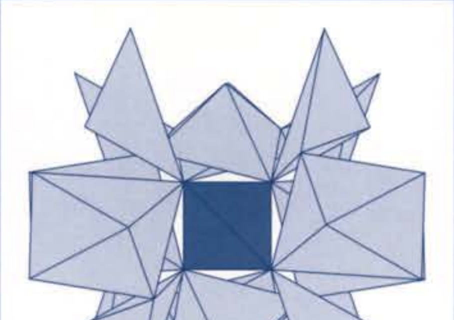
Hugo Strunz
Ernest H. Nickel

Strunz Mineralogical Tables

Chemical Structural Mineral Classification System

9th Edition



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STRUNZ
MINERALOGICAL
TABLES

Chemical-Structural Mineral Classification System

Ninth Edition

by

Hugo Strunz and Ernest H. Nickel

with 226 figures

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Cover Diagram: A fragment of the crystal structure of sillénite – a framework composed of corner-sharing BiO_4 tetrahedra and flat BiO_5 pyramids.

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Preface to the First Edition

The chemical classification of minerals, begun by Berzelius and Rose, was developed into a comprehensive crystallographic-chemical classification over a period of about 100 years, especially by Naumann, Dana, Groth and Hintze, and has been published in well-known manuals and tables. The latest tabular summary, published by P. v. Groth and K. Mieleitner, appeared in 1921. The enormous progress in chemical crystallography since Laue's discovery (1912) requires that a fundamental revision of the current systematics should be undertaken.

It would be desirable to individually name all the authors who have provided the basics for constructing the new classification by their time-consuming X-ray and chemical investigations. However, their numbers are too large to permit this to be done in the available space; I can only point to the *Strukturbericht* of the *Zeitschrift für Kristallographie* with its numerous references and continuing editions. Special mention must be made of the authors Aminoff, W. L. Bragg, V. M. Goldschmidt, Gossner, Machatschki, Niggli, Palache, Pauling, Rinne and W. H. Taylor who, together with their co-workers, conducted outstanding mineralogical-chemical and structural studies. The names Ramdohr and Schneiderhöhn are notable for their contributions to ore microscopy.

In the course of time, incompletely investigated minerals may require reallocation in the system. Similarly, the occasional discredited mineral name may have to be revalidated. Such changes, however, will generally be restricted to the less common minerals, and those that can easily be shifted in collections. Because of the large volume of material in this volume, the occasional literature reference may be overlooked. The author would therefore appreciate all contributions from his professional colleagues and friends of mineralogy.

The development of the classification system grew from several early papers, at the invitation of the German Mineralogical Society.

Berlin, spring, 1941
H. Strunz

Translated, 1999
E. H. Nickel

Preface to the Fifth Edition

Exactly 300 years ago (1669), Nicolaus Steno discovered the law of constant interfacial angles in quartz, and Erasmus Bartholinus discovered the double refraction of light in calcite; about the same time, Robert Boyle (1661) defined the concept of chemical elements by qualitative mineral analyses.

Exactly 150 years ago (1819), Eilhard Mitcherlich discovered isomorphism, and at about the same time, Jakob Berzelius (1824) was the first to propose a chemical system of minerals. In the following years this system was extended by Gustav Rose, Dana, Groth and Hintze.

About 50 years ago (1912), Max von Laue discovered X-ray diffraction by crystals; with the application of the X-ray method to the determination of crystal structures, especially by William Henry Bragg and Sir Lawrence Bragg (since 1913), the development of crystallography took a new direction, thereby making an enormous impact on science and technology.

For the "Classification of Minerals", crystal-structure determinations improved the definitions of mineral species and varieties, assisted in the development of the concept of crystal structure types, helped to establish isotypic series and homeotypic and heterotypic groups, and pointed to the recognition of much broader crystallochemical relationships. The X-ray method appreciably simplified the generally unique characterization of a mineral species and led to a reduction in varieties and the discreditation of many "minerals" accepted up to that time, thereby eliminating countless superfluous "mineral names".

The idea of developing a "classification of minerals based on crystal chemistry" evolved between 1930 and 1940. The basic concepts of this classification, established in the first edition of *Mineralogische Tabellen* (1941) are still valid today, and have been progressively refined and adapted to conform to the latest revelations of structural research. In this 5th edition, 1745 minerals have been classified in tabular form, including the international name (with original author and year of publication), chemical formula, symmetry, lattice constants and cell content, with a brief explanation of the structure type, relationships, etc. In comparison with the fourth edition, 119 new mineral species have been added to the classification, and 55 additional mineral names have been temporarily incorporated into the text. It has not been necessary to make substantial revisions, although some sections of the oxides and silicates have been thoroughly reworked. The main part of the book, namely the actual classification with footnotes citing the original publications, is based on a critical documentation of all the mineral data of structural interest from 1912 to mid-1969.

About 400 varietal names that have been in use for centuries and are still current today (e. g. amethyst, ruby, sapphire, emerald) have been included in the text. Unfortunately it was felt necessary to retain about 300 names of poorly defined or inadequately characterized minerals; it is hoped that my professional colleagues will assist in cleansing the classification by providing more complete data or by completely discrediting such minerals.

To prevent the continuing proliferation of superfluous mineral names by uncritical publication, the *International Mineralogical Association* (IMA) has created a *Commission on New Minerals and Mineral Names* which undertakes regular voting; the chairman of this Commission, Dr. Michael Fleischer, deserves our heartfelt gratitude for his admirable work.

The introduction to the classification comprises an introduction to crystal chemistry, with definitions, rules, tables of crystallochemical importance, a summary of the classification principles, and a description of structure types that are regarded as essential to an understanding of the structural principles and systematics of minerals and of structural relationships between related minerals.

Following the main part of the book is a general index which lists the recognized names of species and varieties, as well as synonyms (more than 4000 in all), and which includes some brief explanations; this is followed by a formula index.

The author is pleased to express his appreciation and gratitude to the publisher and the printing establishment for the careful manner in which five editions of a complicated book have been typeset.

Berlin, 1 January, 1970
Hugo Strunz

Translated, 1999
Ernest H. Nickel

Preface to the 9th Edition

The chemical-structural mineral classification system developed since the first edition of *Mineralogische Tabellen* (1941) evolved from the chemical mineral system of Haüy (1801), which was based on cations, and of Berzelius (1814, 1824), based on anions, followed by the chemical-morphological system of Gustav Rose (1838, 1852), the periodic system of the chemical elements (cf. Introduction), and finally by the developing knowledge of atomic crystal structures (since Laue, 1912, Bragg, 1913).

The classification system used in the first, and subsequent editions of *Mineralogische Tabellen*, combines chemical features with structural principles, such as structure types, cation size and coordination numbers; minerals are generally arranged according to increasing cation size. A characteristic scheme of chemical formulae was introduced, as well as internationalized names, such as *neso*- to *tektosilicates*. International priority principles have always been acknowledged.

Since the last edition (1978), technological developments, such as improved electron microscopy (since Ernst Ruska, 1931), chemical analysis by microprobe (since Raymond Castaing, 1951), scanning electron microscopy (since Oatley & McMullan, 1952), automatic computer-controlled instrumentation and software for structure determination, have made it possible to carry out the chemical, structural, morphological and physical characterization of tiny particles of new minerals (on the scale of micrograms) within a few days or weeks; computerized structural and morphological drawings can be produced within minutes.

As a result, the number of minerals approved by the Commission on New Minerals & Mineral Names of the IMA (International Mineralogical Association) has grown from about 2500 in 1978 to about 4000 at present, with about 60 to 80 new minerals added each year.

In this edition, the world of minerals is divided by chemical features into ten classes, each of which is subdivided, on chemical-structural principles, into divisions, subdivisions, groups of isotypic and homeotypic minerals, or individual minerals with unique structure types; groups with two or more mineral names comprise minerals with similar structure or composition. The classification system and alphanumeric coding scheme used in this 9th edition of the *Strunz Mineralogical Tables* were presented at the 1994 IMA meeting in Pisa. They permit the insertion of thousands of new minerals in the future without changing the basic classification framework.

The authors gratefully acknowledge the contributions to this volume made by a number of mineralogical colleagues, particularly Emil Makovicky for helpful suggestions relating to the sulfide and sulfosalt classification, and Friedrich Liebau for constructive critical reading of the cyclo- and inosilicate portions of the manuscript. We also acknowledge the contribution made by Irmgard Stolle, Berlin, who provided assistance in the preparation of the manuscript.

This contribution to mineralogy is indebted to about seven generations of diligent and active researchers over a period of two hundred years. The authors welcome suggestions for improvements.

February 24th, 2001

Hugo Strunz
Berlin

Ernest H. Nickel
Perth (Wembley)

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Sulfides, etc.

Sulfosalts

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INTRODUCTION

Historical Development

René Just Haüy (1743–1822), in his well-known four-volume work *Traité de Minéralogie* (Paris, 1801), classified minerals on the type of metals they contain, or, as he would say now, on the type of cations, or the electropositive principle.

Jöns Jacob Berzelius (1779–1848), the famous Swedish chemist who introduced chemical formulae into chemistry and mineralogy, classified minerals by the type of anion, *i. e.* the electronegative principle (1814, 1824).

With this background, together with the knowledge about the seven crystal systems (Christian Samuel Weiss, 1815), the recognition of isomorphy and polymorphy (Mitscherlich, 1819, 1824), and the triad rule of chemical elements (Döbereiner, 1829), Gustav Rose (1798–1873) developed a chemical-morphological mineral system (Berlin, 1838, 1852), which looks quite modern, even today:

Class I. ELEMENTS. A. Metals. Cubic: copper, silver, gold, iron, platinum, iridium. – Tetragonal: tin. – Rhombohedral and Hexagonal: arsenic, antimony, bismuth, tellurium, (Os, Ir). – B. Metalloids. Cubic: diamond. – Hexagonal: graphite. – Orthorhombic: sulfur, iodine. – Monoclinic: sulfur, selenium. – **Class II. SULFIDES. – Class III. HALIDES. – Class IV. OXIDES**, divided into **SIMPLE OXIDES** and **COMPLEX OXIDES**, such as **CARBONATES, PHOSPHATES, SILICATES, BORATES** and **SULFATES**.

This mineral system was a precursor to the important discovery of the Periodic System of the chemical elements developed independently by Dmitry Mendeleev and Lothar Meyer (1869). It influenced the further development of Rose's system, especially in the famous 6th edition of the System of Mineralogy by Dana (1892).

Differing from Rose, Paul Groth (1843–1927), Munich, 1912, "the world's most famous authority on crystallography" (Bragg, 1933), inserted the halides between the simple and complex oxides. This was followed by three important works: Hintze *et al.*: *Handbuch der Mineralogie* (1897–1971); Palache *et al.*: *The System of Mineralogy of Dana* (7th ed., 1944, 1951); Hey: *An Index of Mineral Species and Varieties, Arranged Chemically* (2 eds., 1950, 1975), followed by Clark: *Hey's Mineral Index* (3rd ed., 1993). More about this, with full references, has been given in recent publications.*

The discovery of the diffraction of X-rays by the space lattices of crystals (Max von Laue, 1912), and the resulting determination of crystal structures (W. H. and W. L. Bragg, since1913), enabled many more structures to be determined within the next decade and, by about 1933, the general rules governing atomic crystal structures were recognized.

By 1941 it was therefore possible to develop, in *Mineralogische Tabellen*, an extension of the Rose classification scheme, a comprehensive mineral system based on chemistry and structure, applied systematically to the entire mineral domain. Since then, *Min-*

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* H. Strunz, Lapis, 1994 (1), 56–60: Klassifikation der Sulfide (in German); Lapis-Extraedition, 1993: Classification of elements, sulfides, halides (in English), distributed by mail and at the IMA General Meeting in Pisa (1994). – N. Jahrb. Min. Mh., 1996, 435–445 (general historical survey, with references). – Eur. Journ. Min., 1997, 225–232 (borates). – H. Strunz & E. H. Nickel, Zap. Vses. Min. Ob. 1997 (5), 1–14 (tektosilicates).

eralogische Tabellen have gone through many editions, reprints and translations, some with co-author Christel Tennyson.

As this 9th edition was in preparation, two important works comprising all known mineral species were published: **Dana's New Mineralogy** (Gaines *et al.*, 1997) in which the classification is the same as that used in the seventh edition of Dana's System of Mineralogy, vols. 1 and 2 (1944, 1951) by Palache *et al.*, and vol. 3 (silica minerals) by Frondel (1960), except for the silicates which follow the well-known enlarged Bragg classification. The multi-volume **Handbook of Mineralogy** by Anthony *et al.*, vol. I, Elements, Sulfides, Sulfosalts (1990); vol. II, Silica, Silicates (1995), vol. III, Halides, Hydroxides, Oxides (1997); vol. IV, Phosphates, Arsenates, Vanadates (2000); the arrangement in this series is alphabetical by mineral name, and crystal structures are not considered. Also useful is the **Glossary of Mineral Species** (founded by Fleischer, 1971 and continued by Mandarino to 8th edition, 1999).

Chemical Bonding and Crystal Structures

Atoms are the smallest chemical entities of relevance to the crystal structures of minerals. They consist of a nucleus of **protons** and **neutrons** surrounded by a cloud of **electrons** that are constrained within energy levels or "shells". Within each shell, the electrons occupy particular **orbitals** designated by the symbols *s, p, d* and *f*. The *s* orbitals are the outermost ones for all elements, and have the highest energy. They have spherical symmetry and can accommodate two electrons. The *p* orbitals consist of three mutually perpendicular dumbbell-shaped clouds that can accommodate six electrons. The *d* and *f* orbitals have more complex configurations and can accommodate ten and fourteen electrons, respectively. Only the outer orbitals are involved in bonding between atoms, and the electron configurations of these orbitals are shown in the **Periodic System of the Elements** (Table, inside cover). The symbols *s, p,* etc. represent the orbitals, and the *n* on s^n, p^n gives the number of electrons in that orbital. [He], [Ne], etc. represent the stable shells according to the noble gases He, Ne, etc.

Also shown in this version of the Periodic Table is the atomic number of each element, which corresponds to the total number of electrons, and the atomic weight relative to the mass of C^{12} which has been assigned a mass of 12.000 (the atomic weight of carbon shown in the Periodic Table is slightly higher than this because of the additional presence of a small amount of the C^{13} isotope in natural carbon). The atomic weight represents the sum of the numbers of protons and neutrons in the nucleus of the atom. It has long been known that the elements in a vertical column have similar chemical properties because they have the same number of valence electrons. However, the lanthanides and actinides (except for thorium) shown at the bottom of the Table do not fit readily into this scheme because of the effect of *f* orbitals in the outer electron shells.

The electrons of adjoining atoms in a crystal structure interact in several different ways to form chemical bonds, generally classified into ionic, covalent and metallic types, although combinations of these idealized types commonly occur.

In **ionic bonding**, the outer electron(s) are transferred from an electropositive atom (resulting in a positively charged ion) to an electronegative atom (resulting in a negatively charged ion). The resulting ions, respectively termed cations and anions, are attracted to each other by electrostatic forces. The size of an ion depends to a first approximation on the atomic number, and secondarily on the number of electrons in the outer shell. The ionic radii of all the chemical elements is illustrated in the diagram on the inside back cover. In the classification scheme used in this book, the minerals within a group are arranged primarily according to increasing atomic number of the principal cations in the mineral, but those containing Mg^{2+}, Fe^{2+} and Mn^{2+} are arranged according to increasing ionic size, 0.72, 0.78, 0.83Å.

In **covalent bonding**, the orbitals of adjoining atoms interact. During this process, the orbitals are hybridized, and the immediate neighbourhood of the ion is strongly influenced by the electron configuration of this hybridization, resulting in strongly directional bonding. For example, one *s* and three *p* orbitals are commonly hybridized (sp^3) into the shape of a tetrahedron, as in $\mathrm{Si}^{[4]}$. Another common polyhedral configuration in mineral structures is the octahedron, formed by the hybridization of one *s*, three *p* and two *d* orbitals, generally written as d^2sp^3. Examples of the main polyhedral configurations found in minerals are shown in Figure 3.

In **metallic bonding**, the outermost electrons of the atoms are delocalized, and can move about freely within the array of cations. Metals are characterized by their metallic luster, caused by the interaction of light with the electrons, and by good electrical conductivity because of the mobility of electrons within the structure.

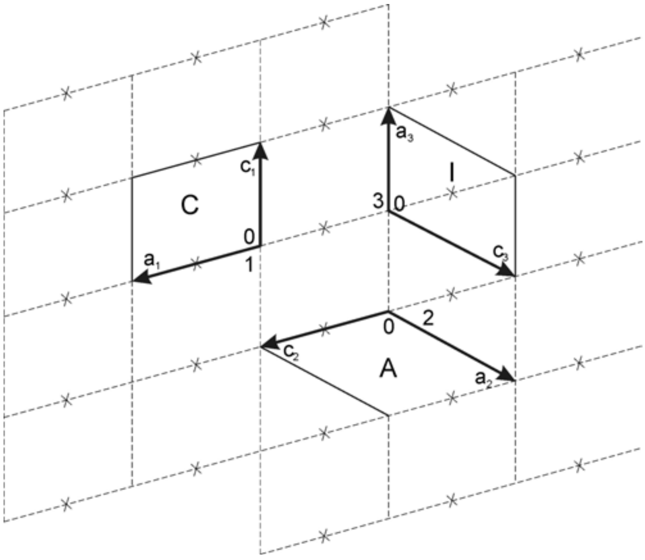


Fig 1. Unit cell settings of a monoclinic crystal with centered Bravais lattice*: Setting 1 = C-centred; setting 2 = A-centred; setting 3 = I-centred. Projection on (010), the b-axis is normal to the plane of the drawing; the cell edges and full lines are at height b = 0; the stars are at height b = ½.*

The bonding between atoms creates three-dimensional crystal structures. These structures can be categorized by their inherent symmetry elements which have been formalized into 230 crystallographic **space groups** (Table 1). The relationship between the different settings of a monoclinic unit cell is illustrated in Fig. 1. The space groups can be derived by combining the 14 **translation types** (Fig. 2) of Bravais (1850) with all possible symmetry operations (Table 2). The relationship between space groups and **crystal classes** is shown in Table 3.

Table 1. Crystal Systems (names), Crystal Classes (symbols), Space Groups (numbers; short symbols for standard and other settings)

Triclinic		
Class	**No.**	**Symbol**
1	1	P1
$\bar{1}$	2	$P\bar{1}$

Normal setting of triclinic minerals: 1) Three shortest lattice parameters; 2) *c*[001] = axis of the main morphological zone; 3) α and β obtuse, γ acute; and 4) $a < b$.

Setting of monoclinic crystals: 1) a:b:c always with *b* as unique axis, β obtuse, in structure and morphology; 2) three shortest lattice parameters; 3) three choices of settings $\mathbf{a_1\ b\ c_1}$, $\mathbf{a_2\ b\ c_2}$ and $\mathbf{a_3\ b\ c_3}$ apply to both P and C Bravais lattices (P = uncentred unit cell; C = C-centred unit cell, demonstrated in Fig. 1 for a centred unit cell); $\mathbf{a_1}$ and $\mathbf{c_1}$, etc. can be exchanged, with -**b**; 4) the symmetry elements and their orientation in the chosen unit cell are derived from the "extinction conditions", and are expressed by the space group symbol. For further details see *International Tables for Crystallography* (Theo Hahn, ed.) Vol. A, 4th ed., 1996, and *Brief Teaching Edition of Vol. A* (Theo Hahn, ed.), 4th revised and enlarged edition, 1996, both published by The International Union of Crystallography. In the monoclinic system, for five space groups (nos. 3, 4, 6, 10 and 11), each setting choice gives the same space group symbol; for two space groups (nos. 9 and 15), six symbols; and for the others, three. The symbol in the first lines and first columns of the tabulations are the "standard short symbols", with the "standard settings", *e.g.* , for no. 5: C2, for no. 7: Pc, etc.

Monoclinic		**Setting**		
Class	**No.**	$\mathbf{a_1\ b\ c_1}$ $\mathbf{c_1\ -b\ a_1}$	$\mathbf{a_2\ b\ c_2}$ $\mathbf{c_2\ -b\ a_2}$	$\mathbf{a_3\ b\ c_3}$ $\mathbf{c_3\ -b\ a_3}$
2	3	P2		
	4	$P2_1$		
	5	C2	A2	I2
m	6	Pm		
	7	Pc	Pn	Pa
	8	Cm	Am	Im
	9	Cc	An	Ia
		Aa	Cn	Ic
2/m	10	P2/m		
	11	$P2_1/m$		
	12	C2/m	A2/m	I2/m
	13	P2/c	P2/n	P2/a
	14	$P2_1/c$	$P2_1/n$	$P2_1/a$
	15	C2/c	A2/n	I2/a
		A2/a	C2/n	I2/c

Orthorhombic				
Class	**No.**	**a b c** **a -c b**	**c a b** **b a -c**	**b c a** **-c b a**
222	16	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$2
	21	C222	A222	B222
	22	F222		
	23	I222		
	24	I2$_1$2$_1$2$_1$		
mm2	25	Pmm2	P2mm	Pm2m
	26	Pmc2$_1$	P2$_1$ma	Pb2$_1$m
		Pm2$_1$b	Pcm2$_1$	P2$_1$am
	27	Pcc2	P2aa	Pb2b
	28	Pma2	P2mb	Pc2m
		Pm2a	Pbm2	P2cm
	29	Pca2$_1$	P2$_1$ab	Pc2$_1$b
		Pb2$_1$a	Pbc2$_1$	P2$_1$ca
	30	Pnc2	P2na	Pb2n
		Pn2b	Pcn2	P2an
	31	Pmn2$_1$	P2$_1$mn	Pn2$_1$m
		Pm2$_1$n	Pnm2$_1$	P2$_1$nm
	32	Pba2	P2cb	Pc2a
	33	Pna2$_1$	P2$_1$nb	Pc2$_1$n
		Pn2$_1$a	Pbn2$_1$	P2$_1$cn
	34	Pnn2	P2nn	Pn2n
	35	Cmm2	A2mm	Bm2m
	36	Cmc2$_1$	A2$_1$ma	Bb2$_1$m
		Bm2$_1$b	Ccm2$_1$	A2$_1$am
	37	Ccc2	A2aa	Bb2b
	38	Amm2	B2mm	Cm2m
		Am2m	Bmm2	C2mm
	39	Abm2	B2cm	Cm2a
		Ac2m	Bma2	C2mb
	40	Ama2	B2mb	Cc2m
		Am2a	Bbm2	C2cm
	41	Aba2	B2cb	Cc2a
		Ac2a	Bba2	C2cb
	42	Fmm2	F2mm	Fm2m
	43	Fdd2	F2dd	Fd2d
	44	Imm2	I2mm	Im2m
	45	Iba2	I2cb	Ic2a
	46	Ima2	I2mb	Ic2m
		Im2a	Ibm2	I2cm

Setting of orthorhombic crystals: 1) three shortest lattice parameters, with $a:b:c$ in agreement with morphology; 2) six choices of settings, **a b c** (first line, first column, standard setting), **c a b** (first line, second column), etc.; transformation **a b c** → **c a b** means that the new **a**-axis corresponds to the old **c**, the new **b** is the old **a**, and the new **c** is the old **b**, etc., and *vice versa*; 4) if, for example, for a chosen unit cell, the "extinction conditions" give a space group symbol C2mm, the transformation **-c b a** → **a b c** gives the standard space group symbol *Amm*2 (no. 38). Further details are given in the *International Tables for Crystallography*, Vol. A (1983, 1996).

In the orthorhombic system, for ten space groups (Nos. 16, 19, 22, etc.), each setting gives the same space group symbol; for two space groups, (Nos. 61, 73) two symbols, for the others three or six.

Setting of orthorhombic crystals: continued

Orthorhombic (continued)				
Class	**No.**	**a b c** **a -c b**	**c a b** **b a -c**	**b c a** **-c b a**
mmm	47	Pmmm		
	48	Pnnn		
	49	Pccm	Pmaa	Pbmb
	50	Pban	Pncb	Pcna
	51	Pmma	Pbmm	Pmcm
		Pmam	Pmmb	Pcmm
	52	Pnna	Pbnn	Pncn
		Pnan	Pnnb	Pcnn
	53	Pmna	Pbmn	Pncm
		Pman	Pnmb	Pcnm
	54	Pcca	Pbaa	Pbcb
		Pbab	Pccb	Pcaa
	55	Pbam	Pmcb	Pcma
	56	Pccn	Pnaa	Pbnb
	57	Pbcm	Pmca	Pbma
		Pcmb	Pcam	Pmab
	58	Pnnm	Pmnn	Pnmn
	59	Pmmn	Pnmm	Pmnm
	60	Pbcn	Pnca	Pbna
		Pcnb	Pcan	Pnab
	61	Pbca		
		Pcab		
	62	Pnma	Pbnm	Pmcn
		Pnam	Pmnb	Pcmn
	63	Cmcm	Amma	Bbmm
		Bmmb	Ccmm	Amam
	64	Cmca	Abma	Bbcm
		Bmab	Ccmb	Acam
	65	Cmmm	Ammm	Bmmm
	66	Cccm	Amaa	Bbmb
	67	Cmma	Abmm	Bmcm
		Bmam	Cmmb	Acmm
	68	Ccca	Abaa	Bbcb
		Bbab	Cccb	Acaa
	69	Fmmm		
	70	Fddd		
	71	Immm		
	72	Ibam	Imcb	Icma
	73	Ibca		
		Icab		
	74	Imma	Ibmm	Imcm
		Imam	Immb	Icmm

Tetragonal

Class	No.	Symbol
4	75	P4
	76	$P4_1$
	77	$P4_2$
	78	$P4_3$
	79	I4
	80	$I4_1$
$\bar{4}$	81	$P\bar{4}$
	82	$I\bar{4}$
4/m	83	P4/m
	84	$P4_2/m$
	85	P4/n
	86	$P4_2/n$
	87	I4/m
	88	$I4_1/a$
422	89	P422
	90	$P42_12$
	91	$P4_122$
	92	$P4_12_12$
	93	$P4_222$
	94	$P4_22_12$
	95	$P4_322$
	96	$P4_32_12$
	97	I422
	98	$I4_122$
4mm	99	P4mm
	100	P4bm
	101	$P4_2cm$
	102	$P4_2nm$
	103	P4cc
	104	P4nc
	105	$P4_2mc$
	106	$P4_2bc$
	107	I4mm
	108	I4cm
	109	$I4_1md$
	110	$I4_1cd$

Tetragonal (continued)

Class	No.	Symbol
$\bar{4}2m$	111	$P\bar{4}2m$
	112	$P\bar{4}2c$
	113	$P\bar{4}2_1m$
	114	$P\bar{4}2_1c$
	115	$P\bar{4}m2$
	116	$P\bar{4}c2$
	117	$P\bar{4}b2$
	118	$P\bar{4}n2$
	119	$I\bar{4}m2$
	120	$I\bar{4}c2$
	121	$I\bar{4}2m$
	122	$I\bar{4}2d$
4/mmm	123	P4/mmm
	124	P4/mcc
	125	P4/nbm
	126	P4/nnc
	127	P4/mbm
	128	P4/mnc
	129	P4/nmm
	130	P4/ncc
	131	$P4_2/mmc$
	132	$P4_2/mcm$
	133	$P4_2/nbc$
	134	$P4_2/nnm$
	135	$P4_2/mbc$
	136	$P4_2/mnm$
	137	$P4_2/nmc$
	138	$P4_2/ncm$
	139	I4/mmm
	140	I4/mcm
	141	$I4_1/amd$
	142	$I4_1/acd$

Trigonal

Class	No.	Symbol
3	143	P3
	144	$P3_1$
	145	$P3_2$
	146	R3
$\bar{3}$	147	$P\bar{3}$
	148	$R\bar{3}$
32	149	P312
	150	P321
	151	$P3_112$
	152	$P3_121$
	153	$P3_212$
	154	$P3_221$
	155	R32
3m	156	P3m1
	157	P31m
	158	P3c1
	159	P31c
	160	R3m
	161	R3c
$\bar{3}m$	162	$P\bar{3}1m$
	163	$P\bar{3}1c$
	164	$P\bar{3}m1$
	165	$P\bar{3}c1$
	166	$R\bar{3}m$
	167	$R\bar{3}c$

Hexagonal

Class	No.	Symbol
6	168	P6
	169	$P6_1$
	170	$P6_5$
	171	$P6_2$
	172	$P6_4$
	173	$P6_3$
$\bar{6}$	174	$P\bar{6}$
6/m	175	P6/m
	176	$P6_3/m$
622	177	P622
	178	$P6_122$
	179	$P6_522$
	180	$P6_222$
	181	$P6_422$
	182	$P6_322$
6mm	183	P6mm
	184	P6cc
	185	$P6_3cm$
	186	$P6_3mc$
$\bar{6}m2$	187	$P\bar{6}m2$
	188	$P\bar{6}c2$
	189	$P\bar{6}2m$
	190	$P\bar{6}2c$
6/mmm	191	P6/mmm
	192	P6/mcc
	193	$P6_3/mcm$
	194	$P6_3/mmc$

Cubic		
Class	**No.**	**Symbol**
23	195	P23
	196	F23
	197	I23
	198	$P2_13$
	199	$I2_13$
$m\bar{3}$	200	$Pm\bar{3}$
	201	$Pn\bar{3}$
	202	$Fm\bar{3}$
	203	$Fd\bar{3}$
	204	$Im\bar{3}$
	205	$Pa\bar{3}$
	206	$Ia\bar{3}$
432	207	P432
	208	$P4_232$
	209	F432
	210	$F4_132$
	211	I432
	212	$P4_332$
	213	$P4_132$
	214	$I4_132$
$\bar{4}3m$	215	$P\bar{4}3m$
	216	$F\bar{4}3m$
	217	$I\bar{4}3m$
	218	$P\bar{4}3n$
	219	$F\bar{4}3c$
	220	$I\bar{4}3d$
$m\bar{3}m$	221	$Pm\bar{3}m$
	222	$Pn\bar{3}n$
	223	$Pm\bar{3}n$
	224	$Pn\bar{3}m$
	225	$Fm\bar{3}m$
	226	$Fm\bar{3}c$
	227	$Fd\bar{3}m$
	228	$Fd\bar{3}c$
	229	$Im\bar{3}m$
	230	$Ia\bar{3}d$

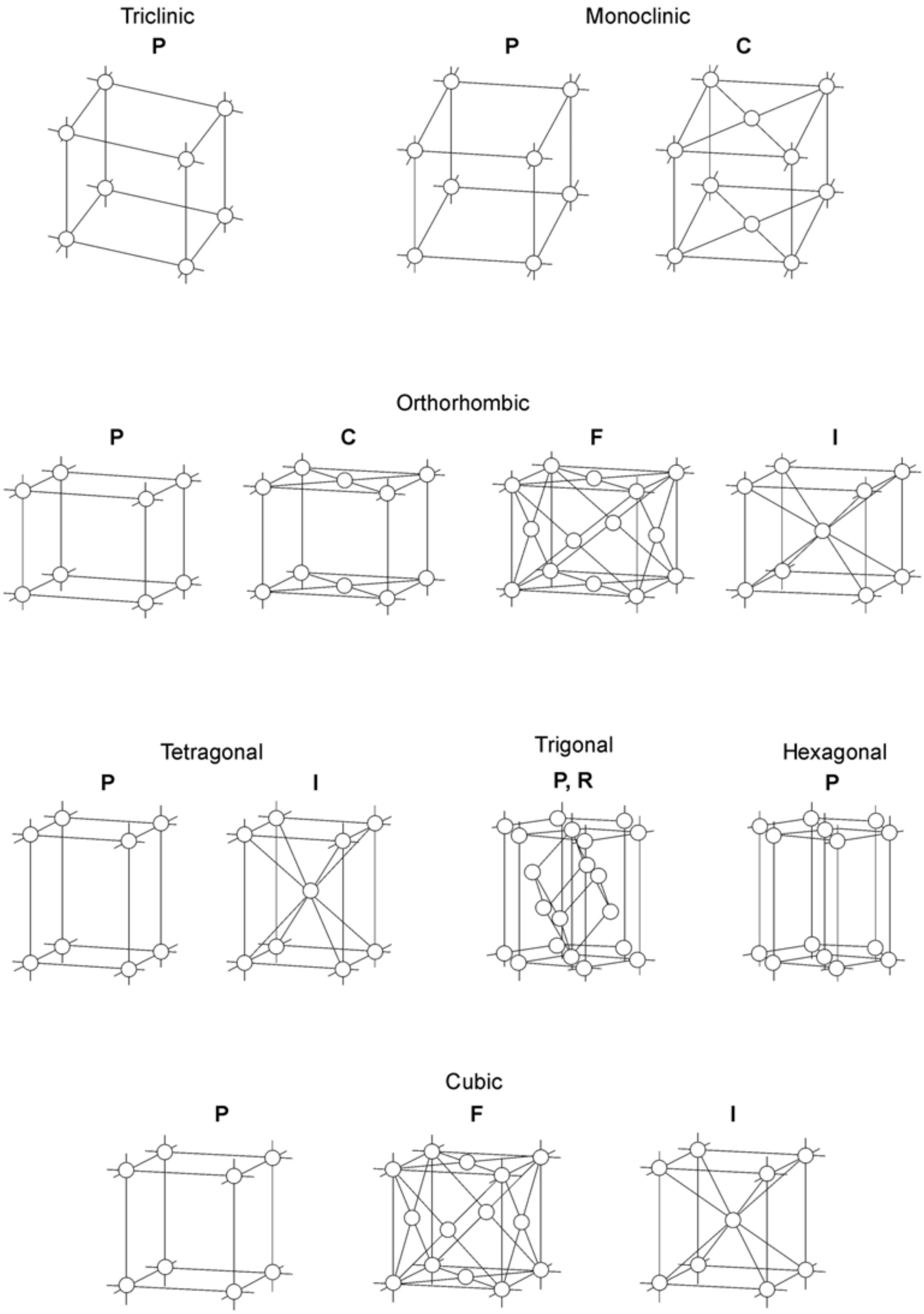


Fig 2. The 14 three-dimensional translation lattice types (Bravais, 1850). *P = primitive; C = c-face centred, F = all face centred, R = rhombohedral (crystals in the 7 rhombohedral space groups are described in relation to hexagonal axes).*

Table 2. Symmetry Operations
Possible symmetry operations which, in combination with the 14 translation lattices, give the 230 space groups. For example, space group no. 62: Pbnm means P = primitive translation lattice; b = axial glide plane // (100) with glide vector b/2; n = diagonal glide plane // (010) with diagonal glide vector a/2 + c/2; m = mirror plane // (001) (see chrysoberyl, triphylite, olivine).

Rotation Axes	Screw Axes	Inversion Axes
1 2 3 4 6	– 2_1 3_1, 3_2 4_1, 4_2, 4_3 6_1, 6_2, 6_3, 6_4, 6_5	$\bar{1} \equiv i$ $\bar{2} \equiv m$ $\bar{3} \equiv 3 + i$ $\bar{4}$ $\bar{6} \equiv 3/m$

Symmetry Planes	Symbol	Glide Vector
Mirror Plane	m	0
Axial Glide Planes	a b c	a/2 b/2 c/2
Diagonal Glide Planes	n	a/2 + b/2 or a/2 + c/2 or b/2 + c/2
Diamond Glide Plane	d	a/4 + b/4 + c/4

Table 3. Crystal Systems, Classes, Space Groups

Crystal System	**Crystal Class**		**Laue Class****	**Range of Space Groups**	
	Names	**Sym-bols***		**Nos.**	**Symbols**
Triclinic	Triclinic-pedial (asymmetric) Triclinic-pinacoidal	1 $\bar{1}$	– +	1 2	P1 P$\bar{1}$
Monoclinic	Monoclinic-sphenoidal Monoclinic-domatic Monoclinic-prismatic	2 m 2/m	– – +	3–5 6–9 10–15	P2 – C2 Pm – Cc P2/m – C2/c
Orthorhombic	Orthorhombic-disphenoidal Orthorhombic-pyramidal Orthorhombic-dipyramidal	222 mm2 mmm	– – +	16–24 25–46 47–74	P222 – I$2_1 2_1 2_1$ Pmm2 – Ima2 Pmmm – Imma

Table 3. Continued

Crystal System	Crystal Class		Laue Class**	Range of Space Groups	
	Names	Symbols*		Nos.	Symbols
Tetragonal	Tetragonal-pyramidal	4	–	75–80	$P4$ – $I4_1$
	Tetragonal-disphenoidal	$\bar{4}$	–	81–82	$P\bar{4}$ – $I\bar{4}$
	Tetragonal-dipyramidal	4/m	+	83–88	P4/m – $I4_1/a$
	Tetragonal-trapezohedral	422	–	89–98	P422 – $I4_122$
	Ditetragonal-pyramidal	4mm	–	99–110	P4mm – $I4_1cd$
	Tetragonal-scalenohedral	$\bar{4}2m$	–	111–122	$P\bar{4}2m$ – $I\bar{4}2d$
	Ditetragonal-dipyramidal	4/mmm	+	123–142	P4/mmm – $I4_1/acd$
Trigonal	Trigonal-pyramidal	3	–	143–146	P3 – R3
	Trigonal-rhombohedral	$\bar{3}$	+	147–148	$P\bar{3}$ – $R\bar{3}$
	Trigonal-trapezohedral	32	–	149–155	P312 – R32
	Ditrigonal-pyramidal	3m	–	156–161	P3m1 – R3c
	Trigonal-scalenohedral	$\bar{3}m$	+	162–167	$P\bar{3}1m$ – $R\bar{3}c$
Hexagonal	Hexagonal-pyramidal	6	–	168–173	P6 – $P6_3$
	Trigonal-dipyramidal	$\bar{6}$	–	174	$P\bar{6}$
	Hexagonal-dipyramidal	6/m	+	175–176	P6/m – $P6_3/m$
	Hexagonal-trapezohedral	622	–	177–182	P622 – $P6_322$
	Dihexagonal-pyramidal	6mm	–	183–186	P6mm – $P6_3mc$
	Ditrigonal-dipyramidal	$\bar{6}m2$	–	187–190	$P\bar{6}m2$ – $P\bar{6}2c$
	Dihexagonal-dipyramidal	6/mmm	+	191–194	P6/mmm – $P6_3/mmc$
Cubic	Cubic-tetartoidal	23	–	195–199	P23 – $I2_13$
	Cubic-disdodecahedral	$m\bar{3}$	+	200–206	$Pm\bar{3}$ – $Ia\bar{3}$
	Cubic-gyroidal	432	–	207–214	P432 – $I4_132$
	Cubic-hex'tetrahedral	$\bar{4}3m$	–	215–220	$P\bar{4}3m$ – $I\bar{4}3d$
	Cubic-hex'octahedral	$m\bar{3}m$	+	221–230	$Pm\bar{3}m$ – $Ia\bar{3}d$

* The class symbols can be derived from the space group symbols by deleting the Bravais symbols (P, C, etc.), dropping all subscripts from screw axes ($2_1, 3_1, 4_1$, etc. → 2, 3, 4, etc.) and replacing all glide plane symbols by the mirror plane symbol, m. Thus $I4_1/acd$ becomes 4/mmm. A slash means perpendicularity of a rotational element and a reflection element.

** The 11 Laue Classes, indicated by +, summarize the preceding classes by introducing an inversion center. Inversion center: – no, + yes.

Crystal systems and crystal axes: C. S. Weiss (1815).
Crystal classes: J. F. C. Hessel (1830); Class names: P. v. Groth (1905), modified in *Min. Tab.* (1941).
Space groups: E. S. v. Fedorov (1891); A. M. Schoenflies (1891).
Laue classes: M. v. Laue (1912); Friedel's Law (1913).
Class and space groups (short) symbols: C. Hermann & C. Mauguin (1935), standard settings. Symbols according to *International Tables for Crystallography* (1996).

Definitions

Crystals. Crystals are solids with a three-dimensional lattice arrangement of atoms, ions or molecules. Ideas about this were independently expressed by Johannes Kepler (1611) in a paper on hexagonal snow crystals, by Christiaan Huygens (1690) in his fundamental work on the wave theory of optics, wherein he ascribed to calcite a structure made up of ellipsoidal particles, by Torbern Olof Bergman (1773), and especially by René Just Haüy (1782) who suggested that all crystals consist of a three-dimensional masonry of equal parallelepipedal building bricks, the "molécules intégrantes" which have the form of tiny cleavage rhombohedra in calcite, and which express the laws governing the symmetry of crystals.

Ludwig August Seeber, a physicist in Freiburg, in his "Erklärung des Baues fester Körper" (1824), in an attempt to find an explanation for the thermal expansion and elasticity of crystals, arrived at a parallelepipedal arrangement, formed by the balance of temperature-dependent attractive and repulsive forces of indivisible parts of matter, thus forming a theory of stable equilibrium in crystals. Max von Laue said that such an arrangement implies a primitive translation lattice (Historical Introduction: *International Tables for X-ray Crystallography*, 1952).

Minerals. A mineral substance is generally regarded as a naturally occurring solid that has been formed by geochemical or geophysical processes, either on earth or in extraterrestrial bodies. Most minerals occur as crystals, and frequently have an external morphology that is a function of the internal arrangement of atoms comprising the crystal.

A mineral species is a mineral substance with well-defined chemical composition and crystallographic properties, and which merits a unique name.

Isotypy. Isotypic substances are those that have the same crystallographic space group and analogous chemical formulae and crystal structures. The terms "isostructural" and "isomorphic" are essentially synonymous with "isotypic".

Homeotypy. Homeotypic substances are those that have similar crystal structures, but with different crystallographic space groups and/or chemical compositions.

Heterotypy. Heterotypic substances are chemically related, but have different chemical compositions and structures.

Polymorphism. Polymorphs are substances with essentially identical compositions, but with different crystal structures.

Polytypism. Polytypes are substances that occur in different structural modifications, each of which can be regarded as being built up by the stacking of layers of (nearly) identical structure and composition, and with the modifications differing only in their stacking sequence.

Diadochy. This refers to the substitution of a chemical element by another one in a crystal lattice, leaving the basic structure unchanged, except for relatively minor variations in the unit-cell parameters. If the substitution occurs over a wide compositional range, such a range is commonly referred to as an isomorphous series or a solid-solution series.

Coupled Replacement. This occurs when two or more chemical elements with different valencies are replaced by other chemical elements that maintain electrostatic neutrality in the crystal.

Coordination. The number of anions surrounding the specified cation in a crystal structure is referred to as the coordination number, and is shown as a numerical digit in square brackets, e. g. [6]; in a chemical formula this symbol is shown as a superscript immediately following the element symbol. The configuration of the coordinating ions is commonly referred to in terms of a polyhedral form; the more common of which are shown in Fig. 3.

The Data in the Tabulations

Each mineral group (or sometimes single mineral) is given an alphanumeric coding, which is explained below in "The Classification System". When the crystal structure is known, a brief description is given, sometimes accompanied by an illustration. Within a group, each mineral is listed by name, chemical formula, space group designation (and number), the author(s) of the original description, crystallographic parameters and unit-cell contents (Z). One or more references relating to the data are given, with the structural reference(s) indicated by a following "(str)".

The chemical formulae are generally end-member formulae, but major substitutions are commonly indicated within round brackets, in decreasing order of abundance. In the first edition of *Mineralogische Tabellen* (1941), a method of writing chemical formulae was introduced whereby subsidiary anions (F,O,OH) were positioned before the complex anions, with both enclosed in square brackets, e. g. *fluorapatite* $Ca_5[F|(PO_4)_3]$, *euchroite* $Cu_2[OH|AsO_4] \cdot 3H_2O$. This procedure was adopted for reasons of specified bonding strength, as all valence electrons of the subsidiary anions are used in bonding to the cations, whereas only a fraction of the valency electrons of the oxygens of the complex ions are involved in bonding to the cations.

Space groups and unit-cell parameters are generally as taken from the published literature, but some have been transformed into alternative settings to maintain consistency within a group or to conform with traditional morphological descriptions.

The Classification System

In this first English edition of *Mineralogical Tables*, the world of minerals is divided by chemical features into 10 Classes which are subdivided on chemical-structural principles, into Divisions, Subdivisions and Groups of isotypic or homeotypic species, or individual minerals of a unique structure type. Groups with a heading containing more than one mineral name include two or more heterotypes of usually unknown structures. Related groups may be designated a Family.

Because of the great diversity of bonding types exhibited by minerals, a variety of criteria has been used to classify minerals within a Class. Some minerals, like the borates and silicates, can be classified mainly on the basis of crystal structure, *ie* the degree of polymerization of the anionic polyhedra. Other minerals, such as the sulfides and oxides,

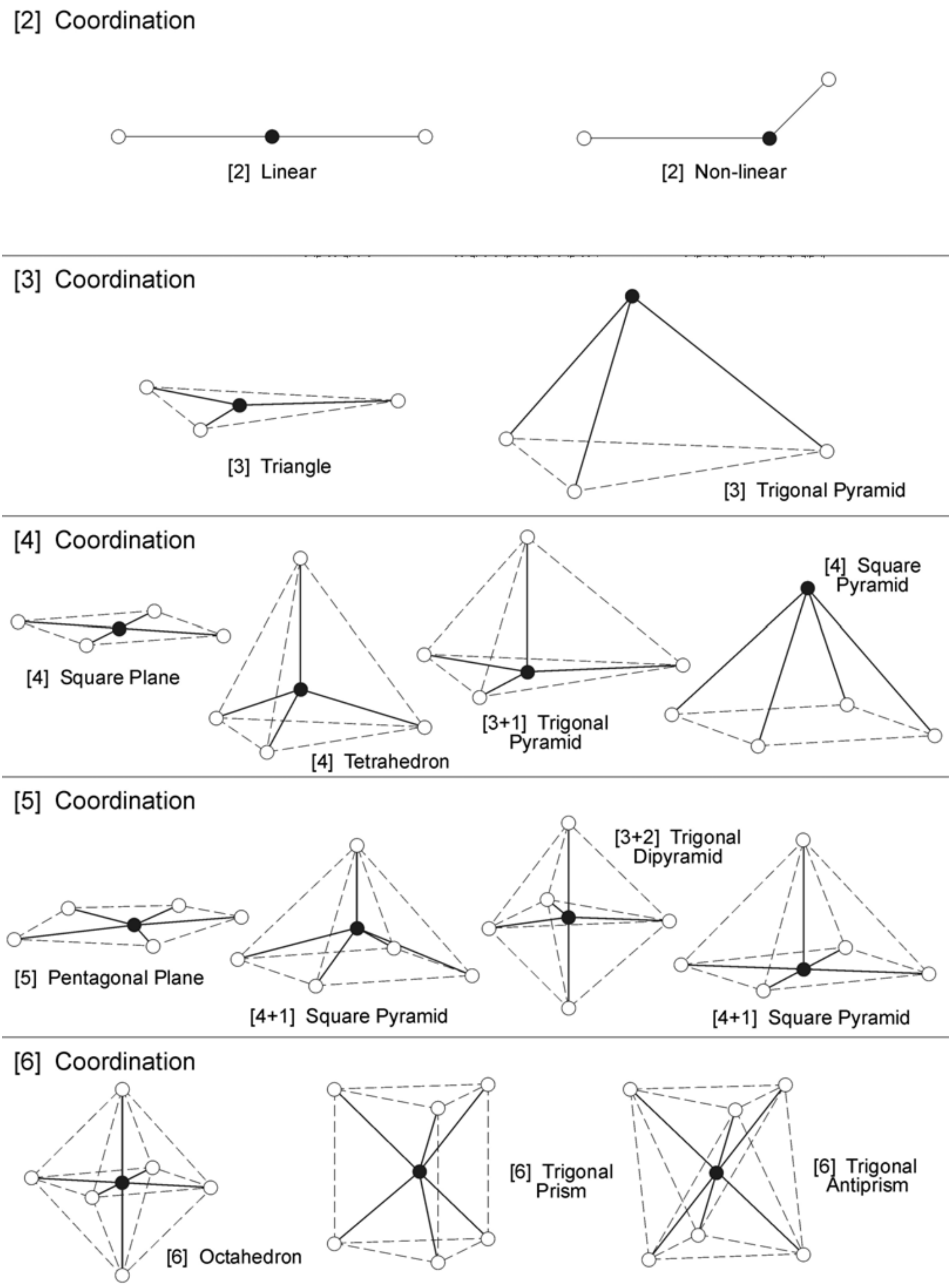
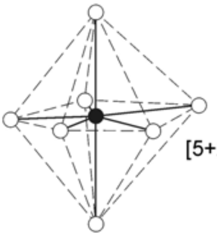
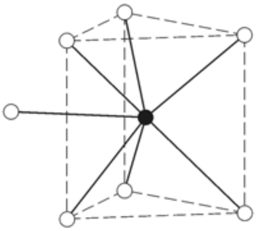


Fig 3. The more common coordination polyhedra*. The black circle represents the central cation; the white circles represent the coordinating anions; cation-anion bonds are shown as solid lines, and polyhedral forms as dashed lines.*

[7] Coordination

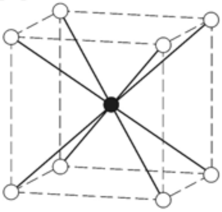


[5+2] Pentagonal Dipyramid

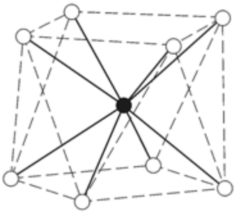


[3+3+1] Monocapped Trigonal Prism

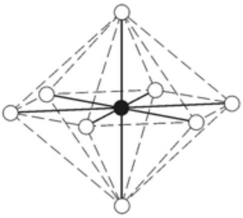
[8] Coordination



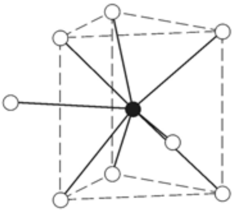
[8] Cube (Hexahedron)



[8] Square Antiprism

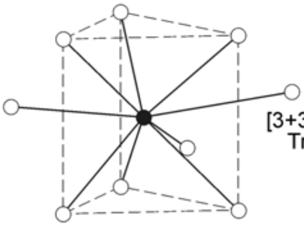


[6+2] Hexagonal Dipyramid

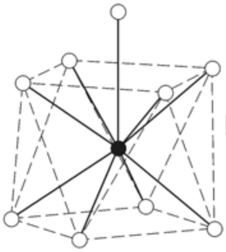


[3+3+2] Bicapped Trigonal Prism

[9] Coordination

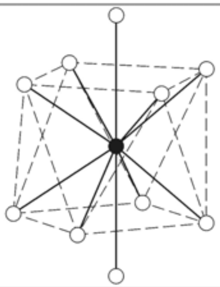


[3+3+3] Tricapped Trigonal Prism



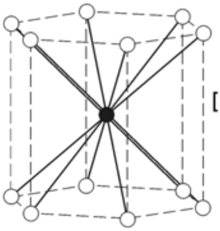
[4+4+1] Monocapped Square Antiprism

[10] Coordination

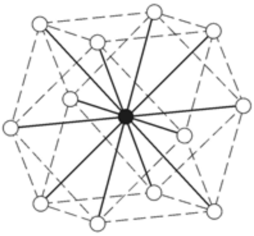


[4+4+2] Bicapped Square Antiprism

[12] Coordination



[12] Hexagonal Prism



[12] Cubooctahedron

can be conveniently grouped according to cation:anion ratio. Still others, such as halides, carbonates, sulfates and phosphates, are classified primarily on the presence or absence of OH and H_2O. The principal motive underlying the classification scheme is to provide a convenient framework to which all minerals can be readily allocated.

An alphanumeric coding scheme, from 1.AA.05 to 1.AA.10 …, etc., encompasses groups rather than individual minerals (as done by Hölzel, 1989). In this scheme, the first numeric digit represents a Class, the first alphabetic character represents a Division, and the second alphabetic character represents a Subdivision. The final two numeric digits represent a Group or individual mineral. In future, new minerals, isotypic or homeotypic with those of known structures can be inserted into an existing group; new minerals with a new structure type can be inserted into the gaps between existing group numbers.

It is hoped that the small number of classes, the logical classification principles, the specific rendition of chemical formulae, and the alphanumeric coding scheme make it relatively easy for scientists and friends of mineralogy to keep the entire system in mind.

Summary of System

1. ELEMENTS (Metals and intermetallic alloys; metalloids and nonmetals; carbides, silicides, nitrides, phosphides)

1.A: Metals and Intermetallic Alloys
    1.AA. Copper-cupalite family
    1.AB. Zinc-brass family
    1.AC. Indium-tin family
    1.AD. Mercury-amalgam family
    1.AE. Iron-chromium family
    1.AF. Platinum group elements
    1.AG. PGE-metal alloys
1.B: Metallic Carbides, Silicides, Nitrides and Phosphides
    1.BA. Carbides
    1.BB. Silicides
    1.BC. Nitrides
    1.BD. Phosphides
1.C: Metalloids and Nonmetals
    1.CA. Arsenic group elements
    1.CB. Carbon-silicon family
    1.CC. Sulfur-selenium-iodine
1.D: Nonmetallic Carbides and Nitrides
    1.DA. Nonmetallic carbides
    1.DB. Nonmetallic nitrides

2. SULFIDES and SULFOSALTS (sulfides, selenides, tellurides; arsenides, antimonides, bismuthides; sulfarsenites, sulfantimonites, sulfbismuthites, etc.)

Sulfides, etc.

2.A: Metal/metalloid alloys

- 2.AA. Alloys of metalloids with Cu, Ag, Au
- 2.AB. Ni-metalloid alloys
- 2.AC. Alloys of metalloids with PGE

2.B: Metal Sulfides, M:S > 1:1 (mainly 2:1)
- 2.BA. With Cu, Ag, Au
- 2.BB. With Ni
- 2.BC. With Rh, Pd, Pt, etc.
- 2.BD. With Hg, Tl
- 2.BE. With Pb (Bi)

2.C: Metal Sulfides, M:S = 1:1 (and similar)
- 2.CA. With Cu
- 2.CB. With Zn, Fe, Cu, Ag, etc.
- 2.CC. With Ni, Fe, Co, etc.
- 2.CD. With Sn, Pb, Hg, etc.

2.D: Metal Sulfides, M:S = 3:4 and 2:3
- 2.DA. M:S = 3:4
- 2.DB. M:S = 2:3
- 2.DC. Variable M:S

2.E: Metal Sulfides, M:S ≤ 1:2
- 2.EA. M:S = 1:2, with Cu, Ag, Au; Ni, Sn, PGE; Mo, W
- 2.EB. M:S = 1:2, with Fe, Co, Ni, PGE, etc.
- 2.EC. M:S = 1: >2

2.F: Sulfides of arsenic, alkalies; sulfides with halide, oxide, hydroxide, H_2O.
- 2.FA. With As, (Sb), S
- 2.FB. With alkalies (without Cl, etc.)
- 2.FC. With Cl, Br, I (halide-sulfides)
- 2.FD. With O, OH, H_2O

Sulfosalts

2.G: Sulfarsenites, sulfantimonites, sulfbismuthites
- 2.GA. Neso-sulfarsenites, etc. without additional S
- 2.GB. Neso-sulfarsenites, etc. with additional S
- 2.GC. Poly-sulfarsenites
- 2.GD. Unclassified sulfosalts

2.H: Sulfosalts of SnS archetype
- 2.HA. With Cu, Ag, Fe (without Pb)
- 2.HB. With Cu, Ag, Fe, Sn and Pb
- 2.HC. With only Pb
- 2.HD. With Tl
- 2.HE. With alkalies, H_2O
- 2.HF. With SnS and PbS archetype structure units

2.J: Sulfosalts of PbS archetype
- 2.JA. Chains, combined into sheets
- 2.JB. Galena derivatives, with Pb
- 2.JC. Galena derivatives, with Tl

2.K: Sulfarsenates

3. HALIDES

3.A: Simple halides, without H_2O
  - 3.AA. M:X = 1:1 and 2:3
  - 3.AB. M:X = 1:2
  - 3.AC. M:X = 1:3

3.B: Simple halides, with H_2O
  - 3.BA. M:X = 1:1 and 2:3
  - 3.BB. M:X = 1:2
  - 3.BC. M:X = 1:3
  - 3.BD. Simple halides with H_2O and additional OH

3.C: Complex halides
  - 3.CA. Borofluorides
  - 3.CB. Neso-aluminofluorides
  - 3.CC. Soro-aluminofluorides
  - 3.CD. Ino-aluminofluorides
  - 3.CE. Phyllo-aluminofluorides
  - 3.CF. Tekto-aluminofluorides
  - 3.CG. Aluminofluorides with CO_3, SO_4, PO_4
  - 3.CH. Silicofluorides
  - 3.CJ. With MX_6 complexes; M = Fe, Mn, Cu

3.D: Oxyhalides, hydroxyhalides and related double halides
  - 3.DA. With Cu, etc., without Pb
  - 3.DB. With Pb, Cu, etc.
  - 3.DC. With Pb (As, Sb, Bi), without Cu
  - 3.DD. With Hg

4. OXIDES (Hydroxides, $V^{[5,6]}$ vanadates, arsenites, antimonites, bismuthites, sulfites, selenites, tellurites, iodates)

4.A: Metal:Oxygen = 2:1 and 1:1
  - 4.AA. Cation:Anion (M:O) = 2:1 (and 1.8:1)
  - 4.AB. M:O = 1:1 (and up to 1:1.25); with small to medium-sized cations only
  - 4.AC. M:O = 1:1 (and up to 1:1.25); with large cations (± smaller ones)

4.B: Metal:Oxygen = 3:4 and similar
  - 4.BA.With small and medium-sized cations
  - 4.BB. With only medium-sized cations
  - 4.BC. With medium-sized and large cations
  - 4.BD. With only large cations

4.C: Metal:Oxygen = 2:3, 3:5, and similar
  - 4.CA. With small cations
  - 4.CB. With medium-sized cations
  - 4.CC. With large and medium-sized cations

4.D: Metal:Oxygen = 1:2 and similar
  - 4.DA. With small cations: Silica family
  - 4.DB. With medium-sized cations; chains of edge-sharing octahedra
  - 4.DC. With medium-sized cations; sheets of edge-sharing octahedra