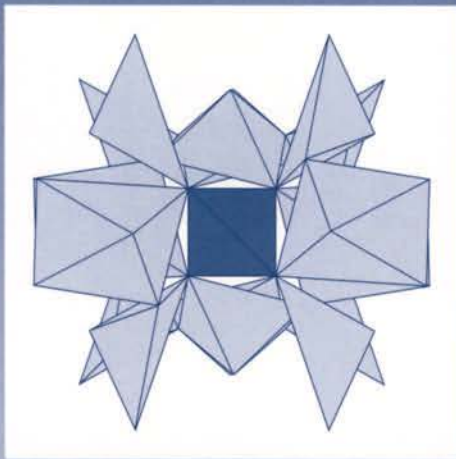


Hugo Strunz
Ernest H. Nickel

Strunz

Mineralogical Tables

Chemical Structural Mineral
Classification System
9th Edition



E. Schweizerbart'sche Verlagsbuchhandlung
(Nägele u. Obermiller) Stuttgart

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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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, since 1913), 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-*

* 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 *sⁿ*, *pⁿ* 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 C¹² 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 C¹³ 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 $\text{Si}^{[4]}$. 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.

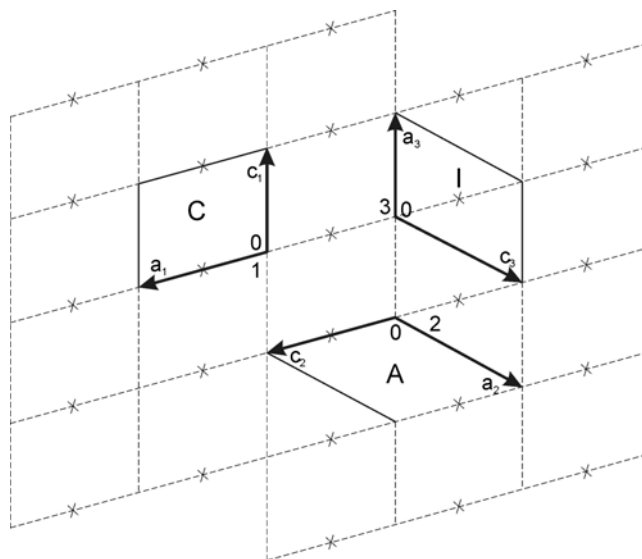


Fig 1. Unit cell settings of a monoclinic crystal with centered Bravais lattice: Setting 1 = C-centred; setting 2 = A-centred; setting 3 = I-centred. Projection on (010), the b -axis is normal to the plane of the drawing; the cell edges and full lines are at height $b = 0$; the stars are at height $b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

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) $a < b$.

Monoclinic		Setting		
Class	No.	$a_1 \ b \ c_1$ $c_1 \ -b \ a_1$	$a_2 \ b \ c_2$ $c_2 \ -b \ a_2$	$a_3 \ b \ c_3$ $c_3 \ -b \ a_3$
2	3 4 5	P2 P2 ₁ C2	A2	I2
m	6 7 8 9	Pm Pc Cm Cc Aa	Pn Am An Cn	Pa Im Ia Ic
2/m	10 11 12 13 14 15	P2/m P2 ₁ /m C2/m P2/c P2 ₁ /c C2/c A2/a	A2/m P2/n P2 ₁ /n A2/n C2/n	I2/m P2/a P2 ₁ /a I2/a I2/c

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 $a_1 \ b \ c_1$, $a_2 \ b \ c_2$ and $a_3 \ b \ c_3$ 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); a_1 and 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.

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
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** \rightarrow **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** \rightarrow **a b c** gives the standard space group symbol *Amm2* (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.

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	Pnbn	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	Pmnm	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	lbam	lmc b	lcma
	73	lbca		
		lcab		
	74	Imma	lbmm	lmcm
		Imam	lmmb	lcmm

Setting of orthorhombic crystals:
continued

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	P4 ₂ 2
	91	P4 ₁ 22
	92	P4 ₁ 2 ₁ 2
	93	P4 ₂ 22
	94	P4 ₂ 2 ₁ 2
	95	P4 ₃ 22
	96	P4 ₃ 2 ₁ 2
	97	I422
	98	I4 ₁ 22
4mm	99	P4mm
	100	P4bm
	101	P4 ₂ cm
	102	P4 ₂ nm
	103	P4cc
	104	P4nc
	105	P4 ₂ mc
	106	P4 ₂ bc
	107	I4mm
	108	I4cm
	109	I4 ₁ md
	110	I4 ₁ cd

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	$\bar{P}3$
	148	R $\bar{3}$
32	149	P312
	150	P321
	151	P3 ₁ 12
	152	P3 ₁ 21
	153	P3 ₂ 12
	154	P3 ₂ 21
	155	R32
3m	156	P3m1
	157	P31m
	158	P3c1
	159	P31c
	160	R3m
	161	R3c
$\bar{3}m$	162	$\bar{P}31m$
	163	$\bar{P}31c$
	164	$\bar{P}3m1$
	165	$\bar{P}3c1$
	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	$\bar{P}6$
6/m	175	P6/m
	176	P6 ₃ /m
622	177	P622
	178	P6 ₁ 22
	179	P6 ₅ 22
	180	P6 ₂ 22
	181	P6 ₄ 22
	182	P6 ₃ 22
6mm	183	P6mm
	184	P6cc
	185	P6 ₃ cm
	186	P6 ₃ mc
$\bar{6}m2$	187	$\bar{P}6m2$
	188	$\bar{P}6c2$
	189	$\bar{P}62m$
	190	$\bar{P}62c$
6/mmm	191	P6/mmm
	192	P6/mcc
	193	P6 ₃ /mcm
	194	P6 ₃ /mmc

Cubic		
Class	No.	Symbol
23	195 196 197 198 199	P23 F23 I23 P2 ₁ 3 I2 ₁ 3
$m\bar{3}$	200 201 202 203 204 205 206	Pm $\bar{3}$ Pn $\bar{3}$ Fm $\bar{3}$ Fd $\bar{3}$ Im $\bar{3}$ Pa $\bar{3}$ Ia $\bar{3}$
432	207 208 209 210 211 212 213 214	P432 P4 ₂ 32 F432 F4 ₁ 32 I432 P4 ₃ 32 P4 ₁ 32 I4 ₁ 32
$\bar{4}3m$	215 216 217 218 219 220	P $\bar{4}3m$ F $\bar{4}3m$ I $\bar{4}3m$ P $\bar{4}3n$ F $\bar{4}3c$ I $\bar{4}3d$
$m\bar{3}m$	221 222 223 224 225 226 227 228 229 230	Pm $\bar{3}m$ Pn $\bar{3}n$ Pm $\bar{3}n$ Pn $\bar{3}m$ Fm $\bar{3}m$ Fm $\bar{3}c$ Fd $\bar{3}m$ Fd $\bar{3}c$ Im $\bar{3}m$ Ia $\bar{3}d$

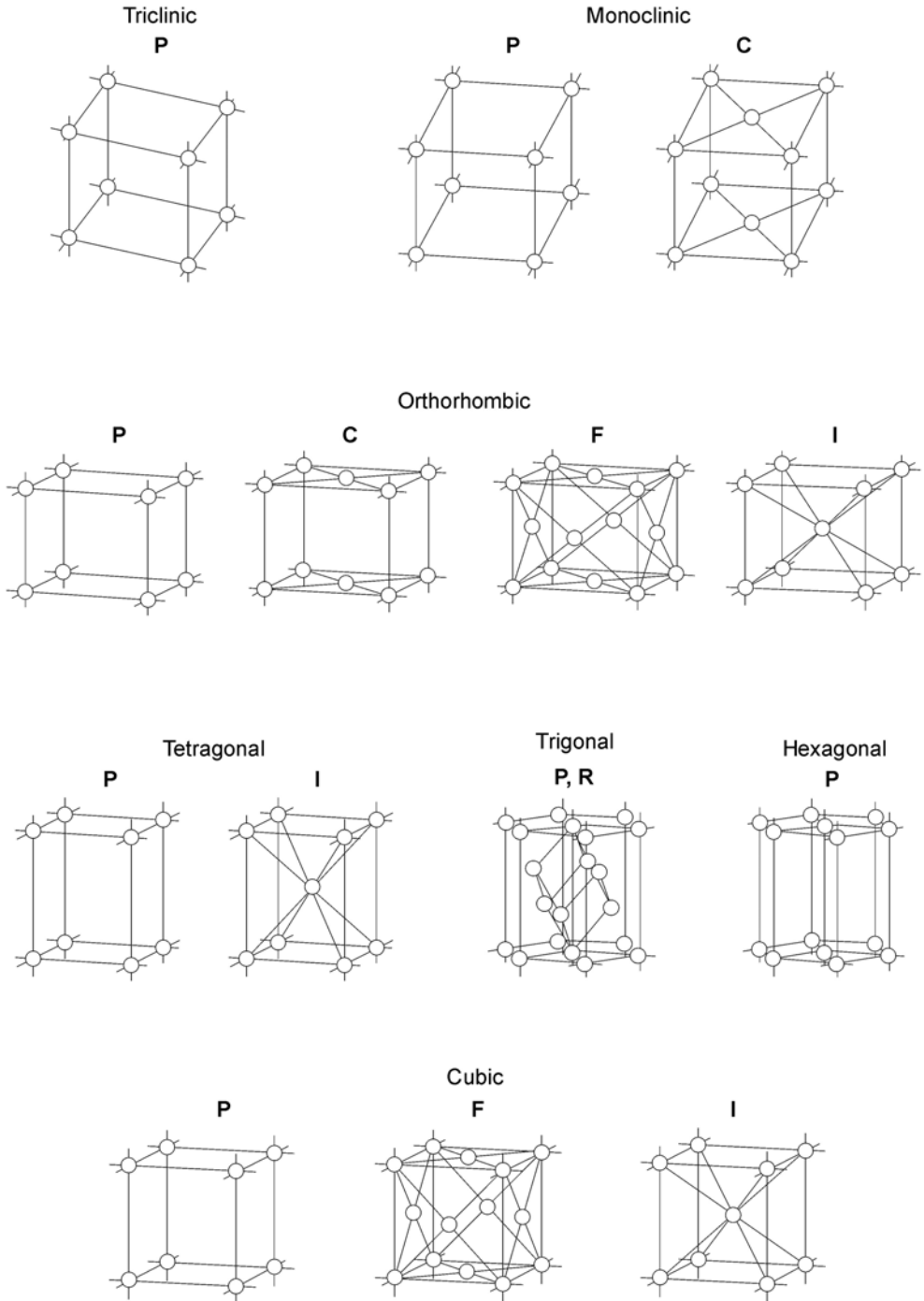


Fig 2. The 14 three-dimensional translation lattice types (Bravais, 1850). P = primitive; C = c-face centred, F = all face centred, R = rhombohedral (crystals in the 7 rhombohedral space groups are described in relation to hexagonal axes).

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

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	Symbols*		Nos.	Symbols
Triclinic	Triclinic-pedial (asymmetric)	1	–	1	P1
	Triclinic-pinacoidal	$\bar{1}$	+	2	$P\bar{1}$
Monoclinic	Monoclinic-sphenoidal	2	–	3–5	P2 – C2
	Monoclinic-domatic	m	–	6–9	Pm – Cc
	Monoclinic-prismatic	$2/m$	+	10–15	$P2/m$ – $C2/c$
Orthorhombic	Orthorhombic-disphenoidal	222	–	16–24	$P222$ – $I2_12_12_1$
	Orthorhombic-pyramidal	mm2	–	25–46	$Pmm2$ – $Ima2$
	Orthorhombic-dipyramidal	mmm	+	47–74	$Pmmm$ – $Imma$

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 ₁ 22
	Ditetragonal-pyramidal	4mm	-	99-110	P4mm - I4 ₁ cd
	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 ₃ 22
	Dihexagonal-pyramidal	6mm	-	183-186	P6mm - P6 ₃ mc
	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 ₁ 3
	Cubic-disdodecahedral	m $\bar{3}$	+	200-206	Pm $\bar{3}$ - Ia $\bar{3}$
	Cubic-gyroidal	432	-	207-214	P432 - I4 ₁ 32
	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 (2₁, 3₁, 4₁, etc. → 2, 3, 4, etc.) and replacing all glide plane symbols by the mirror plane symbol, m. Thus I4₁/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* $\text{Ca}_5[\text{F}(\text{PO}_4)_3]$, *euchroite* $\text{Cu}_2[\text{OH}|\text{AsO}_4] \cdot 3\text{H}_2\text{O}$. 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

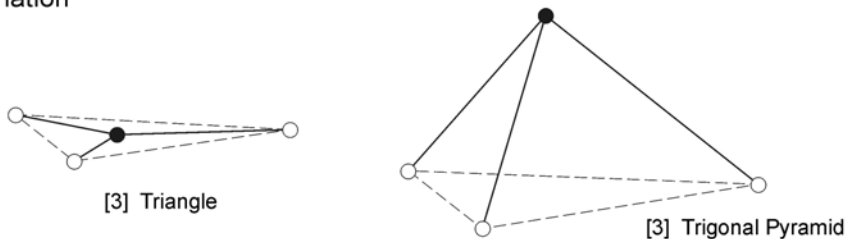
In this first English edition of *Mineralogical Tables*, the world of minerals is divided by chemical features into 10 Classes which are subdivided on chemical-structural principles, into Divisions, Subdivisions and Groups of isotypic or homeotypic species, or individual minerals of a unique structure 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,

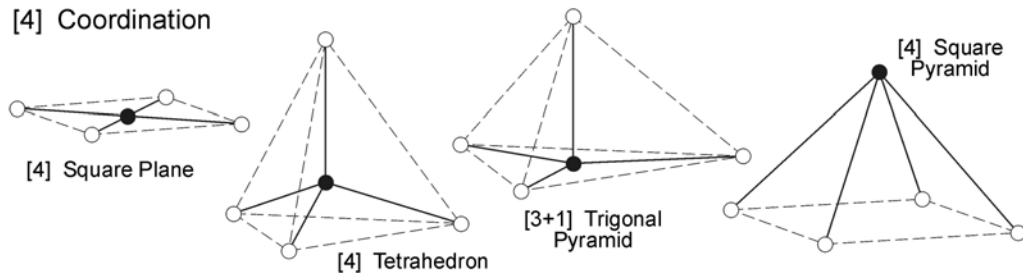
[2] Coordination



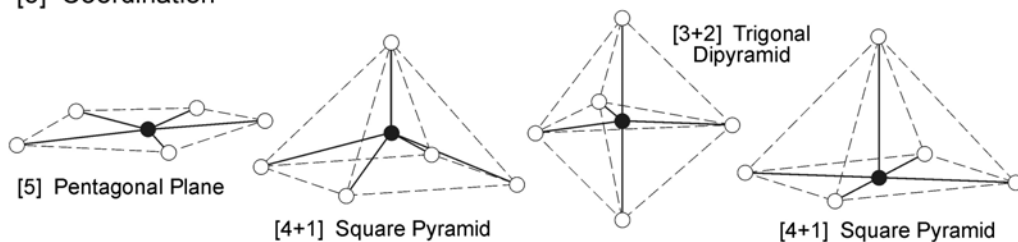
[3] Coordination



[4] Coordination



[5] Coordination



[6] Coordination

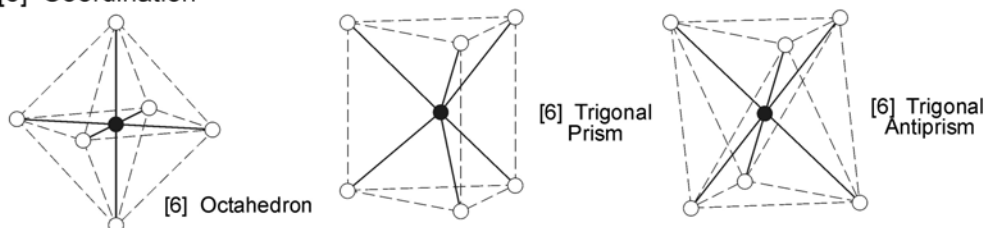
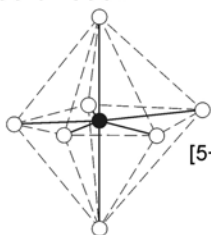
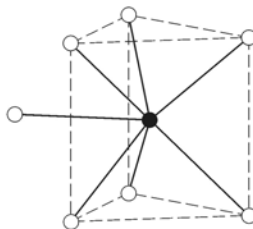


Fig 3. The more common coordination polyhedra. The black circle represents the central cation; the white circles represent the coordinating anions; cation-anion bonds are shown as solid lines, and polyhedral forms as dashed lines.

[7] Coordination

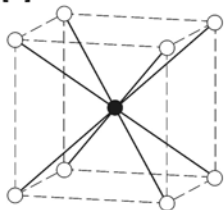


[5+2] Pentagonal Dipyramid

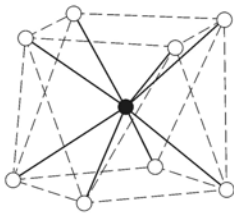


[3+3+1] Monocapped Trigonal Prism

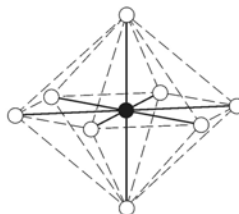
[8] Coordination



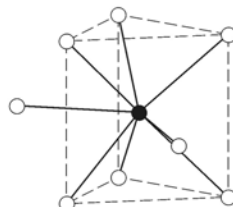
[8] Cube (Hexahedron)



[8] Square Antiprism

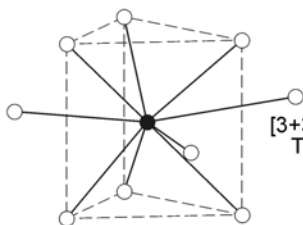


[6+2] Hexagonal Dipyramid

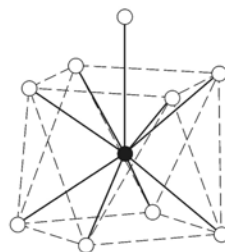


[3+3+2] Bicapped Trigonal Prism

[9] Coordination

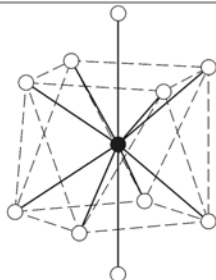


[3+3+3] Tricapped Trigonal Prism



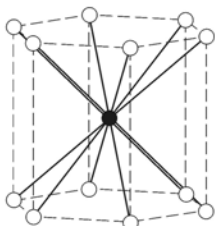
[4+4+1] Monocapped Square Antiprism

[10] Coordination

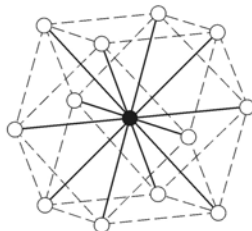


[4+4+2] Bicapped Square Antiprism

[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 H₂O. 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, H₂O.
 - 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, H₂O

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, H₂O
 - 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 H₂O
 - 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 H₂O
 - 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 H₂O 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 CO₃, SO₄, PO₄
 - 3.CH. Silicofluorides
 - 3.CJ. With MX₆ 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 (\pm 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

- 4.DD. With medium-sized cations; frameworks of edge-sharing octahedra
- 4.DE. With medium-sized cations; with various polyhedra
- 4.DF. With large (\pm medium-sized) cations; dimers and trimers of edge-sharing octahedra
- 4.DG. With large (\pm medium-sized) cations; chains of edge-sharing octahedra
- 4.DH. With large (\pm medium-sized) cations; sheets of edge-sharing octahedra
- 4.DJ. With large (\pm medium-sized) cations; polyhedral frameworks
- 4.DK. With large (\pm medium-sized) cations; tunnel structures
- 4.DL. With large (\pm medium-sized) cations; fluorite-type structures
- 4.DM. With large (\pm medium-sized) cations; unclassified
- 4.E: Metal:Oxygen = $< 1:2$
- 4.F: Hydroxides (without V or U)
 - 4.FA. Hydroxides with OH, without H₂O; corner-sharing tetrahedra
 - 4.FB. Hydroxides with OH, without H₂O; insular octahedra
 - 4.FC. Hydroxides with OH, without H₂O; corner-sharing octahedra
 - 4.FD. Hydroxides with OH, without H₂O; chains of edge-sharing octahedra
 - 4.FE. Hydroxides with OH, without H₂O; sheets of edge-sharing octahedra
 - 4.FF. Hydroxides with OH, without H₂O; various polyhedra
 - 4.FG. Hydroxides with OH, without H₂O; unclassified
 - 4.FH. Hydroxides with H₂O \pm (OH); insular octahedra
 - 4.FJ. Hydroxides with H₂O \pm (OH); corner-sharing octahedra
 - 4.FK. Hydroxides with H₂O \pm (OH); chains of edge-sharing octahedra
 - 4.FL. Hydroxides with H₂O \pm (OH); sheets of edge-sharing octahedra
 - 4.FM. Hydroxides with H₂O \pm (OH); unclassified
- 4.G: Uranyl Hydroxides
 - 4.GA. Without additional cations
 - 4.GB. With additional cations (K, Ca, Ba, Pb, etc.); with mainly UO₂(O,OH)₅ pentagonal polyhedra
 - 4.GC. With additional cations; with mainly UO₂(O,OH)₆ hexagonal polyhedra
- 4.H: V^[5,6] Vanadates
 - 4.HA. Nesovanadates
 - 4.HB. Uranyl Sorovanadates
 - 4.HC. [6]-Sorovanadates
 - 4.HD. Inovanadates
 - 4.HE. Phyllovanadates
 - 4.HF. Tektovanadates
 - 4.HG. Unclassified V oxides
- 4.J: Arsenites, antimonites, bismuthites, sulfites, selenites, tellurites; iodates.
 - 4.JA: Arsenites, antimonites, bismuthites; without additional anions, without H₂O
 - 4.JB. Arsenites, antimonites, bismuthites; with additional anions, without H₂O
 - 4.JC. Arsenites, antimonites, bismuthites; without additional anions, with H₂O
 - 4.JD. Arsenites, antimonites, bismuthites; with additional anions, with H₂O
 - 4.JE. Sulfites
 - 4.JF. Selenites without additional anions, without H₂O

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- 4.JG. Selenites with additional anions, without H₂O
 - 4.JH. Selenites without additional anions, with H₂O
 - 4.JJ. Selenites with additional anions, with H₂O
 - 4.JK. Tellurites without additional anions, without H₂O
 - 4.JL. Tellurites with additional anions, without H₂O
 - 4.JM. Tellurites without additional anions, with H₂O
 - 4.JN. Tellurites with additional anions, with H₂O
 - 4.K: Iodates
 - 4.KA. Iodates without additional anions, without H₂O
 - 4.KB. Iodates with additional anions, without H₂O
 - 4.KC. Iodates without additional anions, with H₂O
 - 4.KD. Iodates with additional anions, with H₂O
 - 5. CARBONATES (+ NITRATES)**
 - 5.A: Carbonates without additional anions, without H₂O
 - 5.AA. Alkali carbonates
 - 5.AB. Alkali-earth (and other M²⁺) carbonates
 - 5.AC. Alkali and alkali-earth carbonates
 - 5.AD. With rare-earth elements (REE)
 - 5.B: Carbonates with additional anions, without H₂O
 - 5.BA. With Cu, Co, Ni, Zn, Mg, Mn
 - 5.BB. With alkalis, etc.
 - 5.BC. With alkali-earth cations
 - 5.BD. With rare earth elements (REE)
 - 5.BE. With Pb, Bi
 - 5.BF. With (Cl), SO₄, PO₄
 - 5.C: Carbonates without additional anions, with H₂O
 - 5.CA. With medium-sized cations
 - 5.CB. With large cations (alkali and alkali-earth carbonates)
 - 5.CC. With rare earth elements (REE)
 - 5.D: Carbonates with additional anions, with H₂O
 - 5.DA. With medium-sized cations
 - 5.DB. With large and medium-sized cations
 - 5.DC. With large cations
 - 5.E: Uranyl Carbonates
 - 5.EA. UO₂:CO₃ = 1:1
 - 5.EB. UO₂:CO₃ = < 1:1 to 1:2
 - 5.EC. UO₂:CO₃ = 1:3
 - 5.ED. UO₂:CO₃ = 1:4
 - 5.EE. UO₂:CO₃ = 1:5
 - 5.EF. UO₂:CO₃ > 1:1
 - 5.EG. With SO₄ or SiO₄
 - 5.N: NITRATES
 - 5.NA. Without OH or H₂O
 - 5.NB. With OH

- 5.NC. With H₂O
- 5.ND. With OH (etc.) and H₂O

6. BORATES

6.A: Monoborates

- 6.AA. BO₃, without additional anions; 1(Δ).
- 6.AB. BO₃, with additional anions; 1(Δ) + OH, etc.
- 6.AC. B(O,OH)₄, without and with additional anions; 1(T), 1(T)+OH, etc.

6.B: Diborates

- 6.BA. Neso-diborates with double triangles B₂(O,OH)₅; 2(2 Δ); 2(2 Δ) + OH, etc.
- 6.BB. Neso-diborates with double tetrahedra B₂O(OH)₆; 2(2T)
- 6.BC. Ino-diborates with triangles and/or tetrahedra

6.C: Triborates

- 6.CA. Neso-triborates
- 6.CB. Ino-triborates
- 6.CC. Phyllo-triborates

6.D: Tetraborates

- 6.DA. Neso-tetraborates
- 6.DB. Ino-tetraborates
- 6.DC. Phyllo-tetraborates
- 6.DD. Tekto-tetraborates

6.E: Pentaborates

- 6.EA. Neso-pentaborates
- 6.EB. Ino-pentaborates
- 6.EC. Phyllo-pentaborates
- 6.ED. Tekto-pentaborates

6.F: Hexaborates

- 6.FA. Neso-hexaborates
- 6.FB. Ino-hexaborates
- 6.FC. Phyllo-hexaborates

6.G: Heptaborates and other megaborates

6.H: Unclassified borates

7. SULFATES (selenates, tellurates; chromates, molybdates, wolframates)

7.A: Sulfates (selenates, etc.) without additional anions, without H₂O

- 7.AA. With small cations
- 7.AB. With medium-sized cations
- 7.AC. With medium-sized and large cations
- 7.AD. With only large cations

7.B: Sulfates (selenates, etc.) with additional anions, without H₂O

- 7.BA. With small cations
- 7.BB. With medium-sized cations
- 7.BC. With medium-sized and large cations
- 7.BD. With only large cations

7.C: Sulfates (selenates, etc.) without additional anions, with H₂O

- 7.CA. With small cations
- 7.CB. With only medium-sized cations
- 7.CC. With medium-sized and large cations
- 7.CD. With only large cations
- 7.D: Sulfates (selenates, etc.) with additional anions, with H₂O
 - 7.DA. With small cations
 - 7.DB. With only medium-sized cations; insular octahedra and finite groups
 - 7.DC. With only medium-sized cations; chains of edge-sharing octahedra
 - 7.DD. With only medium-sized cations; sheets of edge-sharing octahedra
 - 7.DE. With only medium-sized cations; unclassified
 - 7.DF. With large and medium-sized cations
 - 7.DG. With large and medium-sized cations; with NO₃, CO₃, B(OH)₄, SiO₄ or IO₃
- 7.E: Uranyl sulfates
 - 7.EA. Without cations
 - 7.EB. With medium-sized cations
 - 7.EC. With medium-sized and large cations
- 7.F: Chromates
 - 7.FA. Without additional anions
 - 7.FB. With additional O, V, S, Cl
 - 7.FC. With PO₄, AsO₄, SiO₄
 - 7.FD. Dichromates
- 7.G: Molybdates and wolframates
 - 7.GA. Without additional anions or H₂O
 - 7.GB. With additional anions and/or H₂O
- 7.H: Uranium and uranyl molybdates and wolframates
 - 7.HA. With U⁴⁺
 - 7.HB. With U⁶⁺

8. PHOSPHATES, ARSENATES, VANADATES

- 8.A: Phosphates, etc. without additional anions, without H₂O
 - 8.AA. With small cations (some also with larger ones)
 - 8.AB. With medium-sized cations
 - 8.AC. With medium-sized and large cations
 - 8.AD. With only large cations
- 8.B: Phosphates, etc., with additional anions, without H₂O
 - 8.BA. With small and medium-sized cations
 - 8.BB. With only medium-sized cations, (OH, etc.):RO₄ ≤ 1:1
 - 8.BC. With only medium-sized cations, (OH, etc.):RO₄ > 1:1 and < 2:1
 - 8.BD. With only medium-sized cations, (OH, etc.):RO₄ = 2:1
 - 8.BE. With only medium-sized cations, (OH, etc.):RO₄ > 2:1
 - 8.BF. With medium-sized and large cations, (OH, etc.):RO₄ < 0.5:1
 - 8.BG. With medium-sized and large cations, (OH, etc.):RO₄ = 0.5:1
 - 8.BH. With medium-sized and large cations, (OH, etc.):RO₄ = 1:1
 - 8.BJ. With medium-sized and large cations, (OH, etc.):RO₄ = 1.5:1
 - 8.BK. With medium-sized and large cations, (OH, etc.):RO₄ = 2:1, 2.5:1

- 8.BL. With medium-sized and large cations, (OH, etc.):RO₄ = 3:1
 8.BM. With medium-sized and large cations, (OH, etc.):RO₄ = 4:1
 8.BN. With only large cations, (OH, etc.):RO₄ = 0.33:1
 8.BO. With only large cations, (OH, etc.):RO₄ ≥ 1:1
 8.C: Phosphates without additional anions, with H₂O
 8.CA. With small and large/medium cations
 8.CB. With only medium-sized cations, RO₄:H₂O = 1:1
 8.CC. With only medium-sized cations, RO₄:H₂O = 1:1.5
 8.CD. With only medium-sized cations, RO₄:H₂O = 1:2
 8.CE. With only medium-sized cations, RO₄:H₂O ≤ 1:2.5
 8.CF. With large and medium-sized cations, RO₄:H₂O > 1:1
 8.CG. With large and medium-sized cations, RO₄:H₂O = 1:1
 8.CH. With large and medium-sized cations, RO₄:H₂O < 1:1
 8.CJ. With only large cations
 8.D: Phosphates, etc. with additional anions, with H₂O
 8.DA. With small (and occasionally larger) cations
 8.DB. With only medium-sized cations, (OH, etc.):RO₄ < 1:1
 8.DC. With only medium-sized cations, (OH, etc.):RO₄ = 1:1 and < 2:1
 8.DD. With only medium-sized cations, (OH, etc.):RO₄ = 2:1
 8.DE. With only medium-sized cations, (OH, etc.):RO₄ = 3:1
 8.DF. With only medium-sized cations, (OH, etc.):RO₄ > 3:1
 8.DG. With large and medium-sized cations, (OH, etc.):RO₄ < 0.5:1
 8.DH. With large and medium-sized cations, (OH, etc.):RO₄ < 1:1
 8.DJ. With large and medium-sized cations, (OH, etc.):RO₄ = 1:1
 8.DK. With large and medium-sized cations, (OH, etc.):RO₄ > 1:1 and < 2:1
 8.DL. With large and medium-sized cations, (OH, etc.):RO₄ = 2:1
 8.DM. With large and medium-sized cations, (OH, etc.):RO₄ > 2:1
 8.DN. With only large cations
 8.DO. With CO₃, SO₄, SiO₄
 8.E: Uranyl phosphates and arsenates
 8.EA. UO₂:RO₄ = 1:2
 8.EB. UO₂:RO₄ = 1:1
 8.EC. UO₂:RO₄ = 3:2
 8.ED. Unclassified
 8.F: Polyphosphates, polyarsenates, [4]-polyvanadates
 8.FA. Diphosphates, etc., without OH and H₂O; dimers of corner-sharing RO₄ tetrahedra
 8.FB. Diphosphates, etc., with OH only
 8.FC. Diphosphates, etc., with H₂O only
 8.FD. Diphosphates, etc., with OH and H₂O
 8.FE. Ino-[4]-vanadates

9. SILICATES (Germanates)

9.A: Nesosilicates

- 9.AA. Nesosilicates without additional anions; cations in tetrahedral [4] coordination

- 9.AB. Nesosilicates without additional anions; cations in [4] and greater coordination
- 9.AC. Nesosilicates without additional anions; cations in octahedral [6] coordination
- 9.AD. Nesosilicates without additional anions; cations in [6] and/or generally greater coordination
- 9.AE. Nesosilicates with additional anions (O, OH, F, H₂O); cations in tetrahedral [4] and mostly greater coordination
- 9.AF. Nesosilicates with additional anions; cations in [4], [5] and/or only [6] coordination
- 9.AG. Nesosilicates with additional anions; cations in mostly [6] and > [6] coordination
- 9.AH. Nesosilicates with CO₃, SO₄, PO₄, etc.
- 9.AJ. Nesosilicates with BO₃ triangles and/or B^[4], Be^[4] tetrahedra, corner-sharing with SiO₄ tetrahedra
- 9.AK. Uranyl neso- and polysilicates
- 9.B: Sorosilicates
- 9.BA. Si₂O₇ groups, without non-tetrahedral anions; cations in tetrahedral [4] coordination
- 9.BB. Si₂O₇ groups, without non-tetrahedral anions; cations in tetrahedral [4] and greater coordination
- 9.BC. Si₂O₇ groups, without non-tetrahedral anions; cations in octahedral [6] and greater coordination
- 9.BD. Si₂O₇ groups, with additional anions; cations in tetrahedral [4] and greater coordination
- 9.BE. Si₂O₇ groups, with additional anions; cations in octahedral [6] and/or other coordination
- 9.BF. Sorosilicates with mixed SiO₄ and Si₂O₇ anions; cations in tetrahedral [4] and greater coordination
- 9.BG. Sorosilicates with mixed SiO₄ and Si₂O₇ groups; cations in octahedral [6] and greater coordination
- 9.BH. Sorosilicates with Si₃O₁₀, or larger anions; cations in tetrahedral [4] and greater coordination
- 9.BJ. Sorosilicates with Si₃O₁₀, Si₄O₁₁, etc. anions; cations in octahedral [6] and/or greater coordination
- 9.BK. Unclassified sorosilicates
- 9.C: Cyclosilicates
- 9.CA. [Si₃O₉]⁶⁻ 3-membered single rings (*dreier-Einfachringe*), without insular complex anions
- 9.CB. [Si₃O₉]⁶⁻ 3-membered single rings, with insular complex anions
- 9.CC. [Si₃O₉]⁶⁻ branched 3-membered single rings
- 9.CD. [Si₃O₉]⁶⁻ 3-membered double rings
- 9.CE. [Si₄O₁₂]⁸⁻ 4-membered single rings (*vierer-Einfachringe*), without insular complex anions
- 9.CF. [Si₄O₁₂]⁸⁻ 4-membered single rings, with insular complex anions

- 9.CG. $[\text{Si}_4\text{O}_{12}]^{8-}$ branched 4-membered single rings
- 9.CH. $[\text{Si}_4\text{O}_{12}]^{8-}$ 4-membered double rings
- 9.CJ. $[\text{Si}_6\text{O}_{18}]^{12-}$ 6-membered single rings (*sechser-Einfachringe*), without insular complex anions
- 9.CK. $[\text{Si}_6\text{O}_{18}]^{12-}$ 6-membered single rings, with insular complex anions
- 9.CL. $[\text{Si}_6\text{O}_{18}]^{12-}$ branched 6-membered single rings
- 9.CM. $[\text{Si}_6\text{O}_{18}]^{12-}$ 6-membered double rings (*sechser-Doppelringe*)
- 9.CN. $[\text{Si}_8\text{O}_{24}]^{16-}$ 8-membered rings
- 9.CO. $[\text{Si}_9\text{O}_{27}]^{18-}$ 9-membered rings
- 9.CP. 12-membered and larger rings
- 9.D: Inosilicates.
 - 9.DA. Inosilicates with 2-periodic single chains, Si_2O_6 ; pyroxene family
 - 9.DB. Inosilicates with 2-periodic single chains, Si_2O_6 ; with additional O, OH, H_2O . Pyroxene-related minerals
 - 9.DC. Inosilicates with branched 2-periodic single chains
 - 9.DD. –9.DE. Inosilicates with 2-periodic double chains; amphibole family
 - 9.DD. Orthoamphiboles
 - 9.DE. Clinoamphiboles
 - 9.DF. Inosilicates with 2-periodic multiple chains
 - 9.DG. Inosilicates with 3-periodic single and multiple chains
 - 9.DH. Inosilicates with 4-periodic single chains
 - 9.DJ. Inosilicates with 4-periodic double and triple chains
 - 9.DK. Inosilicates with 5-periodic single chains
 - 9.DL. Inosilicates with 5-periodic double chains
 - 9.DM. Inosilicates with 6-periodic single chains
 - 9.DN. Inosilicates with 6-periodic double chains
 - 9.DO. Inosilicates with 7-, 8-, 10-, 12- and 14-periodic chains
 - 9.DP. Transitional ino-phyllsilicate structures
 - 9.DQ. Unclassified inosilicates
- 9.E: Phyllosilicates
 - 9.EA. Single nets of tetrahedra with 4-, 5-, (6-), and 8-membered rings
 - 9.EB. Double nets with 4- and 6-membered rings
 - 9.EC. Phyllosilicates with mica sheets, composed of tetrahedral and octahedral nets
 - 9.ED. Phyllosilicates with kaolinite layers composed of tetrahedral and octahedral nets
 - 9.EE. Single tetrahedral nets of 6-membered rings connected by octahedral nets or octahedral bands
 - 9.EF. Single nets with 6-membered rings, connected by $\text{M}^{[4]}$, $\text{M}^{[8]}$, etc.
 - 9.EG. Double nets with 6-membered rings
 - 9.EH. Transitional structures between phyllosilicate and other silicate units
- 9.F: Tektosilicates without zeolitic H_2O
 - 9.FA. Tektosilicates without additional non-tetrahedral anions
 - 9.FB. Tektosilicates with additional anions
- 9.G: Tektosilicates with zeolitic H_2O : zeolite family
 - 9.GA. Zeolites with chains of 4-membered rings connected by a fifth Si
 - 9.GB. Zeolites with chains of single connected 4-membered rings

- 9.GC. Zeolites with chains of doubly-connected 4-membered rings
- 9.GD. Zeolites with chains of 5-membered rings
- 9.GE. Zeolites with sheets with 4-4-1-1 structural units
- 9.GF. Zeolites with Leucite-type frameworks
- 9.GG. Zeolites with Cages and double cages of 4-, 6-, and 8-membered rings
- 9.GH. Unclassified zeolites
- 9.H: Unclassified silicates
 - 9.HA. With Alkali and Alkali-earth Elements
 - 9.HB. With Ti, V, Cr
 - 9.HC. With Mn, Fe
 - 9.HD. With Co, Ni
 - 9.HE. With Cu, Zn
 - 9.HF. With Nb, Ta, Zr
 - 9.HG. With REE, Th
 - 9.HH. With Pb
- 9.J: Germanates

10. ORGANIC COMPOUNDS

- 10.A: Salts of organic acids
 - 10.AA. Acetates
 - 10.AB. Oxalates
 - 10.AC. Benzene Salts
 - 10.AD. Cyanates
- 10.B: Hydrocarbons
- 10.C: Miscellaneous Organic Minerals

In the preparation of the tabulation, which comprises the main portion of this book, we used information from a large number of sources. Most of the data came from primary published sources, but much useful information was also obtained from secondary sources such as the *Mineral Database* produced by Aleph Enterprises, Livermore, California, and various textbooks, notably *Structural Chemistry of Silicates* by F. Liebau (1985), *Natural Zeolites* by G. Gottardi and E. Galli (1985), *Crystallography and Crystal Chemistry* by F. D. Bloss (1994), and *Crystal Structure, I. Patterns and Symmetry* by M. O'Keeffe and B. G. Hyde (1996). Authoritative crystallographic information is provided by *International Tables for Crystallography*, Volume A, fourth, revised and enlarged edition by Theo Hahn (1996), and *Brief Teaching Edition of International Tables for Crystallography*, Volume A, by Theo Hahn, editor (1996), both published by Kluwer Academic, Dordrecht. The structure diagrams were produced by means of the *Atoms* computer program developed by Eric Dowty of Shape Software, Kingsport, Tennessee, USA.

References to published data cited in the tabulations are given in an abbreviated form in the interest of saving space. In general, only the year of publication and the page number are cited, but when several volumes are published within the same year, the volume number is added after the year, e. g. ZK 1987/181. The abbreviations used are as follows:

PERIODICALS

AC	Acta Crystallographica
Accad. Naz. Lincei	Accademia Nazionale dei Lincei
Acta Chem. Scand.	Acta Chemica Scandinavica
Acta Geol. Sinica	Acta Geologica Sinica
Acta Min. Sinica	Acta Mineralogica Sinica
Acta Petr. Min.	Acta Petrologica Mineralogica (Chinese)
Acta Phys. Sinica	Acta Physica Sinica
Ah	Neues Jahrbuch für Mineralogie, Abhandlungen
AM	American Mineralogist
Am. J. Sci.	American Journal of Science
Ann. Phys.	Annalen der Physik
Ark. Kem.	Arkiv för Kemi
Ark. Kem. Min. Geol.	Arkiv för Kemi, Mineralogi och Geologi
Ark. Min. Geol.	Arkiv för Mineralogi och Geologi
Austral. J. Chem.	Australian Journal of Chemistry
Austral. J. Min.	Australian Journal of Mineralogy
Austral. J. Phys.	Australian Journal of Physics
Austral. Min.	Australian Mineralogist
BM	Bulletin Société française de Minéralogie et Crystallographie; Bulletin de Minéralogie
Bull. Geol. Soc. Denmark	Bulletin of the Geological Society of Denmark
Bull. Geol. Soc. Finland	Bulletin of the Geological Society of Finland
Bull. Geol. Soc. Turkey	Bulletin of the Geological Society of Turkey
BYU	Brigham Young University
Can. J. Chem.	Canadian Journal of Chemistry
CA	Chemical Abstracts
Chem. Comm.	Chemical Communications
Chem. Erde	Chemie der Erde
Chem. Lett.	Chemistry Letters
Chem. Mater.	Chemistry of Materials
Chinese Sci. Bull.	Chinese Science Bulletin
CIM Spec. Vol.	Canadian Institute of Mining and Metallurgy, Special Volume
Clay Mins.	Clay Minerals
Clays Cl. Mins.	Clays and Clay Minerals
CM	Canadian Mineralogist
Contr. Min. Pet.	Contributions to Mineralogy and Petrology
CR	Comptes Rendus de l'Académie des Sciences, Paris
Cryst. Struct. Comm.	Crystal Structure Communications
Czech. J. Phys.	Czechoslovak Journal of Physics
Dok. Akad. Nauk	Doklady Akademiy Nauk
Dok. Akad. Nauk SSSR	Doklady Akademiy Nauk SSSR
Dok. Earth Sci.	Transactions (Doklady) of the USSR Academy of Sciences, Earth Science Sections

Ec. Geol.	Economic Geology
EJM	European Journal of Mineralogy
Eur. J. Sol. St. Inorg. Chem.	European Journal of Solid State Inorganic Chemistry
Fortsch. Min.	Fortschritte der Mineralogie
GAC-MAC	Geological Association of Canada – Mineralogical Association of Canada (Annual Meeting)
Geochim. Cosmochim. Acta	Geochimica et Cosmochimica Acta
Geol. För. Förh.	Geologiska Föreningens i Stockholm, Förhandlingar
Grøn. Geol. Undersøg.	Grønlands Geologiske Undersøgelse
Handb. Min.	Handbook of Mineralogy (Anthony <i>et al.</i>)
Helv. Chim. Acta	Helvetica Chimica Acta
IGC	International Geological Congress
IMA	International Mineralogical Association
Inorg. Chem.	Inorganic Chemistry
J. Alloys Comp.	Journal of Alloys and Compounds
J. Am. Chem. Soc.	Journal of the American Chemical Society
J. Appl. Chem.	Journal of Applied Chemistry
J. Appl. Cryst.	Journal of Applied Crystallography
J. Appl. Phys.	Journal of Applied Physics
J. Chem. Soc. Dalt.	Journal of the Chemical Society, Dalton Transactions
J. Chem. Phys.	Journal of Chemical Physics
J. Geol. Soc. Japan	Journal of the Geological Society of Japan
J. Inorg. Nucl. Chem.	Journal of Inorganic and Nuclear Chemistry
JLCM	Journal of Less-Common Metals
J. Min. Soc. Jap.	Journal of the Mineralogical Society of Japan
J. Mol. Struct.	Journal of Molecular Structure
J. Phys.	Journal of Physics
J. Phys. Chem.	Journal of Physical Chemistry
J. Phys. Chem. Sol.	Journal of the Physics and Chemistry of Solids
J. Phys. Soc. Japan	Journal of the Physical Society of Japan
J. Res. NBS	Journal of Research, National Bureau of Standards
J. Sol. St. Chem.	Journal of Solid State Chemistry
Struct. Chem.	Journal of Structural Chemistry
J. Wash. Acad. Sci.	Journal of the Washington Academy of Science
Kali u. Steinsalz	Kali und Steinsalz
Lunar Planet. Sc.	Lunar and Planetary Sciences
MA	Mineralogical Abstracts
Mater. Res. Bull.	Materials Research Bulletin
Medd. Grønland	Meddelelser om Grønland
Mh	Neues Jahrbuch für Mineralogie, Monatshefte
Mh. Chem.	Monatshefte für Chemie
Min. Deposita	Mineralium Deposita
Min. Jour.	Mineralogical Journal (Japan)
Min. Pet.	Mineralogy and Petrology
Min. Polonica	Mineralogica Polonica

Min. Tab.	Mineralogische Tabellen
Min. Zhur.	Mineralogicheskii Zhurnal (Ukraine)
Mitt. Österr. Min. Ges.	Mitteilungen der Österreichischen Mineralogischen Gesellschaft
MM	Mineralogical Magazine
MR	Mineralogical Record
MSA	Mineralogical Society of America (Annual Meeting)
MSA Spec. Pap.	Mineralogical Society of America Special Paper
Nature, Phys. Sci.	Nature, Physical Sciences
Naturw.	Naturwissenschaften
NBS Circ.	National Bureau of Standards, Circular
NBS Monogr.	National Bureau of Standards, Monograph
New Zeal. J. Geol. Geoph.	New Zealand Journal of Geology and Geophysics
Norsk. Geol. Tid.	Norske Geologisk Tidsskrift
Norske Vid.	Norske Videnskapsakademi
PDF	Powder Diffraction File of the International Centre for Diffraction Data (JCPDS)
Per. Min.	Periodico di Mineralogia
Phil. Mag.	Philosophical Magazine
Physik. Z.	Physikalische Zeitschrift
Phys. Chem. Min.	Journal of the Physics and Chemistry of Minerals
Phys. Rev.	Physical Review
Powd. Diff.	Powder Diffraction
Proc. Austral. I.M.M.	Proceedings of the Australasian Institute of Mining and Metallurgy
Proc. Lun. Sci. Conf.	Proceedings of the Lunar Science Conference
Proc. Roy. Soc.	Proceedings of the Royal Society, London
Rend. Accad. Lincei	Rendiconti, Accademia dei Lincei
Rend. Soc. Ital. Min. Pet.	Rendiconti, Societa Italiana di Mineralogia e Petrologia
Rend. Soc. Min. Ital.	Rendiconti, Societa Mineralogica Italiana
Rev. Min.	Reviews in Mineralogy (Mineralogical Society of America)
Rom. J. Min.	Romanian Journal of Mineralogy
Sc. Geol. Sinica	Scientia Geologica Sinica
SB	Strukturberichte
SMPM	Schweizerische Mineralogische und Petrographische Mitteilungen
Sov. Phys. Cryst.	Soviet Physics, Crystallography
Sov. Phys. Dok.	Soviet Physics, Doklady
SR	Structure Reports
Svensk Kem. Tid.	Svensk Kemisk Tidskrift
TMPM	Tschermak's Mineralogische und Petrographische Mitteilungen
Tr. Min. Muz. AN SSSR	Trudy Mineralogicheskogo Muzeya Akademiyi Nauk SSSR
USGS Prof. Pap.	United States Geological Survey, Professional Paper

Vest. Mosk. Univ.	Vestnik Moskovskogo Universiteta
Anorg. Allg. Chem.	Zeitschrift für Anorganische und Allgemeine Chemie
Z. Anorg. Chem.	Zeitschrift für Anorganische Chemie
Z. Elektrochem.	Zeitschrift für Elektrochemie
ZK	Zeitschrift für Kristallographie
Z. Metallk.	Zeitschrift für Metallkunde
Z. Naturf.	Zeitschrift für Naturforschung
Z. Phys. Chem.	Zeitschrift für Physikalische Chemie
ZVMO	Zapiski Vsesoyuznogo Mineralogicheskogo Obshchestva; Zapiski Vserossiyskogo Mineralogicheskogo Obshchestva

CLASS 1. ELEMENTS

(Metals and Intermetallic Alloys; Metalloids and Nonmetals;
Carbides, Silicides, Nitrides, Phosphides)

The minerals in this Class are separated into four Divisions. – **1.A: Metals and Intermetallic alloys.** – **1.B: Metal Carbides, Silicides, Nitrides and Phosphides.** – **1.C: Metalloids and Nonmetals;** and **1.D: Nonmetal Carbides and Nitrides.** The Divisions are further broken down into Subdivisions (or families), based on composition and structure, periodic system and structure types. Within the Subdivisions, the minerals are separated into structural groups; a single group name indicates isotopy or homeotypy of species within the group, and a multiple name indicates compositional or structural similarity.

1.A: Metals and Intermetallic Alloys

In metals and intermetallic alloys, the atoms have lost their valence electrons, resulting in cations in a “sea” of freemoving electrons, constituting metallic bonding. Dense packing of the cations is responsible for high density and thermal conductivity; the free valence electrons are responsible for metallic luster and high electrical conductivity. The metals have typically high coordination numbers [CN], mostly [12] or [8].

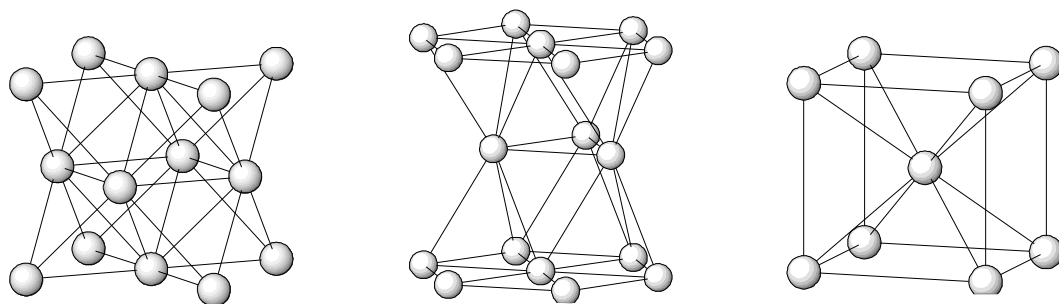


Fig 1.AA.00: The structures of copper (left), zinc (middle) and iron (right).

Subdivisions 1.AA – 1.AG

- | | |
|------------------------------------|-------------------------|
| 1.AA. Copper-cupalite family | 1.AB. Zinc-brass family |
| 1.AA.05. Copper group | 1.AB.05. Zinc group |
| 1.AA.10. Nickel group | 1.AB.10. Brass group |
| 1.AA.15. Cupalite-khatyrkite group | 1.AC. Indium-tin family |
| 1.AA.20. Anyuite-hunchunite group | 1.AC.05. Indium |

- 1.AC.10. Tin
- 1.AC.15. Bronze group
- 1.AD. Mercury-amalgam family
 - 1.AD.05. Mercury
 - 1.AD.10. Copper amalgam group
 - 1.AD.15. Silver amalgam group
 - 1.AD.20. Gold amalgam group
 - 1.AD.25. Palladium amalgam
 - 1.AD.30. Leadamalgam
- 1.AE. Iron-chromium family
 - 1.AE.05. Iron-kamacite group
 - 1.AE.10. Chromium group
 - 1.AE.15. Chromferide group
 - 1.AE.20. Wairauite-awaruite group
 - 1.AE.25. Jedwabite
- 1.AF. Platinum-group elements
 - 1.AF.05. Ruthenium group
 - 1.AF.10. Rhodium group
- 1.AG. PGE-metal alloys
 - 1.AG.05. Hexaferrum
 - 1.AG.10. Zvyagintsevite group
 - 1.AG.15. Taimyrite group
 - 1.AG.20. Paolovite-cabriite group
 - 1.AG.25. Stannopalladinite group
 - 1.AG.30. Reserved
 - 1.AG.35. Isoferroplatinum group
 - 1.AG.40. Tetraferroplatinum group
 - 1.AG.45. Hongshiite
 - 1.AG.50. Yixunite-damiaoite group
 - 1.AG.55. Niggliite

1.AA. Copper-Cupalite Family

1.AA.05. **Copper Group.** M^[12] in cubic closest packing; Cu structure type and derivatives.

Copper (<i>Cuprum</i> ¹)	Cu	Cubic, Fm $\bar{3}m$ (225) a = 3.615 Å	Z = 4
Silver (<i>Argentum</i> ²)	Ag	Cubic, Fm $\bar{3}m$ (225) a = 4.086 Å	Z = 4
Gold (<i>Aurum</i> ³)	Au	Cubic, Fm $\bar{3}m$ (225) a = 4.078 Å	Z = 4
“Electrum” (<i>Plinius</i> , AD 77 ⁴)	Au-Ag (disordered)	Cubic, Fm $\bar{3}m$ (225) a = 4.08 Å	Z = 4

Related Minerals

Silver-2H (Novgorodova <i>et al.</i> , 1979 ⁵)	Ag	Hexagonal, P6 ₃ /mmc (194) (Zn type) a = 2.93, c = 4.78 Å	Z = 2
Silver-4H (Novgorodova <i>et al.</i> , 1979 ⁶)	Ag	Hexagonal, P6 ₃ /mmc (194) (Am type) a = 2.91, c = 9.46 Å	Z = 4

Cu-Au Alloys. Native gold with some Cu in solid solution in plutonic rocks forms ordered phases during slow cooling below ~ 385 °C. In **auricupride**, the Cu coordination is Cu[Cu₈Au₄], and that of Au is Au[Cu₁₂]. In **cuproauride**, these coordinations are reversed. In **tetraauricupride**, the Cu coordination is Cu[Cu₄Au₈] and that of Au is Au[Cu₈Au₄]; alternating (001) planes of Cu and Au atoms.

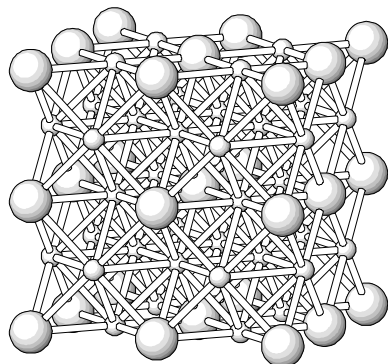


Fig 1.AA.05a. The crystal structure of auricupride. Large spheres = Au; small spheres = Cu.

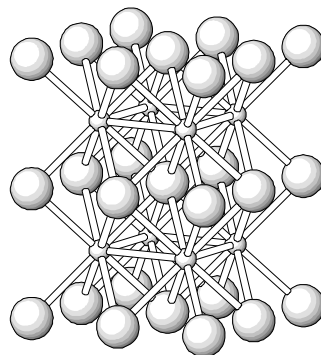


Fig 1.AA.05b. The crystal structure of tetraauricupride. Large spheres = Au; small spheres = Cu.

Auricupride (Ramdohr, 1950 ⁷)	Cu ₃ Au	Cubic, Pm $\bar{3}$ m (221) a = 3.75 Å	Z = 1
Cuproauride (Lozhechkin, 1939 ⁸)	CuAu ₃	Cubic, Pm $\bar{3}$ m (221) a = 3.98 Å	Z = 1
Tetraauricupride (Chen <i>et al.</i> 1982 ⁹)	CuAu	Tetragonal, P4/mmm (123) a = 2.81, c = 3.72 Å	Z = 1

¹ *Latin name.* Plinius: AD 77, *Aes Cyprium*; W. L. Bragg: 1914, SB 1, 35 (str); Batchelder & Simmons: J. Appl. Phys. 1965, 2864 (str)

² *Latin name.* Vegard: 1916, SB 1, 36 (str)

³ *Latin name.* Vegard: 1916, SB 1, 38 (str); Batchelder & Simmons: J. Appl. Phys. 1965, 2864 (str)

⁴ A solid-solution of Au and Ag, in nature usually with ~25–30 at. % Ag

⁵ ZVMO 1979, 552; AM 1980, 1069 (Abst.)

⁶ *idem* (Americium type)

⁷ Fortsch. Min. 1950, 69; Borelius *et al.*: Ann. Phys. 1928, 291; SB 1, 506 (strs. in the Cu-Au system)

⁸ Dokl. Akad. Nauk SSSR 1939/24, 454; Kubiak & Janczak: J. Alloys Compounds 1991/176, 133 (str); Stumpfl & Clark: Trans. Inst. Mining Metall. 1965/74, B933; Oen & Kieft: Mh 1974, 1; Verryn *et al.*: EJM 1991, 451; Knipe & Fleet: CM 1997, 573, with the Cu-Au phase diagram after Okamoto *et al.*, 1987. The name was originally used for Cu₃Au₂, which is not found in the Cu-Au phase diagram.

⁹ Sc. Geol. Sinica 1982, 111; AM 1983, 1250 (Abst.); Borelius *et al.*: *idem* (str)

1.AA.10. Nickel Group. Cu structure type.

Nickel (Ramdohr, 1967 ¹)	Ni	Cubic, Fm $\bar{3}$ m (225) a = 3.52 Å	Z = 4
Aluminium (Oleinikov <i>et al.</i> , 1978 ²)	Al	Cubic, Fm $\bar{3}$ m (225) a = 4.05 Å	Z = 4
Lead (<i>Plumbum</i> ³)	Pb	Cubic, Fm $\bar{3}$ m (225) a = 4.95 Å	Z = 4

¹ AM 1968, 348 (Abst.); Hull: 1917, SB 1, 68 (str)

² Dok. Akad. Nauk SSSR 1978/243, 191; AM 1980, 205 (Abst.); Hull: 1917, SB 1, 45 (str); Straumanis & Ejima: Z. Phys. Chem., 1960, 440 (str)

³ *Latin name*. Vegard: 1916, SB 1, 55 (str); Owen & Yates: Phil. Mag. 1933, 472 (str)

1.AA.15. **Cupalite-Khatyrkite Group.** In **khatyrkite**, columns // [001] of face-sharing AlCu_8 polyhedra are connected into a framework by sharing edges of the polyhedra; copper forms CuAl_4 square planes.

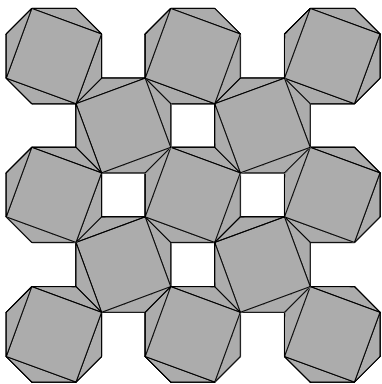


Fig 1.AA.15. A slice // (001) through the khatyrkite structure, showing the AlCu_8 polyhedra.

Cupalite (Razin <i>et al.</i> , 1985 ¹)	CuAl	Orthorhombic $a = 6.94$, $b = 4.16$, $c = 10.04\text{\AA}$	$Z = 10$
Khatyrkite (Razin <i>et al.</i> , 1985 ²)	CuAl_2	Tetragonal, $I4/mcm$ (140) $a = 6.07$, $c = 4.89\text{\AA}$	$Z = 4$

¹ ZVMO 1985, 90; AM 1986, 1278 (Abst.)

² *idem*; Friauf: J. Am. Chem. Soc. 1927, 3107 (str)

1.AA.20. **Anyuïite-Hunchunite Group.** **Anyuïite** is isostructural with khatyrkite. **Hunchunite** is a Laves phase in which $\text{Pb}[\text{Pb}_4]$ tetrahedra form a framework like that of C in diamond, with Au in the interstices; isostructural with maldonite.

Anyuïite (Razin & Sidorenko, 1989 ¹)	AuPb_2	Tetragonal, $I4/mcm$ (140) $a = 7.39$, $c = 5.61\text{\AA}$	$Z = 4$
Hunchunite (Wu <i>et al.</i> , 1992 ²)	Au_2Pb	Cubic, $Fd\bar{3}m$ (227) $a = 7.93\text{\AA}$	$Z = 8$

¹ Min. Zhur. 1989(4), 88; AM 1991, 299 (Abst.); Wallbaum: Z. Metallk. 1943, 200 (str)

² Acta Min. Sinica 1992, 319; AM 1994, 1210 (Abst.); Perlit: 1934, SB 3, 612 (str)

1.AB. Zinc-Brass Family

1.AB.05. **Zinc Group.** $M^{[12]}$ in hexagonal closest packing; Zn structure type.

Zinc (Anon. ¹)	Zn	Hexagonal, $P6_3/mmc$ (194) $a = 2.665$, $c = 4.947\text{\AA}$	$Z = 2$
Cadmium (Oleinikov <i>et al.</i> , 1979 ²)	Cd	Hexagonal, $P6_3/mmc$ (194) $a = 2.98$, $c = 5.62\text{\AA}$	$Z = 2$
Titanium (Trumilina <i>et al.</i> , 1988 ³)	Ti	Hexagonal, $P6_3/mmc$ (194) $a = 2.95$, $c = 4.69\text{\AA}$	$Z = 2$
Rhenium (Rafal'son & Sorokin, 1976 ⁴)	Re	Hexagonal, $P6_3/mmc$ (194) $a = 2.76$, $c = 4.46\text{\AA}$	$Z = 2$

¹ Clarke & Sillitoe: AM 1970, 1019; Hull & Davey: 1921, SB 1, 41 (str)

² Dok. Earth Sci. 1979/248, 182; AM 1980, 1065 (Abst.); Hull & Davey: 1921, SB 1, 42 (str)

³ Dok. Akad. Nauk SSSR 1988/303, 948; AM 1991, 1435 (Abst.); Hull: 1921, SB 1, 53 (str)

⁴ AM 1978, 1283 (Abst.); V. M. Goldschmidt: 1929, SB 1, 759 (str)

1.AB.10. **Brass Group** (Cu-Zn Alloys). In **Zhanghengite** (β -brass), the atoms are in body-centred arrangement, with atoms in 8-fold cubic coordination (Fe structure type). **β' -brass** has the CsCl-type structure, which also gives 8-fold coordination. In **γ -brass**, the atoms are in body-centred cubic close-packing, but with ordering of the Cu and Zn atoms.

α -Brass (Okrugin <i>et al.</i> , 1981 ¹)	α -(Cu,Zn)	(Zn up to 36 %, disordered)	Cubic, $Fm\bar{3}m$ (225) (Cu type) $a = 3.65\text{--}3.69\text{\AA}$	$Z = 4$
Zhanghengite (Wang, 1986 ²)	β -brass)	β -CuZn (1:1, disordered)	Cubic, $Im\bar{3}m$ (229) (Fe type) $a = 2.95\text{\AA}$	$Z = 1$
β' -Brass (Rao & Anantharaman, 1969 ³)	β' -CuZn	(1:1, ordered)	Cubic, $Pm\bar{3}m$ (221) (CsCl type) $a = 2.93\text{--}2.95\text{\AA}$	$Z = 1$
γ -Brass (Bradley & Gregory, 1931 ⁴)	Cu_5Zn_8	(Hume-Rothery phase)	Cubic, $I\bar{4}3m$ (217) $a = 8.85\text{--}8.89\text{\AA}$	$Z = 4$
Danbaite (Yue <i>et al.</i> , 1983 ⁵)	$CuZn_2$		Cubic $a = 7.76\text{\AA}$	$Z = 12$
ϵ -Brass (Westgren & Phragmén, 1925 ⁶)	$CuZn_3$	(ordered)	Hexagonal $a = 2.74$, $c = 8.58\text{\AA}$ (?)	$Z = 1$
η -Brass (Westgren & Phragmén, 1925 ⁷)	η -(Cu,Zn)	(Zn 96–100 %, disordered)	Hexagonal, $P6_3/mmc$ (194) (Zn type) $a = 2.67$, $c = 4.94\text{\AA}$	$Z = 2$

¹ AM 1982, 416 (Abst.); Owen & Preston: 1923, SB 1, 523 (str)

² Acta Min. Sinica 1986, 220; AM 1990, 244 (Abst.); Owen & Preston: *idem* (str);

³ Z. Metallk. 1969/60, 312

⁴ Bradley & Gregory: 1931, SB 2, 693 (str); homeotype of α -Mn, SB 2, 2 (str)

⁵ Kexue Tongbao 1983, 1383; AM 1984, 566 (Abst.)

⁶ Westgren & Phragmén: 1925, SB 1, 535 (str)

⁷ *idem*

1.AC. Indium-Tin Family

1.AC.05. **Indium.** Distorted cubic closest packing of In^[12].

Indium (Ivanov, 1967 ¹)	In	Tetragonal, I4/mmm (139) a = 3.25, c = 4.95 Å	Z = 2
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¹ AM 1967, 299 (Abst.); Hull & Davey: 1921, SB 1, 44 (str); Smith & Schneider: JLCM, 1964, 17 (str)

1.AC.10. **Tin.** Distorted diamond structure type, with Sn^[4] in tetrahedral coordination.

Tin (<i>Stannum</i> ¹)	β -Sn	Tetragonal, I4 ₁ /amd (141) a = 5.82, c = 3.18 Å	Z = 4
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¹ *Latin name*; Ivanov: AM 1967, 299 (Abst.); Mark & Polanyi: 1923, SB 1, 54 (str)

1.AC.15. **Bronze Group.** Nickeline structure type. η' -**Bronze** has the nickeline structure type, but with additional Cu.

η'-Bronze (Clark, 1972 ¹)	Cu _{1.2} Sn	Hexagonal, P6 ₃ /mmc (194) a = 4.23, c = 5.12 Å	Z = 2
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Sorosite (Barkov <i>et al.</i> , 1998 ²)	Cu(Sn,Sb)	Hexagonal, P6 ₃ /mmc (194) (?) a = 4.22, c = 5.12 Å	Z = 2
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Yuanjiangite (Chen <i>et al.</i> , 1994 ³)	AuSn	Hexagonal, P6 ₃ /mmc (194) a = 4.32, c = 5.51 Å	Z = 2
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¹ Mh 1972, 108; Rose: Mh 1981, 117; Bernal: Nature 1928/122, 54 (str)

² AM 1998, 901

³ Acta Petr. Min. 1994, 232; AM 1995, 1330 (Abst.); Preston & Owen: 1927, SB 1, 562 (str)

1.AD. Mercury-Amalgam Family

1.AD.05. **Mercury.** Hg has distorted cubic closest packing, with [3 + 3 + 6] coordination; its structure is related to that of zinc.

Mercury (<i>Hydrargyrium</i> ¹)	Hg (below -38.9 °C)	Trigonal, R $\bar{3}$ m (166) a = 3.46, c = 6.71 Å	Z = 3
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¹ *NewLatin name.* Barrett: AC 1957, 58 (str)

1.AD.10. **Copper Amalgam Group.** The **belendorffite** structure contains Hg^[11] and Cu^[12].

Kolymite (Markova <i>et al.</i> , 1980 ¹)	Cu ₇ Hg ₆	Cubic, Im $\bar{3}$ m (229), I $\bar{4}$ 3m (217), I432 (211) a = 9.42 Å	Z = 4
Belendorffite (Bernhardt & Schmetzer, 1992 ²)	Cu ₇ Hg ₆	Trigonal, R3m (160) (pseudo-cubic) a = 9.41 Å α = 90.5°	Z = 4

¹ ZVMO 1980, 206; AM 1981, 218 (Abst.)

² Mh 1992, 21; AM 1992, 1305 (Abst.); Lindahl & Westman: Acta. Chem. Scand. 1969, 1181 (str)

1.AD.15. **Silver Amalgam Group. “Kongsbergite”** (α-amalgam) has Ag-type structure with Hg up to ~30%. The **schachnerite** structure is a derivative of the zinc structure. In **moschellandsbergite**, the atoms are in body-centred close packing (CsCl structure type), but with two empty Hg sites per unit cell, which lowers the symmetry.

Schachnerite (Seeliger & Mücke, 1972 ¹)	Ag _{1.1} Hg _{0.9} (β-amalgam, disordered)	Hexagonal, P6 ₃ /mmc (194) a = 2.98, c = 4.84 Å	Z = 1
Paraschachnerite (Seeliger & Mücke, 1972 ²)	Ag _{1.2} Hg _{0.8} (β'-amalgam, ordered)	Orthorhombic, Cmcm (63), Cmc2 ₁ (36), C2cm (40) a = 2.96, b = 5.13, c = 4.83 Å	Z = 2
Eugenite (Kucha, 1986 ³)	Ag ₁₁ Hg ₂	Cubic, I $\bar{4}$ 3m (217) a = 10.02 Å	Z = 4
Moschellandsbergite (Berman & Harcourt, 1938 ⁴)	Ag ₅ Hg _{7.5}	Cubic, I23 (197) a = 10.05 Å	Z = 4
Luanheite (Shao <i>et al.</i> , 1984 ⁵)	Ag ₃ Hg	Hexagonal a = 6.61, c = 10.98 Å	Z = 6

¹ Ah 1972/177, 1; AM 1973, 347 (Abst.)

² *idem*

³ Min. Polonica 1986(2), 3; AM 1995, 845 (Abst.)

⁴ AM 1938, 761; Fairhurst & Cohen: AC 1972.B, 371 (str); compare γ-brass

⁵ Acta Min. Sinica 1984, 97; AM 1988, 192 (Abst.)

1.AD.20. **Gold Amalgam Group. Weishanite** appears to have the schachnerite structure. The structure of **goldamalgam** is related to that of moschellandsbergite.

Weishanite (Li <i>et al.</i> , 1984 ¹)	(Au,Ag) _{1.2} Hg _{0.8}	Hexagonal, P6 ₃ /mmc (194) a = 2.93, c = 4.82 Å	Z = 1
Goldamalgam (Chen <i>et al.</i> , 1981 ²)	γ-(Au,Ag) ₂ Hg ₃	Cubic, Im $\bar{3}$ m (229) a = 10.01 Å	Z = 10

¹ Acta Min. Sinica 1984, 102; AM 1988, 196 (Abst.)

² Dizhi Pinglun 1981, 107; AM 1985, 215 (Abst.)

1.AD.25. **Palladium Amalgam.** CuAu structure type.

Potarite (Harrison, 1926 ¹)	PdHg	Tetragonal, P4/mmm (123) a = 3.02, c = 3.71 Å	Z = 1
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¹ Terada & Cagle: AM 1960, 1093 (str)

1.AD.30. **Leadamalgam.** Structure not known.

Leadamalgam (Chen <i>et al.</i> , 1981 ¹)	Pb _{0.7} Hg _{0.3}	Tetragonal, I4/mmm (139) a = 3.55, c = 4.53 Å	Z = 2
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¹ Dizhi Pinglun 1981, 107; AM 1985, 215 (Abst.)

1.AE. Iron-Chromium Family

1.AE.05. **Iron-Kamacite Group.** In **iron** (α -Fe), the Fe^[8] atoms are in a cubic body-centred packing (Fe structure type); it is magnetic up to 769 °C (Curie point). The β -Fe phase, stable above 769 °C, is non-magnetic. The γ -Fe phase is stable above 911 °C. In the high-pressure form, **ϵ -iron**, Fe^[12] has the Zn structure type. **Kamacite** is α -(Fe,Ni), **taenite** is γ -(Fe,Ni) (Cu type), and **tetrataenite** is similar but with Ni-Fe ordering (CuAu structure type).

Iron (<i>Ferrum</i> ¹)	α -Fe	Cubic, Im $\bar{3}$ m (229) a = 2.87 Å	Z = 2
γ-Iron (artificial ²)	γ -Fe	Cubic, Fm $\bar{3}$ m (225) a = 3.65 Å	Z = 4
ϵ-Iron (Ramdohr, 1966 ³)	ϵ -Fe (stable at P > 131 kbar)	Hexagonal, P6 ₃ /mmc (194) a = 2.47, c = 3.96 Å	Z = 2

Kamacite (Reichenbach, 1861 ⁴)	α -(Fe,Ni) with Fe:Ni \geq 3:1	Cubic, $Im\bar{3}m$ (229) a = 2.87–2.88Å	Z = 2
Taenite (Reichenbach, 1861 ⁵)	γ -(Fe,Ni) with Fe:Ni < 3:1	Cubic, $Fm\bar{3}m$ (225) a = 3.60Å	Z = 4
Tetrataenite (Clarke & Scott, 1980 ⁶)	FeNi with Fe:Ni = 1:1	Tetragonal, $P4/mmm$ (123) a = 2.53, c = 3.58Å	Z = 1
Taenite-1M (Tagai & Takeda, 1995 ⁷)	FeNi with Fe:Ni = 1:1	Monoclinic, Pm (6), pseudo-cubic a = 3.58, b = 3.58, c = 3.59Å $\beta = 90.0^\circ$	Z = 2

¹ *Latin name*. Nordenskiöld, 1870 – first reported natural occurrence; Hull: 1917, SB 1, 66 (str)

² Westgren & Lindh: 1921, SB 1, 66 (str); Basinski *et al.*, 1955 (str), from Donnay & Ondik *Crystal Data*, 1973

³ Chem. Erde 1966/25, 259; Takahashi & Basset: Science 1964/145, 483 (str)

⁴ Young: 1926, SB 1, 523 (str); Ramsden & Cameron: AM 1966, 37

⁵ *idem* (str)

⁶ AM 1980, 624; Rubin: MM 1994, 215

⁷ ZK 1995/210, 14 (str)

1.AE.10. **Chromium Group.** The Cr^[8] atoms are in cubic body-centred packing; α -Fe structure type.

Chromium (Yue <i>et al.</i> , 1981 ¹)	Cr	Cubic, $Im\bar{3}m$ (229) a = 2.88Å	Z = 2
Wolfram (Tungsten) (Novgorodova <i>et al.</i> , 1995 ²)	W	Cubic, $Im\bar{3}m$ (229) a = 3.16Å	Z = 2
Tantalum (Seredin <i>et al.</i> , 1998 ³)	Ta	Cubic, $Im\bar{3}m$ (229) a = 3.31Å	Z = 2

¹ Kexue Tongbao 1981, 959; AM 1982, 854 (Abst); Hull: 1921, SB 1, 61 (str)

² Dok. Akad. Nauk SSSR 1995/340, 681; AM 1996, 1284 (Abst.)

³ Dok. Earth Sci. 1998/361, 642; Owen & Iball: 1932, SB 2, 163 (str)

1.AE.15. **Chromferide Group.** Probably ordered phases; CsCl structure type.

Chromferide (Novgorodova <i>et al.</i> , 1986 ¹)	Fe(Fe _{0.5} Cr _{0.2} □ _{0.3})	Cubic, $Pm\bar{3}m$ (221) a = 2.86Å	Z = 1
Ferchromide (Novgorodova <i>et al.</i> , 1986 ²)	Cr(Cr _{0.5} Fe _{0.2} □ _{0.3})	Cubic, $Pm\bar{3}m$ (221) a = 2.88Å	Z = 1

¹ ZVMO 1986, 355; AM 1988, 190 (Abst.)

² *idem*

1.AE.20. **Wairauite-Awaruite Group.** The **wairauite** structure is of the CsCl structure type. The **awaruite** structure is of the auricupride (Cu_3Au) structure type.

Wairauite (Challis & Long, 1964 ¹)	FeCo (ordered)	Cubic, $\text{Pm}\bar{3}\text{m}$ (221) $a = 2.86\text{\AA}$	$Z = 1$
Awaruite (Skey, 1885 ²)	FeNi_3	Cubic, $\text{Pm}\bar{3}\text{m}$ (221) $a = 3.59\text{\AA}$	$Z = 1$

¹ MM 1964, 942; Bayliss: CM 1990, 751

² Nickel: CM 1959, 307; Bayliss: *idem*

1.AE.25. **Jedwabite.** Structure not known.

Jedwabite (Novgorodova <i>et al.</i> , 1997 ¹)	$\text{Fe}_7(\text{Ta},\text{Nb})_3$	Hexagonal, $\text{P6}_3/\text{mmc}$ (194), $\text{P6}_3\text{mc}$ (186), $\text{P}\bar{3}2\text{c}$ (190) $a = 4.81, c = 7.87\text{\AA}$	$Z = 1$
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¹ ZVMO 1997 (2), 100; AM 1998, 654 (Abst.)

1.AF. Platinum-Group Elements (PGE)

1.AF.05. **Ruthenium Group.** Platinum-group elements with hexagonal close packing; Zn structure type.

Ruthenium (Urashima <i>et al.</i> , 1974 ¹)	Ru	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.71, c = 4.28\text{\AA}$	$Z = 2$
Osmium (Berzelius, 1819 ²)	Os	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.73, c = 4.31\text{\AA}$	$Z = 2$
Rutheniridosmine (Aoyama, 1936 ³)	(Os,Ir,Ru)	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.73, c = 4.33\text{\AA}$	$Z = 2$

¹ Hull & Davey: 1921, SB 1, 69 (str); Min. Jour. 1974, 438; AM 1976, 177 (Abst.)

² Hull: 1921, SB 1, 70 (str); Harris & Cabri: CM 1973/12, 104

³ Strunz: Min. Tab. 1966; Cabri: CIM Spec. Vol. 1981/23, 91

1.AF.10. **Rhodium Group.** Platinum-group elements with cubic close packing; Cu structure type.

Rhodium (Cabri & Laflamme, 1974 ¹)	(Rh,Pt)	Cubic, $\text{Fm}\bar{3}\text{m}$ (225) $a = 3.84\text{\AA}$	$Z = 4$
Palladium (Wollaston, 1803 ²)	Pd	Cubic, $\text{Fm}\bar{3}\text{m}$ (225) $a = 3.89\text{\AA}$	$Z = 4$

Iridium (Hausmann, 1813 ³)	Ir	Cubic, Fm $\bar{3}$ m (225) a = 3.84Å	Z = 4
Platinum (Ulloa, 1748 ⁴)	Pt	Cubic, Fm $\bar{3}$ m (225) a = 3.92Å	Z = 4

¹ CM 1974, 399; Hull: 1920: SB 1, 69 (str)

² Hull & Davey: 1921, SB 1, 70 (str)

³ Hull & Davey: *idem* (str); Singh: AC 1968, 469 (str)

⁴ Hull & Davey: 1921, SB 1, 71 (str); Cabri & Feather: CM 1975, 117 (PGE nomenclature); Harris & Cabri: CM 1991, 231 (PGE nomenclature)

1.AG. PGE-Metal Alloys

Ru,Os-M Alloys

1.AG.05. **Hexaferrum**. Hexagonal close-packing; Zn structure type, cf ϵ -Fe.

Hexaferrum (Mochalov <i>et al.</i> , 1998 ¹)	(Fe,Os,Ru,Ir)	Hexagonal, P6 ₃ /mmc (194) a = 2.59, c = 4.17Å	Z = 2
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¹ ZVMO 1998 (5), 41; AM 1999, 1686 (Abst.)

Pd,Pt-M Alloys

1.AG.10. **Zvyagintsevite Group**. **Zvyagintsevite** has the auricupride (Cu₃Au) structure type. **Atokite** and **rustenburgite** may have the Cu structure type.

Zvyagintsevite (Genkin <i>et al.</i> , 1966 ¹)	Pd ₃ (Pb,Sn) (ordered phase)	Cubic, Pm $\bar{3}$ m (221) a = 4.03Å	Z = 1
Atokite (Mihalik <i>et al.</i> , 1975 ²)	(Pd,Pt) ₃ Sn (disordered phase)	Cubic, Fm $\bar{3}$ m (225) a = 3.99Å	Z = 1
Rustenburgite (Mihalik <i>et al.</i> , 1975 ³)	(Pt,Pd) ₃ Sn (disordered phase?)	Cubic, Fm $\bar{3}$ m (225) ? a = 3.99Å	Z = 1

¹ CM 1966, 541; Szymanski *et al.*: CM 1997, 773 (str)

² CM 1975, 146; AM 1976, 340 (Abst.)

³ *idem*

1.AG.15. **Taimyrite Group**. Structures not known. Isotypes.

Taimyrite (Begizov <i>et al.</i> , 1982 ¹)	(Pd,Pt) ₉ Cu ₃ Sn ₄	Orthorhombic a = 7.88, b = 3.89, c = 7.88Å	Z = 1
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Tatyanaité (Pt,Pd)₉Cu₃Sn₄ Orthorhombic
(Barkov *et al.*, 2000²) a = 7.89, b = 4.07, c = 7.73 Å Z = 1

¹ ZVMO 1982, 78; AM 1983, 1252 (Abst.) a, b, c = 16.11, 11.27, 8.64 Å; 12.57, 13.40, 17.09 Å; Barkov *et al.*: EJM 2000, 391 (data from Evstigneeva Nekrasov, 1984, for synthetic taimyrite)

² EJM 2000, 391; AM 2000, 1845 (Abst.)

1.AG.20. **Paolovite-Cabriite Group.** Structures not known.

Paolovite Pd₂Sn Orthorhombic, Pbnm (62)
(Genkin *et al.*, 1974¹) a = 8.11, b = 5.66, c = 4.32 Å Z = 4

Cabriite Pd₂CuSn Orthorhombic, Pmmm (47)
(Evstigneeva & Genkin, 1983²) a = 7.88, b = 7.88, c = 3.94 Å Z = 4

¹ AM 1974, 1331 (Abst.)

² CM 1983, 481; AM 1984, 1190 (Abst.)

1.AG.25. **Stannopalladinite Group.** Structures related to that of nickeline.

Stannopalladinite Pd₃Sn₂ Hexagonal, P6₃/mmc (194)
(Maslenitzki *et al.*, 1947¹) a = 4.38, c = 5.66 Å Z = 1

Plumbopalladinite Pd₃Pb₂ Hexagonal, P6₃mc (186)
(Genkin *et al.*, 1970²) a = 4.47, c = 5.72 Å Z = 1

¹ Shelton *et al.*: CM 1981, 599

² AM 1971, 1121 (Abst.); Shelton *et al.*: CM 1981, 599 (phase relations)

1.AG.30. **Reserved.** For future similar alloys.

1.AG.35. **Isoferroplatinum Group.** Probably auricupride (Cu₃Au) structure type.

Chengdeite Ir₃Fe Cubic, Pm $\bar{3}$ m (221)
(Yu, 1995²) a = 3.79 Å Z = 1

Isoferroplatinum Pt₃Fe Cubic, Pm $\bar{3}$ m (221)
(Cabri & Feather, 1975¹) a = 3.86 Å Z = 1

¹ Acta Geol. Sinica 1995, 215; AM 1996, 516 (Abst.)

² CM 1975, 117; AM 1976, 338 (Abst.)

1.AG.40. **Tetraferroplatinum Group.** Isostructural with tetraauricupride; alternating (001) layers of Pt and (Fe,Cu) atoms.

Tulameenite (Cabri <i>et al.</i> , 1973 ¹)	Pt ₂ FeCu	Tetragonal, P4/mmm (123) a = 3.89, c = 3.58Å	Z = 1
Tetraferroplatinum (Cabri & Feather, 1975 ²)	PtFe	Tetragonal, P4/mmm (123) a = 2.72, c = 3.69Å	Z = 1
Ferronickelplatinum (Rudashevskiy <i>et al.</i> , 1983 ³)	Pt(Ni,Fe)	Tetragonal, P4/mmm (123) a = 2.73, c = 3.64Å	Z = 1

¹ CM 1973, 21; AM 1974, 383 (Abst.); Shahmiri *et al.*: MM 1985, 547 (str)² CM 1975, 117; AM 1976, 341 (Abst.); Tarkian: Min. Petrol. 1987/36, 169³ ZVMO 1983, 487; AM 1984, 1190 (Abst.); Bayliss: CM 1990, 7511.AG.45. **Hongshiite**. Structure not known.

Hongshiite (Yu <i>et al.</i> , 1974 ¹)	PtCu	Trigonal, R $\bar{3}$ m (166), R3m (160), R32 (155) a = 10.71, c = 13.19Å	Z = 48
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¹ AM 1984, 411 (Abst.)1.AG.50. **Yixunite-Damiaioite Group**. **Yixunite** has the auricupride structure; **damiaioite** may be related.

Yixunite (Yu, 1997 ¹)	Pt ₃ In	Cubic, Pm $\bar{3}$ m (221) a = 3.99Å	Z = 1
Damiaioite (Yu, 1997 ²)	PtIn ₂	Cubic, Fm $\bar{3}$ m (225) a = 6.36Å	Z = 4

¹ AM 1998, 655 (Abst.)² AM 1998, 653 (Abst.)1.AG.55. **Niggliite**. Nickeline-type structure; cf. also yuanjiangite, AuSn.

Niggliite (Scholtz, 1936 ¹)	PtSn	Hexagonal, P6 ₃ /mmc (194) a = 4.10, c = 5.43Å	Z = 2
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¹ Yushko-Zakharova & Chernaev: Dok. Earth Sci. 1966/170, 148 (str); Cabri & Harris: MM 1972, 794

1.B: Metal Carbides, Silicides, Nitrides and Phosphides

These can be regarded as interstitial alloys. The non-metal atoms (C, etc.) are located in small empty sites of the metal structures. High hardness, density and reflectivity. Metallic (and covalent) bonding. CN (of the non-metal atoms) is [4] or [6].

Subdivisions 1.BA. – 1.BD.

- | | |
|--|--|
| 1.BA. Carbides | 1.BB.10. Perryite-xifengite group |
| 1.BA.05. Martensite-“austenite”-cohenite group | 1.BB.15. Fersilicite-ferdisilicite group |
| 1.BA.10. Haxonite group | 1.BC. Nitrides |
| 1.BA.15. Tongbaite | 1.BC.05. Roaldite-siderazot group |
| 1.BA.20. Tantalcarbide group | 1.BC.10. Osbornite-carlsbergite group |
| 1.BA.25. Tungsten carbide | 1.BD. Phosphides |
| 1.BB. Silicides | 1.BD.05. Schreibersite group |
| 1.BB.05. Suessite-gupeiite group | 1.BD.10. Barringerite |

1.BA. Carbides

1.BA.05. **Martensite-“Austenite”-Cohenite Group.** In **martensite** (magnetic steel) and **“austenite”** (non-magnetic steel), C^[6] atoms are in octahedral coordination, interstitial in α' - and γ -Fe, whereas in **cohenite**, they are in triangular-prismatic coordination in pleated layers of hexagonal close-packed Fe^[11, 12] atoms. α' -Fe is tetragonally deformed α -Fe.

Martensite (Osmond, 1895, synthetic ¹)	α' -Fe with ~ 0.3–1.5 % C	Tetragonal, I4/mmm (139) a ~ 2.85, c ~ 2.88–3.04Å	Z = 2
“Austenite” (Osmond, 1901, synthetic ²)	γ -Fe with ~ 2–7 % C	Cubic, Fm $\bar{3}$ m (225) a = 3.63Å	Z = 4
Cohenite (Weinschenk, 1889 ³)	Fe ₃ C (cementite in metallurgy)	Orthorhombic, Pnma (62) a = 5.09, b = 6.75, c = 4.52Å	Z = 4

¹ Calvert, 1993: PDF 44–1291; Roberts: J. Met. 1953, 203; Zhang *et al.*: Geochim. Cosmochim. Acta 1993, 3725 (in meteorites)

² Westgren & Phragmén: 1921, SB 1, 577 (str)

³ Westgren & Phragmén: *idem* (str); Fasiska & Jeffrey: AC 1965/19, 463 (str)

1.BA.10. **Haxonite Group.** Isotypes. The structure may be related to γ -Fe and taenite.

Haxonite (Scott, 1971 ¹)	(Fe,Ni) ₂₃ C ₆	Cubic, Fm $\bar{3}$ m (225) a = 10.55Å	Z = 4
Isovit (Generalov <i>et al.</i> , 1998 ²)	(Cr,Fe) ₂₃ C ₆	Cubic, Fm $\bar{3}$ m (225) a = 10.65Å	Z = 4

¹ Nature, Phys. Sci. 1971/229, 61; AM 1974, 209 (Abst.)

² ZVMO 1998 (5), 26; AM 1999, 1686 (Abst.)

1.BA.15. **Tongbaite**. The carbon atoms are at the centres of triangular prisms formed by six Cr atoms; these triangular prisms share faces to form columns// [001] and edges // [001]; the Cr atoms are enclosed by five C atoms in the form of square pyramids.

Tongbaite (Tian <i>et al.</i> , 1983 ¹)	Cr_3C_2	Orthorhombic, Pnam (62) $a = 5.57, b = 11.47, c = 2.82\text{\AA}$	$Z = 4$
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¹ Acta Min. Sinica 1983, 241; AM 1985, 218 (Abst.); Rundqvist & Runnsjö: 1969, SR 34A, 56 (str)

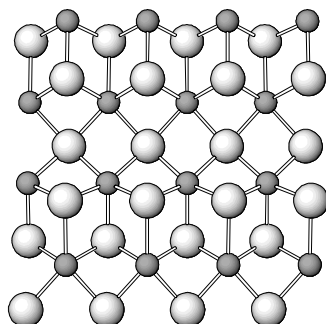


Fig 1.BA.15. A slice through the tongbaite structure approximately // (100), c-axis horizontal. Large spheres = Cr; small spheres = C.

1.BA.20. **Tantalcarbide Group**. Halite structure type.

Khamrabaevite (Novgorodova <i>et al.</i> , 1984 ¹)	TiC	Cubic, $\text{Fm}\bar{3}\text{m}$ (225) $a = 4.32\text{\AA}$	$Z = 4$
Niobocarbide (Novgorodova <i>et al.</i> , 1997 ²)	(Nb,Ta)C	Cubic, $\text{Fm}\bar{3}\text{m}$ (225) $a = 4.45\text{\AA}$	$Z = 4$
Tantalcarbide (FrondeI, 1962 ³)	TaC	Cubic, $\text{Fm}\bar{3}\text{m}$ (225) $a = 4.45\text{\AA}$	$Z = 4$

¹ ZVMO 1984, 697; AM 1985, 1329 (Abst.)

² ZVMO 1997 (1), 76; AM 1998, 1117 (Abst.)

³ AM 1962, 786; Schwarz & Summa: Metallwirtschaft 1933, 298 (str)

1.BA.25. **Tungsten Carbide**. A hexagonal array of W atoms, with $\text{C}^{[6]}$ in trigonal-prismatic interstices.

Tungsten Carbide (Zhang <i>et al.</i> , 1986 ¹)	WC	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.90, c = 2.84\text{\AA}$	$Z = 1$
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¹ AM 1989, 948 (Abst.); Glavatskikh *et al.*: AM 1998, 189 (Abst.); Westgren & Phragmén: 1926, SBI, 575 (str); Leciejewicz: AC 1961, 200 (str)

1.BB. Silicides

1.BB.05. **Suessite-Gupeiite Group.** The structure of **suessite** is similar to that of α -Fe; in **gupeiite**, a is doubled.

Suessite (Keil <i>et al.</i> , 1982 ¹)	Fe _{0.75} Si _{0.25} (disordered α phase)	Cubic, Im $\bar{3}$ m (229) $a = 2.84\text{\AA}$	Z = 2
Gupeiite (Yu, 1984 ²)	Fe ₃ Si (ordered phase)	Cubic, Fm $\bar{3}$ m (225) $a = 5.67\text{\AA}$	Z = 4

¹ AM 1982, 126; Phragmén: 1926, SB 1, 589 (str); Weill: 1945, SR 10, 61 (str)

² AM 1986, 228 (Abst.)

1.BB.10. **Perryite-Xifengite Group.** In **perryite**, layers of Ni^[11-14] atoms // (0001) alternate with layers of Si^[8-12] atoms

Perryite (Frederiksson & Henderson, 1965 ¹)	(Ni,Fe) ₈ (Si,P) ₃	Trigonal, R3c (161) $a = 6.64, c = 37.98\text{\AA}$	Z = 12
Xifengite (Yu, 1984 ²)	Fe ₅ Si ₃ (η phase)	Hexagonal, P6 ₃ /mcm (193) $a = 6.76, c = 4.72\text{\AA}$	Z = 2

¹ MM 1970, 905; Okada *et al.*: AC 1991.C, 1358 (str)

² AM 1986, 228 (Abst.); Weill, 1943, SR 10, 63 (str); Haughton, etc., 1930, 1937; SR 10,62 (Fe-Si phase diagram)

1.BB.15. **Fersilicite-Ferdisilicite Group.** **Fersilicite** has a distorted NaCl-type structure.

Fersilicite (Gevorkyan <i>et al.</i> , 1969 ¹)	FeSi (ϵ phase)	Cubic, P2 ₁ 3 (198) $a = 4.46\text{\AA}$	Z = 4
Ferdisilicite (Gevorkyan <i>et al.</i> , 1969 ²)	FeSi ₂	Tetragonal, P4/mmm (123) $a = 2.69, c = 5.14\text{\AA}$	Z = 1

¹ Geol. Zhur. 1969 (2), 62; AM 1969, 1737 (Abst.); Wever & Möller: 1930, SB 2, 13 and 241 (str); Hanawalt *et al.*: Annal. Chem 1938/10, 475 (str)

² Geol. Zhur. 1969 (2), 62; AM 1969, 1737 (Abst.); Aronsson: Acta Chem. Scand. 1960, 1414 (str); PDF 35-822

1.BC. Nitrides

1.BC.05. **Roaldite-Siderazot Group.** In **roaldite**, the N atoms are ordered in tetrahedral sites, related to the γ -Fe phase. **Siderazot** is related to the ϵ -Fe phase.

Roaldite (Buchwald & Nielsen, 1981 ¹)	Fe ₄ N	Cubic, P $\bar{4}$ 3m (215) a = 3.79Å	Z = 1
Siderazot (Silvestri, 1876 ²)	Fe ₃ N (Fe:N ~ 3:1–3:1.5)	Hexagonal, P6 ₃ 22 (182) a = 4.68, c = 4.37Å	Z = 2

¹ Lunar Planet. Sc. 1981, 112; AM 1981, 1100 (Abst.); Jack: 1948, SR 11, 141 (str)² Hendricks & Kosting: ZK 1930/74, 511; 1930, SB 2, 302 (str)1.BC.10. **Osbornite Group.** Halite structure type.

Osbornite (Maskelyne, 1870 ¹)	TiN	Cubic, Fm $\bar{3}$ m (225) a = 4.24Å	Z = 4
Carlsbergite (Buchwald & Scott, 1971 ²)	CrN	Cubic, Fm $\bar{3}$ m (225) a = 4.16Å	Z = 4

¹ Christensen: Acta Chem. Scand. A1975, 563 (str); Bashir *et al.*: J. Appl. Cryst. 1996, 471 (str)² Nature, Phys. Sci. 1971/233, 113; AM 1972, 1311 (Abst.)**1.BD. Phosphides**

1.BD.05. **Schreibersite Group.** An interstitial sheet structure // (001), with P coordinated by 9 (Fe,Ni) atoms, 8 within the sheets, 1 between the sheets.

Schreibersite (Patera, 1847 ¹)	(Fe,Ni) ₃ P	Tetragonal, I $\bar{4}$ (82) a = 9.04, c = 4.46Å	Z = 8
Nickelphosphide (Britvin <i>et al.</i> , 1999 ²)	(Ni,Fe) ₃ P	Tetragonal, I $\bar{4}$ (82) a = 8.99, c = 4.40Å	Z = 8

¹ Doenitz: ZK 1970/131, 222 (str)² ZVMO 1999 (3), 64; AM 2000, 875 (Abst.)

1.BD.10. **Barringerite.** A close-packed arrangement of PFe₉, FeP₄ and FeP₅ polyhedra.

Barringerite (Buseck, 1969 ¹)	(Fe,Ni) ₂ P	Hexagonal, P $\bar{6}$ 2m (189) a = 5.87, c = 3.46Å	Z = 3
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¹ Science 1969/165, 169; AM 1970, 317 (Abst.); Rundqvist & Jellinek: Acta Chem. Scand. 1959, 425 (str)

1.C: Metalloids and Nonmetals

In the metalloids and nonmetals, the atomic orbitals can be hybridized in different ways to create a variety of structures that can have metalloid or nonmetallic character depending on the electronic interactions between neighbouring atoms. In the non-metals, there is covalent and van der Waals bonding.

Subdivisions 1.CA. – 1.CC.

1.CA. Arsenic group elements	1.CB.10. Diamond group
1.CA.05. Arsenic group	1.CB.15. Silicon
1.CA.10. Arsenolamprite	1.CC. Sulfur-selenium-iodine
1.CA.15. Paradocrasite	1.CC.05. Sulfur group
1.CB. Carbon-silicon family	1.CC.10. Selenium group
1.CB.05. Graphite group	1.CC.15. Iodine

1.CA. Arsenic-Group Elements

1.CA.05. **Arsenic Group.** In **arsenic**, As^[3] atoms form puckered sheets of trigonal 6-membered rings // (0001), with stacking as in graphite-3R. Covalent bonding within the sheets, metalloid bonding between the sheets. The a:c ratio decreases in the order **arsenic-stibarsen-antimony-bismuth**, resulting in increasing metallic character.

Arsenic* (<i>Anon.</i> ¹)	As	Trigonal, R $\bar{3}m$ (166) a = 3.76, c = 10.55Å	Z = 6
Stibarsen (Wretblad, 1941 ²)	AsSb	Trigonal, R $\bar{3}m$ (166) a = 4.02, c = 10.80Å	Z = 3
Antimony (<i>Anon.</i> ³)	Sb	Trigonal, R $\bar{3}m$ (166) a = 4.31, c = 11.27Å	Z = 6
Bismuth (Agricola, 1439 ⁴)	Bi	Trigonal, R $\bar{3}m$ (166) a = 4.54, c = 11.86Å	Z = 6

* In German: As = Arsen, As₂O₃ = Arsenic (highly poisonous).

¹ Schiferl & Barrett: J. Appl. Cryst. 1969, 30 (str); Swanson & Fuyat, 1954: PDF 5–632

² AM 1941, 456 (Abst.); Ferguson: PDF 31–80

³ Barrett *et al.*: AC 1963, 451 (str); Swanson & Fuyat, 1954: PDF 35–732

⁴ Barrett: Austral. J. Phys. 1960, 200 (str); Swanson & Fuyat, 1954: PDF 5–519

1.CA.10. **Arsenolamprite.** The As^[3] atoms are in widely separated double layers // (001). Dimorphs arsenic, arsenolamprite.

Arsenolamprite (Hintze, 1886 ¹)	As (orthorhombic)	Orthorhombic, Bmab (64) a = 3.63, b = 4.45, c = 10.96Å	Z = 8
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¹ Johan: Chem. Erde 1959, 71; Clark: MM 1970, 732; Smith *et al.*: Phil. Mag. 1975, 57 (str)

1.CA.15. **Paradocrasite.** Structure not known.

Paradocrasite (Leonard <i>et al.</i> , 1971 ¹)	$\text{Sb}_2(\text{Sb,As})_2$	Monoclinic, C2 (5) $a = 7.25$, $b = 4.17$, $c = 4.43 \text{ \AA}$ $\beta = 123.1^\circ$	$Z = 1$
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¹ AM 1971, 1127**1.CB. Carbon-Silicon Family**

1.CB.05. **Graphite Group.** In **graphite**, $\text{C}^{[3]}$ atoms form planar sheets of hexagonal rings // (0001); covalent bonding within the sheets (three hybrid sp^2 electrons of each C atom overlap their orbitals with those of three neighbouring C atoms; C-C = 1.42 \AA), metalloid bonding between the sheets by “free” π electrons; (C-C = 3.35 \AA). **Fullerenes**, artificial C_{60} and C_{70} , from hollow spheres composed of 5- and 6-membered rings; the spheres may cristalize in cubic or hexagonal closest packing.

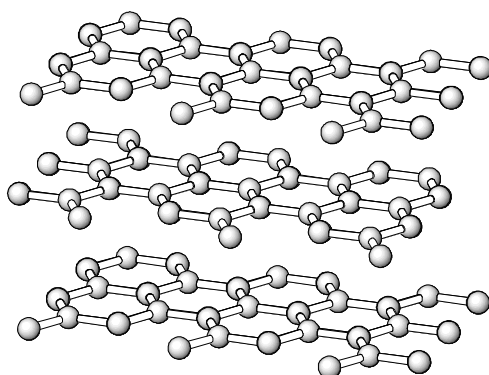


Fig 1.CB.05. The structure of graphite showing the sheets of 6-membered $\text{C}^{[3]}$ rings // (0001).

Graphite-2H (Werner, 1789 ¹)	C	Hexagonal, $P6_3/mmc$ (194) $a = 2.46$, $c = 6.71 \text{ \AA}$	$Z = 4$
Graphite-3R (Lipson & Stokes, 1942 ²)	C	Trigonal, $R\bar{3}m$ (166) $a = 2.46$, $c = 10.06 \text{ \AA}$	$Z = 6$
“Chaoite” (El Goresy, 1970 ³)	C	Hexagonal, $P6/mmm$ (191) ? $a = 8.95$, $c = 14.08 \text{ \AA}$	$Z = 168$
“Fullerite” (Parthasarathy <i>et al.</i> , 1998 ⁴)	C_{60}	Cubic (Cu-type structure) $a = 14.20 \text{ \AA}$	$Z = 4$

¹ Hull: 1917, SB 1, 28 (str); Trucano & Chen: Nature 1975/258, 136 (str)

² Nature 1942/149, 328 (str); Holcombe 1974: PDF 26–1079 (R3)

³ Smith & Buseck: Science 1982/216, 984 (a mixture); AM 1983, 1251 (Abst.)

⁴ Parthasarathy et al., 1998; AM 1999, 1686 (Abst.); Novgorodova: 1999; AM 2000, 629 (Abst.; tetragonal, $\alpha = 14.22$, $c = 13.56\text{\AA}$)

1.CB.10. **Diamond Group.** **Diamond** has a cubic tetrahedral framework structure. Four C atoms at the corners and the three face-centres of the unit cell correspond to cubic closest packing; four of the eight tetrahedral sites in this packing are occupied by C atoms, the remainder are empty. Corner-sharing CC_4 tetrahedra form a framework with channels along the six $\langle 110 \rangle$ directions. Extremely strong covalent bonding (4 hybridized sp^3 electrons of each C atom overlap their orbitals in $\langle 111 \rangle$ directions with those of four neighbouring C atoms; C-C = 1.54\AA); This very strong bonding is responsible for the extreme properties exhibited by this mineral. **Lonsdaleite**, a dimorph of diamond, has a hexagonal tetrahedral framework structure. Members of the sphalerite-wurtzite family are homeotypes of diamond and lonsdaleite.

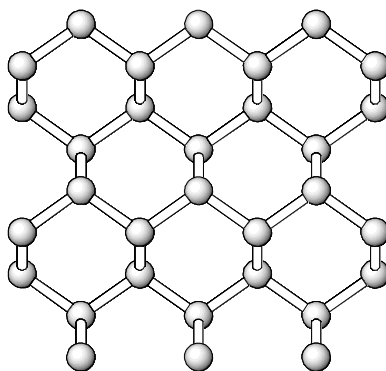


Fig 1.CB.10. The structure of diamond projected on (110).

Diamond (Pliny, A.D. 77 ¹)	C	Cubic, $\text{Fd}\bar{3}\text{m}$ (227) $a = 3.567\text{\AA}$	$Z = 8$
Lonsdaleite (Frondele & Marvin, 1967 ²)	C	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.51$, $c = 4.12\text{\AA}$	$Z = 4$
“Lonsdaleite-4H” (O’Keeffe & Hyde, 1996 ³)	C	Hexagonal, $\text{P6}_3/\text{mmc}$ (194) $a = 2.51$, $c = 8.12\text{\AA}$	$Z = 8$

¹ Hist. Nat. 37,15; W. H. Bragg & W. L. Bragg: Proc. Roy. Soc. 1913, 277 (str); Straumanis & Aka: J. Am. Chem. Soc. 1951, 5643 (str)

² Nature 1967/214, 587; AM 1967, 1579 (Abst.); Ownby *et al.*: J. Am. Ceram. Soc. 1992, 1876 (str)

³ O’Keeffe & Hyde: Crystal Structures I, 1996, 301 (str, synth. product)

1.CB.15. **Silicon.** Diamond structure type.

Silicon (Marshintsev <i>et al.</i> , 1982 ¹)	Si	Cubic, Fd $\bar{3}$ m (227) a = 5.43Å	Z = 8
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¹ Dok. Earth Sci. 1982/262, 163; Novgorodova *et al.*: AM 1991, 668 (Abst.); Debye & Scherrer: 1916, SB 1, 52 (str)

1.CC. Sulfur-Selenium-Iodine

1.CC.05. **Sulfur Group.** Molecules of puckered 8-membered rings of S atoms, with covalent bonding within the molecules and van der Waals bonding between the molecules.

Sulfur (Anon. ¹)	α -S	Orthorhombic Fddd (70) a = 10.44, b = 12.84, c = 24.37Å	Z = 128
β-Sulfur (Panichi, 1912 ²)	β -S	Monoclinic, P2 ₁ /a (14) a = 10.85, b = 10.93, c = 10.95Å β = 96.2°	Z = 48
Rosickyite (Sekanina, 1931 ³)	γ -S	Monoclinic, P2/c (13) a = 8.44, b = 13.02, c = 9.36Å β = 125.0°	Z = 32

¹ Warren & Burwell: J. Chem. Phys. 1935, 6 (str); Rettig & Trotter: AC 1987.C, 2260 (str)

² Burwell: ZK 1937/97, 132; SB 5, 29 (str); Sands: J. Am. Chem. Soc. 1965, 1395 (str)

³ Y. Watanabe: AC 1974.B, 1396 (str)

1.CC.10. **Selenium Group.** Helical chains // [001]; covalent bonding along the chains, metalloid bonding between the chains.

Selenium (Berzelius, 1818 ¹)	γ -Se	Trigonal, P3 ₁ 21 (152) and P3 ₂ 21 (154) a = 4.37, c = 4.95Å	Z = 3
Tellurium (Klaproth, 1802 ²)	γ -Te	Trigonal, P3 ₁ 21 (152) and P3 ₂ 21 (154) a = 4.46, c = 5.92Å	Z = 3

¹ Bradley: 1924. SB1, 31 (str); Marsh *et al.*: AC 1953, 71 (str)

² Cherin & Unger: AC 1967/23, 670 (str)

1.CC.15. **Iodine.** I₂ molecules in sheets // (010).

Iodine (Matteucci, 1897 ¹)	I ₂	Orthorhombic Ccmb (64) a = 4.79, b = 7.27, c = 9.80Å	Z = 4
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¹ Harris *et al.*: J. Am. Chem. Soc. 1928, 1583 (str); SB1, 760

1.D: Nonmetal Carbides and Nitrides

Minerals in this Division have covalent bonding and nonmetallic character.

Subdivisions 1.DA. – 1.DB.

1.DA. Nonmetal Carbides	1.DB.05. Nierite
1.DA.05. Moissanite group	1.DB.10. Sinoite
1.DB. Nonmetal Nitrides	1.DB.15. "Borazon"

1.DA. Nonmetal Carbides

1.DA.05. **Moissanite Group.** Synthetic SiC (carborundum: Acheson, 1893), and the naturally-occurring mineral (Moissan, 1894), **moissanite** (Kunz, 1895), occur as a wide range of polytypes, which are differentiated by crystallographic suffixes (introduced by Ramsdell², 1947). **Moissanite-3C** (β -moissanite) has the sphalerite structure type (β -ZnS), and **moissanite-2H** (α -moissanite), the wurtzite (α -ZnS) structure type (α -moissanite includes all hexagonal and trigonal polytypes). Strong covalent bonding, hardness 9½, an important abrasive.

Moissanite-3C (Regis & Sand, 1958 ¹)	β -SiC	Cubic, $F\bar{4}3m$ (216) a = 4.35 Å	Z = 4
Moissanite-2H (Kunz, 1905 ²)	α -SiC	Hexagonal, $P6_3mc$ (186) a = 3.08, c = 5.05 Å	Z = 2
Moissanite-4H (artificial ³)	SiC	Hexagonal, $P6_3mc$ (186) a = 3.09, c = 10.09 Å	Z = 4
Moissanite-5H (Gevorkyan <i>et al.</i> , 1974 ⁴)	SiC	Hexagonal a = 3.06, c = 12.58 Å	Z = 5
Moissanite-6H (Kunz, 1905 ⁵)	SiC	Hexagonal, $P6_3mc$ (186) a = 3.09, c = 15.17 Å	Z = 6
Moissanite-15R (Marshintsev <i>et al.</i> , 1990 ⁶)	SiC	Trigonal, $R3m$ (160) a = 3.09, c = 37.95 Å	Z = 15
Moissanite-33R (Marshintsev, 1990 ⁷)	SiC	Trigonal a = 3.08, c = 83.0 Å	Z = 33

¹ Bull. Geol. Soc. Am. 1958/69, 1633; Brækken: ZK 1930/75, 573 (str)

² Am. J. Sci. 1905, ser. 4/19, 396 (unspecified polytype); Ott: ZK 1926/63, 1; SB 1, 145 (str); Ramsdell: AM 1947, 64; Shaffer: AC 1969.B, 477 (extended classification of the polytypes)

³ Ott: *idem* (str)

⁴ ZVMO 1974, 106; AM 1976, 1054 (Abst.)

⁵ Am. J. Sci. 1905, ser. 4/19, 396; Ott: *idem* (str); Bauer *et al.*: AM 1963, 620. Strongly prevalent in synthetic products and in nature

⁶ Min. Zhur. 1990 (3), 17; AM 1992, 208 (Abst.); Ott: *idem* (str)

⁷ Min. Zhur. 1990 (3), 17; AM 1992, 208 (Abst.)

1.DB. Nonmetal Nitrides

1.DB.05. **Nierite**. A framework of corner-sharing SiN_4 tetrahedra; each N atom is surrounded by 3 Si atoms in a triangular configuration.

Nierite (Lee <i>et al.</i> , 1995 ¹)	$\alpha\text{-Si}_3\text{N}_4$	Trigonal, P31c (159) a = 7.74, c = 5.61 Å	Z = 4
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¹ Meteoritics 1995, 387; Marchand *et al.*: AC 1969.B, 2157 (str)

1.DB.10. **Sinoite**. A framework of corner-sharing SiN_3O tetrahedra.

Sinoite (Anderson <i>et al.</i> , 1964 ¹)	$\text{Si}_2\text{N}_2\text{O}$	Orthorhombic, Cmc2 ₁ (36) a = 8.84, b = 5.47, c = 4.84 Å	Z = 4
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¹ Science, 1964/146, 256; AM 1965, 521 (Abst.); Brosset & Idrestedt: Nature 1964/201, 1211 (str)

1.DB.15. **“Borazon”**. Sphalerite structure type; a high-pressure product of hexagonal BN.

“Borazon”	BN	Cubic, F $\bar{4}3m$ (216) a = 3.61 Å	Z = 4
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Wentorf: J. Chem. Phys. 1957/26, 956 (synthet.)

CLASS 2. SULFIDES and SULFOSALTS

(Sulfides, selenides, tellurides; arsenides, antimonides, bismuthides; sulfarsenites, sulfantimonites, sulfbismuthites, etc.)

The minerals in this class are compounds of metals with S, Se, Te (chalcogens) and As, Sb, Bi (metalloids). A wide range of bonding types is represented, including metallic, covalent and ionic. The appearance is predominantly metallic, although the minerals in the 2.F division are mainly non-metallic. The classification begins with the **Metal/Metalloid Alloys (2.A)**, followed by the **Simple Sulfides, Selenides, etc. (2.B to 2.F)**, and the complex sulfides or **Sulfosalts (2.G to 2.K)**.

The **Simple Sulfides** are classified into **Divisions** on the basis of the metal:sulfur ratio, M:S = 2:1, 1:1, 3:4 and 2:3, 1:2, and higher. The **Subdivisions** are generally arranged according to the position of the metals in the Periodic System of the Elements, and increasing ionic size or coordination number [CN]. **Groups** combine mineral species with isotypic (or homeotypic) structures; groups with two or more mineral names include heterotypes.

The **Sulfosalts*** are characterized by the presence of trigonal pyramids that represent the fundamental building blocks in the structure. These trigonal pyramids include $[\text{AsS}_3]^{3-}$, $[\text{SbS}_3]^{3-}$ or $[\text{BiS}_3]^{3-}$, and consist of three sulfur atoms forming the base of the pyramid, and the metalloids As, Sb or Bi at the apex. This can be attributed to the lone-electron-pair effect of the metalloid ions. The classification of the sulfosalts is based partly on the chemical-structural scheme developed by Nowacki (*Schweiz. Min. Petr. Mitt.* 1969, 109–156) and Edenharter (*Schweiz. Min. Petr. Mitt.* 1976, 195–217), and partly on the concept of SnS and PbS archetypes and the incorporation of these structural elements into homologous series by Makovicky (*N. Jb. Min., Abh.* 1989, 269–297, etc.).

* Berzelius (1819).

2.A: Metal/Metalloid Alloys

Subdivisions 2.AA – 2.AC.

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| <p>2.AA. Alloys of metalloids with Cu, Ag, Au</p> <p style="padding-left: 20px;">2.AA.05. Algodonite-domeykite group</p> <p style="padding-left: 20px;">2.AA.10. Koutekite</p> <p style="padding-left: 20px;">2.AA.15. Novákite</p> <p style="padding-left: 20px;">2.AA.20. Horsfordite-cuprostibite group</p> <p style="padding-left: 20px;">2.AA.25. Kutinaite</p> <p style="padding-left: 20px;">2.AA.30. Allargentum-dyscrasite group</p> <p style="padding-left: 20px;">2.AA.35. Maldonite</p> <p>2.AB. Ni-metalloid alloys</p> <p style="padding-left: 20px;">2.AB.05. Dienerite</p> <p style="padding-left: 20px;">2.AB.10. Orcelite</p> <p style="padding-left: 20px;">2.AB.15. Maucherite</p> | <p>2.AC. Alloys of metalloids with PGE</p> <p style="padding-left: 20px;">2.AC.05. Atheneite-vincentite group</p> <p style="padding-left: 20px;">2.AC.10. Stillwaterite group</p> <p style="padding-left: 20px;">2.AC.15. Isomertieite</p> <p style="padding-left: 20px;">2.AC.20. Stibiopalladinite-palladoarsenide group</p> <p style="padding-left: 20px;">2.AC.25. Polarite group</p> <p style="padding-left: 20px;">2.AC.30. Rhodarsenide group</p> <p style="padding-left: 20px;">2.AC.35. Polkanovite</p> |
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2.AA. Alloys of Metalloids with Cu, Ag, Au

2.AA.05. **Algodonite-Domeykite Group.** **Algodonite** has hexagonal close-packing of Cu atoms, stabilized by disordered partial replacement of Cu by As; Zn-type derivative. In **domeykite**, the arsenic forms a body-centred cubic lattice with Cu in the interstices; Cu is coordinated by three As and six Cu; As is coordinated by nine Cu. In **β -domeykite**, the arsenic is in hexagonal close packing with Cu in tetrahedral interstices.

Algodonite (Field, 1857 ¹)	α -Cu _{1.7} As _{0.3}	Hexagonal, P6 ₃ /mmc (194) a = 2.59, c = 4.23 Å	Z = 1
Domeykite (Haidinger, 1845 ²)	α -Cu ₃ As	Cubic, I $\bar{4}$ 3d (220) a = 9.62 Å	Z = 16
β-Domeykite (Padera, 1952 ³)	β -Cu ₃ As to Cu _{2.6} As (>225 °C)	Trigonal, P $\bar{3}$ c1 (165) a = 7.14, c = 7.32 Å	Z = 6

¹ Naud & Priest: Mater. Res. Bull. 1972, 782 (str)

² Iglesia & Nowacki: ZK 1977/145, 334 (str)

³ MA 1953/12, 201 (Abst.); Makovicky *et al.*: Ah 1979/135, 221; Mansmann: ZK 1965/122, 399 (str)

2.AA.10. **Koutekite.** The structure is a derivative of the fluorite structure.

Koutekite (Johan, 1958 ¹)	Cu ₅ As ₂	Orthorhombic, Ibam (72) a = 5.98, b = 11.58, c = 5.49 Å	Z = 4
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¹ Nature 1958/181, 1553; AM 1958, 794 (Abst.); Makovicky *et al.*: *idem.*; Liebisch & Shubert: J. Less-Comm. Metals 1971, 231 (str); Abulgazina *et al.*: AM 1993, 677 (Abst.)

2.AA.15. **Novákite.** Structure not known.

Novákite (Johan & Hak, 1961 ¹)	Cu ₂₀ AgAs ₁₀	Monoclinic, C2/m (12), C2 (5) or Cm (8) a = 16.27, b = 11.71, c = 10.01 Å β = 112.7°	Z = 4
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¹ AM 1961, 885; Johan: TMPM 1985/34, 167

2.AA.20. **Horsfordite-Cuprostibite Group.** In **cuprostibite**, there is close-packing of Cu and Sb atoms, with each Cu atom coordinated by 8Cu and 4Sb, and each Sb coordinated by 9Cu.

Horsfordite (Laist & Norton, 1888 ¹)	Cu ₅ Sb	No data known.	
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Cuprostibite (Sörensen <i>et al.</i> , 1969 ²)	Cu_2Sb	Tetragonal, $P4/nmm$ (129) $a = 3.99$, $c = 6.09 \text{ \AA}$	$Z = 2$
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¹ Possibly an unstable high-temperature phase.

² ZVMO 1969, 716; AM 1970, 1810 (Abst.); Elander *et al.*: Ark. Kem. Min. Geol. 1935/12B, 1 (str)

2.AA.25. **Kutinaite**. Structure not known.

Kutinaite (Hak <i>et al.</i> , 1970 ¹)	$\text{Cu}_7\text{Ag}_3\text{As}_{3.5}$	Cubic $a = 11.76 \text{ \AA}$	$Z = 8$
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¹ AM 1970, 1083; Johan: TPM 1985/34, 167

2.AA.30. **Allargentum-Dyscrasite Group**. Approximate hexagonal close-packing of Ag and Sb; Zn-type derivatives. In **allargentum**, the Ag and Sb are disordered. In **dyscrasite**, the Ag and Sb atoms are ordered into alternating pseudo-hexagonal close-packed layers SbAg and AgAg.

Allargentum (Ramdohr, 1950 ¹)	$\text{Ag}_{1-x}\text{Sb}_x$ ($x = 0.09\text{--}0.16$)	Hexagonal, $P6_3/mmc$ (194) $a = 2.95$, $c = 4.77 \text{ \AA}$	$Z = 2$
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Dyscrasite (Beudant, 1832 ²)	Ag_3Sb	Orthorhombic, $Pm2m$ (25) $a = 3.01$, $b = 5.21$, $c = 4.83 \text{ \AA}$	$Z = 1$
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¹ Petruk *et al.*: CM 1970, 163; Weibke & Efinger: Z. Elektrochem. 1940, 53 (str)

² Peacock: Univ. Toronto, Geol. Ser. 1940/44, 31 (str, setting); Scott: CM 1976, 139 (str)

2.AA.35. **Maldonite**. $\text{Bi}[\text{Bi}_4]$ tetrahedra form a framework like that of C in diamond, with Au in the interstices; a Laves phase.

Maldonite (Ulrich, 1869 ¹)	Au_2Bi	Cubic, $Fd\bar{3}m$ (227) $a = 7.98 \text{ \AA}$	$Z = 8$
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¹ Prokuronov *et al.*: ZVMO 1976, 453; Jurriaanse: ZK 1935/90, 322 (str); SB3, 612

2.AB. Ni-Metalloid Alloys

2.AB.05. **Dienerite** (doubtful validity)

Dienerite (Doelter, 1926 ¹)	Ni_3As	Cubic
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¹ No crystallographic data available; original specimen lost.

2.AB.10. **Orcelite.** Structure not known.

Orcelite (Caillère <i>et al.</i> , 1959 ¹)	$\text{Ni}_{5-x}\text{As}_2$ ($x = 0.23$)	Hexagonal, $P6_3cm$ (185) $a = 6.70$, $c = 12.39\text{\AA}$	$Z = 6$
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¹ CR 1959/249, 1771; AM 1960, 753 (Abst.); Oen *et al.*: BM 1980, 198

2.AB.15. **Maucherite.** NiAs_5 square pyramids (as in millerite) and NiAs_6 octahedra share edges and faces to form a framework with short Ni-Ni distances.

Maucherite (Grünling, 1913 ¹)	$\text{Ni}_{11}\text{As}_8$	Tetragonal, $P4_12_12$ (92) or $P4_32_12$ (96) $a = 6.87$, $c = 21.82\text{\AA}$	$Z = 4$
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¹ Fleet: AM 1973, 203 (str)

2.AC. Alloys of Metalloids with Platinum-Group Elements

2.AC.05. **Atheneite-Vincentite Group.** $M:(\text{As,Sb,Bi}) \geq 3.0:1$. Structures not known.

Atheneite (Clark <i>et al.</i> , 1974 ¹)	$(\text{Pd,Hg})_3\text{As}$	Hexagonal, $P6/mmm$ (191) $a = 6.80$, $c = 3.48\text{\AA}$	$Z = 2$
Vincentite (Stumpfl & Tarkian, 1974 ²)	$(\text{Pd,Pt})_3$ (As,Sb,Te)	Monoclinic, $P2/m$ (10) $a = 11.18$, $b = 10.31$, $c = 4.31\text{\AA}$ $\beta = 98.1^\circ$	$Z = 8$

¹ MM 1974, 528; AM 1974, 1330 (Abst.)

² MM 1974, 525 (tetr.); AM 1974, 1332 (Abst.); Bayliss, 1991: PDF 44–1432

2.AC.10. **Stillwaterite Group.** $M:(\text{As,Sb,Sn}) < 3.0:1, > 2.5:1$. Structures not known; **Mertieite-I** is dimorphous with isomertieite.

Stillwaterite (Cabri <i>et al.</i> , 1975 ¹)	Pd_8As_3	Trigonal, $P\bar{3}$ (147) or $P3$ (143) $a = 7.40$, $c = 10.31\text{\AA}$	$Z = 3$
Palarstanide (Begizov <i>et al.</i> , 1981 ²)	$\sim \text{Pd}_8(\text{Sn,As})_3$	Trigonal $a = 7.50$, $c = 10.34\text{\AA}$	$Z = 3$
Mertieite-I (Desborough <i>et al.</i> , 1973 ³)	$\text{Pd}_{11}\text{As}_2\text{Sb}_2$	Pseudo-hexagonal $a = 15.04$, $c = 22.41\text{\AA}$	$Z = 18$
Mertieite-II (Desborough <i>et al.</i> , 1973 ⁴)	$\text{Pd}_8(\text{Sb,As})_3$	Hexagonal $a = 7.55$, $c = 43.18\text{\AA}$	$Z = 12$

Arsenopalladinite $\text{Pd}_8(\text{As}_{2.5}\text{Sb}_{0.5})$ Triclinic, $P1$ (1) or $P\bar{1}$ (2)
 (Claringbull & Hey, 1956⁵) $a = 7.43$, $b = 13.95$, $c = 7.35 \text{ \AA}$
 $\alpha = 92.9$, $\beta = 119.5$, $\gamma = 87.8^\circ$ $Z = 6$

¹ CM 1975, 321; AM 1977, 1060 (Abst.)

² ZVMO 1981, 487; AM 1982, 858 (Abst.); Evstigneeva & Genkin: AM 1989, 1219 (Abst., new data)

³ AM 1973, 1; PDF 25–698

⁴ AM 1973, 1; Cabri *et al.*: CM 1975, 321

⁵ MA 1957/13, 237 (Abst.); Clark *et al.*: MM 1974, 528; Cabri *et al.*: CIM Spec. Vol. 1981/23, 83

2.AC.15. **Isomertieite**. Structure not known.

Isomertieite $\text{Pd}_{11}\text{As}_2\text{Sb}_2$ Cubic, $Fd\bar{3}m$ (227)
 (Clark *et al.*, 1974¹) $a = 12.28 \text{ \AA}$ $Z = 8$

¹ MM 1974, 528; AM 1983, 851 (Abst.)

2.AC.20. **Stibiopalladinite-Palladoarsenide Group**. $M:(\text{As},\text{Sb},\text{Bi}) \leq 2.5:1$, $> 1:1$.
 Structures not known. **Majakite** may be an isotype of barringerite $(\text{Fe},\text{Ni})_2\text{P}$.

Stibiopalladinite Pd_5Sb_2 Hexagonal, $P6_3cm$ (185)
 (Adam, 1927¹) $a = 7.61$, $c = 14.21 \text{ \AA}$ $Z = 6$

Palladoarsenide Pd_2As Monoclinic, $P2/m$ (10)
 (Begizov *et al.*, 1974²) $a = 9.25$, $b = 8.47$, $c = 10.44 \text{ \AA}$
 $\beta = 94^\circ$ $Z = 18$

**Palladobis-
mutharsenide** $\text{Pd}_2\text{As}_{0.8}\text{Bi}_{0.2}$ Orthorhombic, $Pm\bar{c}n$ (62) or $P2_1cn$ (33)
 (Cabri *et al.*, 1976³) $a = 7.50$, $b = 18.88$, $c = 6.84 \text{ \AA}$ $Z = 20$

Majakite PdNiAs Hexagonal, $P\bar{6}2m$ (189) (?)
 (Genkin *et al.*, 1976⁴) $a = 6.07$, $c = 7.20 \text{ \AA}$ $Z = 6$

Genkinite $(\text{Pt},\text{Pd})_4\text{Sb}_3$ Tetragonal
 (Cabri *et al.*, 1977⁵) $a = 7.74$, $c = 24.16 \text{ \AA}$ $Z = 8$

¹ El Boragy *et al.*: J. Less-Comm. Metals 1970/22, 445

² ZVMO 1974, 104; AM 1975, 162 (Abst.)

³ CM 1976, 410

⁴ ZVMO 1976, 698; AM 1977, 1260 (Abst.)

⁵ CM 1977, 389; AM 1979, 654 (Abst.)

2.AC.25. **Polarite Group.** M:(As,Sb,Bi) ≤ 1:1. Structures not known.

Borishanskiite (Razin <i>et al.</i> , 1975 ¹)	Pd(As,Pb) ₂	Orthorhombic, Ccm2 ₁ (36) ? a = 7.18, b = 8.62, c = 10.66Å	Z = 16
Polarite (Genkin <i>et al.</i> , 1969 ²)	Pd(Bi,Pb)	Orthorhombic, Ccm2 ₁ (36) a = 7.19, b = 8.69, c = 10.68Å	Z = 16

¹ ZVMO 1975, 57; AM 1976, 502 (Abst.)² ZVMO 1969, 708; AM 1970, 1810 (Abst.)2.AC.30. **Rhodarsenide Group.** Structure not known.

Rhodarsenide (Tarkian <i>et al.</i> , 1997 ¹)	(Rh,Pd) ₂ As	Orthorhombic a = 5.87, b = 3.89, c = 7.30Å	Z = 4
Palladodymite (Britvin <i>et al.</i> , 1999 ²)	(Pd,Rh) ₂ As	Orthorhombic, Pnma (62) a = 5.91, b = 3.90, c = 7.34Å	Z = 4

¹ EJM 1997, 1321; AM 1998, 909 (Abst.)² ZVMO 1999 (2), 39; AM 2000, 876 (Abst.)2.AC.35. **Polkanovite.** A framework of edge-sharing RhAs₅ square pyramids and RhAs₄ tetrahedra.

Polkanovite (Britvin <i>et al.</i> , 1998 ¹)	Rh ₁₂ As ₇	Trigonal, P6 ₃ /m (176) a = 9.31, c = 3.64Å	Z = 1
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¹ ZVMO 1998 (2), 60; AM 1999, 195 (Abst.); Lambert-Andron *et al.*: J. Less-Comm. Metals 1985/108, 353 (str)**Simple Sulfides, Selenides, etc. (2.B to 2.F)****2.B: Metal Sulfides, M:S > 1:1 (mainly 2:1)**

Subdivisions 2.BA. – 2.BE.

2.BA. With Cu, Ag, Au	2.BA.30. Stromeyerite-jalpaite group
2.BA.05. Chalcocite-digenite group	2.BA.35. Eucairite-naumannite group
2.BA.10. Bornite	2.BA.40. Henryite-hessite group
2.BA.15. Berzelianite-umangite group	2.BA.45. Argyrodite group
2.BA.20. Weissite-rickardite group	2.BA.50. Petzite group
2.BA.25. Acanthite group	2.BA.55. Bezsmeritovite group

- 2.BB. With Ni
 2.BB.05. Heazlewoodite group
 2.BB.10. Hauchecornite group
 2.BB.15. Pentlandite group
- 2.BC. With Rh, Pd, Pt, etc.
 2.BC.05. Prassoite group
 2.BC.10. Oosterboschite
 2.BC.15. Chrisstanleyite
 2.BC.20. Telargpalite-sopcheite group
 2.BC.25. Luberoite
- 2.BD. With Hg, Tl
 2.BD.05. Balkanite-imitérite group
 2.BD.10. Carlinite
 2.BD.15. Thalcusite-sabatierite group
- 2.BE. With Pb(Bi)
 2.BE.05. Betekhtinite-furotobeite group
 2.BE.10. Shandite group

2.BA. With Cu, Ag and/or Au

2.BA.05. **Chalcocite-Digenite Group.** Both **chalcocite** modifications have hexagonal close-packing of S atoms; in **high chalcocite**, the Cu atoms are disordered and statistically distributed between triangular, tetrahedral and 2-coordinated sites; in **low chalcocite**, the Cu atoms are ordered, with most in triangular coordination. The **djurleite** structure is similar. In **tetragonal chalcocite**, the Cu atoms have triangular coordination. Both **digenite** modifications have cubic close-packing of S atoms with Cu in octahedral, tetrahedral and triangular sites.

Chalcocite (Beudant, 1832 ¹)	α -Cu ₂ S (<103 °C)	Monoclinic, P2 ₁ /c (14) (pseudo-hexagonal) a = 15.25, b = 11.88, c = 13.49 Å β = 116.3°	Z = 48
Chalcocite (high) (Buerger, 1941 ²)	β -Cu ₂ S (>103 °C)	Hexagonal, P6 ₃ /mmc (194) a = 3.95, c = 6.75 Å	Z = 2
Chalcocite (tetragonal) (Clark & Sillitoe, 1971 ³)	Cu _{1.96} S	Tetragonal, P4 ₁ 2 ₁ 2 (92) a = 4.00, c = 11.29 Å	Z = 4
Djurleite (Roseboom, 1962 ⁴)	Cu _{1.96} S	Monoclinic, P2 ₁ /n (14) a = 26.90, b = 15.75, c = 13.47 Å β ~ 90.1°	Z = 128
Roxbyite (Mumme <i>et al.</i> , 1988 ⁵)	Cu _{2-x} S (x = 0.18–0.26)	Monoclinic, C2/m (12), C2 (5) or Cm (8) a = 53.79, b = 30.90, c = 13.36 Å β = 90.0°	Z = 4x128
Digenite (Breithaupt, 1844 ⁶)	Cu _{1.8} S	Trigonal, R $\bar{3}m$ (166), pseudo-cubic a = 3.92, c = 48.00 Å	Z = 15
Digenite (high) (Morimoto & Kullerud, 1963 ⁷)	β -Cu _{1.8} S	Cubic, Fm $\bar{3}m$ (225) a = 5.57 Å	Z = 4
Anilite (Morimoto <i>et al.</i> , 1969 ⁸)	Cu _{1.75} S	Orthorhombic, Pnma (62) a = 7.89, b = 7.84, c = 11.01 Å	Z = 16
Geerite (Goble & Robinson, 1980 ⁹)	Cu _{1.6} S	Trigonal (pseudo-cubic, a' = 5.41) a = 3.86, c = 46.1 Å	Z = 15

Structures related to covellite

Spionkopite (Goble, 1980 ¹⁰)	Cu _{1.39} S	Trigonal, P $\bar{3}$ m1 (164), P321 (150), P3m1 (156) a = 22.96, c = 41.43Å	Z = 504
Yarrowite (Goble, 1980 ¹¹)	Cu _{1.12} S	Trigonal, P $\bar{3}$ m1 (164), P321 (150), P3m1 (156) a = 3.80, c = 67.26Å	Z = 24

¹ Evans: ZK 1979/150, 299 (str)² Buerger & Wuensch: Science 1963/141, 276 (str)³ Mh 1971, 418; Skinner: Ec. Geol. 1970, 724; János: AC 1964, 311 (str)⁴ AM 1962, 1181; Evans: ZK 1979/150, 299 (str)⁵ MM 1988, 323; AM 1989, 946 (Abst.)⁶ Donnay *et al.*: AM 1958, 228 (str)⁷ AM 1963, 110 (str)⁸ AM 1969, 1256; Koto & Morimoto: AC 1970.B, 915 (str)⁹ CM 1980, 519; Goble: CM 1985, 61 (may be rhombohedral)¹⁰ CM 1980, 511; AM 1981, 1279 (Abst.); Goble: CM 1985, 61 (str)¹¹ *idem*

2.BA.10. **Bornite**. Face-centred cubic close-packing of S atoms, with an ordered distribution of Cu and Fe atoms in the tetrahedral interstices. The polyhedral configuration can be visualized as two types of cubes alternating along the three crystallographic axes: antiferrotype-type, with eight MS₄ tetrahedra per cube, and sphalerite-type, with four MS₄ tetrahedra and MS₃ triangles per cube. In **bornite (high)**, the Cu and Fe atoms are disordered in the tetrahedral interstices.

Bornite (Haidinger, 1845 ¹)	Cu ₅ FeS ₄ (<228 °C)	Orthorhombic, Pbca (61) a = 10.95, b = 21.86, c = 10.95Å	Z = 16
Bornite (high) (Haidinger, 1845 ²)	β-Cu ₅ FeS ₄ (>228 °C)	Cubic, Fm $\bar{3}$ m (225) a = 5.50Å	Z = 1

¹ Koto & Morimoto: AC 1975.B, 2268 (str)² Morimoto & Kullerud: AM 1961, 1270 (str); Morimoto: AC 1964, 351 (str)

2.BA.15. **Berzelianite-Umangite Group**. **Berzelianite** has face-centred cubic close-packing of Se atoms, with Cu in tetragonal and trigonal sites. In **umangite**, Cu-Cu bonding creates sheets // (001).

Berzelianite (Beudant, 1832 ¹)	Cu ₂ Se	Cubic, Fm $\bar{3}$ m (225) a = 5.69Å	Z = 4
Bellidoite (De Montreuil, 1975 ²)	β-Cu ₂ Se	Tetragonal, P4 ₂ /n (86) a = 11.52, c = 11.74Å	Z = 32
Umangite (Klockmann, 1891 ³)	Cu ₃ Se ₂	Tetragonal, P $\bar{4}$ ₂ m (113) a = 6.40, c = 4.28Å	Z = 2

Athabascaite (Harris <i>et al.</i> , 1970 ⁴)	Cu_5Se_4	Orthorhombic $a = 8.23, b = 11.98, c = 6.44 \text{ \AA}$	$Z = 4$
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¹ Yamamoto & Kashida: J. Sol. St. Chem. 1991, 202 (str)

² Ec. Geol. 1975, 384; AM 1975, 736 (Abst.)

³ Heyding & Murray: Can. J. Chem. 1976, 841 (str)

⁴ CM 1970, 207; AM 1971, 632 (Abst.)

2.BA.20. **Weissite-Rickardite Group.** In **rickardite**, edge-sharing CuTe_4 tetrahedra form sheets // (001) linked by CuTe_{4+1} pyramids.

Weissite (Crawford, 1927 ¹)	Cu_{2-x}Te ($x \leq 0.33$)	Hexagonal, $P6/mmm$ (191) $a = 12.54, c = 21.71 \text{ \AA}$	$Z = 45$
Rickardite (Ford, 1903 ²)	$\text{Cu}_{3-x}\text{Te}_2$ ($x \leq 0.26$)	Orthorhombic, $Cmcm$ (63) $a = 3.97, b = 4.00, c = 6.11 \text{ \AA}$	$Z = 2$

¹ Thompson: AM 1949, 342; Patzak: Z. Metallk. 1956, 418; Bayliss: AM 1990, 751 (space group $P3m1, a = 8.34, c = 21.69 \text{ \AA}$)

² Schutte & DeBoer: AC 1993.B, 398 (str)

With Ag

2.BA.25. **Acanthite Group.** A body-centred array of tetrahedrally coordinated S atoms with AgS_3 triangles in planes nearly // (010); the sheets are linked by $\text{Ag}^{[2]}$. The Ag atoms are ordered in **acanthite**, but disordered in **argentite**.

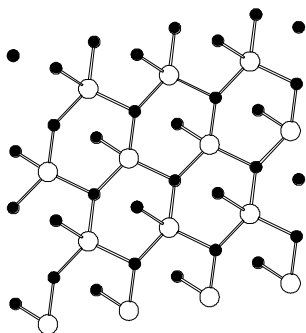


Fig 2.BA.25. A slice // (010) through the acanthite structure. White circles = S; black dots = Ag.

Acanthite (Kenngott, 1855 ¹)	Ag_2S ($<173 \text{ }^\circ\text{C}$)	Monoclinic, $P2_1/n$ (14) $a = 4.23, b = 6.93, c = 7.86 \text{ \AA}$ $\beta = 99.6^\circ$	$Z = 4$
Argentite (Haidinger, 1845 ²)	$\beta\text{-Ag}_2\text{S}$ ($>173 \text{ }^\circ\text{C}$)	Cubic, $Im\bar{3}m$ (229) $a = 4.89 \text{ \AA}$	$Z = 2$

¹ Frueh: ZK 1958/110, 136 (str)

² Sadanaga & Sueno: Min. Jour. 1967, 124

2.BA.30. **Stromeyerite-Jalpaite Group.** **Stromeyerite** has hexagonal close-packed S atoms with $\text{Cu}^{[3]}$ triangles in (001) layers that are bridged by $\text{Ag}^{[2]}$. In **jalpaite**, AgS_6 octahedra share edges to form an open 3-dimensional framework; $\text{Cu}^{[2]}$ atoms are accommodated in the cavities.

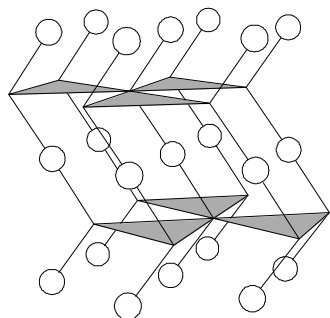


Fig 2.BA.30a. The structure of stromeyerite projected approximately on (100); CuS_3 triangles linked by $\text{Ag}^{[2]}$ spheres.

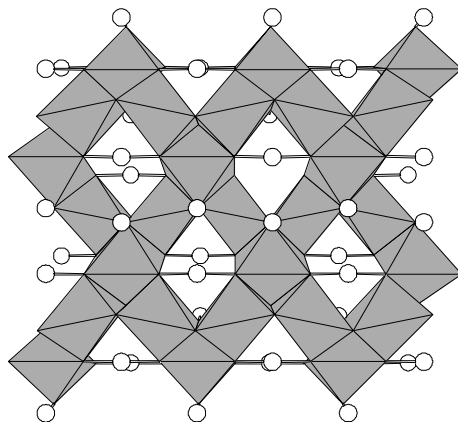


Fig 2.BA.30b. A slice // (100) through the jalpaite structure; AgS_6 octahedra; $\text{Cu}^{[2]}$ spheres with bonds to nearest S atoms.

Stromeyerite (Beudant, 1832 ¹)	CuAgS (<94 °C)	Orthorhombic, $\text{Cmc}2_1$ (36) $a = 4.06$, $b = 6.62$, $c = 7.97 \text{ \AA}$	$Z = 4$
Mckinstryite (Skinner <i>et al.</i> , 1966 ²)	$\text{Cu}_{0.8}\text{Ag}_{1.2}\text{S}$	Orthorhombic, Pnam (62) or $\text{Pna}2_1$ (33) $a = 14.04$, $b = 15.68$, $c = 7.80 \text{ \AA}$	$Z = 32$
Jalpaite (Breithaupt, 1850 ³)	CuAg_3S_2	Tetragonal, $\text{I}4_1/\text{amd}$ (141) $a = 8.69$, $c = 11.76 \text{ \AA}$	$Z = 8$

¹ Baker *et al.*: AC 1991.B, 891 (str)

² Ec. Geol. 1966, 1383; AM 1967, 1253 (Abst.)

³ Grybeck & Finney: AM 1968, 1530; Baker *et al.*: Austral. J. Chem. 1992, 1441 (str)

2.BA.35. **Eucairite-Naumannite Group.** In **eucairite**, sheets of corner-sharing flattened CuSe_4 tetrahedra // (001) alternate with sheets containing Ag atoms coordinated to 4 Ag and 1 Se. The **naumannite** structure is closely related to that of acanthite, with Se in body-centred cubic close-packing and Ag in the interstices; the Ag atoms are in tetrahedral and approximately triangular coordination; Se is surrounded by 9 Ag atoms.

Eucairite (Berzelius, 1818 ¹)	CuAgSe (<190 °C)	Orthorhombic, Pmmn (59)(pseudo-tetragonal) $a = 4.10$, $b = 20.35$, $c = 6.31 \text{ \AA}$	$Z = 10$
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Aguilarite (Genth, 1891 ²)	Ag ₄ SeS	Orthorhombic a = 4.33, b = 7.09, c = 7.76 Å	Z = 2
Naumannite (Haidinger, 1845 ³)	α-Ag ₂ Se (<128 °C)	Orthorhombic, P2 ₁ 2 ₁ 2 ₁ (19) a = 4.33, b = 7.06, c = 7.76 Å	Z = 4

¹ Frueh *et al.*: ZK 1957/108, 389 (str)² Petruk *et al.*: CM 1974, 365³ Wiegers: AM 1971, 1882 (str)

2.BA.40. **Henryite-Hessite Group.** In **hessite**, edge-sharing AgTe₄ tetrahedra form sheets // (100) that are linked by corner-sharing tetrahedra. In **stützite**, highly mobile Ag atoms in a Te framework form Frank-Kasper polyhedra; Te is in tetrahedral sites and also forms Te₂ dumbbells.

Henryite (Criddle <i>et al.</i> , 1983 ¹)	Cu ₄ Ag ₃ Te ₄	Cubic, F-cell a = 12.20 Å	Z = 8
Cervelleite (Criddle <i>et al.</i> , 1989 ²)	Ag ₄ TeS	Cubic, P-cell a = 14.03 Å	Z = 24
Hessite (Fröbel, 1843 ³)	α-Ag ₂ Te (<155 °C)	Monoclinic, P2 ₁ /c (14) a = 8.16, b = 4.47, c = 8.98 Å β = 124.2°	Z = 4
Kurilite (Kovalenker <i>et al.</i> , 1989 ⁴)	Ag ₂ (Te,Se)	Cubic, Pm $\bar{3}$ m (221) or P $\bar{4}3$ n (218) a = 11.27 Å	Z = 24
Stützite (Schrauf, 1878 ⁵)	Ag _{5-x} Te ₃ (x = 0.24–0.36)	Hexagonal, P $\bar{6}2$ m (189) a = 13.46, c = 16.92 Å	Z = 14
Benleonardite (Stanley <i>et al.</i> , 1986 ⁶)	Ag ₈ Te ₂ (Sb,As)S ₃	Tetragonal a = 6.60, c = 12.73 Å	Z = 2
Tsnigriite (Sandomirskaya <i>et al.</i> , 1992 ⁷)	Ag ₉ Te ₃ SbS ₃	Monoclinic, P2/m (10) or Pm (6) a = 8.89, b = 8.29, c = 19.50 Å β = 97.0°	Z = 4

¹ BM 1983, 511; AM 1985, 216 (Abst.)² EJM 1989, 371; AM 1990, 1431 (Abst.)³ Van der Lee & de Boer: AC 1993.C, 1444 (str)⁴ Min. Zhur. 1989(6), 3; AM 1992, 208 (Abst.)⁵ Imamov & Pinsker: Sov. Phys. Cryst. 1966, 182 (str); Peters *et al.*: Z. anorg. allg. Chem. 1996/622, 1823 (str)⁶ MM 1986, 681; AM 1988, 439 (Abst.)⁷ ZVMO 1992(5), 95; AM 1994, 389 (Abst.)

2.BA.45. **Argyrodite Group.** In **argyrodite**, GeS₄ tetrahedra, AgS₄ tetrahedra, AgS₃ triangles, AgS₂ linear units and additional S atoms are connected into a framework.

Argyrodite (Weisbach, 1886 ¹)	Ag ₈ GeS ₆	Orthorhombic, Pna2 ₁ (33) a = 15.15, b = 7.48, c = 10.59Å	Z = 4
Canfieldite (Penfield, 1894 ²)	Ag ₈ SnS ₆ (<172 °C)	Orthorhombic, Pna2 ₁ (33) a = 15.30, b = 7.55, c = 10.70Å	Z = 4

¹ Eulenberg: Mh. Chem. 1977/108, 901 (str)

² Wang: Mh 1978, 269

With Au

2.BA.50. **Petzite Group.** **Petzite** has a garnet-like structure consisting of edge-sharing Ag[Te₄Ag₂Au₂] and Au[Ag₆Te₂] polyhedra.

Uytendogaardite (Barton <i>et al.</i> , 1978 ¹)	Ag ₃ AuS ₂	Tetragonal, P4 ₁ 22 (91) or P4 ₁ (76) a = 9.68, c = 9.81Å	Z = 8
Fischesserite (Johan <i>et al.</i> , 1971 ²)	Ag ₃ AuSe ₂	Cubic, I4 ₁ 32 (214) a = 9.97Å	Z = 8
Petzite (Haidinger, 1845 ³)	Ag ₃ AuTe ₂	Cubic, I4 ₁ 32 (214) a = 10.39Å	Z = 8

Related Minerals

Petrovskaité (Nesterenko <i>et al.</i> , 1984 ⁴)	AgAu(S,Se)	Monoclinic, P2/m (10), Pm (6) or P2 (3) a = 4.94, b = 6.67, c = 7.22Å β = 95.7°	Z = 4
Penzhinite (Bochek <i>et al.</i> , 1984 ⁵)	Ag ₄ Au(S,Se) ₄	Hexagonal, P6 ₃ 22 (182) a = 13.78, c = 16.98Å	Z = 18

¹ CM 1978, 651; AM 1980, 209 (Abst.)

² BM 1971, 381; AM 1972, 1554 (Abst.)

³ Frueh: AM 1959, 693 (str); Chamid *et al.*: Sov. Phys. Cryst. 1978, 267 (str)

⁴ ZVMO 1984, 602; AM 1985, 1331 (Abst.)

⁵ ZVMO 1984, 356; AM 1985, 875 (Abst.)

2.BA.55. **Bezmertnovite Group.** Structures not known.

Bezmertnovite (Spiridonov & Chvileva, 1979 ¹)	Cu(Au,Ag) ₄ (Te,Pb)	Orthorhombic (pseudo-cubic) a = 24.21 b = 4.02, c = 16.24Å	Z = 16
Bogdanovite (Spiridonov <i>et al.</i> , 1979 ²)	(Cu,Fe) ₃ Au ₅ (Te,Pb) ₂	Pseudocubic, probably orthorhombic a' = 4.09Å	Z' = ½
Bilibinskite (Spiridonov <i>et al.</i> , 1978 ³)	Cu ₂ Au ₃ PbTe ₂	Cubic (gold superstructure) a' = 4.10Å	Z' = ½

¹ Dok. Akad. Nauk SSSR 1979/249, 185; AM 1981, 87 (Abst.)

² AM 1979, 1329 (Abst.)

³ ZVMO 1978, 310; AM 1979, 652 (Abst.)

2.BB. With Ni

2.BB.05. **Heazlewoodite Group.** In **heazlewoodite**, Ni occupies tetrahedral sites in a body-centred cubic lattice of S atoms; the NiS₄ tetrahedra share edges, resulting in short Ni-Ni distances.

Heazlewoodite (Petterd, 1896 ¹)	Ni ₃ S ₂	Trigonal, R32 (155) a = 5.74, c = 7.14Å	Z = 3
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Oregonite (Ramdohr & Schmitt, 1959 ²)	Ni ₂ FeAs ₂	Trigonal a = 6.08, c = 7.13Å	Z = 3
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Related Mineral

Vozhminite (Rudashevskiy <i>et al.</i> , 1982 ³)	(Ni,Co) ₄ (As,Sb)S ₂	Hexagonal a = 17.46, c = 7.20Å	Z = 18
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¹ Parise: AC 1980.B, 1179 (str)

² Mh 1959, 239; AM 1960, 1130 (Abst.)

³ ZVMO 1982, 480; AM 1983, 645 (Abst.)

2.BB.10. **Hauchecornite Group.** In **hauchecornite**, NiS₄ square planes share corners and edges to form a 3-dimensional framework strengthened by bonding to Bi^[6] and Sb^[8] atoms.

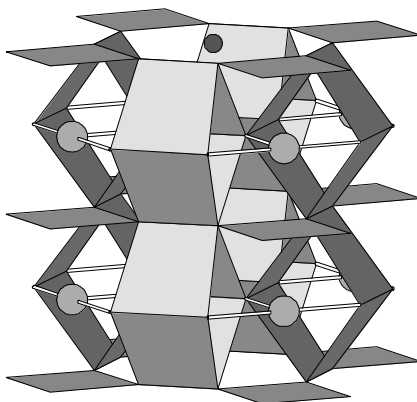


Fig 2.BB.10. The structure of hauchecornite, projected with c-axis vertical. Square planes = NiS₄; light larger spheres with bonds = Bi; smaller dark sphere near top of diagram = Sb.

Arsenohauchecornite (Gait & Harris ¹)	$(As_{0.5}Bi_{0.5})(NiBi)Ni_8S_8$	Tetragonal, I4/mmm (139) a = 10.27, c = 10.81 Å	Z = 4
Hauchecornite (Scheibe, 1892 ²)	$Sb(NiBi)Ni_8S_8$	Tetragonal, P4/mmm (123) a = 7.30, c = 5.40 Å	Z = 1
Bismutohauchecornite (Just, 1980 ³)	$Bi_2Ni_9S_8$	Tetragonal, P4/mmm (123) a = 7.37, c = 5.88 Å	Z = 1
Tellurohauchecornite (Gait & Harris, 1980 ⁴)	$TeBiNi_9S_8$	Tetragonal, P4/mmm (123) a = 14.64, c = 10.87 Å	Z = 8
Tučekite (Just & Feather, 1978 ⁵)	$Sb_2Ni_9S_8$	Tetragonal, P4/mmm (123) a = 7.17, c = 5.40 Å	Z = 1

¹ MM 1980, 877; Grice & Ferguson: CM 1989, 137 (str)

² Kocman & Nuffield: CM 1974, 269 (str)

³ MM 1980, 873; AM 1981, 436 (Abst.)

⁴ MM 1980, 877; AM 1981, 436 (Abst.)

⁵ MM 1978, 278; AM 1979, 465 (Abst.)

2.BB.15. **Pentlandite Group.** The structures are based on cubic close-packed S atoms with metal atoms in the interstices. In **pentlandite**, eight edge-sharing $(Ni,Fe)S_4$ tetrahedra form clusters that are combined into a framework by Fe^{6l} octahedra; each cluster shares corners with 12 neighbouring clusters. The structures of **cobalt pentlandite** and **argentopentlandite** are similar, except that in argentopentlandite, the octahedral site is occupied by Ag. In **godlevskite**, edge-sharing $Ni[S_4]$ tetrahedra form 3-membered chains // [100], [001] and [010]; the [001] and [010] chains form a 5-membered cross; edge-sharing $Ni[S_5]$ square pyramids form 4-fold clusters and chains // [101].

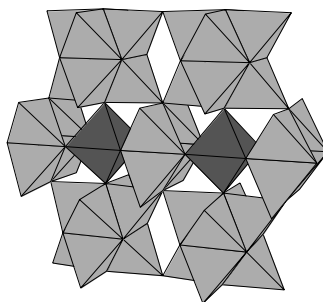


Fig 2.BB.15. A fragment of the pentlandite structure showing clusters of $(Ni,Fe)S_4$ tetrahedra (light) and FeS_6 octahedra (dark).

Pentlandite (Dufrenoy, 1856 ¹)	Fe(Ni,Fe) ₈ S ₈	Cubic, Fm $\bar{3}$ m (225) a = 10.04Å	Z = 4
Cobalt pentlandite (Kouvo <i>et al.</i> , 1959 ²)	(Co,Ni,Fe) ₉ S ₈	Cubic, Fm $\bar{3}$ m (225) a = 9.93Å	Z = 4
Argentopentlandite (Rudashevskiy <i>et al.</i> , 1977 ³)	Ag(Ni,Fe) ₈ S ₈	Cubic, Fm $\bar{3}$ m (225) a = 10.52Å	Z = 4
Shadlunite (Evstigneeva <i>et al.</i> , 1973 ⁴)	(Pb,Cd)(Fe,Cu) ₈ S ₈	Cubic, Fm $\bar{3}$ m (225) a = 10.91Å	Z = 4
Manganese-shadlunite (Evstigneeva <i>et al.</i> , 1973 ⁵)	(Mn,Pb)(Cu,Fe) ₈ S ₈	Cubic, Fm $\bar{3}$ m (225) a = 10.73Å	Z = 4
Geffroyite (Johan <i>et al.</i> , 1982 ⁶)	(Cu,Fe,Ag) ₉ (Se,S) ₈	Cubic, Fm $\bar{3}$ m (225) a = 10.89Å	Z = 4

Related Minerals

Godlevskite (Kulagov <i>et al.</i> , 1969 ⁷)	(Ni _{8.7} Fe _{0.3})S ₈	Orthorhombic, C222 (21) a = 9.34, b = 11.22, c = 9.43Å	Z = 4
Kharaelakhite (Genkin <i>et al.</i> , 1985 ⁸)	(Pt,Cu,Pb,Fe,Ni) ₉ S ₈	Orthorhombic, Pmmm (47), Pmm2 (25) or P222 (16) a = 9.71, b = 8.33, c = 14.50Å	Z = 4

¹ Rajmani & Prewitt: CM 1973, 169 (str)

² AM 1959, 897; Rajmani & Prewitt: CM 1975, 75 (str)

³ ZVMO 1977, 688; MA 79–762 (Abst.); Hall & Stewart: CM 1973, 169 (str)

⁴ ZVMO 1973, 63; AM 1973, 1114 (Abst.)

⁵ *idem*

⁶ Tmpm 1982/29, 151; AM 1982, 107 (Abst.)

⁷ AM 1970, 317 (Abst.); Fleet: AC 1987.C, 2255 (str)

⁸ Min. Zhur. 1985(1), 78; AM 1989, 1215 (Abst.)

2.BC. With Rh, Pd, Pt, etc.

2.BC.05. **Prassoite Group.** In **prassoite**, RhS₆ octahedra and RhS₄ square planes share corners to form a framework. **Palladseite** is isostructural.

Prassoite (Kingston, 1977 ¹)	Rh ₁₇ S ₁₅	Cubic, Pm $\bar{3}$ m (221) a = 9.91Å	Z = 2
Palladseite (Davis <i>et al.</i> , 1977 ²)	Pd ₁₇ Se ₁₅	Cubic, Pm $\bar{3}$ m (221) a = 10.64Å	Z = 2

¹ Cabri: CIMM Spec. Vol. 1981, 132; Geller: AC 1962, 1198 (str)

² MM 1977, 123; AM 1977, 1059 (Abst.); Geller: AC 1962, 713 (str)

2.BC.10. **Oosterboschite**. Structure not known.

Oosterboschite (Pd,Cu)₇Se₅ Orthorhombic
(Johan *et al.*, 1970¹) a = 10.42, b = 10.60, c = 14.43 Å Z = 8

¹ BM 1970, 476; AM 1972, 1553 (Abst.)

2.BC.15. **Chrisstanleyite**. Structure not known.

Chrisstanleyite Pd₃Ag₂Se₄ Monoclinic, P2₁/m (11) or P2₁ (4)
(Paar *et al.*, 1998¹) a = 6.35, b = 10.39, c = 5.68 Å
β = 114.9° Z = 2

¹ MM 1998, 257; AM 1998, 134 (Abst.)

2.BC.20. **Telargpalite-Sopcheite Group** (with Te). In **keithconnite**, the Pd and Te atoms form chains // [0001]. **Vasilite** has a complicated framework structure, with 12 Pd in (nearly) linear 2S coordination, and 4 Pd in trigonal-pyramidal 3S coordination with Pd at the apex.

Vasilite Pd₁₆S₇ (~ 2.5Cu, 0.4Te) Cubic, I $\bar{4}$ 3m (217)
(Atanasov, 1990¹) a = 8.92 Å Z = 2

Oulankite (Pd,Pt)₅(Cu,Fe)₄SnTe₂S₂ Tetragonal
(Barkov *et al.*, 1996²) a = 9.04, c = 4.94 Å Z = 2

Telargpalite (Pd,Ag)₃Te (?) Cubic
(Kovalenker *et al.*, 1974³) a = 12.60 Å Z = 16

Keithconnite Pd₂₀Te₇ Trigonal, R $\bar{3}$ (148)
(Cabri *et al.*, 1979⁴) a = 11.46, c = 11.30 Å Z = 3

Telluropalladinite Pd_{2.25}Te Monoclinic, P2₁/c (14)
(Cabri *et al.*, 1979⁵) a = 7.45, b = 13.95, c = 8.82 Å
β = 91.9° Z = 16

Temagamite Pd₃HgTe₃ Orthorhombic (pseudo-hexagonal)
(Cabri *et al.*, 1973⁶) a = 11.57, b = 12.16, c = 6.76 Å Z = 6

Borovskite Pd₃SbTe₄ Cubic
(Yalovoi *et al.*, 1973⁷) a = 5.79 Å Z = 1

Sopcheite Pd₃Ag₄Te₄ Orthorhombic
(Orsoev *et al.*, 1982⁸) a = 9.65, b = 7.91, c = 11.04 Å Z = 4

¹ CM 1990, 687; AM 1991, 1435 (Abst.); Matković *et al.*: J. Less-Comm. Metals 1976/50, 165 (str, synth. Pd₁₆S₇)

² EJM 1996, 311; AM 1996, 1514 (Abst.)

³ ZVMO 1974, 595; AM 1975, 489 (Abst.); Begizov & Batashev: Dok. Akad. Nauk SSSR 1978/243, 1265

⁴ CM 1979, 589; AM 1981, 1275 (Abst.); Wopersnow & Schubert: J. Less-Comm. Metals 1977/51, 35 (str)

⁵ CM 1979, 589; AM 1981, 1275 (Abst.); Matković & Schubert: J. Less-Comm. Metals 1978/58, P39 (str)

⁶ CM 1973, 193; AM 1975, 947 (Abst.)

⁷ ZVMO 1973, 427; AM 1974, 873 (Abst.)

⁸ ZVMO 1982, 114; AM 1983, 472 (Abst.)

2.BC.25. **Luberoite**. PtSe_6 distorted octahedra and PtSe_5 pyramids share edges and faces to form a dense framework.

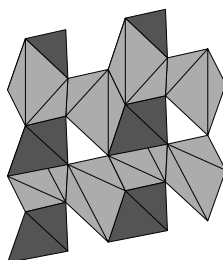


Fig 2.BC.25. The structure of luberoite projected on (010), c-axis vertical. Light polyhedra = PtSe_6 ; dark polyhedra = PtSe_5 .

Luberoite	Pt_5Se_4	Monoclinic, $P2_1/c$ (14)	
(Jedwab <i>et al.</i> , 1992 ¹)		$a = 6.58$, $b = 4.60$, $c = 11.10\text{\AA}$	
		$\beta = 101.6^\circ$	$Z = 2$

¹ EJM 1992, 683; AM 1993, 450 (Abst.); Matković & Schubert: J. Less-Comm. Metals 1977/55, 185 (str)

2.BD. With Hg, Tl

2.BD.05. **Balkanite-Imitérite Group** (with Hg). In **imitérite**, AgS_3 triangles are linked into a framework by linearly coordinated $\text{Hg}^{[2]}$ atoms.

Gortdrumite	$(\text{Cu,Fe})_{19}\text{Hg}_6\text{S}_{16}$	Orthorhombic	
(Steed, 1983 ¹)		$a = 14.96$, $b = 7.90$, $c = 24.10\text{\AA}$	$Z = 4$
Balkanite	$\text{Cu}_9\text{Ag}_5\text{HgS}_8$	Orthorhombic, $Pmmm$ (47), $P222$ (16)	
(Atanassov & Kirov, 1973 ²)		or $Pmm2$ (25)	
		$a = 10.62$, $b = 9.42$, $c = 3.92\text{\AA}$	$Z = 1$
Danielsite	$(\text{Cu,Ag})_{14}\text{HgS}_8$	Orthorhombic	
(Nickel, 1987 ³)		$a = 9.64$, $b = 9.18$, $c = 18.16\text{\AA}$	$Z = 4$
Imitérite	Ag_2HgS_2	Monoclinic, $P2_1/c$ (14)	
(Guillou <i>et al.</i> , 1985 ⁴)		$a = 4.04$, $b = 8.01$, $c = 6.58\text{\AA}$	
		$\beta = 107.1^\circ$	$Z = 2$

Petrovicite (Johan <i>et al.</i> , 1976 ⁵)	$\text{Cu}_3\text{PbHgBiSe}_5$	Orthorhombic, Pnam (62) or Pna2 ₁ (33) a = 16.18, b = 14.68, c = 4.33 Å	Z = 4
Donharrisite (Paar <i>et al.</i> , 1989 ⁶)	$\text{Ni}_8\text{Hg}_3\text{S}_9$	Monoclinic, C2/m (12), Cm (8) or C2 (5) a = 11.66, b = 6.91, c = 10.92 Å $\beta = 97.4^\circ$	Z = 2

¹ MM 1983, 35; AM 1984, 407 (Abst.)

² AM 1973, 11

³ AM 1987, 481; Kato & Nickel: AM 1988, 187

⁴ BM 1985, 457 (str); AM 1986, 1277 (Abst.)

⁵ BM 1976, 310; AM 1977, 594 (Abst.)

⁶ CM 1989, 257; AM 1990, 706 (Abst.)

2.BD.10. **Carlinite.** Structure not known.

Carlinite (Radtke & Dickson, 1975 ¹)	Tl_2S	Trigonal, R3 (146) a = 12.12, c = 18.18 Å	Z = 27
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¹ AM 1975, 559

2.BD.15. **Thalcosite-Sabatierite Group.** The **chalcothallite** structure consists of mackinawite-like layers // (001) of edge-sharing (Cu,Fe)S₄ tetrahedra alternating with layers containing Cu(S₂Sb₂) tetrahedra and CuSb₄ square planes, with short metal-metal distances // (001); the layers are linked by Tl^[8] atoms.

Thalcosite (Kovalenker <i>et al.</i> , 1976 ¹)	$\text{Cu}_3\text{FeTl}_2\text{S}_4$	Tetragonal, I4/mmm (139), etc. a = 3.88, c = 13.25 Å	Z = 1
Murunskite (Dobrovolskaya <i>et al.</i> , 1981 ²)	$\text{K}_2\text{Cu}_3\text{FeS}_4$	Tetragonal, I4/mmm (139), etc. a = 3.88, c = 13.10 Å	Z = 1
Bukovite (Johan & Kvaček, 1971 ³)	$\text{Cu}_3\text{FeTl}_2\text{Se}_4$	Tetragonal, I4/mmm (139) a = 3.98, c = 13.70 Å	Z = 1
Rohaite (Karup-Møller, 1978 ⁴)	$\text{Cu}_5\text{TlSbS}_2$	Orthorhombic, Pmmm (47), etc. (pseudo-tetragonal) a = 3.80, b = 3.80, c = 20.99 Å	Z = 2
Chalcothallite (Semenov <i>et al.</i> , 1967 ⁵)	$(\text{Cu,Fe})_6\text{Tl}_2\text{SbS}_4$	Tetragonal, I4/mmm (139) a = 3.83, c = 34.28 Å	Z = 2
Sabatierite (Johan <i>et al.</i> , 1978 ⁶)	Cu_6TlSe_4	Orthorhombic a = 3.99, b = 5.62, c = 9.78 Å	Z = 1
Crookesite (Nordenskiöld, 1866 ⁷)	Cu_7TlSe_4	Tetragonal, I4̄ (82) a = 10.45, c = 3.93 Å	Z = 2

¹ ZVMO 1976, 202; AM 1977, 396 (Abst.); Makovicky *et al.*: Ah 1980/138, 122

² ZVMO 1981, 468; AM 1982, 624 (Abst.)

³ BM 1971, 529; AM 1972, 1910 (Abst.); Makovicky *et al.*: Ah 1980/138, 122

⁴ AM 1980, 208 (Abst.); Makovicky *et al.*: Ah 1980/138, 122

⁵ AM 1968, 1775 (Abst.); Makovicky *et al.*: Ah 1980/138, 122 (str)

⁶ BM 1978, 557; AM 1979, 1331 (Abst.); Berger: ZK 1987/181, 241

⁷ Johan: CR 1987/304, 1121; Berger: ZK 1987/181, 241

2.BE. With Pb (Bi)

2.BE.05. **Betekhtinite-Furotobeite Group.** In **betekhtinite**, face-sharing (?) PbS_{3+3} trigonal prisms form columns // [001]; corner-sharing CuS_3 triangles form 2-periodic double chains // [001]; both are linked by CuS_4 tetrahedra.

Betekhtinite $(\text{Cu,Fe})_{21}\text{Pb}_2\text{S}_{15}$ Orthorhombic, Immm (71)
(Schüller & Wohlmann, 1955¹) $a = 14.67, b = 22.80, c = 3.86\text{Å}$ Z = 2

Furotobeite $(\text{Cu,Ag})_6\text{PbS}_4$ Monoclinic, C2 (5), Cm (8) or C2/m (12)
(Srigaki *et al.*, 1981²) $a = 20.02, b = 3.96, c = 9.70\text{Å}$
 $\beta = 101.6^\circ$ Z = 4

Arcubisite $\text{CuAg}_6(\text{Bi,Pb})\text{S}_4$
(Karup-Møller, 1976³)

Larosite $(\text{Cu,Ag})_{21}(\text{Pb,Bi})_2\text{S}_{13}$ Orthorhombic (?)
(Petruk, 1972⁴) $a = 22.15, b = 24.03, c = 11.67\text{Å}$ Z = 10

¹ Geologie 1955, 535; AM 1956, 371 (Abst.); Dornberger-Schiff & Höhne: AC 1959, 646 (str)

² BM 1981, 737; AM 1982, 1075 (Abst.)

³ Lithos 1976, 253; AM 1978, 424 (Abst.)

⁴ CM 1972, 886; AM 1974, 382 (Abst.)

2.BE.10. **Shandite Group.** In **parkerite**, face-sharing $\text{Ni}(\text{Bi}_4\text{S}_2)$ octahedra form sheets // (010). **Shandite** has $\text{Ni}(\text{Pb}_4\text{S}_2)$ octahedra.

Shandite $\text{Ni}_3\text{Pb}_2\text{S}_2$ Trigonal, $R\bar{3}m$ (166)
(Ramdohr, 1950¹) $a = 5.59, c = 13.58\text{Å}$ Z = 3

Rhodplumsite $\text{Rh}_3\text{Pb}_2\text{S}_2$ Trigonal, $R\bar{3}m$ (166)
(Genkin *et al.*, 1983²) $a = 5.73, c = 14.00\text{Å}$ Z = 3

Parkerite $\text{Ni}_3\text{Bi}_2\text{S}_2$ Orthorhombic, Pmam (51)
(Scholtz, 1936³) $a = 5.55, b = 5.73, c = 4.05\text{Å}$ Z = 1

¹ Peacock & McAndrew: AM 1950, 425; Claus *et al.*: Mh 1978, 256 (str)

² Min. Zhur. 1983(2), 87; MA 1984, 3588 (Abst.)

³ Fleet: AM 1973, 435 (str); Brower *et al.*: AM 1974, 296 (monoclinic superstructure, Z = 8)

2.C: Metal Sulfides, M:S = 1:1 (and similar)

Subdivisions 2.CA. – 2.CE.

- | | |
|---------------------------------------|--------------------------------------|
| 2.CA. With Cu | 2.CB.65. Argentopyrite group |
| 2.CA.05. Covellite group | 2.CB.70. Sulfanite group |
| 2.CA.10. Nukundamite | 2.CB.75. Vulcanite-empressite group |
| 2.CB. With Zn, Fe, Cu, Ag, etc. | 2.CC. With Ni, Fe, Co, etc. |
| 2.CB.05. Sphalerite group | 2.CC.05. Nickeline group |
| 2.CB.10. Chalcopyrite group | 2.CC.10. Pyrrhotite group |
| 2.CB.15. Stannite-kesterite group | 2.CC.15. Westerveldite group |
| 2.CB.20. Luzonite-briartite group | 2.CC.20. Millerite group |
| 2.CB.25. Hemusite-morozeviczite group | 2.CC.25. Mackinawite |
| 2.CB.30. Vinciennite group | 2.CC.30. Braggite group |
| 2.CB.35. Germanite-mooihoekite group | 2.CD. With Sn, Pb, Hg, etc. |
| 2.CB.40. Lautite | 2.CD.05. Herzenbergite group |
| 2.CB.45. Wurtzite group | 2.CD.10. Galena group |
| 2.CB.50. Enargite group | 2.CD.15. Matildite group |
| 2.CB.55. Cubanite-mohite group | 2.CD.20. Aramayoite-diaphorite group |
| 2.CB.60. Raguinite-picotpaulite group | 2.CD.25. Cinnabar |

2.CA. With Cu

2.CA.05. **Covellite Group.** In **covellite**, double sheets of CuS_4 tetrahedra // (0001) connected by S-S bonds // [0001] alternate with sheets of Cu in triangular coordination. The **klockmannite** structure is similar.

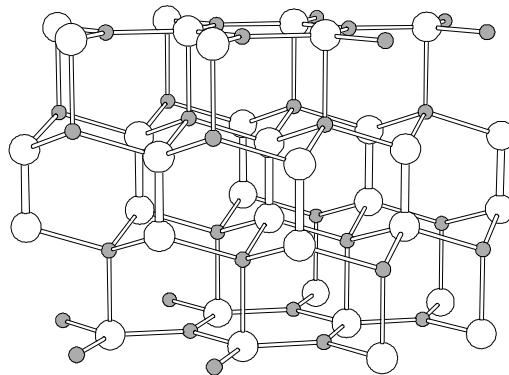


Fig 2.CA.05. Clinographic projection of the covellite structure. Large spheres = S; small dark spheres = Cu; the S-S bond is shown as a wider rod than the Cu-S bonds.

Covellite
(Beudant, 1832¹)

CuS

Hexagonal, $P6_3/mmc$ (194)
 $a = 3.79$, $c = 16.34 \text{ \AA}$

$Z = 6$

Klockmannite (Ramdohr, 1928 ²)	CuSe	Hexagonal, $P6_3/mmc$ (194) $a = 3.94$, $c = 17.25\text{\AA}$	$Z = 6$
Idaite (Frenzel, 1958 ³)	$\sim \text{Cu}_5\text{FeS}_6$	Hexagonal $a = 3.90$, $c = 16.95\text{\AA}$	$Z = 1$

¹ Berry: AM 1954, 504 (str); Evans & Konnert: AM 1976, 996 (str)

² Berry, idem; Effenberger & Pertlik: Mh 1981, 197 (str)

³ Mh 1958, 142; AM 1958, 1219 (Abst.); Yund: AM 1963, 672; Frenzel: AM 1963, 676

2.CA.10. **Nukundamite**. Thick layers of edge- and corner-sharing $(\text{Cu,Fe})\text{S}_4$ tetrahedra // (0001) alternate with S_2 sheets.

Nukundamite (Rice <i>et al.</i> , 1979 ¹)	$\sim \text{Cu}_{3.4}\text{Fe}_{0.6}\text{S}_4$	Trigonal, $P\bar{3}m1$ (164) $a = 3.78$, $c = 11.19\text{\AA}$	$Z = 1$
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¹ MM 1979, 193; AM 1980, 407 (Abst.); Sugaki *et al.*: AM 1981, 398 (str)

2.CB. With Zn, Fe, Cu, Ag, etc.

2.CB.05. **Sphalerite Group**. Corner-sharing $\text{M}^{[4]}$ and $\text{X}^{[4]}$ tetrahedra form cubic or pseudo-cubic frameworks; viewed along $[111]$, the layers are stacked A-B-C (*cf* wurtzite, 2.CB.45). Homeotype of diamond.

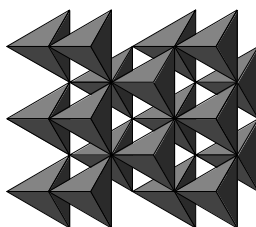


Fig 2.CB.05. Two layers of the sphalerite structure projected on (111), showing corner-sharing ZnS_4 tetrahedra.

Sphalerite (Glocker, 1847 ¹)	ZnS	Cubic, $F\bar{4}3m$ (216) $a = 5.41\text{\AA}$	$Z = 4$
Hawleyite (Traill & Boyle, 1955 ²)	CdS	Cubic, $F\bar{4}3m$ (216) $a = 5.82\text{\AA}$	$Z = 4$

Metacinnabar (Moore, 1870 ³)	HgS	Cubic, $F\bar{4}3m$ (216) $a = 5.87\text{\AA}$	$Z = 4$
Stilleite (Ramdohr, 1956 ⁴)	ZnSe	Cubic, $F\bar{4}3m$ (216) $a = 5.67\text{\AA}$	$Z = 4$
Tiemannite (Naumann, 1855 ⁵)	HgSe	Cubic, $F\bar{4}3m$ (216) $a = 6.08\text{\AA}$	$Z = 4$
Coloradoite (Genth, 1877 ⁶)	HgTe	Cubic, $F\bar{4}3m$ (216) $a = 6.45\text{\AA}$	$Z = 4$

Related Mineral

Isocubanite (Caye <i>et al.</i> , 1988 ⁷)	CuFe_2S_3 ($>200\text{--}210\text{ }^\circ\text{C}$)	Cubic, $Fm\bar{3}m$ (225) $a = 5.30\text{\AA}$	$Z = 4/3$
Sakuraiite (Kato, 1965 ⁸)	$(\text{Cu,Zn,Fe,In,Sn})\text{S}$	Cubic, $P432$ (207), $P\bar{4}3m$ (215) or $Pm\bar{3}m$ (221) $a = 5.46\text{\AA}$	$Z = 4$

¹ Ewald: Ann. Phys. 1914, 257 (str)² AM 1955, 555³ Aurivilius: Acta Chem. Scand. 1964, 1552 (str)⁴ AM 1957, 584 (Abst.); McIntyre *et al.*: AC 1980.A, 482 (str)⁵ Earley: AM 1950, 337; deJong: ZK 1926/63, 466 (str)⁶ Thompson: AM 1949, 342; deJong: *idem*⁷ MM 1988, 509; AM 1989, 503 (Abst.)⁸ AM 1968, 1421 (Abst.); Kissin & Owens: CM 1986, 679

2.CB.10. **Chalcopyrite Group.** Corner-sharing $M^{[4]}$ and $X^{[4]}$ tetrahedra form cubic or pseudo-cubic frameworks, as in sphalerite, but with cation ordering.

Chalcopyrite (Henckel, 1725 ¹)	CuFeS_2	Tetragonal, $I\bar{4}2d$ (122) $a = 5.29, c = 10.42\text{\AA}$	$Z = 4$
Gallite (Strunz <i>et al.</i> , 1958 ²)	CuGaS_2	Tetragonal, $I\bar{4}2d$ (122) $a = 5.35, c = 10.48\text{\AA}$	$Z = 4$
Roquésite (Picot & Pierrot, 1963 ³)	CuInS_2	Tetragonal, $I\bar{4}2d$ (122) $a = 5.51, c = 11.05\text{\AA}$	$Z = 4$
Eskebornite (Ramdohr, 1949 ⁴)	CuFeSe_2	Tetragonal, $P\bar{4}2c$ (112) $a = 5.53, c = 10.48\text{\AA}$	$Z = 4$
Lenaite (Amuzinsky <i>et al.</i> , 1995 ⁵)	AgFeS_2	Tetragonal, $P4_2mc$ (105) ? $a = 5.64, c = 10.34\text{\AA}$	$Z = 4$
Laforêtite (Meisser <i>et al.</i> , 1999 ⁶)	AgInS_2	Tetragonal, $I\bar{4}2d$ (122) $a = 5.88, c = 11.21\text{\AA}$	$Z = 4$

Related Mineral

Isochalcopyrite (Missack <i>et al.</i> , 1989 ⁷)	CuFeS ₂ (>~550 °C)	Cubic, I $\bar{4}3m$ (217) a = 10.61 Å	Z = 16
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¹ Hall & Stewart: AC 1973.B, 579 (str)

² Mh 1958, 241; AM 1959, 906 (Abst.)

³ BM 1963, 7; AM 1963, 1178 (Abst.)

⁴ Delgado *et al.*: Mater. Res. Bull. 1992, 367 (str)

⁵ ZVMO 1995 (5), 85; AM 1996, 1283 (Abst.)

⁶ EJM 1999, 891; AM 2000, 875 (Abst.)

⁷ Min. Deposita 1989, 82; AM 1990, 432 (Abst.); Hiller & Probsthain: ZK 1956/108, 108 (str)

2.CB.15. **Stannite-Kesterite Group.** Corner-sharing M^[4] and X^[4] tetrahedra, as in sphalerite, but with cation ordering.

Kuramite (Kovalenker <i>et al.</i> , 1979 ¹)	Cu ₃ SnS ₄	Tetragonal, I $\bar{4}2m$ (121) a = 5.45, c = 10.75 Å	Z = 2
Stannite (Beudant, 1832 ²)	Cu ₂ FeSnS ₄	Tetragonal, I $\bar{4}2m$ (121) a = 5.45, c = 10.76 Å	Z = 2
Černýite (Kissin <i>et al.</i> , 1978 ³)	Cu ₂ CdSnS ₄	Tetragonal, I $\bar{4}2m$ (121) a = 5.49, c = 10.85 Å	Z = 2
Velikite (Kaplunnik <i>et al.</i> , 1977 ⁴)	Cu ₂ HgSnS ₄	Tetragonal, I $\bar{4}$ (82) a = 5.57, c = 10.88 Å	Z = 2
Hocartite (Caye <i>et al.</i> , 1968 ⁵)	Ag ₂ FeSnS ₄	Tetragonal, I $\bar{4}2m$ (121) a = 5.74, c = 10.96 Å	Z = 2
Pirquitasite (Johan & Picot, 1982 ⁶)	Ag ₂ ZnSnS ₄	Tetragonal, I $\bar{4}2m$ (121) or I $\bar{4}$ (82) a = 5.79, c = 10.83 Å	Z = 2
Ferrokesterite (Kissin & Owens, 1989 ⁷)	Cu ₂ (Fe,Zn)SnS ₄	Tetragonal, I $\bar{4}$ (82) a = 5.43, c = 10.88 Å	Z = 2
Kesterite (Orlova, 1956 ⁸)	Cu ₂ (Zn,Fe)SnS ₄	Tetragonal, I $\bar{4}$ (82) a = 5.43, c = 10.87 Å	Z = 2

Related Mineral

Stannoidite (Kato, 1969 ⁹)	Cu ₈ (Fe,Zn) ₃ Sn ₂ S ₁₂	Orthorhombic, I222 (23) a = 5.41, b = 10.77, c = 16.12 Å	Z = 2
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¹ ZVMO 1979, 564; AM 1980, 1067 (Abst.)

² Brockway: ZK 1934/89, 434 (str); Hall *et al.*: CM 1978, 131 (str)

³ CM 1978, 139; AM 64 (1979), 653 (Abst.); Szymanski: CM 1978, 147 (str)

⁴ AM 1977, 1260 (Abst.); Gruzdev *et al.*: ZVMO 1997 (4), 71; Kabalov *et al.*: Cryst Repts. 1998, 16 (str)

⁵ BM 1968, 383; AM 1969, 573 (Abst.)

⁶ BM 1982, 229; AM 1983, 1249 (Abst.)

⁷ CM 1989, 673; AM 1990, 1432 (Abst.)

⁸ AM 1959, 1329 (Abst.); Hall *et al.*: CM 1978, 131 (str)

⁹ AM 1969, 1495 (Abst.); Kudoh & Takéuchi: ZK 1976/144, 145 (str)