

APPENDIX 5

CRYSTAL STRUCTURE DATA

A5.1 Introduction

In this volume we have been almost exclusively concerned with structure, and have paid little attention to the chemical compositions that have a given structure. There are several reasons for this approach. One is that some common structure types occur for a rather wide range of compounds; another is our belief that it is important to have some feeling for structures in general without being too weighed down with the baggage of theories that pretend to explain the occurrence of certain structure types for different compositions.

Nevertheless chemists, at least, should have some idea of the sorts of compounds that adopt the common structure types described in the text, so here we indicate some typical compositions for these. Of course many compounds are polymorphic, and in particular many transform under pressure. The general rule (there are some exceptions) is that increasing pressure causes a transformation to a structure with higher coordination numbers. Thus **sphalerite** compounds with 4-coordination generally transform to **NaCl** with 6-coordination; and **NaCl** compounds transform under pressure to **CsCl** with 8-coordination with, of course, an increase in density in each case.¹

Crystal data for some compounds, referred to in the text, are given in the final section.

A5.2 Elements

The metallic elements are nearly all either **cp** or **bcc** (Mn, and the early actinides are exceptions and they have generally rather complex structures). Periodic trends are fairly well developed; for example Ni, Pd, Pt and Cu, Ag, Au are all **ccp** and V, Nb, Ta and Cr, Mo, W are all **bcc**. However many metals are polymorphic; for example Fe is **bcc** at low temperature, **fcc** at higher temperature, and **hcp** under pressure. It should be noted that for most polymorphic metals the **bcc** and **cp** forms have very similar densities; in particular the **cp** forms are not always the densest modification.

C (at high pressure), Si, Ge and Sn (at low temperature) are **diamond** with 4-coordination. The remaining non-metallic elements have "covalent" structures with low coordination numbers (3 for P, As, Sb, Bi; 2 for S, Se, Te; 1 for N, O, F, Cl, Br, I).

¹But note that although the density is greater in the high-pressure phase, the A-X bond length is also greater; indeed the driving force for the transformation under pressure is to reduce the repulsion between atoms forced to be close together. Notice also in the examples we have given, that the structure of AX combined is **diamond** for **sphalerite**, **pc** (primitive cubic) for **NaCl** and **bcc** for **CsCl** so the overall array is transforming to a more efficient packing under pressure.

A5.3 Composition AB (AX)

There are hundreds of different AB (or AX) structure types. Some different structures we have mentioned briefly are those of AuCd, BaCu, FeSi, LiGe, LiP, MoB, NaP, NaPb, NbO, PbO and WC. These have either just one or at most a few representatives. Other structure types such as **ZnS**, **NaCl**, **NiAs**, **CuZn** (**CsCl**), **CuAu**, **CrB** and **FeB** have dozens or even hundreds of examples and we discuss them below.

A5.3.1 Sphalerite and wurtzite

The polymorphs of ZnS (see § 4.6.4 and § 6.1.5) lend their names to the two common structure types with atoms in tetrahedral coordination.

Wurtzite is based on **hcp** arrays of both cations and anions (each in tetrahedral holes of the other array) and occurs mainly for oxides and nitrides such as BeO, ZnO, AlN and GaN. Very many ternary, quaternary, etc. compounds such as β -NaFeO₂, LiSiON, etc. have derived structures.

Sphalerite is more common and occurs for many binary compounds particularly of elements of columns 13-17 of the periodic table with eight valence electrons (excluding d electrons) per atom pair. Examples are "III-V" compounds AX with A = Al, Ga, In and X = P, As, Sb. and "II-VI" compounds AX with A = Be, Zn, Cd and X = S, Se and Te. Some compounds have both structures (ZnS!) and then it is common also to find polytypes based on more complex close packings. SiC is notable in this regard (see § 7.11.4). Interestingly, SiC is the only known "IV-IV" compound—GeC is unstable (has not yet been made) and GeSi is a disordered composition in the Ge_xSi_{1-x} solid solution series. Just as for **wurtzites** there are many derived ternary, etc. structures; the most common type is **chalcopyrite** (CuFeS₂).

A5.3.2 NaCl and NiAs

NaCl and **NiAs** (see § 6.1.5) are the 6-coordinated analogs of **sphalerite** and **wurtzite** which are based on **ccp** and **hcp** respectively.

NaCl (also known as **rock salt**) is of course one of the more common structure types. It is often considered the prototypical "ionic" crystal structure and at normal pressures and temperatures it is that of all the alkali hydrides and halides other than CsCl, CsBr and CsI. Other **NaCl** compounds are the alkaline earth chalcogenides (MgO, SrS, BaTe etc.) other than MgTe and Be compounds (these have ZnS structures). Further examples are compounds AX with A = Sc, Y and lanthanide and X = N, P, As, Sb. Carbide examples include ThC and TiC. Hundreds of ternary compounds ABX₂ with the α -NaFeO₂ structure (Na and Fe order) are also known. These are mainly oxides and sulfides, but also include antistructure compounds with ordered anions such as Ba₂PBr and Ca₂NCl.

NiAs is also a very common structure type. For most of the compounds AX, A is a transition metal and X is S, Se, Te, V, As or Sb. Recall that the structure is hexagonal (see § 4.6.3) and it should be noted that many compounds have an axial ratio (*c/a*) rather

different from the ideal value for **hcp As**. Many of the compounds assigned to this type also have a wide range of stoichiometry and some authors include compositions in the range A_2X to AX_2 in the **NiAs** classification.

A5.3.3 **CuZn (CsCl) and CuAu**

CsCl ionic crystals are rare (**CsCl**, **CsBr** and **CsI** are the only alkali halides) at normal pressures, but many **NaCl** compounds transform to **CsCl** under pressure. The structure type, now often called **CuZn** is found for about a hundred intermetallic compounds such as **LiAg**, **BeCu**, **CaTi**, **YIn**, **MnNi**, etc. We saw in § 6.6.2 that the structure is in sense a special case of **AuCu** (which appears to be confined to intermetallic examples)

A5.3.4 **CrB and FeB**

CrB and **FeB** were described briefly in § 6.4.2. Together they comprise the structures of another large group (well over 100 binary examples) of intermetallic compounds. These orthorhombic structures have a number of free parameters (see data below) and the trigonal prisms (occupied by **B**) can vary significantly in shape from one compound to another and some authors recognize subgroups according to the shapes of the trigonal prisms (e.g. "short and fat" or "tall and skinny"). Some **CrB** compounds are **CaAg**, **BaSi**, **ScGa**, **LaNi**, **VB** and **NiB**; some **FeB** compounds are **BaAg**, **LaSi**, **ZrGe**, **LuNi**, **TiB** and **MnB**. Some have been found to transform to **CuZn** with increasing temperature and/or pressure. Although common as silicide and boride structures, no isostructural carbides are known.

A5.4 Composition AB_2 (AX_2 and A_2X)

Just as for compounds AB , the composition AB_2 give rise to hundreds of structure types. Some like **cuprite** (known only for **Cu₂O** and **Ag₂O**) and **quartz** (known only for forms of **SiO₂**, **GeO₂** and **BeF₂**) have only a few examples. Notice that silica (**SiO₂**) and water (**H₂O**) are perhaps the most intensively studied of all binary compounds and the structures of their crystalline forms have much in common (§ 7.3.13).

We give examples of compositions belonging to some of the larger families below. We should point out here that **BaMgSi (PbFCl)** is also called **Cu₂Sb**, and **SrMgSi** is called either **PbCl₂** or **Co₂Si**. Both these very large groups are really ternary structure types. Another large group of compounds is known as **Fe₂P** and in fact this is really a quaternary structure type $A_3B_3X_2Y$ although most reported compositions are ABX (i.e. $X = Y$).

A5.4.1 AB_2 compounds with $\{A\}B_6$ octahedra or trigonal prisms

An important structure type with $\{A\}B_6$ octahedra is **rutile** (**TiO₂**) which is found for oxides (e.g. of **Ti**, **Ge** and **Sn**) and also for fluorides of (e.g. of **Mg**, **Mn**, and **Zn**) and for **MgH₂**. It is closely related to **CaCl₂** (see Exercise 6.9.7) which is found only for a form

of **PtO₂** and for halides other than fluorides.

A second group of structures is that of **CdCl₂** and **CdI₂** with respectively **ccp** and **hcp** anions and all the octahedral sites in alternate layers filled with cations (§ 6.1.5). These are mostly halides (but not fluorides) but also include a few chalcogenides. Examples of **CdCl₂** compounds are **MgCl₂**, **NiCl₂** and **ZnBr₂**; some anti-structure compositions are **Cs₂O**, **Sr₂N**, **Y₂C** and **Ag₂F**. **CdI₂** compositions include **MgBr₂**, **MgI₂**, **TiS₂**, **PtSe₂** and **IrTe₂**; anti-structure compositions are **W₂C** and **Ti₂O**. If the H atoms are ignored, then hydroxides such as **Mg(OH)₂** (brucite) and **Ca(OH)₂** are **CdI₂**.

A related series of structures has trigonal prism layers. These are mostly compounds of the early transition elements (**Nb**, **Ta**, **Mo** and **W**) with **S**, **Se** and **Te** and most compounds are polymorphic—the simplest forms are $2H_a$, $2H_b$ and $3R$ described in § 6.4.1.

A5.4.2 Fluorite and antifluorite compounds

Fluorite (§ 6.1.5) compounds form a large group of mainly "ionic" crystals such as **CaF₂**, **SrCl₂**, **ThO₂**, **UO₂** but the family also includes compounds such as **CoSi₂** and **NiSi₂**. The group of **antifluorite** compounds is also large; typical "ionic" compositions are **Li₂O**, **Rb₂O**, **K₂S**, **Rb₂Se**. Some other isostructural phases are **Be₂C**, **Mg₂Si**, **Mg₂Sn**, **PtAl₂** and **PtIn₂**.

A5.4.3 Intermetallic structures: AlB_2 , $CuAl_2$ and $MgCu_2$

These three structure types are probably the largest groups of intermetallic AB_2 structures. There are hundreds of AlB_2 compounds with the characteristic **graphite**-like honeycomb layers of **B** (§ 5.3.5), typical compositions are **ThAg₂**, **ThAl₂**, **CrB₂**, **MgB₂**, **CaGa₂**, **Li₂Pt**, **ScSi₂**, **YHg₂** and **ThNi₂**. The largest group of compounds is that of borides and gallides, but as the examples given show, a rather wide range of intermetallic compositions occur.

Some **CuAl₂** compounds (§ 6.4.3) are **Th₂Ag**, **Th₂Al**, **Cr₂B**, **Zr₂Ni**, **Th₂Cu** and **Ta₂Si**. Notice that the first three examples contain the same elements, but in different proportion, as the first three AlB_2 compounds.

The **MgCu₂** (§ 6.6.3) group is the largest. *Pearson's Handbook* (Book List) has many hundreds of entries under this heading (not all binary compounds). Most compositions involve one or two transition elements, but there are also compounds such as **CaAl₂** and **CsBi₂** with the same structure; some other compositions are **PbAu₂**, **TaCo₂**, **DyPt₂**, **ZrW₂**, and **ZrZn₂**.

A5.5 Other binary structure types

It would take a sizable book to do justice to binary structures in general.¹ Important

¹The classic reference is *Kristallstrukturen zweikomponentiger Phasen* by K. Schubert [Springer-Verlag, Berlin (1964)].

structure types we have met include **corundum** ($\alpha\text{-Al}_2\text{O}_3$ —§ 6.1.6) which is mainly an oxide structure (of Al, Cr, Fe, etc.) with 6^3 layers of Al in octahedral sites of **hcp O**. A derivative structure is **ilmenite** (FeTiO_3) in which Al is replaced by alternate layers of Fe and Ti.

Th₃P₄ (§ 6.3.7) is the structure of a large group of compounds A_3X_4 with $\text{A} = \text{Th}, \text{U}, \text{Y}, \text{Ln}$ and $\text{X} = \text{P}, \text{As}, \text{Sb}, \text{S}, \text{Se}$ and Te . Antistructure compounds A_4X_3 are also common, typical compositions are La_4As_3 (contrast La_3S_4) and La_4Ge_3 . The structure type is notable for existing over a range of composition with (presumably) incomplete occupation of one set of atomic sites. Notable compounds of this sort are compositions in the range Ln_2S_3 – Ln_3S_4 .

A5.6 Ternary structure types

With over 10^2 elements, there are over $10^6/3!$ different combinations of three elements; in many of these cases compounds of several different stoichiometries are formed, and these in turn are often polymorphic. It may be seen therefore, that to give a *comprehensive* account of crystal chemistry would be a daunting task. Here we just mention typical compositions of some popular ternary structure types that have been met in the text.

A5.6.1 Oxide structures: spinel and perovskite

The prototypical **spinel** (§ 6.1.6) composition is MgAl_2O_4 ; other compositions AB_2X_4 (with A in one eighth of the tetrahedral sites and B in one half of the octahedral sites of **ccp X**) are Mn_2GeO_4 , Na_2WO_4 , ZnAl_2S_4 and CdCr_2Se_4 . “Inverse” spinels are compounds AB_2X_4 with B on tetrahedral and half the octahedral sites and A on the other half of the octahedral sites; examples are Li_2NiF_4 and ZnTi_2O_4 . Notice that there are now two kinds of B atom (with different coordination) and the structure is really quaternary and compositions such as LiZnNbO_4 are also included as **spinel**s (but in some, at least, of these last compositions, cation ordering occurs to produce a lower-symmetry structure). In magnetite, Fe_3O_4 , the tetrahedral sites are occupied by Fe^{3+} and the octahedral sites are a disordered combination of Fe^{2+} and Fe^{3+} .

The mineral perovskite is CaTiO_3 ; its structure is a small orthorhombic distortion of the cubic ABX_3 structure (described in § 6.6.2 and § 5.3.4) with 12-coordinated A and 6-coordinated B . Many perovskites have the orthorhombic structure, usually known as **GdFeO₃**. Examples are NaMgF_3 , KpF_3 , CaZrO_3 , SmAlO_3 and NaUO_3 . MgSiO_3 at high-pressure has the same structure and is thought to be the major component of the earth's lower mantle, and thus to be the major phase in the planet. Other cubic **perovskite** compositions are compounds AB_3X with A and B being metallic elements with **Cu₃Au** arrangement and $\text{X} = \text{B}, \text{C}$ or N in $\{\text{X}\}\text{B}_6$ octahedra. Examples are ScIr_3B , ZnCo_3C and SnMn_3N . An anti-perovskite composition is Na_3ClO (with $\{\text{Cl}\}\text{Na}_{12}$ and $\{\text{O}\}\text{Na}_6$).

A5.6.2 Intermetallic structures: BaMgSi (PbFCl), SrMgSi (PbCl₂) and ThCr₂Si₂

BaMgSi or **PbFCl** (§ 6.4.1) is also known as **Cu₂Sb** or **Fe₂As**, but the first two designations are preferred as they emphasize the ternary nature of the structure. There are two main groups of compounds. In the first group there are two “anions” as in **PbFCl**, **YOCl**, **BaHl** and **UAsSe** with the smaller (given first) in tetragonal layers of (e.g.) $\{\text{F}\}\text{Pb}_4$ tetrahedra. The second group are antistructure compounds with two metal atoms such as **BaMgSi**, **NaLiS** and **YFeSi**; **Cu₂Sb** and **Fe₂As** are in this category also.

SrMgSi (§ 5.3.7) is also known as **PbCl₂** or **Co₂Si**, but again we prefer the first name which makes the ternary nature of the structure clear. In compounds with two crystallographically-distinct “anions,” these are often the same element as in **PbCl₂**, **BaH₂**, **BaI₂**, **US₂** and **ThP₂**. Compounds like **SrMgSi**, **NbFeP** and **ReCoB** are formally the antistructure, but often the composition consists of two or three metallic elements as in **Lu₂Au** and **LuCoSn**.

ThCr₂Si₂ (§ 6.4.2) is also named after a chemically binary composition viz. **BaAl₄**, but again we use the ternary designation. This has the most known examples of all structure types and we just mention a few typical compositions here. In **ThCr₂Si₂** there are layers of $\{\text{Cr}\}\text{Si}_4$ tetrahedra. In the following formulas the tetrahedrally-coordinated atom is second: **BaAg₂Sn₂**, **UOs₂Si₂**, **CaCo₂As₂**, **LaPt₂Ge₂**, **YNi₂P₂**, **TiNi₂S₂**. Some compounds with two elements are **BaAl₄**, **CaGa₄**, **RbIn₄** and **ThZn₄**. In the anti-structure type, **Th₂TeN₂**, there are $\{\text{N}\}\text{Th}_4$ tetrahedral layers; another composition is **La₂TeO₂**.

A5.7 Crystallographic data

Crystallographic data for some of the simpler structures discussed in Chapters 5–7 are given here in condensed form (the *International Tables* or some other source should be consulted for equivalent positions). The listing is in alphabetical order of the chemical formula as normally written. See the Book List part D for sources of data.

AlB_2	$P6/mmm$, $a = 3.005$, $c = 3.245 \text{ \AA}$. Al 1 a , 0,0,0; B 2 d , $1/3, 2/3, 1/2$
Al_2O_3	$R\bar{3}c$, $a = 4.759$, $c = 12.991 \text{ \AA}$. Al 12 c , 0,0,0.3523; O 18 e , 0.3064,0,1/4
AuCd (HT)	$Pm\bar{3}m$, $a = 3.323 \text{ \AA}$. $V = 36.7 \text{ \AA}^3$. Au 0,0,0; Cd $1/2, 1/2, 1/2$ (CuZn structure)
AuCd (LT)	$Pmma$, $a = 4.765$, $b = 3.154$, $c = 4.864 \text{ \AA}$. $V = 2 \times 35.5 \text{ \AA}^3$ Au 2 f : $1/4, 0, 0.312$; Cd 2 e : $1/4, 1/2, 0.812$
AuZn_3	$Pm\bar{3}n$, $a = 7.903 \text{ \AA}$. Au(1) 2 a , 0,0,0; Au(2) 6 c , $1/4, 0, 1/2$; Zn 24 k , 0,0.165,0.300
B_2O_3	$P3_1$, $a = 4.336$, $c = 8.340 \text{ \AA}$, all atoms in 3 a B(1), 0.223,0.393,0.980; B(2), 0.828,0.603,0.092 O(1), 0.547,0.397,0.0; O(2), 0.149,0.600,0.078; O(3), 0.005,0.161,0.871
BaCu	$P6_3/mmc$, $a = 4.499$, $c = 16.25 \text{ \AA}$, $c/a = 3.61$ Ba 4 f , $1/3, 2/3, 0.1217$; Cu(1) 2 b , 0,0,1/4; Cu(2) 2 d , $1/3, 2/3, 3/4$

BaCu ₂ P ₄	<i>Fddd</i> , <i>a</i> = 5.345, <i>b</i> = 18.973, <i>c</i> = 10.244 Å. Ba 8 <i>a</i> , 1/8, 1/8, 1/8; Cu 16 <i>f</i> , 1/8, 0.5048, 1/8; P 32 <i>h</i> , 0.195, 0.1789, 0.817	FeSi	<i>P2₁3</i> , <i>a</i> = 4.517 Å. Fe 4 <i>a</i> , 0.136, 0.136, 0.136; Si 4 <i>a</i> , 0.844, 0.844, 0.844
β-BaFe ₂ S ₄	<i>I4/m</i> , <i>a</i> = 7.678, <i>c</i> = 5.292 Å Ba 2 <i>a</i> , 0, 0, 0; Fe 4 <i>d</i> , 0, 1/2, 1/4; S 8 <i>h</i> , 0.6196, 0.1986, 0	γ-Ge	<i>P4₃2₁2</i> , <i>a</i> = 5.93, <i>c</i> = 6.98 Å. [origin chosen for comparison with SiO ₂ —keatite] Ge(1) 4 <i>a</i> , 0.4088, 0.4088, 0; Ge(2) 8 <i>b</i> , 0.3270, 0.1216, 0.2486
BaMgSi	<i>P4/nmm</i> , <i>a</i> = 4.610, <i>c</i> = 7.870 Å Ba 2 <i>c</i> , 1/4, 1/4, 0.339; Mg 2 <i>a</i> , 3/4, 1/4, 0; Si 2 <i>c</i> , 1/4, 1/4, 0.794	Hg ₃ NbF ₆	<i>P3m1</i> , <i>a</i> = 5.02, <i>c</i> = 7.68 Å. Hg(1) 1 <i>b</i> , 0, 0, 1/2; Hg(2) 2 <i>d</i> , 1/3, 2/3, 0.500; Nb 1 <i>a</i> , 0, 0, 0; F 6 <i>h</i> , 0.309, 0, 0.143
BaNiO ₃	<i>P6₃/mmc</i> , <i>a</i> = 5.629, <i>c</i> = 4.811 Å Ba 2 <i>c</i> , 1/3, 2/3, 1/4; Ni 2 <i>a</i> , 0, 0, 0; O 6 <i>h</i> , 0.1462, 0.2924, 1/4	Hg ₂ 9SbF ₆	<i>I4₁/amd</i> , <i>a</i> = 7.655, <i>c</i> = 12.558 Å. Hg disordered in positions 16 <i>h</i> : 0, <i>y</i> , <i>z</i> with <i>z</i> = 0 Sb: 4 <i>b</i> , 0, 1/4, 3/8; F(1) 8 <i>e</i> , 0, 1/4, 0.230; F(2) 16 <i>g</i> , 0.672, 0.922, 1/4
BaTiO ₃ (200 °C)	<i>Pm3m</i> , <i>a</i> = 4.012. Ba 1 <i>a</i> , 0, 0, 0; Ti 1 <i>b</i> , 1/2, 1/2, 1/2; O 3 <i>c</i> , 0, 1/2, 1/2	KInTe ₂	<i>I4/mcm</i> , <i>a</i> = 8.52, <i>c</i> = 7.39 Å K 4 <i>a</i> , 0, 0, 1/4; In 4 <i>b</i> , 0, 1/2, 1/4; Te 8 <i>h</i> , 0.177, 0.678, 0
β-BeO	<i>P4₂/nmm</i> , <i>a</i> = 4.75, <i>c</i> = 2.74 Å. Be 4 <i>g</i> , 0.164, 0.836, 0; O 4 <i>f</i> , 0.190, 0.190, 0	K ₂ MgF ₄	<i>I4/mmm</i> , <i>a</i> = 3.995, <i>c</i> = 13.706 Å K 4 <i>e</i> , 0, 0, 0.350; Mg 2 <i>a</i> , 0, 0, 0; F(1) 4 <i>c</i> , 0, 1/2, 0; F(2) 4 <i>e</i> , 0, 0, 0.150
C graphite	<i>P6₃/mmc</i> , <i>a</i> = 2.461, <i>c</i> = 6.709 Å. C(1) 2 <i>b</i> , 0, 0, 1/4; C(2) 2 <i>c</i> , 1/3, 2/3, 1/4	K ₃ V ₅ O ₁₄	<i>P31m</i> , <i>a</i> = 8.680, <i>c</i> = 4.991 Å. K 3 <i>c</i> , 0.605, 0, 0.000; V(1) 3 <i>c</i> , 0.231, 0, 0.472 V(2) 2 <i>b</i> , 1/3, 2/3, 0.472; O(1) 2 <i>b</i> , 1/3, 2/3, 0.796; O(2) 3 <i>c</i> , 0.240, 0, 0.782 O(3) 3 <i>c</i> , 0.838, 0, 0.367; O(4) 6 <i>d</i> , 0.469, 0.177, 0.366
CaB ₆	<i>Pm3m</i> , <i>a</i> = 4.151 Å. Ca 1 <i>b</i> , 1/2, 1/2, 1/2; B 6 <i>e</i> , 0.302, 0, 0	LaB ₂ C ₂	<i>P4₂c</i> , <i>a</i> = 3.822, <i>c</i> = 7.924 Å La 2 <i>e</i> , 0, 0, 0; B 4 <i>h</i> , 1/2, 0.226, 1/4; C 4 <i>i</i> , 0.173, 1/2, 1/4
CdCl ₂	<i>R3m</i> , <i>a</i> = 3.846, <i>c</i> = 17.493 Å. Cd 3 <i>a</i> , 0, 0, 0; Cl 6 <i>c</i> , 0, 0, 0.2519	La ₂ O ₃	<i>P3m1</i> , <i>a</i> = 3.938, <i>c</i> = 6.136 Å. La 2 <i>d</i> , 1/3, 2/3, 0.2467 O(1) 1 <i>a</i> , 0, 0, 0; O(2) 2 <i>d</i> , 1/3, 2/3, 0.6470
CdI ₂	<i>P3m1</i> , <i>a</i> = 4.224, <i>c</i> = 6.859 Å. Cd 1 <i>a</i> , 0, 0, 0; I 2 <i>d</i> , 1/3, 2/3, 0.2492	LiP	<i>P2₁/c</i> , <i>a</i> = 5.582, <i>b</i> = 4.940, <i>c</i> = 10.255 Å, β = 118.15°. All atoms in 4 <i>e</i> Li(1): 0.2151, 0.3876, 0.3299; Li(2): 0.2257, 0.6597, 0.0293 P(1): 0.3165, 0.8952, 0.2920; P(2): 0.3050, 0.1565, 0.1125
Co ₉ S ₈	<i>Fm3m</i> , <i>a</i> = 9.927 Å. Co(1) 4 <i>b</i> , 1/2, 1/2, 1/2; Co(2) 32 <i>f</i> , 0.1266, 0.1266, 0.1266 S(1) 8 <i>c</i> , 1/4, 1/4, 1/4; S(2) 24 <i>e</i> , 0.2624, 0, 0	LiY ₂ Si ₂	<i>P4/mbm</i> , <i>a</i> = 7.105, <i>c</i> = 4.144 Å. Li 2 <i>a</i> , 0, 0, 0; Y 4 <i>h</i> , 0.181, 0.681, 1/2; Si 4 <i>g</i> , 0.383, 0.883, 0
CrB	<i>Cmcm</i> , <i>a</i> = 2.978, <i>b</i> = 7.870, <i>c</i> = 2.935 Å Cr 4 <i>c</i> , 0, 0.1453, 1/4; B 4 <i>c</i> , 0, 0.4360, 1/4	Mn ₂ Hg ₅	<i>P4/mbm</i> , <i>a</i> = 9.758, <i>c</i> = 2.998 Å Mn 4 <i>h</i> , 0.180, 0.680, 1/2; Hg(1) 2 <i>d</i> , 0, 1/2, 0; Hg(2) 8 <i>i</i> , 0.063, 0.204, 0
CrB ₄	<i>Immm</i> , <i>a</i> = 4.744, <i>b</i> = 5.477, <i>c</i> = 2.866 Å. Cr 2 <i>a</i> , 0, 0, 0; B 8 <i>n</i> , 0.175, 0.346, 0	α-MoB	<i>I4₁/amd</i> , <i>a</i> = 3.105, <i>c</i> = 16.97 Å. Mo 8 <i>e</i> , 0, 1/4, 0.071; B 8 <i>e</i> , 0, 1/4, 0.227
CuAl ₂	<i>I4/mcm</i> , <i>a</i> = 6.067, <i>c</i> = 4.877 Å. Cu 4 <i>a</i> , 0, 0, 1/4; Al 8 <i>h</i> , 0.1581, 0.6851, 0	MoS ₂ (2H _b)	<i>P6₃/mmc</i> , <i>a</i> = 3.161, <i>c</i> = 12.295 Å. Mo 2 <i>d</i> , 1/3, 2/3, 3/4; S 4 <i>f</i> , 1/3, 2/3, 0.1275
CuFeS ₂	<i>I4₂d</i> , <i>a</i> = 5.289, <i>c</i> = 10.423 Å Cu 4 <i>a</i> , 0, 0, 0; Fe 4 <i>b</i> , 0, 0, 1/2; S 8 <i>d</i> , 0.2574, 1/4, 1/8	MoS ₂ (3R)	<i>R3m</i> , <i>a</i> = 3.166, <i>c</i> = 18.41 Å Mo 3 <i>c</i> , 0, 0, 0; S(1) 3 <i>c</i> , 0, 0, 0.2477; S(2) 3 <i>c</i> , 0, 0, 0.4190
CuFe ₂ S ₃	<i>Pnma</i> , <i>a</i> = 6.231, <i>b</i> = 11.117, <i>c</i> = 6.467 Å Cu 4 <i>c</i> , 0.123, 1/4, 0.417; Fe 8 <i>d</i> , 0.137, 0.0870, 0.915 S(1) 4 <i>c</i> , 0.258, 1/4, 0.087; S(2) 8 <i>d</i> , 0.267, 0.0846, 0.588	NaP	<i>P2₁2₁2₁</i> , <i>a</i> = 6.038, <i>b</i> = 5.643, <i>c</i> = 10.142 Å. All atoms in 4 <i>a</i> Na(1): 0.4174, 0.9089, 0.0318; Na(2): 0.1338, 0.6367, 0.3313 P(1): 0.3086, 0.1404, 0.2838; P(2): 0.4287, 0.4020, 0.1341
Fe ₂ AlB ₂	<i>Cmmm</i> , <i>a</i> = 2.923, <i>b</i> = 11.034, <i>c</i> = 2.870 Å Al 2 <i>a</i> , 0, 0, 0; Fe 4 <i>j</i> , 0, 0.3540, 1/2; B 4 <i>i</i> , 0, 0.2071, 0	NaPb	<i>I4₁/acd</i> , <i>a</i> = 10.580, <i>c</i> = 17.466 Å. Na(1) 16 <i>e</i> , 0.375, 0, 1/4 Na(2) 16 <i>f</i> , 0.375, 0.625, 1/8; Pb 32 <i>g</i> , 0.0694, 0.3814, 0.4383
FeB	<i>Pnma</i> , <i>a</i> = 5.495, <i>b</i> = 2.946, <i>c</i> = 4.053 Å Fe 4 <i>c</i> , 0.180, 1/4, 0.125; B 4 <i>c</i> , 0.036, 1/4, 0.610		
Fe ₂ P	<i>P3m</i> , <i>a</i> = 5.868, <i>c</i> = 3.465 Å. Fe(1) 3 <i>f</i> , 0.2568, 0, 0; Fe(2) 3 <i>g</i> , 0.5946, 0, 1/2 P(1) 1 <i>b</i> , 0, 0, 1/2; P(2) 2 <i>c</i> , 1/3, 2/3, 0		
FeS ₂ (pyrite)	<i>Pa3</i> , <i>a</i> = 5.418 Å. Fe 4 <i>a</i> , 0, 0, 0; S 8 <i>c</i> , 0.384, 0.384, 0.384		

$\text{Na}_3\text{Pt}_4\text{Ge}_4$	$\bar{I}43m$, $a = 7.614 \text{ \AA}$ Na 6 b , 0, 1/2, 1/2; Pt 8 c , 0.1366, 0.1366, 0.1366; Ge 8 c , 0.3136, 0.3136, 0.3136	TbB_2C	$P4_2/mbc$, $a = 6.791$, $c = 7.522 \text{ \AA}$. Tb 8 g , 0.313, 0.813, 1/4 B(1) 8 h , 0.095, 0.595, 0; B(2) 8 h , 0.140, 0.035, 0; C 8 h , 0.456, 0.322, 0
NaZn_{13}	$Fm\bar{3}c$, $a = 12.284 \text{ \AA}$ Na 8 a , 1/4, 1/4, 1/4; Zn(1) 8 b , 0, 0, 0; Zn(2) 96 i , 0, 0.1806, 0.1192	ThB_4	$P4/mbm$, $a = 7.256$, $c = 4.113 \text{ \AA}$. Th 4 g , 0.313, 0.813, 0 B(1) 4 e , 0, 0, 0.212; B(2) 4 h , 0.087, 0.587, 1/2; B(3) 8 j , 0.170, 0.042, 1/2
Nb_6F_{15}	$Im\bar{3}m$, $a = 8.19 \text{ \AA}$. Nb 12 e , 0.242, 0, 0; F(1) 6 b , 0, 1/2, 1/2; F(2) 24 h , 0, 0.25, 0.25	ThB_2C	$R\bar{3}m$, $a = 6.700$, $c = 14.467 \text{ \AA}$ Th(1) 3 a , 0, 0, 0; Th(2) 6 c , 0, 0, 0.3156; B 18 g , 0.276, 0, 1/2; C 9 d , 1/2, 0, 1/2
NbO	$Pm\bar{3}m$, $a = 4.21 \text{ \AA}$. Nb 3 c , 0, 1/2, 1/2; O 3 d , 0, 0, 1/2	ThCr_2Si_2	$I4/mmm$, $a = 4.043$, $c = 10.577 \text{ \AA}$ Th 2 a , 0, 0, 0; Cr 4 d , 0, 1/2, 1/4; Si 4 e , 0, 0, 0.374
$\text{NbSe}_2 (2H_a)$	$P6_3/mmc$, $a = 3.445$, $c = 12.554 \text{ \AA}$. Nb 2 b , 0, 0, 1/4; Se 4 f , 1/3, 2/3, 0.1172	ThMoB_4	$Cmmm$, $a = 7.481$, $b = 9.658$, $c = 3.771 \text{ \AA}$. Mo 4 g , 0.171, 0, 0; Th 4 i , 0, 0.302, 0 B(1) 4 h , 0.379, 0, 1/2; B(2) 4 j , 0, 0.093, 1/2; B(3) 8 g , 0.234, 0.155, 1/2
PbFCl	$P4/nmm$, $a = 4.106$, $c = 7.230 \text{ \AA}$ Pb 2 c , 1/4, 1/4, 0.800; F 2 a , 3/4, 1/4, 0; Cl 2 c , 1/4, 1/4, 0.350	Th_3P_4	$\bar{I}43d$, $a = 8.618 \text{ \AA}$. Th 12 a , 3/8, 0, 1/4; P 16 c , 0.083, 0.083, 0.083
PbO	$P4/nmm$, $a = 3.972$, $c = 5.018$. Pb 2 c , 1/4, 1/4, 0.7615; O 2 a , 3/4, 1/4, 0	Th_3Pd_5	$P\bar{6}2m$, $a = 7.149$, $c = 3.899 \text{ \AA}$ Th 3 g , 0.350, 0, 1/2; Pd(1) 2 c , 1/3, 2/3, 0; Pd(2) 3 f , 0.780, 0, 0
PdF_2	$Pa\bar{3}$, $a = 5.239 \text{ \AA}$. Pd 4 a , 0, 0, 0; F 8 c , 0.343, 0.343, 0.342	ThSi_2	$I4_1/amd$, $a = 4.134$, $c = 14.375 \text{ \AA}$. Th 4 a , 0, 3/4, 1/8; Si 8 e , 0, 1/4, 0.2915
$\text{Pd}_{17}\text{Se}_{15}$	$Pm\bar{3}m$, $a = 10.606 \text{ \AA}$. Pd(1) 2 b , 1/2, 1/2, 1/2; Pd(2) 3 d , 1/2, 0, 0 Pd(3) 6 e , 0.238, 0, 0; Pd(4) 24 m , 0.352, 0.352, 0.150; Se(1) 6 f , 0.257, 1/2, 1/2 Se(2) 12 i , 0, 0.230, 0.230; Se(3) 12 j , 1/2, 0.168, 0.168	Th_2TeN_2	$I4/mmm$, $a = 4.094$, $c = 13.014 \text{ \AA}$ Th 4 c , 0, 0, 0.344; Te 2 a , 0, 0, 0; N 4 d , 0, 1/2, 1/4
$\text{Pr}_3\text{Rh}_4\text{Sn}_{13}$	$Pm\bar{3}n$, $a = 9.698 \text{ \AA}$. Pr 6 d , 1/4, 1/2, 0; Rh 8 e , 1/4, 1/4, 1/4 Sn(1) 2 a , 0, 0, 0; Sn(2) 24 k , 0, 0.3073, 0.1535	Ti_3VS_4	$\bar{I}43m$, $a = 7.51 \text{ \AA}$. Ti 6 b , 0, 1/2, 1/2; V 2 a , 0, 0, 0; S 8 c , 0.175, 0.175, 0.175
Re_3B	$Cmcm$, $a = 2.890$, $b = 9.313$, $c = 7.258 \text{ \AA}$. Re(1) 4 c , 0, 0.426, 1/4; Re(2) 8 f , 0, 0, 0.135, 0.062; B 4 c , 0, 0.744, 1/4.	WAl_{12}	$Im\bar{3}$, $a = 7.580 \text{ \AA}$. W 2 a , 0, 0, 0; Al 24 g , 0, 0, 0.184, 0.309
$\text{Sc}_2\text{O}_2\text{S}$	$P6_3/mmc$, $a = 3.520$, $c = 12.519 \text{ \AA}$, $c/a = 3.56$ Sc 4 f , 1/3, 2/3, 0.3930; O 4 f , 1/3, 2/3, 0.0661; S 2 b , 0, 0, 1/4	WC	$P\bar{6}m2$, $a = 2.906$, $c = 2.837 \text{ \AA}$. W 1 a , 0, 0, 0; C 1 d , 1/3, 2/3, 1/2
$\gamma\text{-Si}$	$Ia\bar{3}$, $a = 6.636 \text{ \AA}$. Si 16 c , 0.1003, 0.1003, 0.1003	YCrB_4	$Pbam$, $a = 5.972$, $b = 11.46$, $c = 3.461 \text{ \AA}$. Y 4 g , 0.125, 0.150, 0; Cr 4 g , 0.125, 0.419, 0; B(1) 4 h , 0.280, 0.315, 1/2 B(2) 4 h , 0.340, 0.465, 1/2; B(3) 4 h , 0.385, 0.050, 1/2; B(4) 4 h , 0.485, 0.180, 1/2
SiO_2 (coesite)	$C2/c$, $a = 7.135$, $b = 12.372$, $c = 7.173 \text{ \AA}$, $\beta = 120.36^\circ$ Si(1) 8 f , 0.140, 0.1084, 0.072; Si(2) 8 f , 0.506, 0.1590, 0.540 O(1) 4 a , 0, 0, 0; O(2) 4 e , 0, 0.3839, 1/4; O(3) 8 f , 0.266, 0.1233, 0.940 O(4) 8 f , 0.311, 0.1037, 0.328; O(5) 8 f , 0.018, 0.2119, 0.478	Y_2ReB_6	$Pbam$, $a = 9.175$, $b = 11.55$, $c = 3.673 \text{ \AA}$ Y(1) 4 g , 0.823, 0.087, 0; Y(2) 4 g , 0.445, 0.131, 0; Re 4 g , 0.138, 0.178, 0 B(1) 4 h , 0.050, 0.060, 1/2; B(2) 4 h , 0.250, 0.075, 1/2; B(3) 4 h , 0.300, 0.240, 1/2 B(4) 4 h , 0.140, 0.310, 1/2; B(5) 4 h , 0.480, 0.290, 1/2; B(6) 4 h , 0.110, 0.470, 1/2
SiO_2 (keatite)	$P4_32_12$, $a = 7.464$, $c = 8.620 \text{ \AA}$. Si(1) 4 a , 0.410, 0.410, 0 Si(2) 8 b , 0.326, 0.120, 0.248; O(1) 8 b , 0.445, 0.132, 0.400 O(2) 8 b , 0.117, 0.123, 0.296; O(3) 8 b , 0.344, 0.297, 0.143	Zn(CN)_2	$P\bar{4}3m$, $a = 5.928 \text{ \AA}$. Zn(1) 1 a , 0, 0, 0; Zn(2) 1 b , 1/2, 1/2, 1/2 C 4 e , 0.1938, 0.1938, 0.1938; N 4 e , 0.3092, 0.3092, 0.3092
SiO_2 (moganite)	$I2/a$, $a = 8.758$, $b = 4.786$, $c = 10.715 \text{ \AA}$, $\beta = 90.08^\circ$. Si(1) 4 c , 1/4, 0.9908, 0 Si(2) 8 f , 0.0115, 0.2533, 0.1678; O(1) 8 f , 0.9686, 0.0680, 0.2860 O(2) 8 f , 0.1711, 0.1770, 0.1050; O(3) 8 f , 0.8657, 0.2148, 0.0739	ZnO	$P6_3mc$, $a = 3.250$, $c = 5.207 \text{ \AA}$. Zn 2 b , 1/3, 2/3, 0, 0; O 2 b , 1/3, 2/3, 0.3819
SrMgSi	$Pnma$, $a = 7.78$, $b = 4.56$, $c = 8.49 \text{ \AA}$. Sr 4 c , 0.515, 1/4, 0.683 Mg 4 c , 0.640, 1/4, 0.057; Si 4 c , 0.276, 1/4, 0.110	ZrFe_4Si_2	$P4_2/mnm$, $a = 7.004$, $c = 3.755 \text{ \AA}$ Zr 2 b , 0, 0, 1/2; Fe 8 i , 0.0920, 0.3468, 0; Si 4 g , 0.2201, 0.7799, 0
SrSi_2	$P4_332$, $a = 6.540 \text{ \AA}$. Sr 4 a , 1/8, 1/8, 1/8; Si 8 c , 0.428, 0.428, 0.428		

Crystallographic point groups

system	point group	Schoenflies	spacegroups	center?
triclinic (anorthic)	1 $\bar{1}$	C_1 C_i	1 2	no yes
monoclinic	2 m $2/m$	C_2 C_s C_{2h}	$3-5$ $6-9$ $10-15$	no no yes
orthorhombic	222 $mm2$ mmm	D_2 C_{2v} D_{2h}	$16-24$ $25-46$ $47-74$	no no yes
tetragonal	4 $\bar{4}$ $4/m$ 422 $4mm$ $42m$ $4/mmm$	C_4 S_4 C_{4h} D_4 C_{4v} D_{2d} D_{4h}	$75-80$ $81-82$ $83-88$ $89-98$ $99-110$ $111-122$ $123-142$	no no yes no no no yes
trigonal	3 $\bar{3}$ 32 $\bar{3}m$ $3m$	C_3 C_{3i} D_3 C_{3v} D_{3d}	$143-146$ $147-148$ $149-155$ $156-161$ $162-167$	no yes no no yes
hexagonal	6 $\bar{6}$ $6/m$ 622 $6mm$ $\bar{6}m2$ $6/mmm$	C_6 C_{3h} C_{6h} D_6 C_{6v} D_{3h} D_{6h}	$168-173$ 174 $175-176$ $177-182$ $183-186$ $187-190$ $191-194$	no no yes no no no yes
cubic (isometric)	23 $m\bar{3}$ 432 $\bar{4}3m$ $m\bar{3}m$	T T_h O T_d O_h	$195-199$ $200-206$ $207-214$ $215-220$ $221-230$	no yes no no yes

In the following list the first symbol in each row is "standard" and those on the right of it are other possibilities. It is a common practice to omit the "1" space markers when **b** is the unique axis (so that, e.g. *C12/c1* becomes *C2/c*). The number is the space group number in the *International Tables*. For numbers 9 and 15 interchanging the labels of the oblique axes results in additional "legal" symbols not used in the *Tables*.

	b unique			c unique		
3	P121			P112		
4	P12 ₁ 1			P112 ₁		
5	C121	A121	I121	A112	B112	I112
6	P1m1			P11m		
7	P1c1	P1n1	P1a1	P11a	P11n	P11b
8	C1m1	A1m1	I1m1	A11m	B11m	I11m
9	C1c1	A1n1	I1a1	A11a	B11n	I11b
	A1a1	C1n1	I1c1	B11b	A11n	I11a
10	P12/m1			P112/m		
11	P12 ₁ /m1			P112 ₁ /m		
12	C12/m1	A12/m1	I12/m1	A112/m	B112/m	I112/m
13	P12/c1	P12/n1	P12/a1	P112/a	P112/n	P112/b
14	P12 ₁ /c1	P12 ₁ /n1	P12 ₁ /a1	P112 ₁ /a	P112 ₁ /n	P112 ₁ /b
15	C12/c1	A12/n1	I12/a1	A112/a	B112/n	I112/b
	A12/a1	C12/n1	I12/c1	B112/b	A112/n	I112/a

The following table gives orthorhombic space groups for various choices of axes. The second column headed **a b c** is the "standard" setting. The remaining columns are the symbols for different labeling of the axes. For example in the column headed **c a b**, the new **a** axis corresponds to the old **c** (in the standard setting), the new **b** is the old **a** and the new **c** is the old **b**.

[illegible]

	a b c	c a b	b c a	a -c b	b a -c	-c b a
25	<i>Pmm2</i>	<i>P2mm</i>	<i>Pm2m</i>	<i>Pm2m</i>	<i>Pmm2</i>	<i>P2mm</i>
26	<i>Pmc2₁</i>	<i>P2₁ma</i>	<i>Pb2₁m</i>	<i>Pm2₁b</i>	<i>Pcm2₁</i>	<i>P2₁am</i>
27	<i>Pcc2</i>	<i>P2aa</i>	<i>Pb2b</i>	<i>Pb2b</i>	<i>Pcc2</i>	<i>P2aa</i>
28	<i>Pma2</i>	<i>P2mb</i>	<i>Pc2m</i>	<i>Pm2a</i>	<i>Pbm2</i>	<i>P2cm</i>
29	<i>Pca2₁</i>	<i>P2₁ab</i>	<i>Pc2₁b</i>	<i>Pb2₁a</i>	<i>Pbc2₁</i>	<i>P2₁ca</i>
30	<i>Pnc2</i>	<i>P2na</i>	<i>Pb2n</i>	<i>Pn2b</i>	<i>Pcn2</i>	<i>P2an</i>
31	<i>Pmn2₁</i>	<i>P2₁mn</i>	<i>Pn2₁m</i>	<i>Pm2₁n</i>	<i>Pnm2₁</i>	<i>P2₁nm</i>
32	<i>Pba2</i>	<i>P2cb</i>	<i>Pc2a</i>	<i>Pc2a</i>	<i>Pba2</i>	<i>P2cb</i>
33	<i>Pna2₁</i>	<i>P2₁nb</i>	<i>Pc2₁n</i>	<i>Pn2₁a</i>	<i>Pbn2₁</i>	<i>P2₁cn</i>
34	<i>Pnn2</i>	<i>P2nn</i>	<i>Pn2n</i>	<i>Pn2n</i>	<i>Pnn2</i>	<i>P2nn</i>
35	<i>Cmm2</i>	<i>A2mm</i>	<i>Bm2m</i>	<i>Bm2m</i>	<i>Cmm2</i>	<i>A2mm</i>
36	<i>Cmc2₁</i>	<i>A2₁ma</i>	<i>Bb2₁m</i>	<i>Bm2₁b</i>	<i>Ccm2₁</i>	<i>A2₁am</i>
37	<i>Ccc2</i>	<i>A2aa</i>	<i>Bb2b</i>	<i>Bb2b</i>	<i>Ccc2</i>	<i>A2aa</i>
38	<i>Amn2</i>	<i>B2mn</i>	<i>Cm2m</i>	<i>Am2m</i>	<i>Bmn2</i>	<i>C2mm</i>
39	<i>Abm2</i>	<i>B2cm</i>	<i>Cm2a</i>	<i>Ac2m</i>	<i>Bma2</i>	<i>C2mb</i>
40	<i>Ama2</i>	<i>B2mb</i>	<i>Cc2m</i>	<i>Am2a</i>	<i>Bmb2</i>	<i>C2cm</i>
41	<i>Aba2</i>	<i>B2cb</i>	<i>Cc2a</i>	<i>Ac2a</i>	<i>Bba2</i>	<i>C2cb</i>
42	<i>Fmm2</i>	<i>F2mm</i>	<i>Fm2m</i>	<i>Fm2m</i>	<i>Fmm2</i>	<i>F2mm</i>
43	<i>Fdd2</i>	<i>F2dd</i>	<i>Fd2d</i>	<i>Fd2d</i>	<i>Fdd2</i>	<i>F2dd</i>
44	<i>Imn2</i>	<i>I2mn</i>	<i>Im2m</i>	<i>Im2m</i>	<i>Imn2</i>	<i>I2mn</i>
45	<i>Iba2</i>	<i>I2cb</i>	<i>Ic2a</i>	<i>Ic2a</i>	<i>Iba2</i>	<i>I2cb</i>
46	<i>Ima2</i>	<i>I2mb</i>	<i>Ic2m</i>	<i>Im2a</i>	<i>Ibm2</i>	<i>I2cm</i>
47	<i>Pmmn</i>	<i>Pnmn</i>	<i>Pmmn</i>	<i>Pmmn</i>	<i>Pmmn</i>	<i>Pmmn</i>
48	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>
49	<i>Pccm</i>	<i>Pmaa</i>	<i>Pbmb</i>	<i>Pbmb</i>	<i>Pccm</i>	<i>Pmaa</i>
50	<i>Pban</i>	<i>Pncb</i>	<i>Pcna</i>	<i>Pcna</i>	<i>Pban</i>	<i>Pncb</i>
51	<i>Pmna</i>	<i>Pbmna</i>	<i>Pmcm</i>	<i>Pmam</i>	<i>Pmnb</i>	<i>Pcmn</i>
52	<i>Pnna</i>	<i>Pbnna</i>	<i>Pncn</i>	<i>Pnan</i>	<i>Pnnb</i>	<i>Pcnn</i>
53	<i>Pmna</i>	<i>Pbmna</i>	<i>Pncm</i>	<i>Pman</i>	<i>Pnmb</i>	<i>Pcnm</i>
54	<i>Pcca</i>	<i>Pbaa</i>	<i>Pbcb</i>	<i>Pbab</i>	<i>Pccb</i>	<i>Pcaa</i>
55	<i>Pbam</i>	<i>Pmcb</i>	<i>Pcma</i>	<i>Pcma</i>	<i>Pbam</i>	<i>Pmcb</i>
56	<i>Pccn</i>	<i>Pnaa</i>	<i>Pbnb</i>	<i>Pbnb</i>	<i>Pccn</i>	<i>Pnaa</i>
57	<i>Pbcm</i>	<i>Pmca</i>	<i>Pbma</i>	<i>Pcmb</i>	<i>Pcam</i>	<i>Pmab</i>
58	<i>Pnmn</i>	<i>Pmnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnmn</i>	<i>Pmnn</i>
59	<i>Pmmn</i>	<i>Pnmn</i>	<i>Pmmn</i>	<i>Pmmn</i>	<i>Pmmn</i>	<i>Pnmn</i>
60	<i>Pbcn</i>	<i>Pnca</i>	<i>Pbna</i>	<i>Pcnb</i>	<i>Pcan</i>	<i>Pnmb</i>
61	<i>Pbca</i>	<i>Pbca</i>	<i>Pbca</i>	<i>Pcab</i>	<i>Pcab</i>	<i>Pcab</i>
62	<i>Pnma</i>	<i>Pbnm</i>	<i>Pmcm</i>	<i>Pnam</i>	<i>Pmnb</i>	<i>Pcnn</i>
63	<i>Cmcm</i>	<i>Amma</i>	<i>Bbmm</i>	<i>Bmmb</i>	<i>Ccmm</i>	<i>Amam</i>
64	<i>Cmca</i>	<i>Abma</i>	<i>Bbcm</i>	<i>Bmab</i>	<i>Ccmb</i>	<i>Acam</i>
65	<i>Cmmm</i>	<i>Ammm</i>	<i>Bmmn</i>	<i>Bmmn</i>	<i>Cmmm</i>	<i>Ammm</i>
66	<i>Cccm</i>	<i>Amaa</i>	<i>Bbmb</i>	<i>Bbmb</i>	<i>Cccm</i>	<i>Amaa</i>
67	<i>Cmma</i>	<i>Abmm</i>	<i>Bmcm</i>	<i>Bmam</i>	<i>Cmmb</i>	<i>Acmm</i>
68	<i>Ccca</i>	<i>Abaa</i>	<i>Bbcb</i>	<i>Bbab</i>	<i>Cccb</i>	<i>Acaa</i>
69	<i>Fmmn</i>	<i>Fmmn</i>	<i>Fmmn</i>	<i>Fmmn</i>	<i>Fmmn</i>	<i>Fmmn</i>
70	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>
71	<i>Immm</i>	<i>Immm</i>	<i>Immm</i>	<i>Immm</i>	<i>Immm</i>	<i>Immm</i>
72	<i>Ibam</i>	<i>Ibcb</i>	<i>Icma</i>	<i>Ibma</i>	<i>Ibcb</i>	<i>Icma</i>
73	<i>Ibca</i>	<i>Ibca</i>	<i>Ibca</i>	<i>Icab</i>	<i>Icab</i>	<i>Icab</i>
74	<i>Imma</i>	<i>Ibmm</i>	<i>Imcm</i>	<i>Imam</i>	<i>Immb</i>	<i>Icmm</i>

Tetragonal space groups

75	<i>P4</i>	76	<i>P4₁</i>	77	<i>P4₂</i>	78	<i>P4₃</i>
79	<i>I4</i>	80	<i>I4₁</i>				
81	<i>P4̄</i>	82	<i>I4̄</i>				
83	<i>P4/m</i>	84	<i>P4₂/m</i>	85	<i>P4/n</i>	86	<i>P4₂/n</i>
87	<i>I4/m</i>	88	<i>I4₁/a</i>				
89	<i>P422</i>	90	<i>P42₁2</i>	91	<i>P4₁22</i>	92	<i>P4₁2₁2</i>
93	<i>P4₂22</i>	94	<i>P4₂2₁2</i>	95	<i>P4₃22</i>	96	<i>P4₃2₁2</i>
97	<i>I422</i>	98	<i>I4₁22</i>				
99	<i>P4mm</i>	100	<i>P4bm</i>	101	<i>P4₂cm</i>	102	<i>P4₂nm</i>
103	<i>P4cc</i>	104	<i>P4nc</i>	105	<i>P4₂mc</i>	106	<i>P4₂bc</i>
107	<i>I4mm</i>	108	<i>I4cm</i>	109	<i>I4₁md</i>	110	<i>I4₁cd</i>
111	<i>P4̄2m</i>	112	<i>P4̄2c</i>	113	<i>P4̄2₁m</i>	114	<i>P4̄2₁c</i>
115	<i>P4m2</i>	116	<i>P4̄c2</i>	117	<i>P4̄b2</i>	118	<i>P4̄n2</i>
119	<i>I4m2</i>	120	<i>I4c2</i>	121	<i>I4̄2m</i>	122	<i>I4̄2d</i>
123	<i>P4/mmm</i>	124	<i>P4/mcc</i>	125	<i>P4/nbm</i>	126	<i>P4/nnc</i>
127	<i>P4/mbm</i>	128	<i>P4/mnc</i>	129	<i>P4/nmm</i>	130	<i>P4/ncc</i>
131	<i>P4₂/mmc</i>	132	<i>P4₂/mcm</i>	133	<i>P4₂/nbc</i>	134	<i>P4₂/nmm</i>
135	<i>P4₂/mbc</i>	136	<i>P4₂/mnm</i>	137	<i>P4₂/nmc</i>	138	<i>P4₂/ncm</i>
139	<i>I4/mmm</i>	140	<i>I4/mcm</i>	141	<i>I4₁/amd</i>	142	<i>I4₁/acd</i>

Trigonal space groups

143	<i>P3</i>	144	<i>P3₁</i>	145	<i>P3₂</i>	146	<i>R3</i>
147	<i>P3̄</i>	148	<i>R3̄</i>				
149	<i>P312</i>	150	<i>P321</i>	151	<i>P3₁12</i>	152	<i>P3₁21</i>
153	<i>P3₂12</i>	154	<i>P3₂21</i>	155	<i>R32</i>		
156	<i>P3m1</i>	157	<i>P31m</i>	158	<i>P3c1</i>	159	<i>P31c</i>
160	<i>R3m</i>	161	<i>R3c</i>				
162	<i>P3̄1m</i>	163	<i>P3̄1c</i>	164	<i>P3̄m1</i>	165	<i>P3̄c1</i>
166	<i>R3̄m</i>	167	<i>R3̄c</i>				

Hexagonal space groups

168 P_6 172 P_{64}	169 P_{61} 173 P_{63}	170 P_{65}	171 P_{62}
174 $P\bar{6}$			
175 P_6/m	176 P_{63}/m		
177 P_{622} 181 P_{6422}	178 P_{6122} 182 P_{6322}	179 P_{6522}	180 $P_{62}22$
183 P_6mm	184 P_6cc	185 $P_{63}cm$	186 $P_{63}mc$
187 $P\bar{6}m2$	188 $P\bar{6}c2$	189 $P\bar{6}2m$	190 $P\bar{6}2c$
191 P_6/mmm	192 P_6/mcc	193 P_{63}/mcm	194 P_{63}/mmc

Cubic space groups

195 P_{23} 199 I_{213}	196 F_{23}	197 I_{23}	198 P_{213}
200 $Pm\bar{3}$ 204 $Im\bar{3}$	201 $Pn\bar{3}$ 205 $Pa\bar{3}$	202 $Fm\bar{3}$ 206 $Ia\bar{3}$	203 $Fd\bar{3}$
207 $P432$ 211 $I432$	208 $P4_232$ 212 $P4_332$	209 $F432$ 213 $P4_132$	210 $F4_132$ 214 $I4_132$
215 $P\bar{4}3m$ 219 $F\bar{4}3c$	216 $F\bar{4}3m$ 220 $I\bar{4}3d$	217 $I\bar{4}3m$	218 $P\bar{4}3n$
221 $Pm\bar{3}m$ 225 $Fm\bar{3}m$ 229 $Im\bar{3}m$	222 $Pn\bar{3}n$ 226 $Fm\bar{3}c$ 230 $Ia\bar{3}d$	223 $Pm\bar{3}n$ 227 $Fd\bar{3}m$	224 $Pn\bar{3}m$ 228 $Fd\bar{3}c$

BOOK LIST

Here is a short list of books mostly in English that we have found particularly useful. Some more-specialized books we have referred to in the text. References to all the crystal structure data given in this book are to be found in the various compilations listed in D (this is where they came from).

A. INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

These are: Volume A: Space-Group Symmetry, 3rd ed. 1992 [the indispensable reference]. Volume B: Reciprocal Space, 1993. Volume C: Mathematical, Physical and Chemical Tables, 1992. Kluwer Academic, Dordrecht.

B. Some books on crystallography and crystal chemistry

BLOSS, F. D.

Crystallography and Crystal Chemistry, reprinted by Mineral. Soc. Amer., Washington, D.C. (1994). Very clear exposition of the crystallographic point groups.

BURNS, G & GLAZER, A. M.

Space Groups for Solid State Scientists 2nd Ed., Academic Press, New York (1990). A good informal account of space groups with useful tables.

BOISEN, M. B. & GIBBS, G. V.

Mathematical Crystallography, Reviews in Mineralogy 15, Mineral. Soc. of Amer., Washington, D.C. (Revised, 1990). A systematic account of how to do crystallographic calculations, and a derivation of the three-dimensional point and space groups.

DE JONG, W. F.

General Crystallography. Freeman, San Francisco (1959). Subtitled "A brief compendium" this useful little book contains a wide variety of information. Particularly useful for geometric aspects.

HYDE, B. G. & ANDERSSON, S.

Inorganic Crystal Structures, John Wiley & Sons, New York (1989). Systematic description of crystal structures with special emphasis on the development of "complex" structures from simpler ones using simple building principles. Numerous tables of data.

MEGAW, H. D.

Crystal Structures: A Working Approach, Saunders, Philadelphia (1973). Clear descriptions of symmetry and the crystallographic description of structures.

PEARSON, W. B.

The Crystal Chemistry and Physics of Metals and Alloys, John Wiley & Sons, New York (1972). A comprehensive account of the subject at the time and still very useful.

SMITH, J. V.

Geometrical and Structural Crystallography, John Wiley & Sons, New York (1982). A good introduction to formal crystallography. Intended for those who are prepared to work through a number of carefully considered examples.

WELLS, A. F.

Structural Inorganic Chemistry. 5th Ed., Clarendon Press, Oxford (1984). Contains a wealth of organized structural information with due attention to crystal structures. Introductory chapters discuss polyhedra, sphere packings etc. Every chemist should own a copy.