

Dictionary of Inorganic Compounds

VOLUME FOUR

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643-770
D511

Dictionary of Inorganic Compounds

VOLUME FOUR

INDEX OF COMMONLY OCCURRING
STRUCTURAL TYPES

NAME INDEX

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Supplements to *Dictionary of Inorganic Compounds* will be published each year subsequent to publication of the Main Work. The first annual supplement will be published in Autumn 1993.

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Introduction to Index of Commonly Occurring Structural Types

Among inorganic compounds a comparatively limited number of structural types are the basis for very many compounds. This index includes the most commonly occurring structures and compounds which – precisely or approximately – exemplify them.

The types included are intended to function as structural formulae, explaining as simply as possible the spatial relationships among the atoms or ions in the structure. They are not intended as a crystallographically definitive listing.

Many solids which resemble one or other of the common structural types, turn out to be slightly distorted forms. In a set of interatomic distances which are all equal in the regular structure, some slight inequalities appear. Such slightly distorted structures have sometimes been included in the list (in the case of distortions from cubic symmetry mostly under separate headings) because the interatomic relationships are the same to a first approximation.

The greater part of the list comprises structures – of elements and then compounds – where the whole structure is defined. These include elements, metallic phases, and simple ionic compounds. The later part is of commonly occurring structure fragments which may be identified as component parts of structures although occurring in structures which are different overall. The majority of these are the chains or layers of silicate structures, or cages of atoms in compounds of boron.

The sequence of entries is primarily determined by formula type. First come the structures of solid elements with, of course, only one kind of atom. These are followed by phases where replacements in sometimes variable proportions or ratios give metallic alloy phases having a common overall structure.

The list then follows a sequence according to formula type. After AX, AX₂, etc. there are the structure types where three or more kinds of atom are involved.

No separate types are allocated which may be described as, for example, A₂X, where the positions of anion and cation are interchanged from the

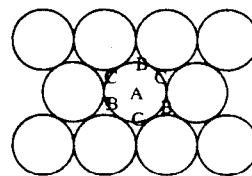
common pattern. Although sometimes described as “anti-” structures, these have been listed under the commoner heading. For example Li₂O comes under AX₂ fluorite type.

Under some formula types are listed compounds of apparently discordant stoichiometry. The relationship to the formula type may come about in a number of different ways. One of these is by rotation of ions in higher temperature forms, for example in caesium cyanide which has the AX caesium chloride structure. In other cases, the presence of a proportion of lattice vacancies, randomly distributed over a set of lattice sites, may produce the appearance of higher symmetry. In this way the high temperature phase δ-Bi₂O₃ has the AX₂ fluorite structure, while γ-Ga₂S₃ has the AX zinc blende structure.

Brief descriptions are given below for the majority of headings in the index.

Close-packed layers

Many structures of widely different bond character have a geometry based upon layers of close-packed atoms, all of the same size. Each atom in the layer has six neighbours. If extended indefinitely, such a layer has twice as many three-fold joins (B and C locations) as there are atoms (centres labelled A locations) in the layer. Two such layers may enclose between them another kind of atom forming layer structures such as AX₂ cadmium chloride, or AX₃ yttrium chloride. Regular stacking of such layers gives rise to the hexagonal close-packed and cubic close-packed structures.

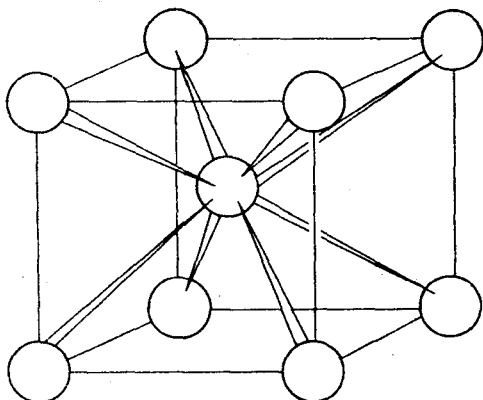


Body-centred cubic metallic

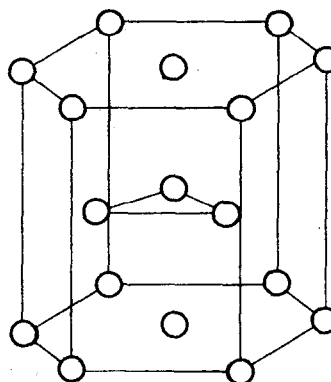
Each atom is surrounded by eight nearest neighbours, at the corners of an enclosing cube, with

Introduction

six other near neighbours having centres slightly (15.5%) farther away.

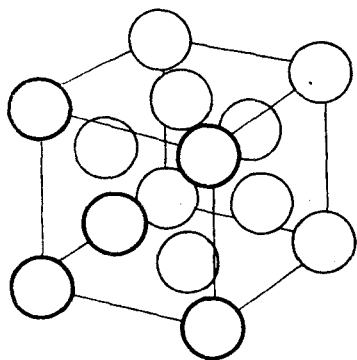


such that atomic centres are located in a sequence ABABAB...



Cubic close-packed metallic

Each atom is surrounded by twelve equivalent nearest neighbours, in a structure which corresponds with stacking close-packed layers so that each atom comes above a join of three in the next layer below, and the centres of atoms in successive layers are located in the sequence ABCABCABC... The axis of sixfold symmetry visible in a single close-packed layer coincides with a body-diagonal of the cubic unit cell.

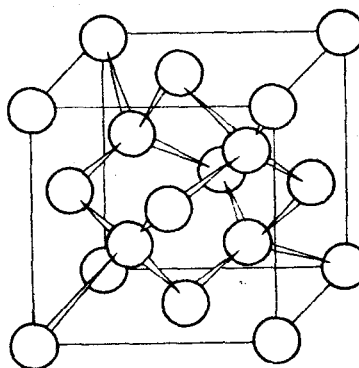


Hexagonal close-packed metallic

Each atom is surrounded by twelve equivalent nearest neighbours, in a structure which corresponds with stacking close-packed layers with each atom above a join between three in the layer below, and

Diamond

The atoms are each surrounded by four others at the corners of an enclosing tetrahedron, corresponding with the formation of four covalent bonds. The structure may also be described as a cubic close-packed array of carbon atoms, with an equal number of carbon atoms located regularly in half the tetrahedral sites between them; nevertheless all the atoms are in an identical environment.



Body-centred alloy (β brass)

If all the atoms were regarded as equivalent, the structure would be that of a body-centred cubic element. In alloy systems this structure is often found when the ratio of valence electrons to atoms is approximately 3:2. The different atoms may be randomly distributed over all the available sites, as in β -brass, CuZn, above 468°C, or ordered with one kind of atom surrounded by eight of the other as in β -brass below 454°C, as in AX caesium chloride. Other ordered arrangements of the different atoms are also possible, for example in NaTl (see below).

β -Manganese alloy

This structure is often formed, as an alternative to the β -brass structure, in intermetallic alloy systems with the ratio of valence electrons to atoms close to 3:2. There are two sets of atoms, each having twelve near neighbours, but at distances which are not precisely the same.

Cubic alloy close-packed

If all the atoms were identical, the structure would be that of cubic close-packed elements. In intermetallic compounds, the different kinds of atom may be arranged in some orderly way over the lattice sites, as with CuAu below 380°C, and Cu₃Au below 300°C. An ordered structure may show slight distortion from strict cubic symmetry.

Cubic alloy (γ brass)

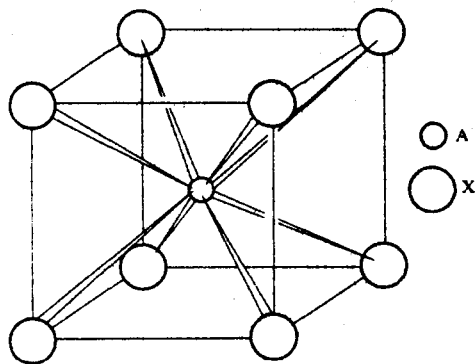
This structure is often formed when the ratio of valence electrons to atoms is approximately 21:13. The cubic unit cell contains 52 atoms; the distances between neighbouring atoms are not all precisely the same.

Hexagonal close-packed alloy (ϵ -brass)

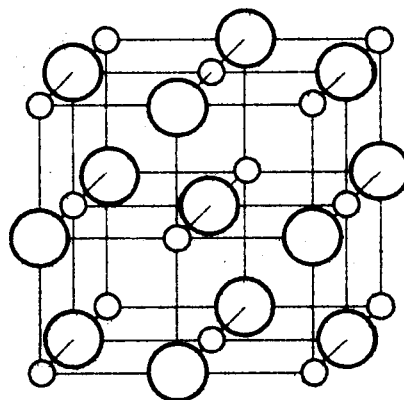
This is found in alloy systems with a ratio of valence electrons to atoms of approximately 7:4. If no distinction is made between different kinds of atom then the arrangement is the elemental structure. In the alloy phase each atom is surrounded by twelve others; the number of each kind depends upon the composition – differing for example between CuZn₃ and Ag₅Al₃.

AX Caesium chloride (CsCl)

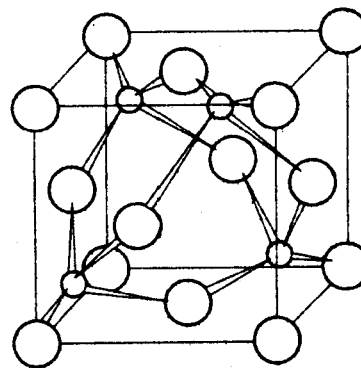
Each atom or ion is closely surrounded by eight of the other kind. It corresponds with a primitive cubic unit cell with one kind of ion at the corners, and the counter-ion at the centre.

**AX Sodium chloride (NaCl)**

Each atom or ion is closely surrounded by six of the other kind, at the corners of an enclosing octahedron. The structure may be described as cubic close-packed X atoms, with A atoms in all the intervening octahedral sites; however if relative sizes are ignored, the same description applies with A and X interchanged.

**AX Zinc blende (ZnS)**

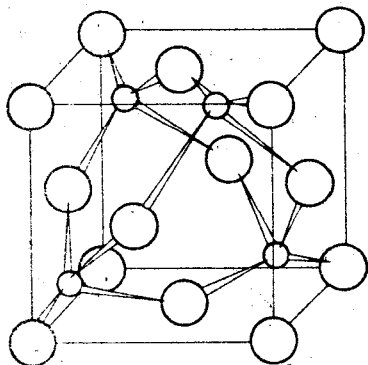
Each atom of one kind is surrounded by four of the other kind at the corners of an enclosing tetrahedron. The structure may be described as having a cubic close-packed array of one kind of atom with the other kind in an orderly arrangement in half the intervening tetrahedral sites. If the distinction between A and X atoms is ignored, the structure is that of diamond.

**AX Wurtzite (ZnS)**

Each atom of one kind is surrounded tetrahedrally by four of the other kind as in zinc blende, but adjacent tetrahedra have a different angular relationship. The structure may be described as one kind of atom in

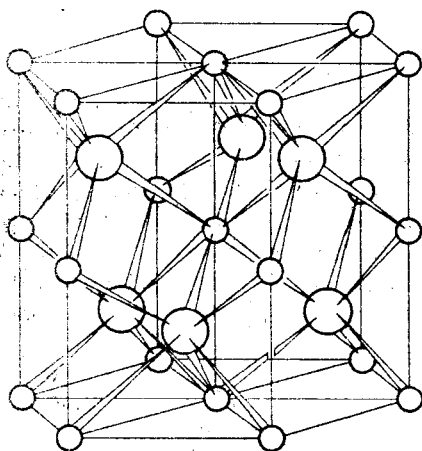
Introduction

hexagonal close-packing, with the other kind ordered in half the intervening tetrahedral sites.



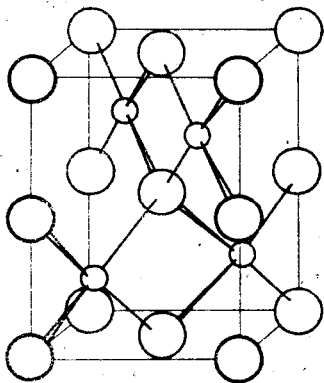
AX Nickel arsenide (NiAs)

The structure may be derived from a hexagonal close-packed array of X atoms, altered by insertion of A atoms in all the sites of octahedral six-coordination. In addition to the six X neighbours, each A atom is close to two atoms of its own kind.



AX Cooperite (PtS)

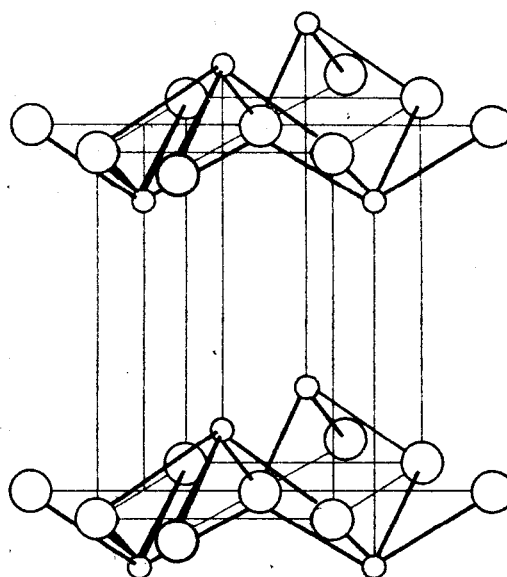
The structure consists of chains of platinum atoms in



which each is at the centre of four coplanar sulfur atoms which, in pairs, link it to the two neighbours in the chain. Each sulfur atom is surrounded by an irregular tetrahedron of platinum atoms; two of these belong to one platinum atom chain, the others to a chain at right angles to the first.

AX Tetragonal lead oxide (PbO)

Each lead atom is at the apex of a pyramid, slightly distorted from square, of four oxygen atoms at the base. Each oxygen atom is linked, not always at the same distance, to four lead atoms. As the PbO pyramid is quite flat, the result is a layer structure.



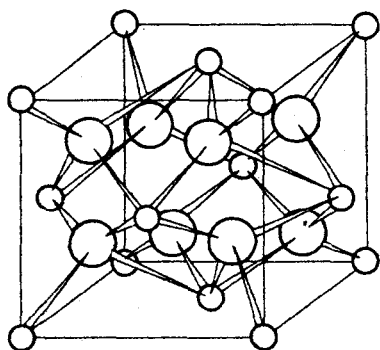
AX β -Thallium iodide (TlI)

The structure may be related to a deformed version of the octahedral 6:6 coordination of sodium chloride, where by displacement of neighbouring parts, one A atom is left close to five X atoms, while around the direction of the missing sixth are a set of four other X atoms at somewhat greater and unequal distances.

AX₂ Fluorite (CaF₂)

The structure may be derived from a close-packed assembly of A atoms, with X atoms in all the sites of

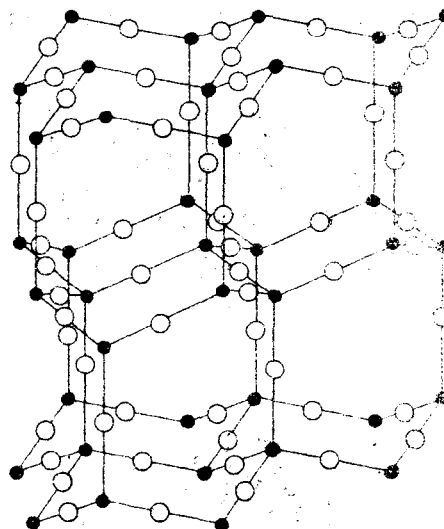
tetrahedral four-coordination. Thus any A atom is surrounded by eight X atoms, each X by four A.



corners of an enclosing tetrahedron; each X is linked to two A atoms, with a bond angle close to 144° . Part of the structure forms a helical chain which may be left handed or right handed in individual crystals.

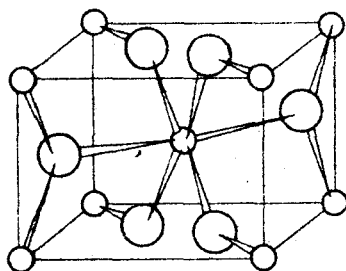
AX₂ Tridymite (SiO₂)

The AX₄ tetrahedra, as in the quartz structure, are linked with A-X-A angles of about 147° in the prototype, to give a different and somewhat lower density network than quartz.



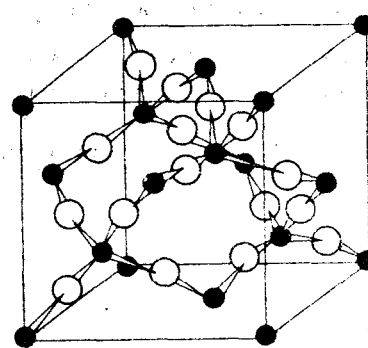
AX₂ Rutile (TiO₂)

Each A atom is associated with six X atoms, at corners of a surrounding octahedron, while each X atom is surrounded by three coplanar A atoms. The interatomic distances in a set may differ slightly.



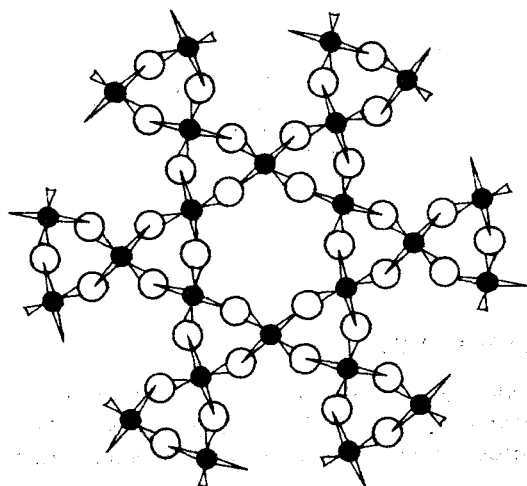
AX₂ Cristobalite (SiO₂)

Again the structure involves AX₄ tetrahedra linked into a lower density network, with A-X-A bond angles of about 147° .



AX₂ Quartz (SiO₂)

Each A atom is surrounded by four X atoms at the



AX₂ Cadmium chloride (CdCl₂)

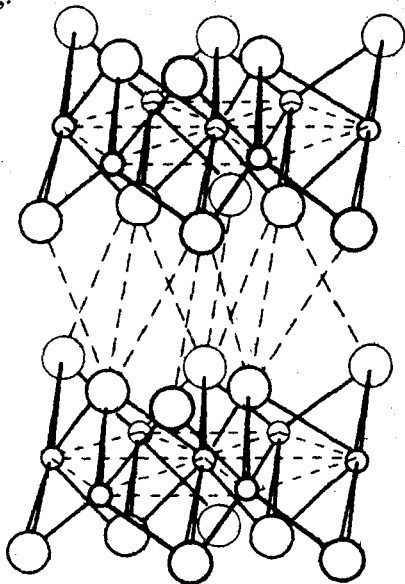
Between two single close-packed layers of X atoms, the A atoms are located in all the sites of octahedral

Introduction

six-coordination. Each X atom is joined, pyramidally, to three A atoms. The crystal is made up by stacking these AX_2 layers. If the A atoms are ignored, the arrangement of X atoms approximates to cubic close-packed.

AX_2 Cadmium iodide (CdI_2)

The A atoms are located in all the sites of octahedral six-coordination between two single close-packed layers of X atoms. The AX_2 layers are stacked parallel. If the A atoms are ignored, the arrangement of X atoms approximates to that of hexagonal close-packing.

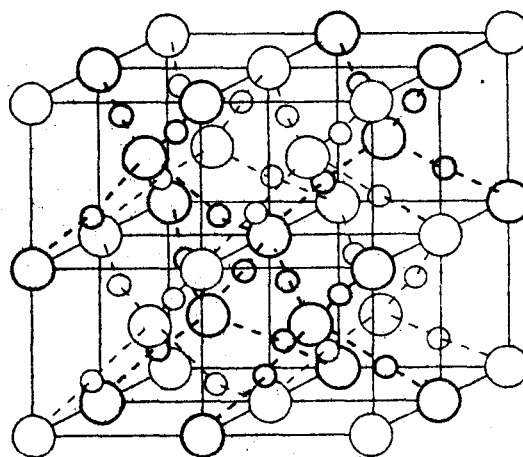


AX_2 Orthorhombic lead chloride ($PbCl_2$)

Each A atom is associated with nine X atoms as near neighbours with a range of interatomic distances, while some X atoms are associated with four and some with five A atoms, at similar but varying distances.

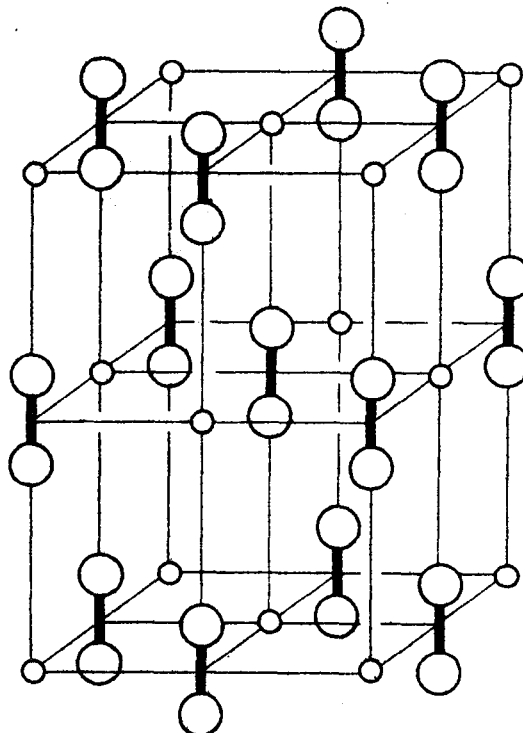
AX_2 Cuprite (Cu_2O)

In this structure each A atom (oxygen) is surrounded by four X atoms (copper), while each X atom is joined to two A atoms to give a continuous open framework. The A-X-A sets are co-linear. There are two such frameworks, interpenetrating and unlinked, in the crystal.



AX_2 Calcium carbide (CaC_2)

In the tetragonal crystal, the closely bonded X_2 pairs, all parallel, are located in positions corresponding with the X atoms in the sodium chloride structure.

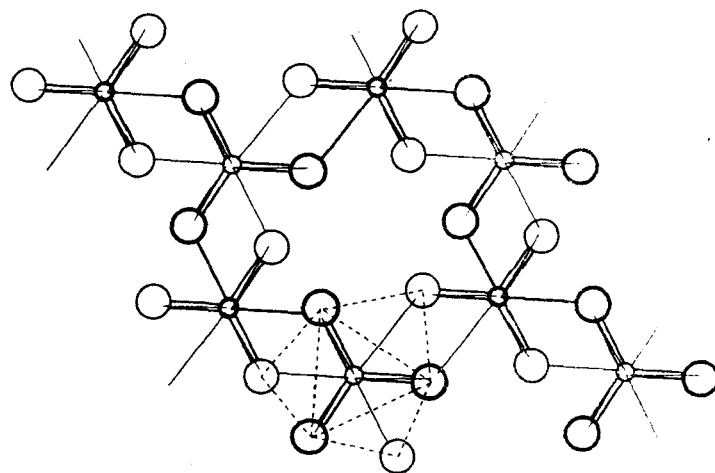


AX_2 Pyrite (FeS_2)

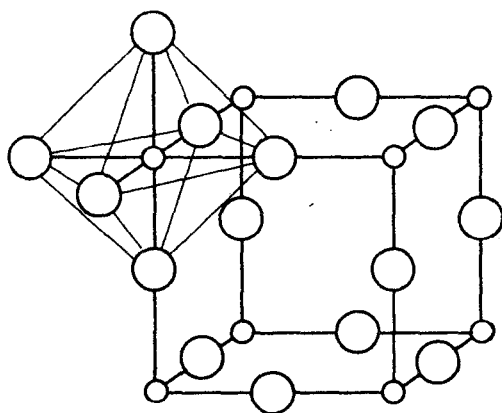
The closely bonded X_2 pairs are located so that their centres correspond with the X atoms in the sodium chloride structure, but the X-X bond orientations vary.

AX₂ Marcasite (FeS₂)

In the orthorhombic crystal, the bonded X₂ pairs have two different orientations. Each X is close to one X atom and three A, each A to six X atoms.

**AX₃ Rhenium oxide (ReO₃)**

Each A atom is surrounded by six X atoms at the corners of an enclosing octahedron, and each X atom lies on a line between two A atoms, so that the A atoms form a primitive cubic lattice with X atoms at the centres of the cube edges.

**AX₃ Plutonium bromide (PuBr₃)**

This is a layer structure in which the A atoms are 8-coordinate.

AX₃ Tysonite (LaF₃)

This is a complicated structure in which the A atoms can be considered as having 11 or 9 coordination since the X atoms are at varying distances.

AX₃ Yttrium chloride (YCl₃)

Between two single close-packed layers of X atoms, the A atoms are located in two-thirds of the octahedral sites, so that each A atom is surrounded by six X atoms while each X atom is close to two A atoms. If the A atoms were removed, the structure would approximate to a cubic close-packed array of X atoms.

AX₄ Uranium fluoride (UF₄)

The structure comprises 8-coordinate A atoms in two non-equivalent approximately square antiprismatic environments and 2-coordinate X atoms.

AX₄ Uranium chloride (UCl₄)

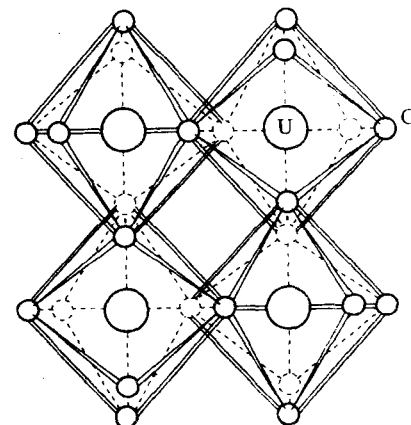
This is a 3D structure of 8:2 coordination with A atoms in a dodecahedral environment.

AX₃ Bismuth iodide (BiI₃)

As in YCl₃ the A atoms are located in two-thirds of the octahedral sites between two single close-packed layers of X atoms, with six X atoms round each A atom and two A atoms close to each X. If the A atoms were removed, the structure would approximate to hexagonal close-packing of X atoms.

AX₃ Uranium chloride (UCl₃)

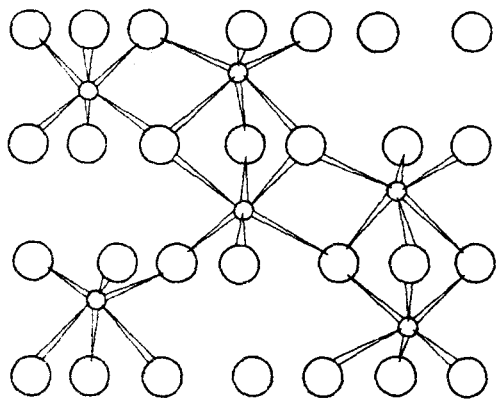
In this structure the A atoms are co-ordinated by a tricapped trigonal prism of nine X atoms which are approximately equidistant.



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A_2X_3 Corundum (α -aluminium oxide)

This structure may be regarded as a hexagonal close packed net of X atoms with A atoms regularly disposed in 2/3 of the octahedral holes with approximately octahedral coordination of A and tetrahedral coordination of X. It contains pairs of face-sharing AX_6 octahedra.

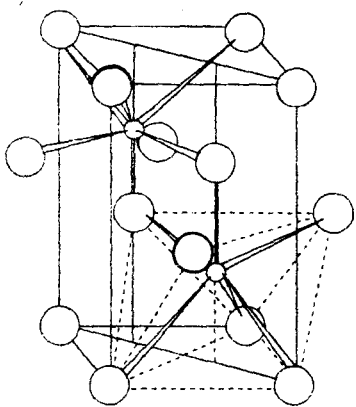


A_2X_3 γ -Aluminium oxide

This is essentially a defect spinel structure (*v.i.*) with cubic close packed X atoms and A atoms randomly distributed between octahedral and tetrahedral sites in the ratio 2 : 1.

A_2X_3 Rare earth sesquioxide A (hexagonal)

This structure contains 7-coordinate A atoms in an approximately face-capped octahedral environment.



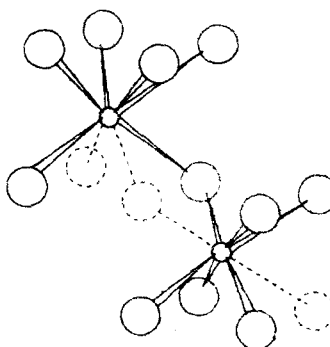
A_2X_3 Rare earth sesquioxide B (monoclinic)

This is a complicated structure containing a mixture

of 6-coordinate (octahedral) and 7-coordinate (monocapped trigonal prismatic) A atoms.

A_2X_3 Rare earth sesquioxide C (cubic)

This structure may be derived from that of fluorite (CaF_2) by removing one quarter of the anions in such a way as to generate 6-coordinate A atoms of two kinds. For one quarter of A, the missing neighbours are at the ends of a body diagonal and for the other three quarters, at the ends of a face diagonal. Both environments are distorted octahedra. The coordination of X is tetrahedral.

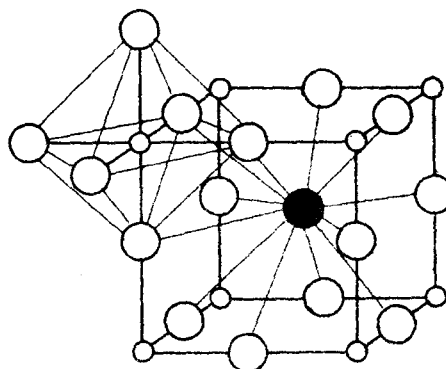


ABX_2 Iron sodium oxide ($FeNaO_2$)

This may be described as a sodium chloride superstructure, having approximately cubic close-packed X atoms with A and B atoms distributed regularly in the octahedral sites.

ABX_3 Perovskite ($CaTiO_3$)

The perovskite structure may perhaps be most easily envisaged as related to the ReO_3 structure with the additional metal atom in the void between vertex-sharing TiO_6 octahedra as shown below:



An alternative description is as a cubic close-packed set of A (Ca) and X (O) atoms arranged in such a way that the B (Ti) atoms occupy octahedral sites formed only by X atoms.

ABX₃ Ilmenite (FeTiO₃)

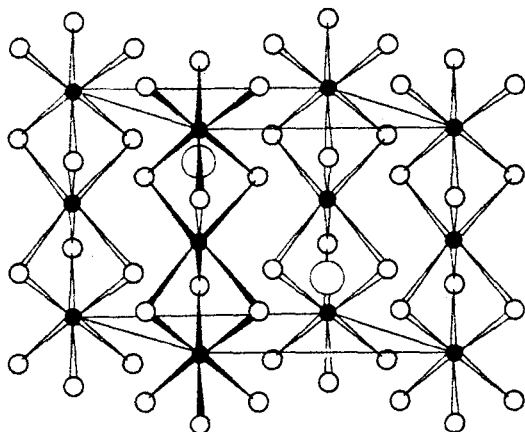
This structure comprises a hexagonal close-packed array of X (O) with A (Fe) and B (Ti) each occupying one third of the octahedral holes, and as such it can also be described as a corundum superstructure.

A₂B₂X₆ Deficit pyrochlore

This structure is described under A₂B₂X₇, Pyrochlore.

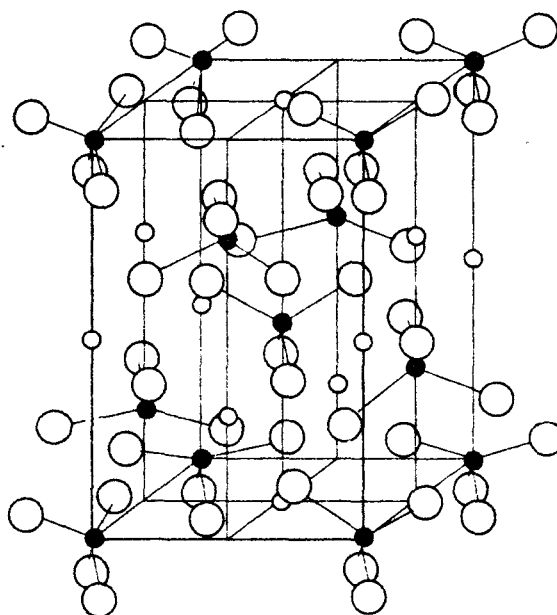
ABX₃ Caesium nickel chloride (CsNiCl₃)

This hexagonal structure contains chains of octahedral BX₆ groups sharing opposite faces. The A atoms are located between the chains.



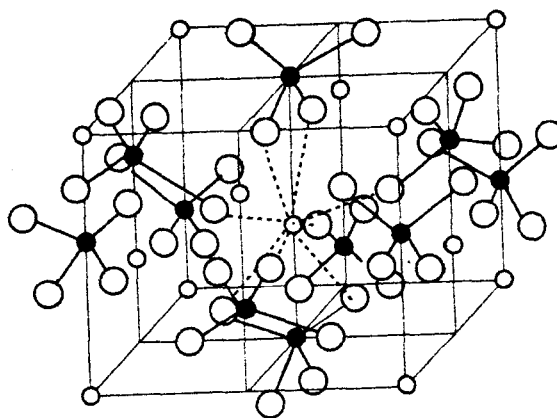
ABX₄ Scheelite (CaWO₄)

This tetragonal structure contains flattened BX₄ tetrahedra with 8-coordinate A (Ca) atoms in the interstices.



ABX₄ Zircon (ZrSiO₄)

This tetragonal structure contains regular BX₄ tetrahedra with 8-coordinate A (Zr) atoms in the interstices.



ABX₄ Monazite (CePO₄)

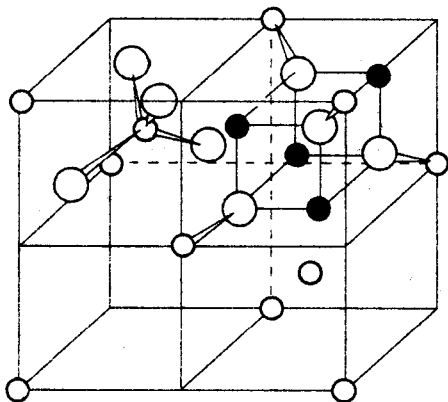
This monoclinic structure contains BX₄ tetrahedra with 8-coordinate A (Ce) in the interstices.

AB₂X₄ Spinel (MgAl₂O₄)

This structure consists of cubic close-packed X atoms with A atoms in tetrahedral sites and B atoms in octahedral sites. The unit cell contains 32 X atoms

Introduction

and although there are 64 tetrahedral and 32 octahedral sites, there are equivalent positions for only 8 and 16 of these respectively as required by the spinel structure. Each X atom has tetrahedral coordination with three neighbours from the octahedrally coordinated B atom and one from the tetrahedrally coordinated A atom.



AB_2X_4 Inverse spinel

This differs from the normal spinel structure by the occupancy of the tetrahedral sites by half the B atoms, and the octahedral sites by the rest of B and all the A atoms, and is therefore sometimes indicated by the formula $B[AB]X_4$. The arrangement of A and B in the octahedral sites may be random or ordered. Additionally, some spinels have completely random occupation across the tetrahedral and octahedral sites.

AB_2X_6 Potassium hexafluoromanganate (K_2MnF_6)

This structure may be described as a close-packed array of $2B + 6X$ atoms in an alternating cubic-hexagonal sequence with the A (Mn) atoms in certain octahedral sites between groups of six X atoms. The K_2GeF_6 and K_2PtCl_6 structures are closely related but differ in the sequence of close-packing.

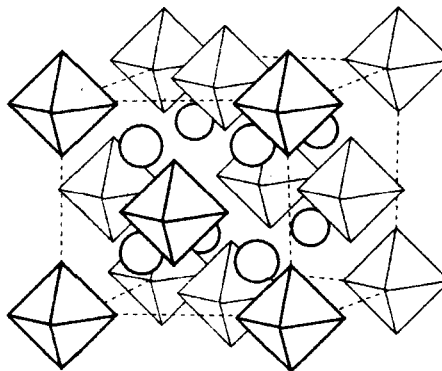
AB_2X_6 Potassium hexafluorogermanate (K_2GeF_6)

This structure may be described as a hexagonal close-packed array of $2B + 6X$ atoms with A (Ge) atoms in certain octahedral sites between groups of six X atoms.

AB_2X_6 Potassium hexachloroplatinate (K_2PtCl_6)

This structure may be described as a cubic close-packed array of $2B + 6X$ atoms with A (Pt) atoms in

certain octahedral sites. Each B atom is surrounded by 12 equidistant X atoms. It is equivalent to the fluorite (CaF_2) structure with Ca replaced by AX_6 and F by B.



AB_3X_6 Cryolite (Na_3AlF_6)

This structure may be described as a cubic close-packed array of $2B + 6X$ with the remaining A and B atoms in octahedral holes such that the close-packed B atoms each have 12 equidistant neighbours. It is closely related both to K_2PtCl_6 and perovskite. Cryolite itself is slightly distorted from cubic symmetry.

AB_2CX_6 Elpasolite (NaK_2AlF_6)

This is cubic and closely related to cryolite, but with the replacement of one third of the B atoms by atoms of a different kind.

$A_2B_2X_7$ Pyrochlore

This cubic structure may be described as two interpenetrating frameworks. The first is a network of BX_6 octahedra linked through their vertices in such a way that their centres form a tetrahedral diamond-like array. A group of four such octahedra is depicted below. Each BX_6 unit is linked to six others. This array has stoichiometry B_2X_6 and the deficit pyrochlore structure, $A_2B_2X_6$, simply has A atoms placed in voids in the network. In $A_2B_2X_7$ structures, however, the A_2X atoms form a second network, typically of a cuprite-like kind, which interpenetrates the voids in the B_2X_6 framework.

