Data in each entry

A variety of crystallographic, chemical, and physical data are given that can be used to characterize a material. In addition, bibliographic data and indications of further information in the literature reference are given. The data include:

Material classifications

- Inorganic
 - Mineral
 - Intermetallic (including the Pearson structure code)
- Organic (including chemical class designations)

Abstracted data

- Unit-cell dimensions and space group
- Z (number of formula units per unit cell)
- Calculated and observed densities
- Compound name and chemical formula

- Literature reference
- Indication of the degree to which the structure has been determined
- Additional information such as structure type, locality for minerals, crystal habit, color, melting point, temperature of data collection, information on sub-, super-, and pseudocells, and an indication if cleavage, twinning, or powder data is included in the original literature reference

Derived data

- Crystal Data cell, space group, and Z
- Reduced cell and reduced form type
- Empirical formula and molecular weight
- Recalculated x-ray density

The detailed database contents are given in the Database Specifications.

c. Evaluation of the data

The scientific and numerical nature of the data permits extensive computer analysis. The NBS Crystal Data Center has developed computer programs that assist the Editors in building and evaluating the database, incorporating years of editorial experience, the results of research in lattice theory, and knowledge gained from analysis of the data as a set.

The FORTRAN program NBS*AIDS83, developed by NBS scientists and widely distributed to the crystallographic community and to data centers, was designed to build a database entry, transform data to standard settings, calculate derived parameters, evaluate parameters for reasonableness and for consistency within an entry, and check for required data items and proper formats. The program also checks items for legality (e.g., space groups and chemical element symbols) and performs cross-checks; for example, the inorganic chemical name and formula must be consistent, the recalculated x-ray density must agree with the reported densities (if any) and with a density approximated by average atomic volumes, and the metric symmetry as determined by reduced form type is compared with the reported crystal symmetry.

As the database now exceeds 100,000 entries, and is growing at the rate of approximately 7,000 entries per year, the evaluation of data between entries is becoming increasingly important. New analysis functions are being developed through the use of independent programs or database management systems. Any specified parameters may be examined using the entire database; for example, an analysis of the frequencies of occurrence for each of the 230 space groups has revealed that many space groups are rarely occupied. Thus any compound reported in a rare space group is a candidate for special editorial scrutiny.

CLASSIFICATION AND STANDARDIZATION OF CELLS

The various data items in each entry in the database have been rigorously defined and standardized using the software described above. All types of physical, chemical, and crystallographic data have been processed. Once the

data items have been standardized, it is possible to sort and classify the materials in a variety of different ways depending on how one wishes to use the database.

In particular, many practical applications result when materials are classified on the basis of the *Crystal Data cell* and the *reduced cell*. Computer programs now exist to transform any cell of the lattice to these standard cells (Mighell, Hubbard, and Stalick, 1981). In fact, many automated commercial x-ray diffractometers routinely calculate the reduced cell and a cell that is the same as, or closely related to, the Crystal Data cell.

a. The Crystal Data cell

The Crystal Data cell is a uniquely-defined primitive or centered cell, with cell parameters assigned on the basis of the symmetry elements of the crystal system. Reduction procedures are used to select the cell parameters not fixed by symmetry (i.e., a , c , and β in the monoclinic system and a , b , c , α , β , and γ in the triclinic system).

A classification of materials based on the Crystal Data cell is used if one wishes to compare lattices within a crystal system. This cell can conveniently be used for comparing similar materials, for identifying unknown substances, for locating isostructural materials, and for studying systematic changes in related materials where the cell orientation remains the same. The Crystal Data cell also provides an ideal conventional cell orientation for the reporting of unit cells in the literature. The complete rules for choice and orientation of the Crystal Data cell are given in Appendix A.

b. The reduced cell

The reduced cell is a unique, primitive cell based on the three shortest lattice translations. If the initial lattice is defined by a centered (F, I, A, B, C) cell, then this cell is converted to a primitive cell which is then reduced.

A classification of materials based on the reduced cell is ideal for identification by lattice-matching techniques (Mighell, 1976), since all cells are defined by the same rules that are independent of the crystal symmetry and cell centering. This method of classification enables one to locate related lattices in spite of certain experimental errors or subtle changes in symmetry. For example, the reduced cell remains invariant even if the experimenter misses the true symmetry of the lattice or if the lattice symmetry varies with site substitution (a common occurrence for minerals).

Once classified by reduced cell, one can determine the metric symmetry of the lattice. It has been shown that for over 95 percent of the entries in the database, the metric symmetry is the same as the crystal symmetry reported by the authors (Mighell and Rodgers, 1980). Thus a convenient procedure to determine the crystal symmetry starts with the determination of any cell defining the lattice. This is followed by transformation to a reduced cell, determination of the reduced form, transformation of the reduced cell to the

conventional cell, and verification of crystal symmetry by checking equivalent intensities.

The mathematical conditions necessary to define the reduced cell and the transformation matrices that relate the reduced cell to the conventional Bravais lattice are given in Appendix B, along with the classification of reduced forms.

APPLICATIONS

The information contained in the database is of interest to scientists in many diverse disciplines, as it includes data from the entire spectrum of well-characterized solid-state materials. These disciplines include analytical chemistry, materials science, crystallography, mineralogy, ceramics, metallurgy, organic chemistry, biochemistry, physical chemistry, and inorganic chemistry. The database may be searched to find one or several materials with specified physical or chemical properties; alternatively, known or measured properties may be used to identify an unknown material.

a. Searching the database

The NBS *Crystal Data* database is a highly evaluated, standardized, and organized collection of formatted scientific data. It is therefore possible to carry out searches on all of the data parameters using computer programs. To perform a wide variety of sophisticated searches, it is most convenient to put the entire database under a database management system. The general search strategy using such a system is based on Boolean operations, and consists of three basic steps: 1) the search question is analyzed and framed into the form of several discrete search parameters; 2) for each parameter, the database is searched and the subset of data consisting of the "hits" is saved; and 3) to find the answer, the subsets of data are intersected using Boolean 'AND', 'OR', and 'NOT' operations. If the resulting data subset is not sufficiently specific, additional search parameters may be formulated to find the desired answer. Surprisingly, several "rough" or rather limited pieces of information (e.g., a partial chemical analysis, a single cell parameter, and an approximate density determination) are commonly sufficient to solve the problem. Typical searches are:

- Find all rare earth binary oxides that crystallize in the hexagonal or monoclinic crystal systems.
- Find all references within the years 1977-1983 that contain data on antibiotics with greater than 30 carbon atoms in the molecule.
- Find all materials with a density between 3.0 and 4.0, with a cell volume in the range 900-1000 Å³, and with only Co, S, and one other chemical element in the formula.
- Find all organic substances that have the character string 'pen' in the chemical name, that have three Ni atoms in the molecule, and that crystallize in the anorthic (triclinic) or monoclinic crystal systems.
- Find all compounds with an *a*-cell parameter (from electron diffraction) in the range 3.5-3.7 Å that contain Pm and O.

- Find all references to steroids in the monoclinic space group $P2_1$ that have four molecules in the asymmetric unit (to search for hydrogen bonds between molecules not symmetrically related).
- Find all materials containing Na and S that have calculated densities 15% greater than the density estimated by formula alone.
- Find the space group frequencies for binary oxides.
- Find references to all cyclophosphamides that have had the full structure determined.
- Find all organic compounds in the 40 least-populated space groups.

The above examples illustrate that, using the database along with a database management system, one can carry out a great variety of highly-selective searches. The search capability can be greatly broadened if the database management system is coupled with scientific software designed specifically for the type of data in the database.

b. Compound identification by lattice matching

The database is a valuable resource for compound characterization and identification, as all of the lattices for materials in the database have been classified on the basis of the reduced cell and the Crystal Data cell. An unknown may be identified by matching the unknown lattice against all of the lattices in the database. For a discussion of the theory of lattice-matching techniques see Himes and Mighell (1985), and for a historical discussion of identification based on cell parameters see the Introduction to the third edition of *Crystal Data Determinative Tables* (Donnay and Ondik, 1972, 1973).

Several recent developments have converged to make identification based on lattice matching even more attractive for routine use in both industrial and analytical laboratories. These include: (a) the large and rapidly expanding file of well-characterized compounds; (b) the high quality of cell data in the file, especially the new data which have often been based on a least-squares refinement; (c) the increasing use of automated diffractometers which makes it easier to obtain a refined cell of the lattice; (d) the development of theory and of computer algorithms to convert any given cell to a standard cell suitable for identification; (e) the fact that low-symmetry organic and inorganic compounds can conveniently be characterized and identified on the basis of their cell parameters (a class of compounds for which the powder method has only limited applicability).

In order to identify an unknown material in conjunction with the database, the following sequence of steps may be used:

1. Mount the unknown crystal on the diffractometer.
2. Determine any cell of the lattice.
3. Refine the cell.
4. Determine the reduced cell (or determine the crystal symmetry and transform to the Crystal Data cell).
5. Check the database for a match.

To make an identification in spite of experimental errors and/or to find all related materials, appropriate sub- and supercells should be calculated (Santoro and Mighell, 1972) and checked for a match. The unit cell and crystal symmetry may equally well be determined by other techniques, e.g., powder diffraction or single-crystal film methods. The identification may be confirmed based on known chemical or physical properties. A computer program for lattice matching has been developed (Himes and Mighell, 1985) for use in conjunction with a file derived from the database.

DATABASE SPECIFICATIONS

The NBS *Crystal Data* database consists of one or more entries for each substance included, and is divided into two separate files. The *inorganic* file includes elements, inorganic substances, intermetallic compounds, and minerals. Also included are a few classes of materials containing carbon (i.e., carbonates, carbides, cyanides, cyanates, carbonyls, and carbon-bearing minerals). Solid solutions are, in general, excluded. The *organic* file contains information on organic compounds, organometallic compounds, and metal complexes containing organic ligands. Solid solutions, proteins, and high polymers are excluded.

Each entry in the database consists of up to 16 record types, beginning with record type 1 and ending with record type K. All records contain units of 80 ASCII characters, and some contain multiple units. The following table gives a summary of record types, with the maximum number of units for each type.

<u>Record Type</u>	<u>Maximum Number of Units</u>	<u>Information in the Record</u>
1	1	Original cell parameters
2	1	Cell parameter standard deviations
3	1	Space group, Z, and density
4	1	Crystal Data space group, Z, and density
5	5	Material, class, and registration indicators
6	5	Compound name
7	5	Chemical formula (dot or structural formula)
8*	1	Empirical formula
9	10	Literature reference
A*	1	Structure type
B*	20	Comments
C	1	Matrix for initial cell → Crystal Data cell
D	1	Reduced cell
E	1	Crystal Data cell
J*	5	Update or revision
K	1	Processing history and entry termination

*Optional

The format for each record type and a complete description of the record contents follow.

RECORD TYPE 1 *Original cell parameters*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
*1-9	F9.5	a (original data) in Angstroms ($1 \text{ \AA} = 10^{-10}\text{m}$)
*10-18	F9.5	b
*19-27	F9.5	c
*28-35	F8.3	α (original data) in degrees
*36-43	F8.3	β
*44-51	F8.3	γ
*52	A1	Editorial code for cell Blank = cell given by author; normal temperature and pressure E = cell inserted by Crystal Data editor C = cell is Crystal Data cell (not necessarily the author's original cell) T = cell data is at high or low temperature P = cell data is at high pressure (may also be at high or low temperature)
53-64	12X	Blank
*65	A1	Radiation of study Blank = not specified X = x-ray N = neutron E = electron G = gamma
66	1X	Blank
*67	A1	Source of unit cell data Blank = not specified S = single crystal P = powder diffraction R = Rietveld or profile fit analysis
68	1X	Blank
*69	A1	Structure code N = no information about structure is given L = limited structure information is given (partial structure determined or assigned by type) T = total structure determined (excluding H atoms)

70-71	2X	Blank
*72-78	7A1	Crystal Data reference code
*79	A1	Crystal system code A = anorthic (triclinic) M = monoclinic O = orthorhombic T = tetragonal H = hexagonal R = rhombohedral (hexagonal or rhombohedral axes) C = cubic
*80	A1	1 (Record Type 1)

Notes:

- (1) Data items for character numbers preceded by an asterisk (*) on this and all subsequent record types are input from the literature reference; all other data items are generated by computer analysis.
- (2) The cell parameters are, in general, those given by the authors, maintaining the reported significance; angles in degrees and minutes have been converted to decimal degrees.
- (3) Only those cell parameters required to define the cell are given:

anorthic	a, b, c, α , β , γ
monoclinic (a-unique)	a, b, c, α
monoclinic (b-unique)	a, b, c β
monoclinic (c-unique)	a, b, c γ
orthorhombic	a, b, c
tetragonal	a c
hexagonal	a c
rhombohedral (H axes)	a c
rhombohedral (R axes)	a α
cubic	a

- (4) The Crystal Data reference code and the crystal system code for character numbers 72-79 are repeated on all subsequent data record types for the entry.

RECORD TYPE 2 *Cell parameter standard deviations*

<u>Character</u> <u>Numbers</u>	<u>FORTTRAN</u> <u>Format</u>	<u>Item</u>
*1-9	F9.5	$\sigma(a)$
*10-18	F9.5	$\sigma(b)$
*19-27	F9.5	$\sigma(c)$
*28-35	F8.3	$\sigma(\alpha)$
*36-43	F8.3	$\sigma(\beta)$
*44-51	F8.3	$\sigma(\gamma)$
52	1X	Blank
53-56	I4	Average error in axial lengths in parts per 10^5
57	A1	Editorial code for average error Blank = standard deviations reported by the authors E = editorial errors assigned (see notes)
59-60	A2	Quality index code for cell
61-71	11X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	2 (Record Type 2)

Notes:

- (1) Only those standard deviations reported by the authors are given.
- (2) If no errors are reported by the authors, then a standard deviation of 5 in the least significant digit of the axial lengths is assumed in the calculation of the average error and the quality index code; an 'E' is then inserted for character number 57.

(3) The quality index code is assigned as follows:

<u>Average error (parts per 10⁵)</u>	<u>QI code</u>
0 - 1	A
2 - 5	A-
6 - 10	B
11 - 50	B- (typical single-crystal diffractometer data)
51 - 100	C
101 - 500	C-
501 - 1000	D
1001 - 5000	D-
5001 - 9999	F

(4) The maximum average error stored in the database is 9999.

RECORD TYPE 3 *Space group, Z, and density*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
*1-8	8A1	Author's space group, aspect in Laue class, or cell centering (left-justified)
*9	A1	Editorial code for space group Blank = space group given by author E = space group inserted by Crystal Data editor T = space group orientation corresponds to that of the Crystal Data cell (rare; orthorhombic only)
10	1X	Blank
11	A1	Aspect code Blank = normal * = aspect number has been assigned
12-14	I3	Space group or aspect number (see notes)
15	A1	Orientation code for space group or aspect
16-19	4X	Blank
*20-25	F6.0	Z (number of formula units per unit cell)
*26	A1	Editorial code for Z Blank = Z given by author E = Z has been inserted by the Crystal Data editor G = Z has been guessed
27-29	3X	Blank
*30-35	F6.3	Dm (author's measured density) in Mg/m ³ (g/cm ³)
36-37	2X	Blank
*38-43	F6.3	Dx (author's calculated density) in Mg/m ³
44-60	17X	Blank
61-69	F9.2	Input cell volume
70-71	2X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	3 (Record Type 3)

Notes:

- (1) The space groups are given in the Hermann-Mauguin notation (*International Tables for X-ray Crystallography*, 1969). Space groups and aspects are written with subscripts appearing on the line (no spaces), and with bars over numbers represented by a minus sign (-) preceding the number.

Examples: $P2_1/c \rightarrow P21/c$

$P4_12_12_1 \rightarrow P412121$

$R\bar{3}m \rightarrow R-3m$

$P\bar{3}cm \rightarrow P-3cm$

- (2) Diffraction aspects are those in the Laue class as given by Donnay and Kennard (1964) and reprinted in Supplement II of the third edition of *Crystal Data Determinative Tables*, Volumes 1 and 2 (Donnay and Ondik, 1972, 1973).

Exceptions: The four aspects that begin with the Laue group symmetry have been rewritten so that the lattice type appears first, e.g.

$\bar{1}P^* \rightarrow P^*, -1$

$\bar{3}P^* \rightarrow P^*, -3$

$\bar{3}mP^*cl \rightarrow P^*cl, -3m$

$\bar{3}mP^*lc \rightarrow P^*lc, -3m$

- (3) If no space group or aspect is given, but the cell centering is known, the appropriate symbol (P, C, F, etc.) is given under space group. If no centering is indicated, a primitive cell is assumed for cell reduction and transformation, although this may not be correct.
- (4) Space group numbers and orientation codes are given in Appendix C. Aspects are given the number corresponding to the highest possible symmetry space group, with a '*' for character number 11.
- (5) The value given for Z corresponds to the chemical and empirical formulas given.

RECORD TYPE 4 *Crystal Data space group, Z, and density*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
1-8	8A1	Crystal Data space group, aspect, or cell centering (left-justified)
9	A1	Editorial code for space group Blank = normal E = original space group (Record Type 3) is editorial
10	1X	Blank
11	A1	Aspect code Blank = normal * = aspect number assigned
12-14	I3	Space group or aspect number
15	A1	Orientation code for space group or aspect
16-19	4X	Blank
20-25	F6.0	Z for Crystal Data cell
26	A1	Editorial code for Crystal Data Z Blank = normal E = original Z (Record Type 3) is editorial G = original Z (Record Type 3) is guessed
27-29	3X	Blank
30-34	F5.2	Density approximated by atomic volumes in Mg/m ³
35	A1	A (editorial code for approximate density)
36-37	2X	Blank
38-43	F6.3	Dx (program calculated density) in Mg/m ³
44	A1	Editorial code for Dx Blank = normal G = Dx is questionable due to guessed or missing Z, or to approximation of empirical formula
45-50	6X	Blank
51-58	F8.2	Molecular or formula weight

59	A1	Editorial code for molecular weight Blank = normal G = molecular weight is questionable due to approximation of empirical formula
60	1X	Blank
61-69	F9.2	Volume of Crystal Data cell
70-71	2X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
80	A1	4 (Record Type 4)

Notes:

- (1) If no value for Z is given on Record Type 3, a value of 1 for the Crystal Data Z is assumed for the calculation of Dx, and a 'G' is given for character number 44. The Crystal Data Z is left blank in the database.
- (2) For the rhombohedral crystal system, if no space group, aspect, or cell centering is given on Record Type 3, an 'R' will be inserted for character number 1.
- (3) See notes 1-4 for Record Type 3 for information on space group numbers and orientation codes.
- (4) The approximate density in character numbers 30-34 is based solely on the empirical formula given on Record Type 8, using average atomic volumes derived from the database. It may be compared, with caution, with the crystallographic calculated density to assess the validity of the cell, formula, and Z; similar materials should show similar agreement.
- (5) The program calculated density in character numbers 38-43 is calculated using a value of 6.0220943×10^{23} mole⁻¹ for Avogadro's number (Deslattes et al., 1974) and the atomic weights of the IUPAC Commission on Atomic Weights (1979). More recent published values for the atomic weights (Holden and Martin, IUPAC Commission on Atomic Weights and Isotopic Abundances, 1984) would not, with very few exceptions, result in a noticeable change in the program calculated density. New recommended values for fundamental constants are expected to be available in the Fall of 1986 through a CODATA report, and these values will be used in future data processing.

RECORD TYPE 5 *Material, class, and registration indicators*

Character	FORTRAN	
<u>Numbers</u>	<u>Format</u>	<u>Item</u>
*1	A1	I for inorganic material (blank if not)
*2	A1	O for organic material (blank if not)
*3	A1	M for mineral (blank if not)
*4	A1	A for alloy, metal, intermetallic material (blank if not)
5-24	20X	Blank
*25-52	7(A1,A3)	Chemical class indicators (organic) or mineral group codes (inorganic) (see notes)
53	1X	Blank
*54-64	I6,1H-,2A1, 1H-,A1	Chemical Abstracts Service (CAS) registry number
65-70	6X	Blank
*71	I1	Sequence number n (1,2 . .), maximum 5 Blank if only one unit of Record Type 5 exists (normal) 'n' if more than one unit of Record Type 5 exists because of multiple CAS registry numbers
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	5 (Record Type 5)

Notes:

- (1) The chemical class indicators for organic materials consist of two parts, where the A1 field indicates the residue number of the corresponding chemical formula (see Record Type 7) and the A3 field gives the number of the associated chemical class. For example, 1023 indicates chemical class 23 for residue 1. Up to 7 classes may be assigned for a single substance. Appendix D gives a listing of the 86 chemical classes currently defined by the Cambridge Crystallographic Data Centre.
- (2) The mineral codes are those defined by the JCPDS--International Centre for Diffraction Data and are given in Appendix E. If an 'm' is given in the A1 field then a mineral group code follows in the A3 field; if an 's' is given in the A1 field then a mineral subgroup code follows.

Character FORTRAN
Numbers Format

Item

*1-67	67A1	Compound name (left justified)
68	1X	Blank
*69	A1	Index code Blank = Crystal Data index name M = mineral name N = chemical name for a mineral C = common or trivial name D = name to be omitted from index
*70	A1	Continuation code Blank = no continuation unit C = compound name is continued on the next unit (character numbers 1-67)
*71	11	Sequence number n (1, 2 . .), maximum 5 Blank if only one unit of Record Type 6 exists 'n' if more than one unit of Record Type 6 exists due to continuations or multiple names (see notes)
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	6 (Record Type 6)

Notes:

- (1) An entry may have more than one name for a given compound.
- (2) A mineral name will be given (character number 69 = 'M') only if the mineral indicator (Record Type 5, character number 3) is 'M'.
- (3) Most inorganic chemical names have been rewritten to facilitate searching as follows:
 1. Numbers are separated from the components of the chemical name. The chemical name for BaCl_2 in this scheme is Barium chloride (1^2), where the relative proportions of the constituents are given within the parentheses, separated by the symbol '^'.
 2. Ligands are named alphabetically following the central atom and are separated by commas. For example, $\text{Co}(\text{CN})_2(\text{NH}_3)_4$ is named Cobalt, ammine, cyano (1,4,2).

3. Oxygen "ligands" are treated differently. These ligands are given only as a number added to the number of central atoms, e.g., (P₃O₉) = phosphate (3+9) and (PO₃S) = phosphate,thio (1+3,1); if the normal number of oxygen ligands is present, it is not indicated, e.g., Potassium sulfate (2¹), not (2¹⁺⁴).
4. Prefixes such as di, iso, etc. are separated from the chemical group name by a slash, e.g., Potassium chromate/di (2¹).
5. Mixed-site occupancy is indicated by a dash, e.g., (Al,Si)₂Nd = Aluminum-silicon neodymium (2¹).
6. The central atoms in heteropoly anions are separated by an asterisk, e.g., K₈(SiW₁₁O₃₉)·12H₂O = Potassium silicate*tungsto hydrate (8¹,11+39¹²).

- (4) Organic compound names are generally those assigned by the authors, provided that they are correct and conform reasonably well to accepted nomenclature rules. In some cases, systematic names have been devised or synonyms are given to cater for trivial and alternative names. In the database, *superscripts* and *subscripts* are bracketed by the symbols '#' and '\$', where '#' indicates 1/2-line down and '\$' indicates 1/2-line up; *Greek letters* are spelled out, e.g., α = alpha.
- (5) Names in the inorganic file (Record Type 5, character number 1 = 'I') are continued at word breaks only; thus blanks may occur at the end of the first unit for the continued name. Organic names are concatenated without respect to word breaks and the first unit uses the full 67-character field.
- (6) Example of continuation and sequencing for the inorganic file:

1234567890123456789012345678901234567890123456789012345678901234567890

Afghanite	M 1 000001M6
Sodium-calcium chloride-sulfate-carbonate silicate-aluminate	NC2 000001M6
hydrate (12 ⁴ 16+34 ¹)	N 3 000001M6

- (7) Example of continuation and sequencing for the organic file:

1234567890123456789012345678901234567890123456789012345678901234567890

bis(mu#2\$-Glutarato)-octacarbonyl-tetrakis(tri-n-butylphosphine)-te	C1 000002M6
tra-ruthenium	2 000002M6

RECORD TYPE 7 *Chemical formula (dot or structural formula)*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
*1-67	67A1	Chemical formula (left justified)
*68	A1	Formula approximation code Blank = normal G = editor has simplified formula or composition is approximate (e.g. for minerals)
*69	A1	Index code Blank = normal A = formula is absent D = omit from index X = pseudo-empirical formula index (organic only) P = permuted formula index (organic only)
*70	A1	Continuation code Blank = no continuation unit C = formula will be continued on the next unit
*71	I1	Sequence number n (1, 2 . . .), maximum 5 Blank if only one unit of Record Type 7 exists 'n' if more than one unit of Record Type 7 exists due to continuations or to multiple formulas
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	7 (Record Type 7)

Notes:

- (1) More than one formula may be given for a compound.
- (2) The first formula given is used to calculate the empirical formula unless the empirical formula on Record Type 8 has an 'E' for character number 69.
- (3) Organic chemical formulas are expressed in terms of residues, e.g. $C_{10}H_8NO_2^- \cdot C_{11}H_{15}N_2O^+$ for the complex between indole-3-acetic acid and 5-methoxytryptamine. The arrangement of symbols within a residue is that used by *Chemical Abstracts*: carbon atoms first, followed by hydrogen atoms (if present) and other elements in alphabetic sequence, typically $C_xH_yA_aB_b\dots$, followed if necessary by the net charge on the residue. Postmultipliers are reserved for polymeric residues, e.g. $(C_{10}H_{14}CdO_4)_n$.

(4) The formula is expressed by a sequence of discrete units. Each unit ends with a space. The following symbols are allowed:

1. Chemical element and number. Each element-number unit is terminated with a space. If the number of atoms of a given element is 1, the 1 is omitted.

Ba Cl2 Na2 S O4

2. Parentheses. A left parenthesis is always preceded and followed by a blank. A right parenthesis is always preceded by a blank and may be followed by a multiplier.

Al2 (S O4)3 Co (C O)6 (N H4)2 S O4

3. Brackets. These are treated the same as parentheses.

Ni3 [Co (C N)6]2 Mg3 [B (O H)4]2 F (O H) S O4

4. Exclamation point. This symbol is used to indicate a center dot. It may be followed by a multiplier.

Rb2 Zn (Be F4)2 !6 H2 O 2 (N H4)2 S O4 ! H2 O

5. Comma. A comma is used to indicate mixed-site occupancy, and is always preceded and followed by a space.

(Cu , Ge)2 Ho K3 Sc (O , O H)10

6. Charges. A + or - charge is always preceded by a space and may be followed by a multiplier.

C17 H31 N7 Ni +2 !2 (C24 H20 B -) ! C2 H3 N

- (5) The variable subscripts or multipliers x and z are used.

Na2 S O4 !x H2 O Fe2-x S W Cx Nx-z

- (6) The polymer subscript n is used; for the calculation of the empirical formula n = 1 is assumed.

(C14 H14 Cd N2 O5)n !2n (H2 O)

- (7) The symbols Ln or TR may be used for unspecified rare earth elements.

- (8) A formula may be continued on more than one unit (character numbers 1-67). No breaks are made between an element and its multiplier or a symbol and its multiplier. Thus zero or more blanks at the end of the formula field of the first unit should always be interpreted as one blank.

Example of continuation and sequencing:

```
1234567890123456789012345678901234567890123456789012345678901234567890
( Mg , Na , Ca , K )2 ( Mg , Al , Fe , Ti )5 ( Si , Al )8 O22 ( O GDC1 000003H7
H )2 GD 2 000003H7
( Mg , Na )2 ( Mg , Al )5 ( Si , Al )8 O22 ( O H )2 G 3 000003H7
```

Character	FORTTRAN	
<u>Numbers</u>	<u>Format</u>	<u>Item</u>
*1-67	67A1	Empirical formula (left justified)
*68	A1	Approximation code for empirical formula Blank = normal G = formula is approximate or simplified
*69	A1	Editorial code for empirical formula Blank = empirical formula was generated from the chemical formula given on Record Type 7 E = empirical formula inserted by editor
70-71	2X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	8 (Record Type 8)

Notes:

- (1) The empirical formula is automatically generated from the chemical formula given on Record Type 7 unless the variable subscripts x or z are present, or if the empirical formula is input by the Crystal Data editor with an 'E' for character number 69. When mixed-site occupancy is given on Record Type 7, e.g. (Mo , W), the empirical formula is based on the first element only, e.g. Mo, and a 'G' is given for character number 68.
- (2) The empirical formula is consistent with Z, and uses the same conventions as the chemical formula on Record Type 7 except that only the chemical element and number units are allowed.
- (3) The elements appear in alphabetical order, except for organics where C, H, D, and T appear first.

Cl2 H18 N2 O3 S (organic)

As3.72 Fe1.95 H 09 (inorganic)

RECORD TYPE 9 *Literature reference*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
*1-6	6A1	Journal CODEN as given by <i>Chemical Abstracts</i>
*7-10	4A1	Journal volume number (right justified)
*11-15	5A1	Journal page number (right justified)
16	1X	Blank
*17-20	4A1	Year of journal reference
21	1X	Blank
*22-67	46A1	Authors (left justified)
*68-69	2A1	Code for reference Blank = primary journal reference CD = reference from Volume 1 or 2 of <i>Crystal Data</i> Determinative Tables
*70	A1	Continuation code Blank = no continuation unit C = authors will be continued on the next unit (character numbers 22-67)
*71	I1	Sequence number n (1, 2 . .), maximum 10 Blank if only one unit of Record Type 9 exists 'n' if more than one unit of Record Type 9 exists due to continuations or to multiple references. For sequence number 10, n = 0.
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	9 (Record Type 9)

Notes:

- (1) The database contains only the journal CODEN as given by *Chemical Abstracts* or as assigned by the Crystal Data editors when no published CODEN was available. A file of CODEN vs. journal name accompanies the database; names in the file are abbreviated according to the conventions of *Chemical Abstracts* or the *Bibliographic Guide for Editors and Authors*, published in 1974 by the American Chemical Society.

- (2) For the primary reference, all authors' names are given, in the following format: Smith, W.G., Brown, R., Green, P.W.R.C.
- (3) If an author has no initials, the name is terminated with a period, e.g. Vovan Tien., Tran-Qui-Duc.
- (4) No umlauts or accent marks are indicated.
- (5) Words are not split between one unit and the next. Extra blanks will, in general, be left at the end of the first unit and are to be interpreted as one blank.
- (6) Example of continuation and sequencing:

1234567890123456789012345678901234567890123456789012345678901234567890

IVNMAW	4	899	1968	Baranov, I.A., Bychov, Yu.F., Evstyukhin,	C1	000005C9
				A.I., Kruglov, V.S., Rastov, N.N.	2	000005C9
ZSTKAI	7	461	1966	Voronkov, A.A., Shumyatskaya, N.G., Pyatenko,	C3	000005C9
				Yu.A.	4	000005C9

RECORD TYPE A *Structure type*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
*1-9	2A1,F7.2	Pearson symbol for alloys, metals, and intermetallics
*10	A1	Editorial code for Pearson symbol Blank = normal (generated from empirical formula and Z) E = Pearson symbol inserted by Crystal Data editor
11-17	7X	Blank
*18-67	50A1	Structure type (formula, name, or Strukturbericht designation)
68-71	4X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	A (Record Type A)

Notes:

- (1) The Pearson symbol (Pearson, 1967) consists of three parts: the crystal system code (lower case) for character number 1, the lattice centering code (upper case) for character number 2, and the number of atoms per unit cell (character numbers 3-9). Numbers of atoms greater than 9999.99 are set to 9999.99. The following symbols are allowed:

<u>Crystal System</u>	<u>Code</u>	<u>Centering</u>
Anorthic	a	P
Monoclinic	m	P, C
Orthorhombic	o	P, C, F, I
Tetragonal	t	P, I
Hexagonal	h	P
Rhombohedral	h	R
Cubic	c	P, F, I

When only the centering is unknown, the symbol '?' is used for the lattice centering code.

Note that for the rhombohedral crystal system, the number of atoms per unit cell is based on the primitive rhombohedral cell.

Examples: mP 128.00 cF 96.00 oC 16.00

- (2) The structure type given will usually be the formula or name of the isostructural type material. Formulas are enclosed in back slashes (\), e.g. \Cr₂₃ C₆\. Note that more than one type of designation may be given, e.g. E8(1), pyrochlore.

Character	FORTTRAN	
<u>Numbers</u>	<u>Format</u>	<u>Item</u>
*1-67	67A1	Comments
68-69	2X	Blank
*70	A1	Continuation code Blank = no continuation unit C = comments will be continued on the next unit (character numbers 1-67)
*71	I1	Sequence number n (1, 2 . .), maximum 20 Blank if only one unit of Record Type B 'n' if more than one unit of Record Type B occurs due to continuations. For sequence numbers > 9, the last digit only is used for 'n' (e.g., for sequence number 14, n = 4)
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	B (Record Type B)

Notes:

- (1) The following types of information might be included: solid state form, locality for minerals, temperature of cell determination, habit, color, melting point, chemical analysis, information on optics, cleavage, twinning, and powder data, and information on sub-, super-, and pseudo-cells.
- (2) Formulas are enclosed in back slashes (\), e.g. \Cu Pt Cl6 !6 H2 O\, and space groups are enclosed in back apostrophes ('), e.g. 'R-3m'.
- (3) Words are not split between one unit and the next. Extra blanks will, in general, be left at the end of the first unit.
- (4) Example of continuation and sequencing:

1234567890123456789012345678901234567890123456789012345678901234567890

From Sar-e-Sang, Badakhshan Province, Afghanistan. Bluish,	C1 000006AB
transparent. Cleavage and optical data given. Powder data	C2 000006AB
indexed. Chem. anal. Cell is very close to a quadruple multiple	C3 000006AB
of the cancrinite cell.	4 000006AB

RECORD TYPE C *Matrix for initial cell → Crystal Data cell*

Character <u>Numbers</u>	FORTTRAN <u>Format</u>	<u>Item</u>
1-4	F4.2	Determinant of transformation matrix
5	1H	:
6	1X	Blank
7-24	3(F5.2,1X)	First row of transformation matrix
25	1H	/
26-43	3(F5.2,1X)	Second row of transformation matrix
44	1H	/
45-62	3(F5.2,1X)	Third row of transformation matrix
63-71	9X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
80	A1	C (Record Type C)

RECORD TYPE D *Reduced cell*

<u>Character</u> <u>Numbers</u>	<u>FORTTRAN</u> <u>Format</u>	<u>Item</u>
1-8	F8.3	a (reduced cell) in Angstroms (\AA)
9-16	F8.3	b
17-24	F8.3	c
25-31	F7.2	α (reduced cell) in degrees
32-38	F7.2	β
39-45	F7.2	γ
46-54	F9.2	Volume (reduced cell)
55-65	11X	Blank
66-67	I2	Reduced form number
68	A1	Metric symmetry code Blank = normal X = metric symmetry exceeds crystal symmetry
69-71	3X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
80	A1	D (Record Type D)

Note: See Appendix B for the definition of the reduced cell, the classification of reduced forms, and the assignment of reduced form numbers.

RECORD TYPE E *Crystal Data cell*

<u>Character Numbers</u>	<u>FORTTRAN Format</u>	<u>Item</u>
1-8	F8.3	a (Crystal Data cell) in Angstroms (Å)
9-16	F8.3	b
17-24	F8.3	c
25-31	F7.2	α (Crystal Data cell) in degrees
32-38	F7.2	β
39-45	F7.2	γ
46-54	F9.4	First determinative ratio
55-62	F8.4	Second determinative ratio
63-71	9X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
80	A1	E (Record Type E)

Notes:

- (1) The first determinative ratio is a/b for the anorthic, monoclinic, and orthorhombic crystal systems; c/a for the tetragonal, hexagonal, and rhombohedral (H axes) systems; and a for the cubic system. The second determinative ratio is c/b for the anorthic, monoclinic, and orthorhombic systems; it is blank for the tetragonal, hexagonal, rhombohedral, and cubic systems.
- (2) See Appendix A for the rules defining the Crystal Data cell.

RECORD TYPE J *Update or revision*

<u>Character Numbers</u>	<u>FORTTRAN Format</u>	<u>Item</u>
*1-8	8A1	Revision date (year/month/day)
9	1X	Blank
*10-12	3A1	Initials (revision by)
13	1X	Blank
*14-68	55A1	Information on items revised or corrected
69	1X	Blank
*70	A1	Continuation code Blank = no continuation unit C = information is continued on the next unit (character numbers 14-68)
*71	I1	Sequence number n (1,2 . .), maximum 5 Blank if only one unit of Record Type J exists 'n' if more than one unit of Record Type J exists due to continuations or to multiple revisions
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	J (Record Type J)

Note: This Record Type is for internal database management use only and should be ignored for all other purposes.

RECORD TYPE K *Processing history and entry termination*

<u>Character</u> <u>Numbers</u>	<u>FORTTRAN</u> <u>Format</u>	<u>Item</u>
*1-8	8A1	Entry date (inorganic) or accession date (organic) in the form year/month/day (e.g. 86/03/15)
9-10	2X	Blank
*11-18	8A1	Keyboarding date (inorganic) or modification date (organic) (year/month/day)
19	1X	Blank
*20-22	3A1	Initials of keyboarder
23	1X	Blank
24-31	8A1	Processing date (year/month/day)
32-34	I3	Number of warnings
35-37	I3	Number of errors
38	1X	Blank
39-40	I2	NBS*AIDS83 revision number
41	1X	Blank
42-49	8A1	Revision date (year/month/day)
50	1X	Blank
*51-57	7A1	PDF number (reference to the Powder Diffraction File of the JCPDS--International Centre for Diffraction Data)
58	1X	Blank
*59-66	8A1	Alternate reference code (Cambridge code, metals code, or inorganic structural code)
67-71	5X	Blank
72-79	8A1	Crystal Data reference and system codes (see Record Type 1)
*80	A1	K (Record Type K)

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APPENDIX A

CHOICE AND ORIENTATION OF THE CRYSTAL DATA CELL

General Rules-- The cell chosen to define the lattice should obey the following rules (Donnay, 1943), to be applied in the sequence given:

- (1) Whenever possible the cell edges should coincide with symmetry directions¹ 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 unique axis ($n \geq 3$) is called *c*. Cell edges not governed by the lattice symmetry should obey the inequalities $c < a < b$.
- (6) The axes of coordinates should be directed, along the cell edges, so as to form a right-handed system with nonacute interedge 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.

In the *anorthic* (triclinic) system Rule 1 does not apply as symmetry directions do not exist. 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) to comply with Rule 3. Its edges must be the shortest three noncoplanar lattice translations (Rule 4) that define the reduced cell (Niggli, 1928; Santoro and Mighell, 1970). The cell edges are labeled so as to have $c < a < b$ (Rule 5) and oriented so that the angles α and β are nonacute (Rule 6).

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 nonacute (Rule 4) and $c < a$ (Rule 5). The resulting cell may be primitive (P) or centered (C, A, or I).

¹By definition a *symmetry direction* is either a symmetry axis, or the normal to a symmetry plane ($1/m = 2$), or both. This concept is used in dealing with point-group symmetries, of either polyhedra or 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, namely a spatial assemblage of points that are the termini of the vectors $L(uvw) = ua + vb + wc$, where *u*, *v*, and *w* are integers positive, negative, or zero.

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. The cell, in accordance with Rule 3, is the smallest possible one that obeys the first rule. All interedge 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 $mmm2$ may have to be oriented as $2mm$ or $m2m$.

The point-group symmetry of the *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 unique 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 unique 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 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). Of the four symmetry directions, one is perpendicular to a plane containing the other three. This unique 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 ($\gamma = 120^\circ$, $\alpha = \beta = 90^\circ$). 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 $1/3\ 2/3\ 2/3$ and $2/3\ 1/3\ 1/3$.

The point-group symmetry of a *cubic* lattice is $4/m\ \bar{3}\ 2/m$. The three 4-fold axes are the symmetry directions taken as edges of the cubic cell. The cell may be primitive (P), body centered (I), or face centered (F).

APPENDIX B

REDUCED CELLS AND REDUCED FORMS

The *reduced cell* (Niggli, 1928) is defined as a unique, primitive cell that is based on the three shortest noncoplanar vectors of the lattice and satisfies a specified set of mathematical conditions. These conditions are given in Table 1. The main conditions assure that one has a cell based on the three shortest lattice translations, while the special conditions assure that the cell is unique. The user should be aware that not all reduction algorithms currently in use satisfy the special conditions given in Table 1. It has been shown that in some lattices more than one cell is based on the three shortest lattice translations (Santoro and Mighell, 1970); Gruber (1973) has shown that at most five different cells of this type may exist in the same lattice. Techniques to obtain the reduced cell from an unreduced cell that is based on the three shortest translations are given in Himes and Mighell (1985).

The *reduced form* is defined by the vector dot products of the reduced cell: $a \cdot a \ b \cdot b \ c \cdot c / b \cdot c \ a \cdot c \ a \cdot b$. From the reduced form, the reduced form type (1-44) may be assigned. Table 2 gives the conditions for the 44 reduced forms, as well as the matrices relating each reduced form to a corresponding conventional cell of the Bravais lattice. In order for the reduced form type to be properly assigned, it is essential that the experimental cell of the lattice be determined as accurately as possible. Also, if the reduced form exhibits more specialization than is required to define the lattice type, it may signify that a subcell of the lattice has been determined or that the material is twinned.

Table 1. *Conditions for a reduced cell*

The reduced cell is specified by three noncoplanar vectors a , b , and c . To be reduced, the cell must be in a normal representation (type I or II) and all the main and special conditions for the given cell type must be satisfied. The main conditions are used to establish that a cell is based on the three shortest lattice translations. The special conditions are used to select a unique cell when two or more cells in the lattice have the same numerical values for the cell edges.

A. Positive reduced form, type I cell, all angles $< 90^\circ$

Main conditions: $a \cdot a \leq b \cdot b \leq c \cdot c$; $b \cdot c \leq \frac{1}{2} b \cdot b$;
 $a \cdot c \leq \frac{1}{2} a \cdot a$; $a \cdot b \leq \frac{1}{2} a \cdot a$

Special conditions: (a) if $a \cdot a = b \cdot b$ then $b \cdot c \leq a \cdot c$
 (b) if $b \cdot b = c \cdot c$ then $a \cdot c \leq a \cdot b$
 (c) if $b \cdot c = \frac{1}{2} b \cdot b$ then $a \cdot b \leq 2 a \cdot c$
 (d) if $a \cdot c = \frac{1}{2} a \cdot a$ then $a \cdot b \leq 2 b \cdot c$
 (e) if $a \cdot b = \frac{1}{2} a \cdot a$ then $a \cdot c \leq 2 b \cdot c$

B. Negative reduced form, type II cell, all angles $\geq 90^\circ$

Main conditions: (a) $a \cdot a \leq b \cdot b \leq c \cdot c$; $|b \cdot c| \leq \frac{1}{2} b \cdot b$;
 $|a \cdot c| \leq \frac{1}{2} a \cdot a$; $|a \cdot b| \leq \frac{1}{2} a \cdot a$
 (b) $(|b \cdot c| + |a \cdot c| + |a \cdot b|) \leq \frac{1}{2} (a \cdot a + b \cdot b)$

Special conditions: (a) if $a \cdot a = b \cdot b$ then $|b \cdot c| \leq |a \cdot c|$
 (b) if $b \cdot b = c \cdot c$ then $|a \cdot c| \leq |a \cdot b|$
 (c) if $|b \cdot c| = \frac{1}{2} b \cdot b$ then $a \cdot b = 0$
 (d) if $|a \cdot c| = \frac{1}{2} a \cdot a$ then $a \cdot b = 0$
 (e) if $|a \cdot b| = \frac{1}{2} a \cdot a$ then $a \cdot c = 0$
 (f) if $(|b \cdot c| + |a \cdot c| + |a \cdot b|) = \frac{1}{2} (a \cdot a + b \cdot b)$
 then $a \cdot a \leq 2 |a \cdot c| + |a \cdot b|$

Table 2. Metric classification of the 44 reduced forms*

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice	Cell Transformation Reduced → Conventional
	First Row	Second Row					
		a·a b·b c·c	b·c	a·c			
a = b = c							
1	a·a a·a a·a	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	+	Cubic F	111/111/111
2	a·a a·a a·a	b·c	b·c	b·c	+	Rhombohedral hR	110/101/111
3	a·a a·a a·a	0	0	0	-	Cubic P	100/010/001
4	a·a a·a a·a	- b·c	- b·c	- b·c	-	Rhombohedral hR	110/101/111
5	a·a a·a a·a	$-\frac{a \cdot a}{3}$	$-\frac{a \cdot a}{3}$	$-\frac{a \cdot a}{3}$	-	Cubic I	101/110/011
6	a·a a·a a·a	$\frac{-a \cdot a + a \cdot b }{2}$	$\frac{-a \cdot a + a \cdot b }{2}$	- a·b	-	Tetragonal I	011/101/110
7	a·a a·a a·a	- b·c	$\frac{-a \cdot a + b \cdot c }{2}$	$\frac{-a \cdot a + b \cdot c }{2}$	-	Tetragonal I	101/110/011
8	a·a a·a a·a	- b·c	- a·c	-(a·a - b·c - a·c)	-	Orthorhombic I	110/101/011
a = b							
9	a·a a·a c·c	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	+	Rhombohedral hR	100/110/113
10	a·a a·a c·c	b·c	b·c	a·b	+	Monoclinic C**	110/110/001
11	a·a a·a c·c	0	0	0	-	Tetragonal P	100/010/001
12	a·a a·a c·c	0	0	$-\frac{a \cdot a}{2}$	-	Hexagonal P	100/010/001
13	a·a a·a c·c	0	0	- a·b	-	Orthorhombic C	110/110/001
14	a·a a·a c·c	- b·c	- b·c	- a·b	-	Monoclinic C**	110/110/001
15	a·a a·a c·c	$-\frac{a \cdot a}{2}$	$-\frac{a \cdot a}{2}$	0	-	Tetragonal I	100/010/112
16	a·a a·a c·c	- b·c	- b·c	-(a·a - 2 b·c)	-	Orthorhombic F	110/110/112
17	a·a a·a c·c	- b·c	- a·c	-(a·a - b·c - a·c)	-	Monoclinic I††	101/110/011
b = c							
18	a·a b·b b·b	$\frac{a \cdot a}{4}$	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	+	Tetragonal I	011/111/100
19	a·a b·b b·b	b·c	$\frac{a \cdot a}{2}$	$\frac{a \cdot a}{2}$	+	Orthorhombic I	100/011/111
20	a·a b·b b·b	b·c	a·c	a·c	+	Monoclinic C†	011/011/100
21	a·a b·b b·b	0	0	0	-	Tetragonal P	010/001/100
22	a·a b·b b·b	$-\frac{b \cdot b}{2}$	0	0	-	Hexagonal P	010/001/100
23	a·a b·b b·b	- b·c	0	0	-	Orthorhombic C	011/011/100
24	a·a b·b b·b	$\frac{b \cdot b - \frac{a \cdot a}{3}}{2}$	$-\frac{a \cdot a}{3}$	$-\frac{a \cdot a}{3}$	-	Rhombohedral hR	121/011/100
25	a·a b·b b·b	- b·c	- a·c	- a·c	-	Monoclinic C†	011/011/100

Table 2. Metric classification of the 44 reduced forms (continued)

Reduced Form No.	Reduced Form Matrix				Reduced Form Type	Bravais Lattice	Cell Transformation Reduced → Conventional
	First Row†††	Second Row					
		a·a b·b c·c	b·c	a·c			
a ≤ b ≤ c 26	a·a b·b c·c	$\frac{a·a}{4}$	$\frac{a·a}{2}$	$\frac{a·a}{2}$	+	Orthorhombic F	100/ $\bar{1}$ 20/ $\bar{1}$ 02
27	a·a b·b c·c	b·c	$\frac{a·a}{2}$	$\frac{a·a}{2}$	+	Monoclinic I***	0 $\bar{1}$ 1/ $\bar{1}$ 00/ $\bar{1}$ $\bar{1}$
28	a·a b·b c·c	$\frac{a·b}{2}$	$\frac{a·a}{2}$	a·b	+	Monoclinic C	$\bar{1}$ 00/ $\bar{1}$ 02/010
29	a·a b·b c·c	$\frac{a·c}{2}$	a·c	$\frac{a·a}{2}$	+	Monoclinic C	100/ $\bar{1}$ 20/00 $\bar{1}$
30	a·a b·b c·c	$\frac{b·b}{2}$	$\frac{a·b}{2}$	a·b	+	Monoclinic C	010/012/ $\bar{1}$ 00
31	a·a b·b c·c	b·c	a·c	a·b	+	Triclinic P	100/010/001
32	a·a b·b c·c	0	0	0	-	Orthorhombic P	100/010/001
33	a·a b·b c·c	0	- a·c	0	-	Monoclinic P	100/010/001
34	a·a b·b c·c	0	0	- a·b	-	Monoclinic P	$\bar{1}$ 00/00 $\bar{1}$ /010
35	a·a b·b c·c	- b·c	0	0	-	Monoclinic P	0 $\bar{1}$ 0/ $\bar{1}$ 00/00 $\bar{1}$
36	a·a b·b c·c	0	$-\frac{a·a}{2}$	0	-	Orthorhombic C	100/ $\bar{1}$ 02/010
37	a·a b·b c·c	- b·c	$-\frac{a·a}{2}$	0	-	Monoclinic C*	102/100/010
38	a·a b·b c·c	0	0	$-\frac{a·a}{2}$	-	Orthorhombic C	$\bar{1}$ 00/120/00 $\bar{1}$
39	a·a b·b c·c	- b·c	0	$-\frac{a·a}{2}$	-	Monoclinic C**	$\bar{1}$ 20/ $\bar{1}$ 00/00 $\bar{1}$
40	a·a b·b c·c	$-\frac{b·b}{2}$	0	0	-	Orthorhombic C	0 $\bar{1}$ 0/012/ $\bar{1}$ 00
41	a·a b·b c·c	$-\frac{b·b}{2}$	- a·c	0	-	Monoclinic C†	0 $\bar{1}$ 2/0 $\bar{1}$ 0/ $\bar{1}$ 00
42	a·a b·b c·c	$-\frac{b·b}{2}$	$-\frac{a·a}{2}$	0	-	Orthorhombic I	$\bar{1}$ 00/0 $\bar{1}$ 0/112
43	a·a b·b c·c	$-\frac{b·b - a·b }{2}$	$-\frac{a·a - a·b }{2}$	- a·b	-	Monoclinic I	$\bar{1}$ 00/ $\bar{1}$ 12/0 $\bar{1}$ 0
44	a·a b·b c·c	- b·c	- a·c	- a·b	-	Triclinic P	100/010/001

† If $a·a < 4|a·c|$ }
 * If $b·b < 4|b·c|$ } Premultiply Table Matrix by 00 $\bar{1}$ /010/101 (I centered)
 ** If $c·c < 4|b·c|$ }

†† If $3a·a < c·c + 2|a·c|$ }
 *** If $3b·b < c·c + 2|b·c|$ } Premultiply Table Matrix by $\bar{1}$ 0 $\bar{1}$ /010/100 (C centered)

††† No required relationships between symmetrical scalars for reduced forms 26-44.

*Reprinted from Mighell and Rodgers (1980). Based on Table 5.1.3.1 of the *International Tables for X-ray Crystallography* (1969) and published revisions.

APPENDIX C

SPACE GROUPS AND ASPECTS

The following tables give the space groups and diffraction aspects, along with the space group and aspect numbers, that appear in the NBS *Crystal Data* database. Although additional orientations may be used on Record Type 3 for the authors' space group or aspect, *only* those listed in these tables (in addition to cell centering symbols) will appear on Record Type 4 for the Crystal Data space group or aspect. If no space group or aspect is given, or if the orientation of the authors' space group or aspect is unusual, a space group number of 0 is assigned.

Part I (Space Groups)

The space group numbers correspond to those given in the *International Tables for X-ray Crystallography* (1969). The assigned number is followed by an orientation code when more than one orientation is permitted for a given space group in the monoclinic or orthorhombic crystal systems. These codes are A, B, and C for the monoclinic system (*b*-unique); D, E, and F for the monoclinic system (*c*-unique, used on Record Type 3 only); and A, B, C, D, E, and F for the orthorhombic system.

Part II (Aspects)

The diffraction aspect is given when the space group is not uniquely defined. The diffraction aspects for each Laue class have been given by Donnay and Kennard (1964) and are reprinted in Supplement II of the third edition of *Crystal Data*, Volumes 1 and 2 (Donnay and Ondik, 1972, 1973). The aspect number, preceded by an asterisk (*), corresponds to the number of the highest symmetry space group that is consistent with the diffraction aspect. The aspects for enantiomorphic space groups (e.g. $P4_12_12$ and $P4_32_12$) are assigned the number corresponding to the lower-numbered space group of the pair. The orientation codes for the monoclinic and orthorhombic systems are the same as those assigned to the space groups.

PART I

SPACE GROUPS

Anorthic (Triclinic) System

Space Group No.	Aspect No.	Space Group Symbols
1	2	P1
2	2	$\overline{P}1$

Monoclinic System

Space Group No.	Aspect No.	Space Group Symbols					
		A*	B	C	D	E	F
3	10	P2			P2		
4	11	P2 ₁			P2 ₁		
5	12	C2	A2	I2	B2	A2	I2
6	10	Pm			Pm		
7	13	Pc	Pa	Pn	Pb	Pa	Pn
8	12	Cm	Am	Im	Bm	Am	Im
9	15	Cc	Aa	Ia	Bb	Aa	Ia
10	10	P2/m			P2/m		
11	11	P2 ₁ /m			P2 ₁ /m		
12	12	C2/m	A2/m	I2/m	B2/m	A2/m	I2/m
13	13	P2/c	P2/a	P2/n	P2/b	P2/a	P2/n
14		P2 ₁ /c	P2 ₁ /a	P2 ₁ /n	P2 ₁ /b	P2 ₁ /a	P2 ₁ /n
15	15	C2/c	A2/a	I2/a	B2/b	A2/a	I2/a

*Orientation code. For the monoclinic system, codes A, B, and C are for *b*-unique, and codes D, E, and F are for *c*-unique.

Orthorhombic System

Space Group No.	Aspect No.	Space Group Symbols					
		A	B	C	D	E	F
16	47	P222					
17		P222 ₁	P2 ₁ 22	P22 ₁ 2			
18		P2 ₁ 2 ₁ 2	P22 ₁ 2 ₁	P2 ₁ 22 ₁			
19		P2 ₁ 2 ₁ 2 ₁					
20		C222 ₁	A2 ₁ 22	B22 ₁ 2			
21	65	C222	B222	A222			
22	69	F222					
23	71	I222					
24	71	I2 ₁ 2 ₁ 2 ₁					
25	47	Pmm2	Pm2m	P2mm			
26	51	Pmc2 ₁	P2 ₁ ma	P2 ₁ am	Pb2 ₁ m	Pcm2 ₁	Pm2 ₁ b
27	49	Pcc2	Pb2b	P2aa			
28	51	Pma2	P2cm	P2mb	Pbm2	Pc2m	Pm2a
29	57	Pca2 ₁	P2 ₁ ca	Pb2 ₁ a	P2 ₁ ab	Pc2 ₁ b	Pbc2 ₁
30	53	Pnc2	Pcn2	Pn2b	Pb2n	P2na	P2an
31	59	Pmn2 ₁	Pnm2 ₁	P2 ₁ nm	Pn2 ₁ m	Pm2 ₁ n	P2 ₁ mn
32	55	Pba2	P2cb	Pc2a			
33	62	Pna2 ₁	Pbn2 ₁	P2 ₁ cn	P2 ₁ nb	Pn2 ₁ a	Pc2 ₁ n
34	58	Pnn2	Pn2n	P2nn			
35	65	Cmm2	Bm2m	A2mm			
36	63	Cmc2 ₁	A2 ₁ am	A2 ₁ ma	Bm2 ₁ b	Bb2 ₁ m	Ccm2 ₁
37	66	Ccc2	A2aa	Bb2b			
38	65	Amn2	Am2m	B2mm	C2mm	Bmn2	Cm2m

Orthorhombic System (cont.)

Space Group No.	Aspect No.	Space Group Symbols					
		A	B	C	D	E	F
39	67	Abm2	Bma2	C2ma	Ab2m	Cm2a	B2am
40	63	Ama2	C2cm	Bbm2	B2mb	Cc2m	Am2a
41	64	Aba2	Ab2a	C2ca	B2ab	Cc2a	Bba2
42	69	Fmm2	Fm2m	F2mm			
43		Fdd2	Fd2d	F2dd			
44	71	Imm2	Im2m	I2mm			
45	72	Iba2	Ib2a	I2aa			
46	74	Ima2	Im2a	Ibm2	I2am	Ib2m	I2ma
47	47	Pmmm					
48		Pnnn					
49	49	Pccm	Pmaa	Pbmb			
50		Pban	Pncb	Pcna			
51	51	Pmma	Pmcm	Pcmm	Pmam	Pbmm	Pmmb
52		Pnna	Pnnb	Pnan	Pncn	Pbnn	Pcnn
53	53	Pmna	Pncm	Pbmn	Pman	Pcnm	Pnmb
54		Pcca	Pbaa	Pbcb	Pccb	Pbab	Pcaa
55	55	Pbam	Pcma	Pmcb			
56		Pccn	Pbnb	Pnaa			
57	57	Pbcm	Pcmb	Pbma	Pcam	Pmab	Pmca
58	58	Pnmm	Pnmn	Pmnn			
59	59	Pmmn	Pnmn	Pmnn			
60		Pbcn	Pnab	Pnca	Pbna	Pcan	Pcnb
61		Pbca	Pcab				

Orthorhombic System (cont.)

Space Group No.	Aspect No.	Space Group Symbols					
		A	B	C	D	E	F
62	62	Pnma	Pmnb	Pbnm	Pmcn	Pcmn	Pnam
63	63	Cmcm	Bbmm	Amam	Amma	Cmmm	Bmmb
64	64	Cmca	Abam	Ccma	Abma	Bmab	Bbam
65	65	Cmmm	Bmmm	Ammm			
66	66	Cccm	Amaa	Bbmb			
67	67	Cmma	Abmm	Bmam			
68		Ccca	Bbab	Abaa			
69	69	Fmmm					
70		Fddd					
71	71	Immm					
72	72	Ibam	Imaa	Ibma			
73		Ibca					
74	74	Imma	Ibmm	Imam			

Tetragonal System

Space Group No.	Aspect No.	Space Group Symbols	Space Group No.	Aspect No.	Space Group Symbols
75	83	P4	76	76	P4 ₁
77	84	P4 ₂	78	76	P4 ₃
79	87	I4	80		I4 ₁
81	83	P4 ⁻	82	87	I4 ⁻
83	83	P4/m	84	84	P4 ₂ /m
85		P4/n	86		P4 ₂ /n
87	87	I4/m	88		I4 ₁ /a

Tetragonal System (cont.)

<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>	<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>
89	123	P4 ₂ 2	90	113	P4 ₂ 1 ₂
91	91	P4 ₁ 22	92	92	P4 ₁ 2 ₁ 2
93		P4 ₂ 22	94		P4 ₂ 2 ₁ 2
95	91	P4 ₃ 22	96	92	P4 ₃ 2 ₁ 2
97	139	I4 ₂ 2	98		I4 ₁ 22
99	123	P4mm	100	127	P4bm
101	132	P4 ₂ cm	102	136	P4 ₂ nm
103	124	P4cc	104	128	P4nc
105	131	P4 ₂ mc	106	135	P4 ₂ bc
107	139	I4mm	108	140	I4cm
109	122	I4 ₁ md	110		I4 ₁ cd
111	123	P $\bar{4}$ ₂ m	112	131	P $\bar{4}$ ₂ c
113	113	P $\bar{4}$ ₂ 1 ₂ m	114		P $\bar{4}$ ₂ 1 ₂ c
115	123	P $\bar{4}$ m2	116	132	P $\bar{4}$ c2
117	127	P $\bar{4}$ b2	118	136	P $\bar{4}$ n2
119	139	I $\bar{4}$ m2	120	140	I $\bar{4}$ c2
121	139	I $\bar{4}$ ₂ m	122	122	I $\bar{4}$ ₂ d
123	123	P4/mmm	124	124	P4/mcc
125		P4/nbm	126		P4/nnc
127	127	P4/mbm	128	128	P4/mnc
129		P4/nmm	130		P4/ncc
131	131	P4 ₂ /mmc	132	132	P4 ₂ /mcm
133		P4 ₂ /nbc	134		P4 ₂ /nnm

Tetragonal System (cont.)

Space Group <u>No.</u>	Aspect <u>No.</u>	Space Group <u>Symbols</u>	Space Group <u>No.</u>	Aspect <u>No.</u>	Space Group <u>Symbols</u>
135	135	$P4_2/mbc$	136	136	$P4_2/mnm$
137		$P4_2/nmc$	138		$P4_2/ncm$
139	139	$I4/mmm$	140	140	$I4/mcm$
141		$I4_1/amd$	142		$I4_1/acd$

Hexagonal and Rhombohedral Systems

Space Group <u>No.</u>	Aspect <u>No.</u>	Space Group <u>Symbols</u>	Space Group <u>No.</u>	Aspect <u>No.</u>	Space Group <u>Symbols</u>
143	147	$P3$	144	144	$P3_1$
145	144	$P3_2$	146	148	$R3$
147	147	$P\bar{3}$	148	148	$R\bar{3}$
149	162	$P312$	150	164	$P321$
151	151	$P3_112$	152	152	$P3_121$
153	151	$P3_212$	154	152	$P3_221$
155	166	$R32$	156	164	$P3m1$
157	162	$P31m$	158	165	$P3c1$
159	163	$P31c$	160	166	$R3m$
161	167	$R3c$	162	162	$P\bar{3}1m$
163	163	$P\bar{3}1c$	164	164	$P\bar{3}m1$
165	165	$P\bar{3}c1$	166	166	$R\bar{3}m$
167	167	$R\bar{3}c$	168	175	$P6$
169	169	$P6_1$	170	169	$P6_5$
171	171	$P6_2$	172	171	$P6_4$

Hexagonal and Rhombohedral Systems (cont.)

<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>	<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>
173	176	P6 ₃	174	175	P ₆ ⁻
175	175	P6/m	176	176	P6 ₃ /m
177	191	P622	178	178	P6 ₁ 22
179	178	P6 ₅ 22	180	180	P6 ₂ 22
181	180	P6 ₄ 22	182		P6 ₃ 22
183	191	P6mm	184	192	P6cc
185	193	P6 ₃ cm	186	194	P6 ₃ mc
187	191	P ₆ m2	188	193	P ₆ c2
189	191	P ₆ 2m	190	194	P ₆ 2c
191	191	P6/mmm	192	192	P6/mcc
193	193	P6 ₃ /mcm	194	194	P6 ₃ /mmc

Cubic System

<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>	<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>
195	200	P23	196	202	F23
197	204	I23	198		P2 ₁ 3
199	204	I2 ₁ 3	200	200	Pm3
201		Pn3	202	202	Fm3
203		Fd3	204	204	Im3
205		Pa3	206		Ia3
207	221	P432	208		P4 ₂ 32
209	225	F432	210		F4 ₁ 32
211	229	I432	212	212	P4 ₃ 32

Cubic System (cont.)

<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>	<u>Space Group No.</u>	<u>Aspect No.</u>	<u>Space Group Symbols</u>
213	212	$P4_132$	214		$I4_132$
215	221	$P\bar{4}3m$	216	225	$F\bar{4}3m$
217	229	$I\bar{4}3m$	218	223	$P\bar{4}3n$
219	226	$F\bar{4}3c$	220		$I\bar{4}3d$
221	221	$Pm3m$	222		$Pn3n$
223	223	$Pm3n$	224		$Pn3m$
225	225	$Fm3m$	226	226	$Fm3c$
227		$Fd3m$	228		$Fd3c$
229	229	$Im3m$	230		$Ia3d$

PART II

ASPECTS

Anorthic (Triclinic) System

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
$P^*, \bar{1}$	2	$P\bar{1}$ (2), $P1$ (1)

Monoclinic System

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
$P^*/^*$	10	$P2/m$ (10), $P2$ (3), Pm (6)
$P^*/^*$	10D*	$P2/m$ (10D), $P2$ (3D), Pm (6D)
$P2_1/^*$	11	$P2_1/m$ (11), $P2_1$ (4)
$P2_1/^*$	11D	$P2_1/m$ (11D), $P2_1$ (4D)
$C^*/^*$	12A	$C2/m$ (12A), $C2$ (5A), Cm (8A)
$A^*/^*$	12B	$A2/m$ (12B), $A2$ (5B), Am (8B)
$I^*/^*$	12C	$I2/m$ (12C), $I2$ (5C), Im (8C)
$B^*/^*$	12D	$B2/m$ (12D), $B2$ (5D), Bm (8D)
$A^*/^*$	12E	$A2/m$ (12E), $A2$ (5E), Am (8E)
$I^*/^*$	12F	$I2/m$ (12F), $I2$ (5F), Im (8F)
P^*/c	13A	$P2/c$ (13A), Pc (7A)
P^*/a	13B	$P2/a$ (13B), Pa (7B)
P^*/n	13C	$P2/n$ (13C), Pn (7C)
P^*/b	13D	$P2/b$ (13D), Pb (7D)
P^*/a	13E	$P2/a$ (13E), Pa (7E)
P^*/n	13F	$P2/n$ (13F), Pn (7F)

*Orientation code. For the monoclinic system, codes A, B, and C are for *b*-unique, and codes D, E, and F are for *c*-unique.

Monoclinic System (cont.)

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
C*/c	15A	C2/c (15A), Cc (9A)
A*/a	15B	A2/a (15B), Aa (9B)
I*/a	15C	I2/a (15C), Ia (9C)
B*/b	15D	B2/b (15D), Bb (9D)
A*/a	15E	A2/a (15E), Aa (9E)
I*/a	15F	I2/a (15F), Ia (9F)

Orthorhombic System

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
P***	47	Pmmm (47), P222 (16), Pmm2 (25A), Pm2m (25B), P2mm (25C)
Pcc*	49A	Pccm (49A), Pcc2 (27A)
P*aa	49B	Pmaa (49B), P2aa (27C)
Pb*b	49C	Pbmb (49C), Pb2b (27B)
P**a	51A	Pmna (51A), P2 ₁ ma (26B), Pm2a (28F)
P*c*	51B	Pmcm (51B), Pmc2 ₁ (26A), P2cm (28B)
Pc**	51C	Pcmm (51C), Pcm2 ₁ (26E), Pc2m (28E)
P*a*	51D	Pmam (51D), P2 ₁ am (26C), Pma2 (28A)
Pb**	51E	Pbmm (51E), Pb2 ₁ m (26D), Pbm2 (28D)
P**b	51F	Pmmb (51F), Pm2 ₁ b (26F), P2mb (28C)
P*na	53A	Pmna (53A), P2na (30E)
Pnc*	53B	Pncm (53B), Pnc2 (30A)
Pb*n	53C	Pbmn (53C), Pb2n (30D)
P*an	53D	Pman (53D), P2an (30F)
Pcn*	53E	Pcnm (53E), Pcn2 (30B)
Pn*b	53F	Pnmb (53F), Pn2b (30C)

Orthorhombic System (cont.)

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
Pba*	55A	Pbam (55A), Pba2 (32A)
Pc*a	55B	Pcma (55B), Pc2a (32C)
P*cb	55C	Pmcb (55C), P2cb (32B)
Pbc*	57A	Pbcm (57A), Pbc2 ₁ (29F)
Pc*b	57B	Pcmb (57B), Pc2 ₁ b (29E)
Pb*a	57C	Pbma (57C), Pb2 ₁ a (29C)
Pca*	57D	Pcam (57D), Pca2 ₁ (29A)
P*ab	57E	Pmab (57E), P2 ₁ ab (29D)
P*ca	57F	Pmca (57F), P2 ₁ ca (29B)
Pnn*	58A	Pnnm (58A), Pnn2 (34A)
Pn*n	58B	Pnmm (58B), Pn2n (34B)
P*nn	58C	Pmnn (58C), P2nn (34C)
P**n	59A	Pmnn (59A), Pm2 ₁ n (31E), P2 ₁ mn (31F)
Pn**	59B	Pnmm (59B), Pnm2 ₁ (31B), Pn2 ₁ m (31D)
P*n*	59C	Pmnm (59C), Pmn2 ₁ (31A), P2 ₁ nm (31C)
Pn*a	62A	Pnma (62A), Pn2 ₁ a (33E)
P*nb	62B	Pmnb (62B), P2 ₁ nb (33D)
Pbn*	62C	Pbnm (62C), Pbn2 ₁ (33B)
P*cn	62D	Pmcn (62D), P2 ₁ cn (33C)
Pc*n	62E	Pcmn (62E), Pc2 ₁ n (33F)
Pna*	62F	Pnam (62F), Pna2 ₁ (33A)
C*c*	63A	Cmcm (63A), Cmc2 ₁ (36A), C2cm (40B)
Bb**	63B	Bbmm (63B), Bb2 ₁ m (36E), Bbm2 (40C)
A*a*	63C	Amam (63C), A2 ₁ am (36B), Ama2 (40A)

Orthorhombic System (cont.)

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
A**a	63D	Amma (63D), A2 ₁ ma (36C), Am2a (40F)
Cc**	63E	Ccmm (63E), Ccm2 ₁ (36F), Cc2m (40E)
B**b	63F	Bmmb (63F), Bm2 ₁ b (36D), B2mb (40D)
C*ca	64A	Cmca (64A), C2ca (41G)
Aba*	64B	Abam (64B), Aba2 (41A)
Cc*a	64C	Ccma (64C), Cc2a (41E)
Ab*a	64D	Abma (64D), Ab2a (41B)
B*ab	64E	Bmab (64E), B2ab (41D)
Bba*	64F	Bbam (64F), Bba2 (41F)
C***	65A	Cmmm (65A), C222 (21A), Cmm2 (35A), C2mm (38D), Cm2m (38F)
B***	65B	Bmmm (65B), B222 (21B), Bm2m (35B), B2mm (38C), Bmm2 (38E)
A***	65C	Ammm (65C), A222 (21C), A2mm (35C), Amm2 (38A), Am2m (38B)
Ccc*	66A	Cccm (66A), Ccc2 (37A)
A*aa	66B	Amaa (66B), A2aa (37B)
Bb*b	66C	Bbmb (66C), Bb2b (37C)
C**a	67A	Cmma (67A), C2ma (39C), Cm2a (39E)
Ab**	67B	Abmm (67B), Abm2 (39A), Ab2m (39D)
B*a*	67C	Bmam (67C), Bma2 (39B), B2am (39F)
F***	69	Fmmm (69), F222 (22), Fmm2 (42A), Fm2m (42B), F2mm (42C)
I***	71	Immm (71), I222 (23), I2 ₁ 2 ₁ 2 ₁ (24), Imm2 (44A), Im2m (44B), I2mm (44C)
Iba*	72A	Ibam (72A), Iba2 (45A)
I*aa	72B	Imaa (72B), I2aa (45C)
Ib*a	72C	Ibma (72C), Ib2a (45B)

Orthorhombic System (cont.)

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
I**a	74A	Imma (74A), Im2a (46B), I2ma (46F)
Ib**	74B	Ibmm (74B), Ib2 (46C), Ib2m (46E)
I*a*	74C	Imam (74C), Ima2 (46A), I2am (46D)

Tetragonal System

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
P ₄ _{1,3}	76	P ₄ ₁ (76), P ₄ ₃ (78)
P ₄ /*	83	P ₄ /m (83), P ₄ (75), P ₄ [−] (81)
P ₄ ₂ /*	84	P ₄ ₂ /m (84), P ₄ ₂ (77)
I ₄ /*	87	I ₄ /m (87), I ₄ (79), I ₄ [−] (82)
P ₄ _{1,3} ₂₂	91	P ₄ ₁ ₂₂ (91), P ₄ ₃ ₂₂ (95)
P ₄ _{1,3} ₂₁ ₂	92	P ₄ ₁ ₂₁ ₂ (92), P ₄ ₃ ₂₁ ₂ (96)
P ₄ ₂ ₁ *	113	P ₄ ₂ ₁ [−] m (113), P ₄ ₂ ₁ ₂ (90)
I ₄ *d	122	I ₄ ₂ d (122), I ₄ ₁ md (109)
P ₄ /**	123	P ₄ /mmm (123), P ₄ ₂₂ (89), P ₄ mm (99), P ₄ ₂ [−] m (111), P ₄ ₂ [−] m (115)
P ₄ /*cc	124	P ₄ /mcc (124), P ₄ cc (103)
P ₄ /*b*	127	P ₄ /mbm (127), P ₄ bm (100), P ₄ ₂ [−] b ₂ (117)
P ₄ /*nc	128	P ₄ /mnc (128), P ₄ nc (104)
P ₄ /**c	131	P ₄ ₂ /mmc (131), P ₄ ₂ mc (105), P ₄ ₂ [−] c (112)
P ₄ /*c*	132	P ₄ ₂ /mcm (132), P ₄ ₂ cm (101), P ₄ ₂ [−] c ₂ (116)
P ₄ /*bc	135	P ₄ ₂ /mbc (135), P ₄ ₂ bc (106)
P ₄ /*n*	136	P ₄ ₂ /mnm (136), P ₄ ₂ nm (102), P ₄ ₂ [−] n ₂ (118)
I ₄ /**	139	I ₄ /mmm (139), I ₄ ₂₂ (97), I ₄ mm (107), I ₄ ₂ [−] m (119), I ₄ ₂ [−] m (121)
I ₄ /*c*	140	I ₄ /mcm (140), I ₄ cm (108), I ₄ ₂ [−] c ₂ (120)

Hexagonal and Rhombohedral Systems

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
$P3_{1,2}$	144	$P3_1$ (144), $P3_2$ (145)
$P^*,\bar{3}$	147	$P\bar{3}$ (147), $P3$ (143)
R^*	148	$R\bar{3}$ (148), $R3$ (146)
$P3_{1,2}12$	151	$P3_112$ (151), $P3_212$ (153)
$P3_{1,2}21$	152	$P3_121$ (152), $P3_221$ (154)
$P31^*$	162	$P\bar{3}1m$ (162), $P312$ (149), $P31m$ (157)
$P^*1c,\bar{3}m$	163	$P\bar{3}1c$ (163), $P31c$ (159)
$P3^*1$	164	$P\bar{3}m1$ (164), $P321$ (150), $P3m1$ (156)
$P^*c1,\bar{3}m$	165	$P\bar{3}c1$ (165), $P3c1$ (158)
R^{**}	166	$R\bar{3}m$ (166), $R32$ (155), $R3m$ (160)
R^*c	167	$R\bar{3}c$ (167), $R3c$ (161)
$P6_{1,5}$	169	$P6_1$ (169), $P6_5$ (170)
$P6_{2,4}$	171	$P6_2$ (171), $P6_4$ (172)
$P6/*$	175	$P6/m$ (175), $P6$ (168), $P\bar{6}$ (174)
$P6_3/*$	176	$P6_3/m$ (176), $P6_3$ (173)
$P6_{1,5}22$	178	$P6_122$ (178), $P6_522$ (179)
$P6_{2,4}22$	180	$P6_222$ (180), $P6_422$ (181)
$P6/***$	191	$P6/mmm$ (191), $P622$ (177), $P6mm$ (183), $P\bar{6}m2$ (187), $P\bar{6}2m$ (189)
$P6/*cc$	192	$P6/mcc$ (192), $P6cc$ (184)
$P6/*c^*$	193	$P6_3/mcm$ (193), $P6_3cm$ (185), $P\bar{6}c2$ (188)
$P6/**c$	194	$P6_3/mmc$ (194), $P6_3mc$ (186), $P\bar{6}2c$ (190)

Cubic System

<u>Aspect</u>	<u>Number</u>	<u>Space Groups (Space Group Numbers)</u>
P*3	200	Pm3 (200), P23 (195)
F*3	202	Fm3 (202), F23 (196)
I*3	204	Im3 (204), I23 (197), I2 ₁ 3 (199)
P4 ₁ ,3 ³²	212	P4 ₃ 32 (212), P4 ₁ 32 (213)
P*3*	221	Pm3m (221), P432 (207), P ⁻ 4 ₃ m (215)
P*3n	223	Pm3n (223), P ⁻ 4 ₃ n (218)
F*3*	225	Fm3m (225), F432 (209), F ⁻ 4 ₃ m (216)
F*3c	226	Fm3c (226), F ⁻ 4 ₃ c (219)
I*3*	229	Im3m (229), I432 (211), I ⁻ 4 ₃ m (217)

APPENDIX D

ORGANIC CHEMICAL CLASSES

The classification of substances containing organic carbon, as developed by the Cambridge Crystallographic Data Centre and given in *Molecular Structures and Dimensions* (Kennard et al., 1984), is given below.

- 1 Aliphatic carboxylic acids and their derivatives (cyclic acid derivatives, e.g. anhydrides and lactones, are classified in the appropriate hetero class)
- 2 Aliphatic carboxylic acid salts (ammonium, IA, IIA metals; in a few cases where the cation is organic, the anion is classified in class 2)
- 3 Aliphatic amines
- 4 Aliphatic (N and S) compounds (must contain -C-N-S or -C-S-N-)
- 5 Aliphatic miscellaneous
- 6 Enolates (aliphatic and aromatic)
- 7 Nitriles (aliphatic and aromatic)
- 8 Urea compounds (aliphatic and aromatic)
- 9 Nitrogen-nitrogen compounds (aliphatic and aromatic; must contain -C-N-N-)
- 10 Nitrogen-oxygen compounds (aliphatic and aromatic; must contain -C-N-O- or -C-O-N-)
- 11 Sulfur and selenium compounds
- 12 Carbonium ions, carbanions, radicals
- 13 Benzoic acid derivatives (cyclic acid derivatives, e.g. anhydrides and lactones, are classified in the appropriate hetero class)
- 14 Benzoic acid salts (ammonium IA, IIA metals)
- 15 Benzene nitro compounds
- 16 Anilines
- 17 Phenols and ethers
- 18 Benzoquinones
- 19 Benzene miscellaneous
- 20 Monocyclic hydrocarbons (3, 4, 5-membered rings)
- 21 Monocyclic hydrocarbons (6-membered rings)
- 22 Monocyclic hydrocarbons (7, 8-membered rings)
- 23 Monocyclic hydrocarbons (9- and higher-membered rings)
- 24 Naphthalene compounds (fully unsaturated)
- 25 Naphthoquinones (fully unsaturated)
- 26 Anthracene compounds (fully unsaturated)
- 27 Polycyclic hydrocarbons (2 fused rings)
- 28 Polycyclic hydrocarbons (3 fused rings)
- 29 Polycyclic hydrocarbons (4 fused rings)
- 30 Polycyclic hydrocarbons (5 or more fused rings)
- 31 Bridged ring hydrocarbons
- 32 Hetero-nitrogen (3, 4, 5-membered monocyclic)
- 33 Hetero-nitrogen (6-membered monocyclic)
- 34 Hetero-nitrogen (7- and higher-membered monocyclic)
- 35 Hetero-nitrogen (2 fused rings)
- 36 Hetero-nitrogen (more than 2 fused rings)
- 37 Hetero-nitrogen (bridged ring system)

- 38 Hetero-oxygen
- 39 Hetero-sulfur and hetero-selenium
- 40 Hetero-(nitrogen and oxygen)
- 41 Hetero-(nitrogen and sulfur)
- 42 Miscellaneous heterocycles
- 43 Barbiturates
- 44 Pyrimidines and purines (the ring system must conform to the unmodified pyrimidine or purine skeleton)
- 45 Carbohydrates
- 46 Phosphates
- 47 Nucleosides and nucleotides
- 48 Alpha-amino-acids and peptides (reserved for peptides and α -amino-acids, whether or not the amino-acid possesses biological properties; thus a β -amino-acid would be classified in the appropriate acid and amine classes)
- 49 Porphyrins and corrins
- 50 Antibiotics (a cross-reference to a structural class is always provided)
- 51 Steroids
- 52 Monoterpenes
- 53 Sesquiterpenes
- 54 Diterpenes
- 55 Sesterterpenes
- 56 Triterpenes
- 57 Tetraterpenes
- 58 Alkaloids
- 59 Miscellaneous natural products (a cross-reference to a structural class is always provided)
- 60 Molecular complexes
- 61 Clathrates
- 62 Boron compounds
- 63 Silicon compounds
- 64 Phosphorus compounds
- 65 Arsenic compounds
- 66 Antimony and bismuth compounds
- 67 Groups IA and IIA compounds (reserved for compounds containing covalently bonded metals of groups IA and IIA)
- 68 Group III compounds
- 69 Germanium, tin, lead compounds
- 70 Tellurium compounds
- 71 Transition metal-C compounds
- 72 Metal π -complexes (open-chain)
- 73 Metal π -complexes (cyclopentadiene)
- 74 Metal π -complexes (arene)
- 75 Metal π -complexes (miscellaneous ring systems)
- 76 Metal complexes (ethylenediamine)
- 77 Metal complexes (acetylacetone)
- 78 Metal complexes (salicylic derivatives)
- 79 Metal complexes (thiourea)
- 80 Metal complexes (thiocarbamate or xanthate)
- 81 Metal complexes (carboxylic acid)
- 82 Metal complexes (amino-acid)
- 83 Metal complexes (nitrogen ligand)

- 84 Metal complexes (oxygen ligand)
- 85 Metal complexes (sulfur or selenium ligand)
- 86 Metal complexes (P, As, Sb ligand)

APPENDIX E

MINERAL GROUP AND SUBGROUP CODES

The mineral group and subgroup codes as defined by the JCPDS--International Centre for Diffraction Data are given below. For each mineral group with subgroups, the subgroups are indented.

ADA	Adamite	ART	Arthurite
ADA	Adamite	ASS	Arseniosiderite
AND	Andalusite	AST	Astrophyllite
AEN	Aenigmatite	AUT	Autunite
RST	Related structures	AUT	Autunite
ALM	Alum	URS	Uranospinite
ALN	Alunite	AXI	Axinite
ALN	Alunite	BAR	Barite
BEU	Beudantite	BAS	Bastnaesite
CRA	Crandallite	BAS	Bastnaesite
DUS	Dussertite	PAR	Parisite
AMB	Amblygonite	SYN	Synchysite
AMO	Amorphous	BEC	Becquerelite
NCR	Noncrystalline	BEC	Becquerelite
MTM	Metamict	CCU	Calciouranoite
AMP	Amphibole	MCU	Metacalciouranoite
OAM	Orthoamphibole	RST	Related structures
AFM	Fe-Mg-Mn	BEN	Benitoite
ACA	Ca	RST	Related structures
ACN	Ca-Na	BER	Beryl
ANA	Na	BET	Betpakdalite
RST	Related structures	BIS	Bischofite
ANC	Analcime	BIX	Bixbyite
ANH	Anhydrite	BJA	Bjarebyite
APA	Apatite	BOR	Boracite
APA	Apatite	BOR	Boracite
BRI	Britholite	CON	Congolite
CES	Cesanite	D'A	D'Ansite
PYM	Pyromorphite	HIL	Hilgardite
VAN	Vanadinite	PRH	Parahilgardite
RST	Related structures	BOU	Bournonite
APO	Apophyllite	BRA	Bradleyite
RST	Related structures	BRK	Brackebuschite
ARA	Aragonite		
RST	Related structures		

BRU	Brucite	CRI	Crichtonite
BRU	Brucite	CRP	Carpholite
MLN	Melonite	CUB	Cubanite
BSM	Bismutite	CYL	Cylindrite
BUT	Buttgenbachite	DAT	Datolite
CAL	Calcite	DES	Descloizite
CAL	Calcite	DIA	Diaspore
DOL	Dolomite	DLF	Delafoosite
RST	Related structures	DUF	Dufrenite
CAN	Cancrinite	DUN	Dundasite
CAR	Carnotite	EKA	Ekanite
CUR	Curienite	EPI	Epidote
RST	Related structures	EPI	Epidote
CCT	Chalcanthite	ZOI	Zoisite
CHC	Chalcoalumite	EPS	Epsomite
CHL	Chlorite	ETT	Ettringite
CDD	Di/dioctahedral	FAI	Fairfieldite
CTD	Tri/dioctahedral	FER	Fergusonite
CTT	Tri/trioctahedral	FLE	Fleischerite
MLO	Mixed-layer	FLU	Fluorite
CHP	Chalcopyrite	FLU	Fluorite
CHP	Chalcopyrite	URN	Uraninite
STN	Stannite	RST	Related structures
BUK	Bukovite	FOR	Fornacite
RST	Related structures	FSP	Feldspar
CLP	Chlorophoenicite	ORT	Orthoclase
CLP	Chlorophoenicite	PLG	Plagioclase
PHN	Phoenicite	PRC	Paracelsian
RST	Related structures	RST	Related structures
CLV	Calaverite	GAR	Garnet
CNF	Canfieldite	BRZ	Berzeliite
COL	Columbite	CRL	Cryolithionite
AES	Aeschynite	GAR	Garnet
COL	Columbite	GOL	Gold
IXI	Ixiolite	RST	Related structures
STC	Stibiocolumbite	GYP	Gypsum
COM	Combeite		
RST	Related structures		
COP	Copiapite		
COR	Corundum		
COR	Corundum		
ILM	Ilmenite		
CRD	Cordierite		

HAL Halite
GAL Galena
HAL Halite
PER Periclase
RST Related structures

HEL Helvite

HEX Hexahydrite

HLT Halotrichite

HOG Hogbomite

HRZ Herzenbergite

HUM Humite

CHD Chondrodite

CLH Clinohumite

HUM Humite

LEU Leucophoenicite

NOR Norbergite

RST Related structures

IRN Iron

JAH Jahnsite

JOA Joaquinite

JOA Joaquinite

OJQ Orthojoaquinite

K-S Kaolinite-Serpentine

DI Dioctahedral

TRI Trioctahedral

MLR Mixed-layer

KIE Kieserite

LAN Lanthanite

LAZ Lazulite

LIL Lillianite

LIL Lillianite

RAM Ramdohrite

LUD Ludwigite

LUD Ludwigite

RST Related structures

MAR Marcasite

ASP Arsenopyrite

LOE Loellingite

MAR Marcasite

RST Related structures

MAT Matlockite

MCK Mckelveyite

MIC Mica

DI Dioctahedral

TRI Trioctahedral

MLO Mixed-layer

MIX Mixite

MLL Melilite

RST Related structures

MLT Melanterite

MOL Molybdenite

MON Monazite

CRO Crocoite

HUT Huttonite

MON Monazite

MTA Meta-autunite

MTA Meta-autunite

MTU Meta-uranospinite

MXL Mixed-layer

MLR Random

MLO Regular

NEP Nepheline

NIC Nickeline

RST Related structures

NOW Nowackiite

OLV Olivine

ARC Arcanite

CHR Chrysoberyl

OLV Olivine

SIN Sinhalite

TPH Triphylite

RST Related structures

OSU Osumilite

RST Related structures

OVE Overite

PEN Pentlandite

PHE Phenakite

PHF Phosphoferrite

PHM Pharmacosiderite

PHU Phosphuranylite

RST Related structures

PIC Picromerite

POL Polybasite

PRC Paracelsian

PRK	Parkerite	SCA	Scapolite
PRV	Perovskite	SCH	Scheelite
PRX	Paravauxite	SEI	Seidozerite
PSB	Pseudobrookite	RST	Related structures
PUM	Pumpellyite	SEP	Sepiolite
PX2	Pyroxene	PAL	Palygorskite
CPX	Clinopyroxene	SEP	Sepiolite
OPX	Orthopyroxene	SJO	Sjogrenite
PXD	Pyroxenoid	COA	Coalingite
PX3	Dreierkette	HYD	Hydrotalcite
PX4	Viererkette	PYA	Pyroaurite
PX5	Funferkette	SJO	Sjogrenite
PX6	Secherkette	STC	Stichtite
PX7	Siebenerkette	RST	Related structures
PXT	Zwolferkette	SME	Smectite
PYA	Pyrargyrite	DI	Diocahedral
PYC	Pyrochlore	TRI	Triocahedral
BTF	Betafite	MLR	Random mixed-layer
JIX	Jixianite	MLO	Regular mixed-layer
MCR	Microlite	SOD	Sodalite
PYC	Pyrochlore	SOH	Sohngeite
STB	Stibiconite	SOH	Sohngeite
RST	Related structures	STT	Stottite
PYR	Pyrite	RST	Related structures
CBT	Cobaltite	SPH	Sphalerite
PYR	Pyrite	MIE	Miersite
ULL	Ullmannite	SPH	Sphalerite
PYS	Pyrosmalite	RST	Related structures
RST	Related structures	SPL	Spinel
QTZ	Quartz	LIN	Linnaeite
RET	Retzian	SPI	Spinel
REY	Reyerite	RST	Related structures
RHB	Rhabdophane	STB	Stibnite
RSA	Rosasite	RST	Related structures
RSA	Rosasite	STK	Starkeyite
RST	Related structures	TAL	Talc
RSL	Roselite	DI	Diocaheral
RUT	Rutile	TRI	Triocahedal.
RUT	Rutile	MLR	Mixed-layer
DIR	Dirutile	THO	Thortveitite
TRR	Trirutile	TIL	Tilasite
RST	Related structures	TOU	Tourmaline
		TPL	Triplite

TRU	Truscottite	WLK	Wilkmanite
TTD	Tetradymite	WOF	Wolframite
ALE	Aleksite	WOH	Wohlerite
ARS	Arsenic	WTZ	Wurtzite
HED	Hedleyite	IOD	Iodargyrite
TEL	Tellurium	MOI	Moissanite
TTD	Tetradymite	WTZ	Wurtzite
JOS	Joseite	ZNC	Zincite
TSU	Tsumoite	RST	Related structures
TTH	Tetrahedrite	WYL	Wyllieite
GER	Germanite	ZEO	Zeolite
TTH	Tetrahedrite	CHB	Chabazite
TUR	Turquoise	ERI	Erionite
TYC	Tychite	HAR	Harmotome
URP	Uranophane	HEU	Heulandite
VAL	Valleriite	MOR	Mordenite
VIV	Vivianite	NAT	Natrolite
RST	Related structures	UNC	Unclassified
VRL	Varulite	RST	Related structures
VRS	Variscite	ZIN	Zinc
PHS	Phosphosiderite	ZIP	Zippeite
VRS	Variscite	ZIR	Zircon
WAR	Wardite	XEN	Xenotime
WEE	Weeksite	ZIR	Zircon

APPENDIX F

EXAMPLES OF ENTRIES

Inorganic file:

5.797	4.803	7.514		112.68			X P L	124007M1
					85E C			124007M2
P21/c	14A	4E	4.330	4.320		193.03		124007M3
P21/a	14B	4E	4.79A	4.318	125.49	193.03		124007M4
I A								124007M5
Copper phosphide (1 ²)								124007M6
Cu P2								124007M7
Cu P2								124007M8
INOC AJ 17	283	1978	Odile, J.P.,	Soled, S.,	Castro, C.A.,	Wold, A.		124007M9
mP 12.00			\Pd P2\					124007MA
Powder data only.								124007MB
1.00:	0.00	0.00	1.00 /	0.00	-1.00	0.00 /	1.00	0.00
	4.803	5.797	7.514	112.68	90.00	90.00	193.03	40X
	7.514	4.803	5.797	90.00	112.68	90.00	1.5644	1.2070
	86/04/18	JKS	86/04/18	0	0	10	85/12/26	

6.297	6.464	6.565	74.14	61.58	61.26		X S N	127348A1
.001	.001	.001	.01	.01	.01	15 B-		127348A2
P1	1	1	2.690	2.670		205.72		127348A3
P1	1	1	2.40A	2.671	330.89	205.72		127348A4
I M		mBOR						127348A5
Cl-tyretskite							M 1	127348A6
Calcium borate,hydroxo chloride (2 ⁵ +8,2 ¹)							N 2	127348A6
Ca2 B5 O8 (O H)2 Cl							G	127348A7
B5 Ca1.99 Cl H1.86 O9.93 Sr0.01							E	127348A8
KASTAL 7	165	1977	von Hodenberg, R.,	Kuhn, R.				127348A9
From nodules of the Boulby K mine, England. In rosette-like							C1	127348AB
aggregates. White. Powder data indexed. Chem. anal. Trimorphous							C2	127348AB
with hilgardite and parahilgardite.							3	127348AB
1.00:	0.00	-1.00	0.00 /	0.00	-1.00 /	1.00	0.00	0.00
	6.297	6.464	6.565	74.14	61.58	61.26	205.72	31
	6.464	6.565	6.297	118.42	118.74	74.14	.9846	.9592
	86/04/18	JKS	86/04/18	1	0	10	85/12/26	

Organic file:

23.164	25.609	8.495				X S T	50049301	
.010	.010	.006			50 B-		50049302	
Fdd2	43A	8	1.030	1.040		5039.29	50049303	
Fdd2	43A	8	1.05A	1.050	398.49	5039.29	50049304	
O		102810122003					50049305	
Lithium acenaphthylene-di-ide bis(N,N,N',N'-tetramethyl-ethylenedia							C1	50049306
mine)							2	50049306
C12 H8 -2 !2 (C6 H16 N2) !2 (Li +)								50049307
C24 H40 Li2 N4								50049308
JORCAI 134 139 1977 Rhine, W.E., Davis, J.H., Stucky, G.								50049309
1.00: 1.00 0.00 0.00 / 0.00 1.00 0.00 / 0.00 0.00 1.00								5004930C
8.495 12.336 13.491 83.78 71.65 69.86 1259.82							26	5004930D
23.164 25.609 8.495 90.00 90.00 90.00 .9045 .3317								5004930E
77/12/13 84/03/13 86/04/18 0 0 10 85/12/26 ACNYLI								5004930K

11.762	5.961	19.363		103.89		X S T	553692M1	
.002	.002	.003		.01	22 B-		553692M2	
P21	4	4		1.169		1317.90	553692M3	
P21	4	4	1.14A	1.171	232.32	1317.91	553692M4	
O		1053					553692M5	
5alpha-Hydroxy-10beta-selina-1,4(15),7-trien-6-one							1	553692M6
Stemonolone							2	553692M6
C15 H20 O2								553692M7
C15 H20 O2								553692M8
JCPRB4	937	1984	Phadnis, A.P., Patwardhan, S.A., Gupta, A.S.,			C1	553692M9	
			Acharya, K.R., Tavale, S.S., Guru Row, T.N.			2	553692M9	
"Mp. 112-114deg.C. "Color: white. "Source: Pogostemon							C1	553692MB
plectranthoides (Desf.).							2	553692MB
1.00: 0.00 0.00 1.00 / 0.00 -1.00 0.00 / 1.00 0.00 0.00								553692MC
5.961 11.762 19.363 103.89 90.00 90.00 1317.90							35	553692MD
19.363 5.961 11.762 90.00 103.89 90.00 3.2483 1.9732								553692ME
85/03/02 85/03/02 86/04/18 0 0 10 85/12/26 CIKTUL								553692MK

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