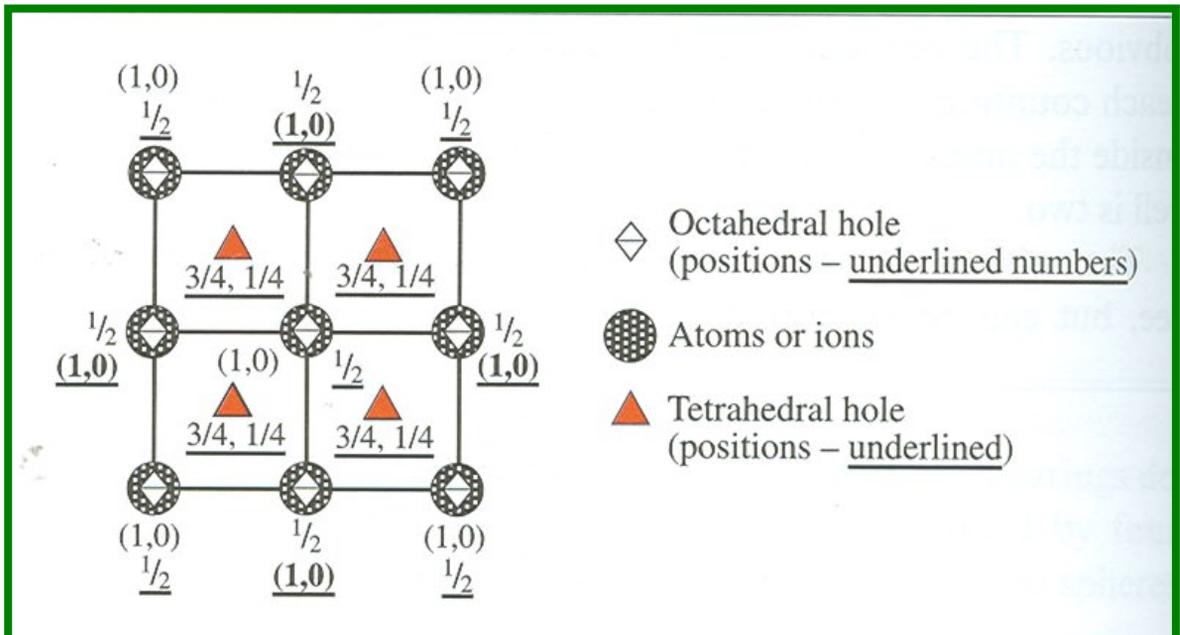
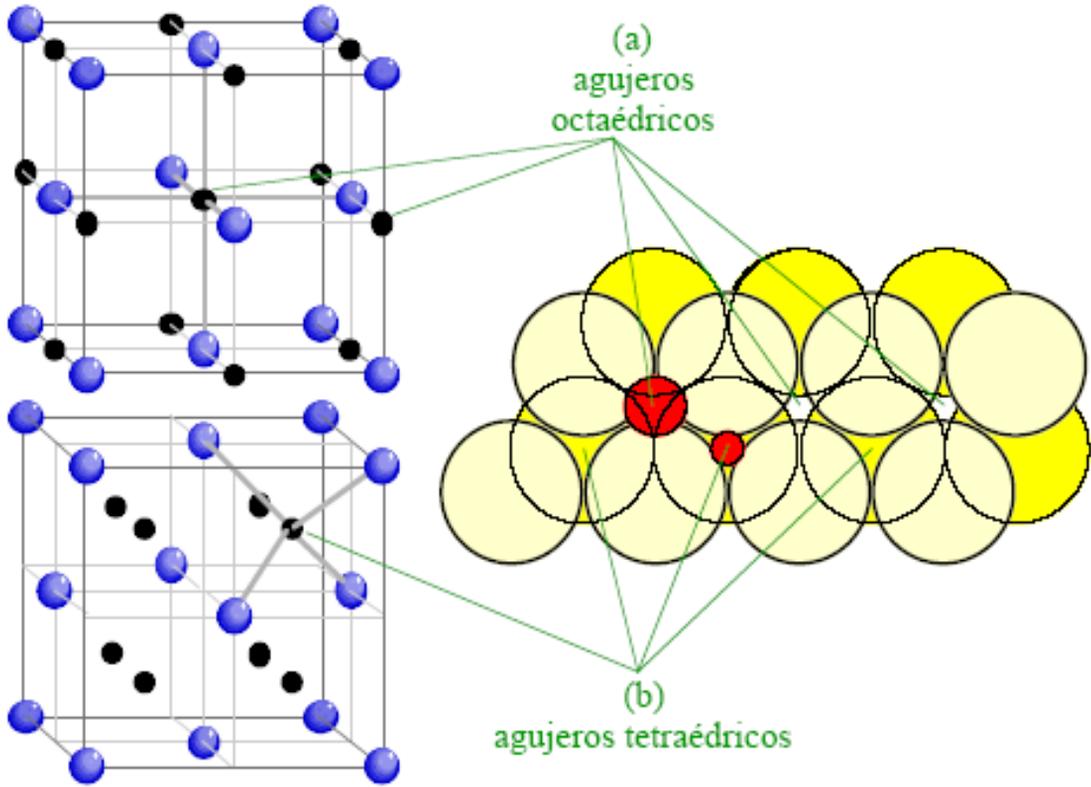
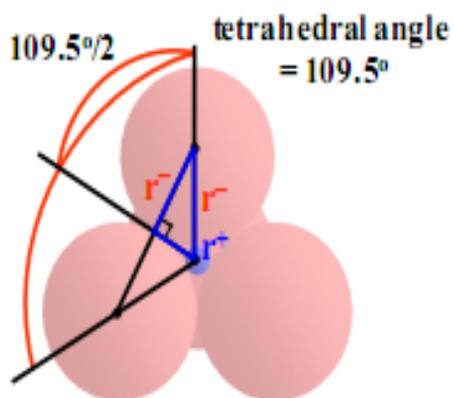


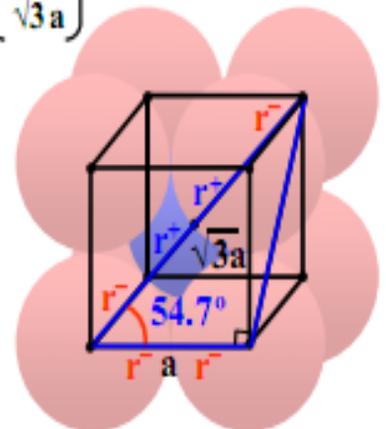
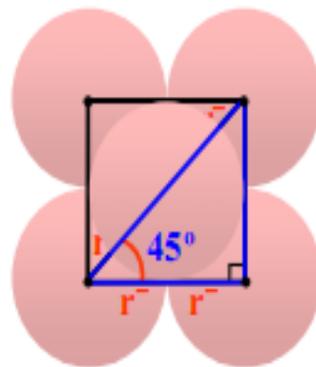
Consideraciones sobre estructuras representativas



Tetrahedral, Octahedral, Cubic Hole Radius Ratio



$$\cos^{-1}\left(\frac{a}{\sqrt{3}a}\right) = 54.7^\circ$$



$$\frac{r^+}{r^- + r^+} = \sin \frac{109.5^\circ}{2} = 0.817$$

$$\frac{2r^+}{2r^- + 2r^+} = \cos 45^\circ = 0.707$$

$$\frac{2r^+}{2r^- + 2r^+} = \cos 54.7^\circ = 0.577$$

$$r^+ = 0.817r^- + 0.817r^+$$

$$r^+ = 0.707r^- + 0.707r^+$$

$$r^+ = 0.577r^- + 0.577r^+$$

$$0.183r^+ = 0.817r^-$$

$$0.293r^+ = 0.707r^-$$

$$0.423r^+ = 0.577r^-$$

$$\frac{r^+}{r^-} = 0.225$$

$$\frac{r^+}{r^-} = 0.414$$

$$\frac{r^+}{r^-} = 0.732$$

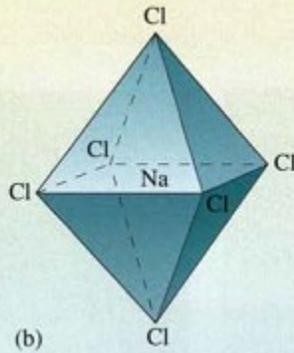
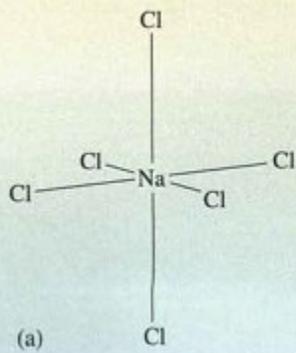
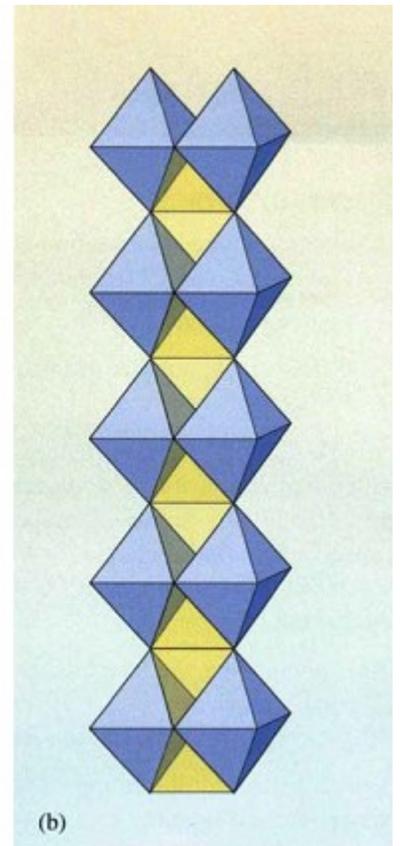
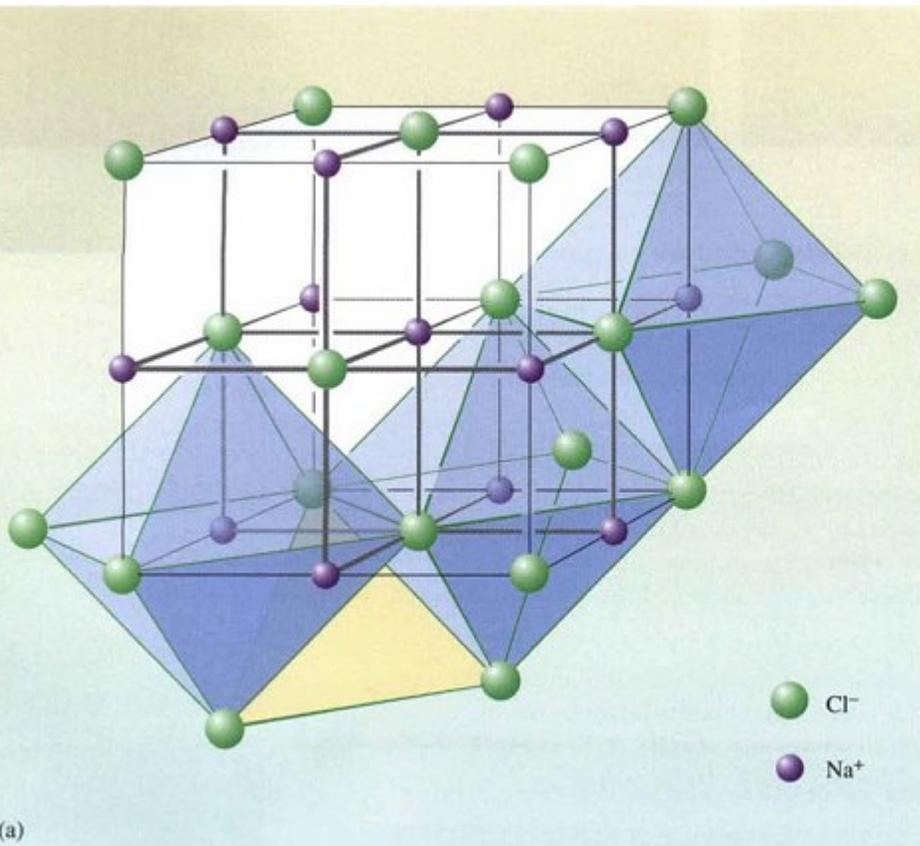


Figure 4.7 (a) An octahedron of chloride ions around a sodium ion in the NaCl crystal; (b) an NaCl_6 octahedron, shown as a solid shape.

Figure 4.8 (a) The NaCl structure, showing edge-sharing of (blue) octahedra (a tetrahedral space is also shown, shaded in yellow); (b) extended NaCl structure showing edge-sharing octahedra, and also depicting adjacent tetrahedral holes (in yellow).

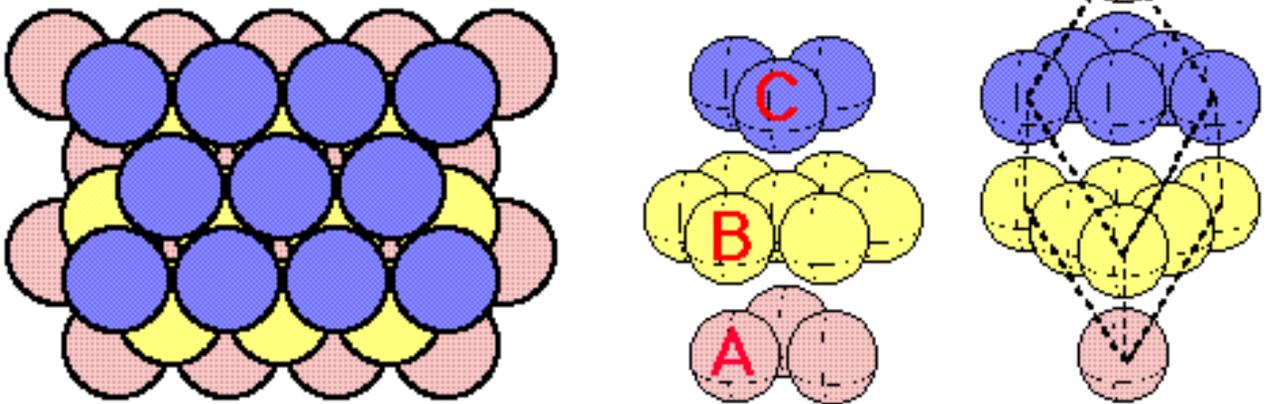


CONSIDERACIONES SOBRE ESTRUCTURAS REPRESENTATIVAS:

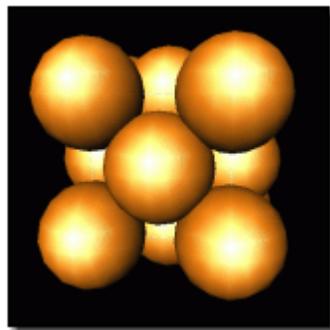
- *En el empaquetamiento compacto hcp y ccp el número de coordinación es 12*
- *Los elementos metálicos son los que tienen preferencia por esta estructura, muchos también son bcc*
- *La eficiencia del empaquetamiento es del 74 % (el 74% del espacio está ocupado)*
- *Se presentan huecos intersticiales tetraédricos y octaédricos. Para los tetraédricos $r = 0.225$ (dos por cada esfera) y para los octaédricos $r = 0.414$ (uno por cada esfera)*

como llegaría usted a este número ?? Inténtelo

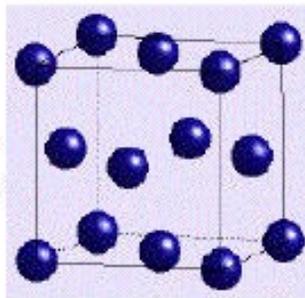
Cubic close packing (ABCABC...)



Tres vistas del empaquetamiento cúbico compacto.
También aquí se ven 8 huecos tetraédricos y 6 octaédricos
alrededor de cada esfera del empaquetamiento

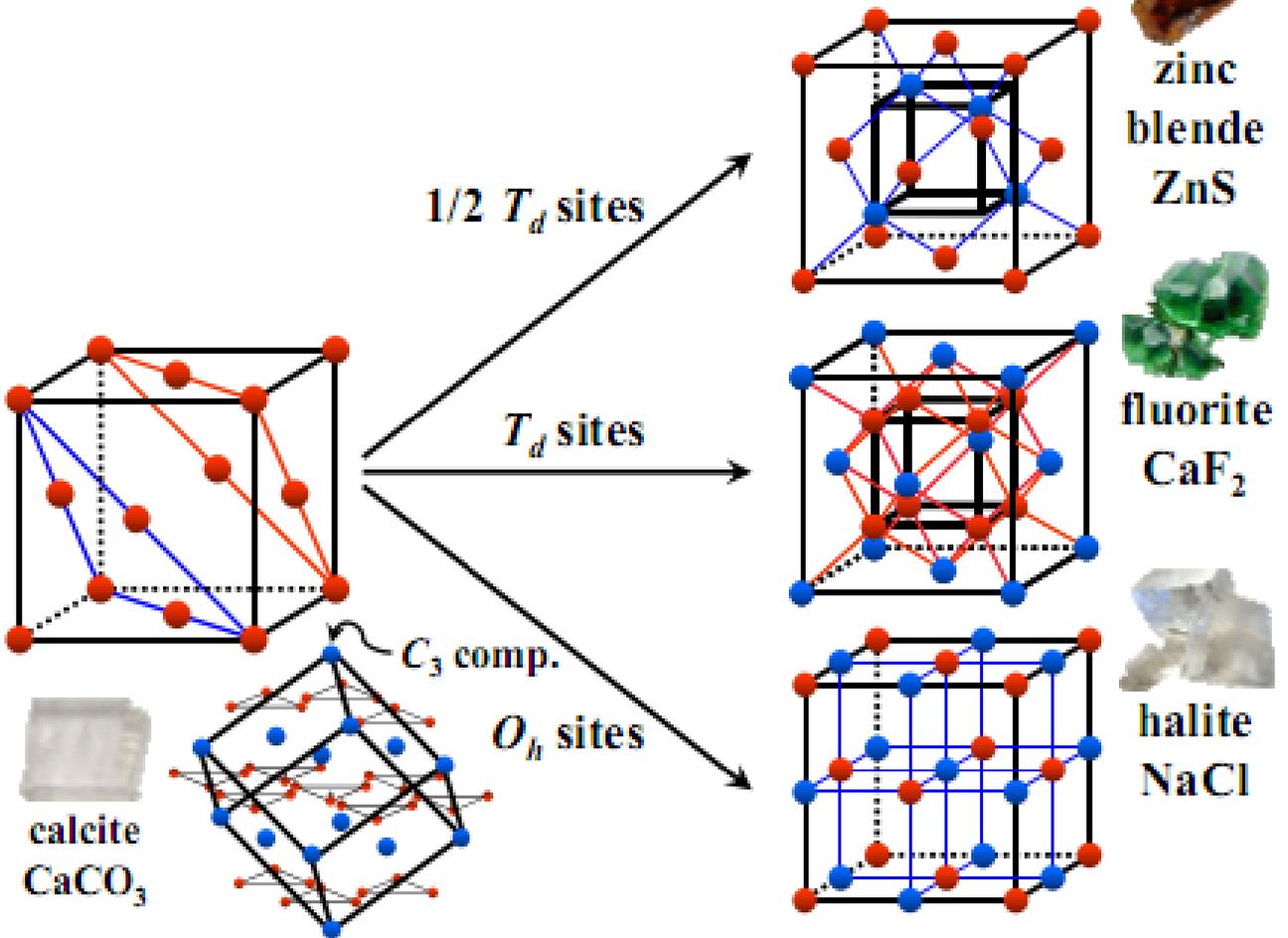


Algunas estructuras típicas pueden observarse si uno piensa que un tipo de átomos están arreglados en un empaquetamiento ccp o hcp y que el otro átomo ocupa huecos (la totalidad o una fracción de ellos) T u O



CCP

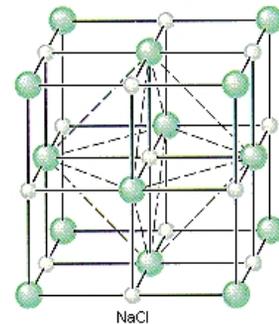
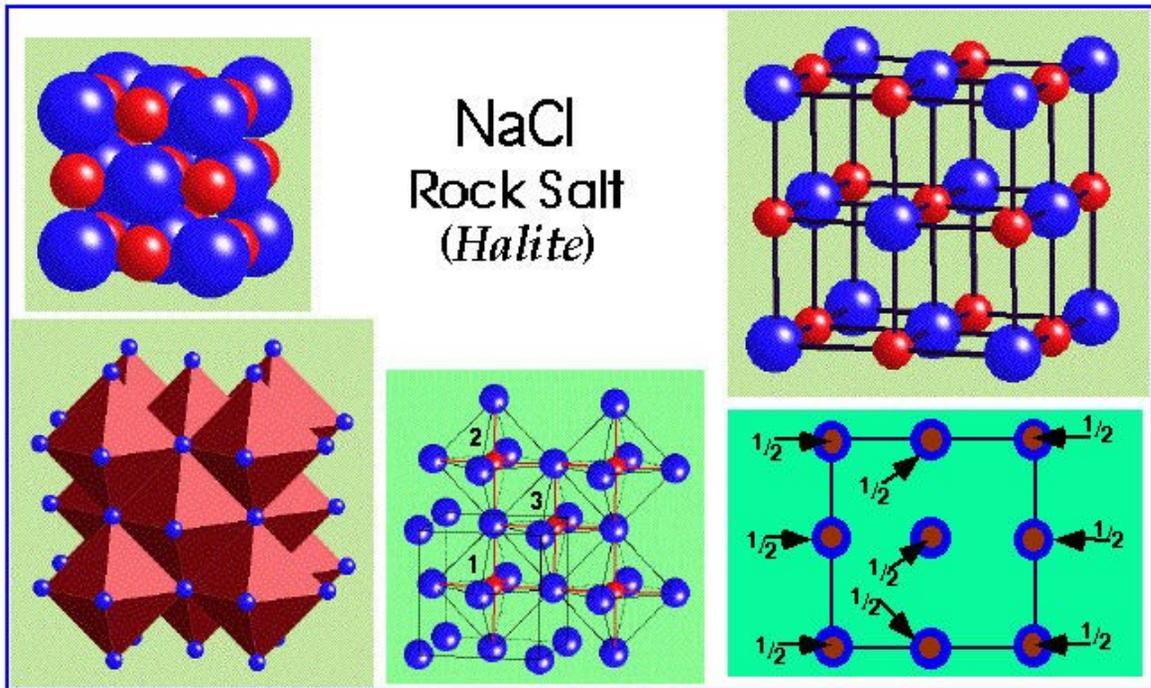
Cubic Derived Lattices



Algunas estructuras binarias que se derivan del llenado de huecos por un tipo de átomo en el arreglo ccp o hcp de otros

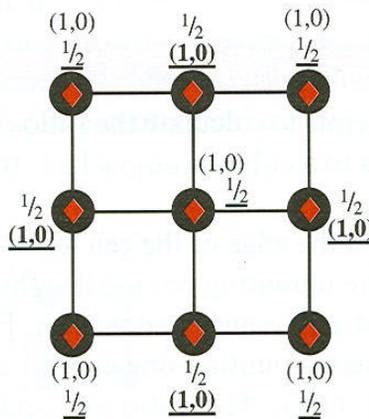
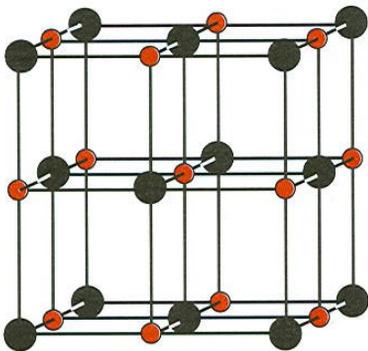
Fórmula	Tipo y fracción de sitios ocupados	CCP Empacamiento cúbico	HCP Empacamiento hexagonal
AB	Todos los octaédricos	<u>NaCl</u> <i>Sal de roca</i>	<u>NiAs</u> <i>Arseniuro de Níquel</i>
	La mitad de los tetraédricos (T+ or T-)	<u>ZnS</u> <i>Blenda de Zinc (Sphalerite)</i>	<u>ZnS</u> <i>Wurtzita</i>
AB ₂	Todos los tetraédricos	<u>Na₂O</u> <i>Anti-Fluorita</i> <u>CaF₂</u> <i>Fluorita</i>	No se conoce
AB ₃	Todos los tetraédricos y octaédricos	<u>Li₃Bi</u>	No se conoce
A ₂ B	La mitad de los octaédricos (alternando capas de ocupados/vacío)	<u>CdCl₂</u> (<i>cloruro de cadmio</i>)	<u>CdI₂</u> (<i>yoduro de cadmio</i>)
	La mitad de los octaédricos (arreglo ordenado de mallas)	<u>TiO₂</u> (<i>Anatasa</i>)	<u>CaCl₂</u> <u>TiO₂</u> (<i>Rutilo</i>)
A ₃ B	Un tercio de octaedros alternan capas, 2/3 ocupados/vacío	<u>YCl₃</u>	<u>BiI₃</u>

ESTRUCTURAS DERIVADAS DEL ARREGLO CCP

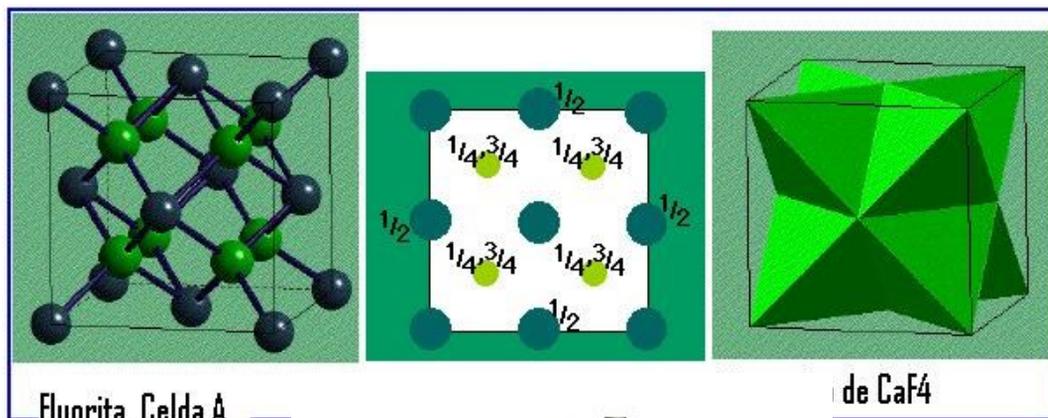


- Arreglo compacto CCP de Cloros (Cl^-) con Na^+ ocupando todos los huecos octaédricos.
- La malla es FCC
- El motivo es Cl en $(0,0,0)$ Na en $(1/2,0,0)$
- 4 unidades NaCl por celda unitaria.
- Coordinación 6:6 (octaédrica)
- Los cationes y aniones son topológicamente idénticos

- La estructura tipo NaCl es adoptada por sistemas “iónicos covalente e intermetálicos, indistintamente. La mayor parte de los haluros de metales alcalinos la adopta (excepto CsCl, CsBr y CsI)
- La adoptan también la mayor parte de los óxidos metálicos y calcogenuros de tierras alcalinas
- También la adoptan los nitruros, carburos e hidruros (ZrN, TiC, NaH).



ESTRUCTURAS DE FLUORITA CaF_2 Y ANTIFLUORITA Na_2O



- Arreglo CCP de Ca_2^+ con F^- en los huecos tetraédricos
- El tipo de malla es FCC
- Motivo: Ca^{2+} en $(0,0,0)$ y 2F^- en $(1/4,1/4,1/4)$ y $(3/4,3/4,3/4)$
- 4 Unidades de CaF_2 por celda unitaria $Z=4$
- La coordinación de Ca^{2+} es 8 (cúbica) y la de F^- es 4 (tetraédrica)
- En la celda de la antifluorita se invierten las posiciones de cationes y aniones

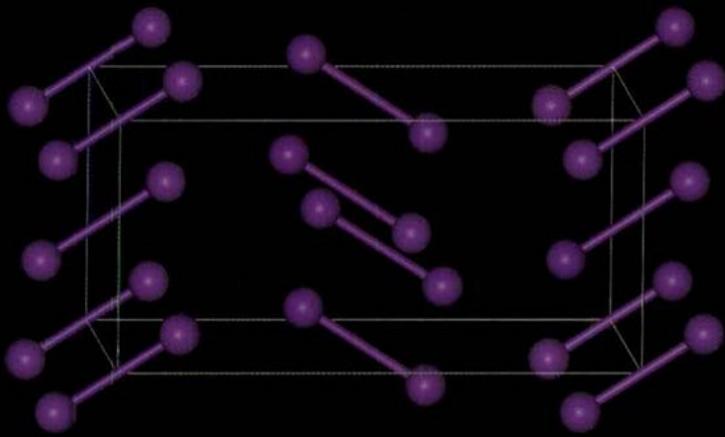
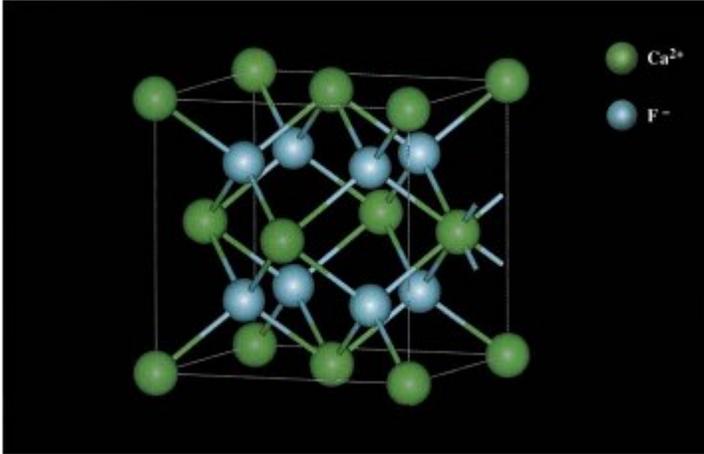
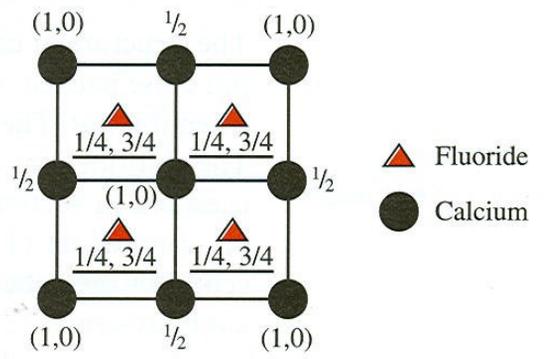
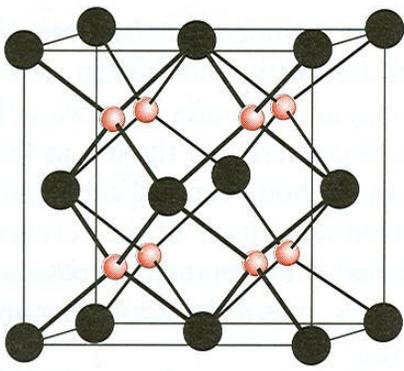
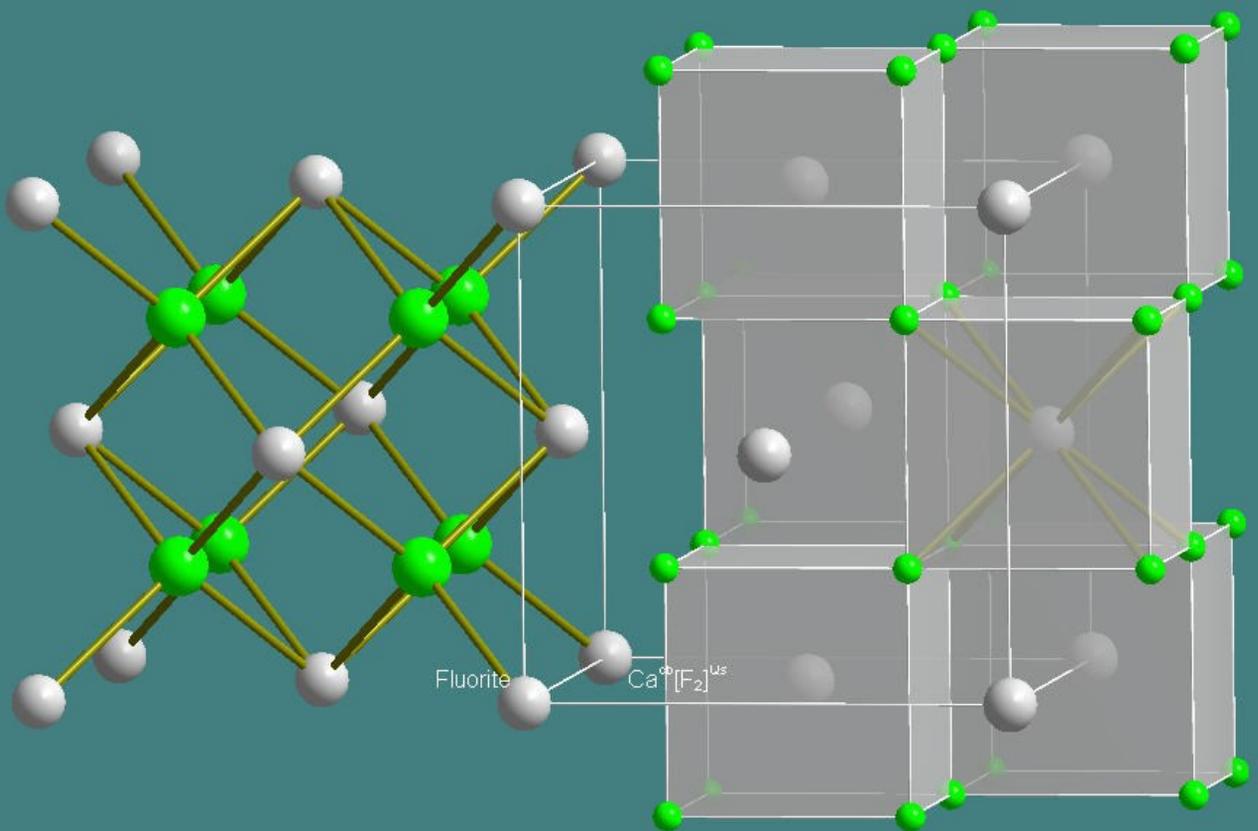
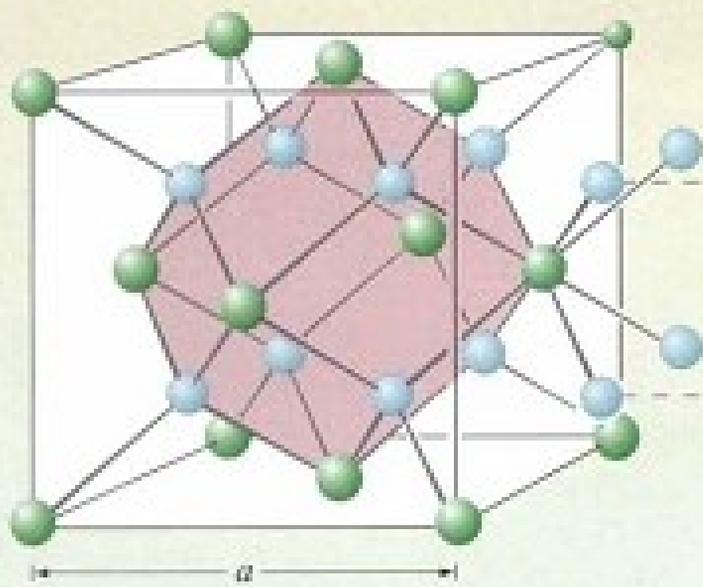


Figure 1.4
(a) Crystals of iodine;
(b) the structure of solid iodine.

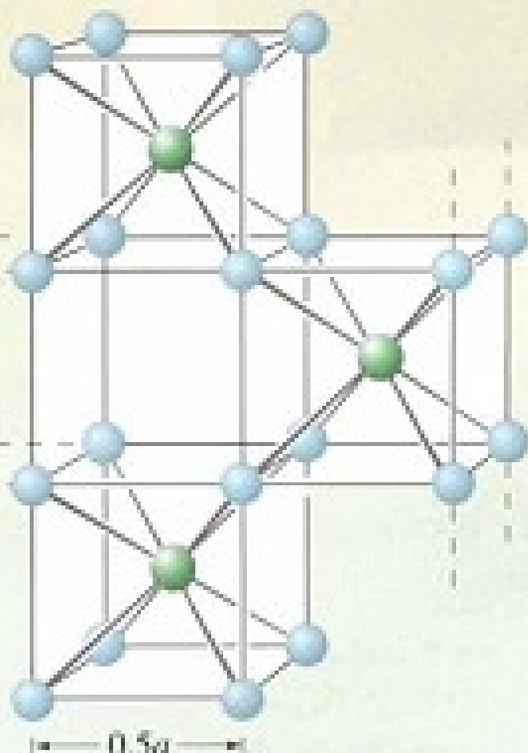


Estructura de CaF_2

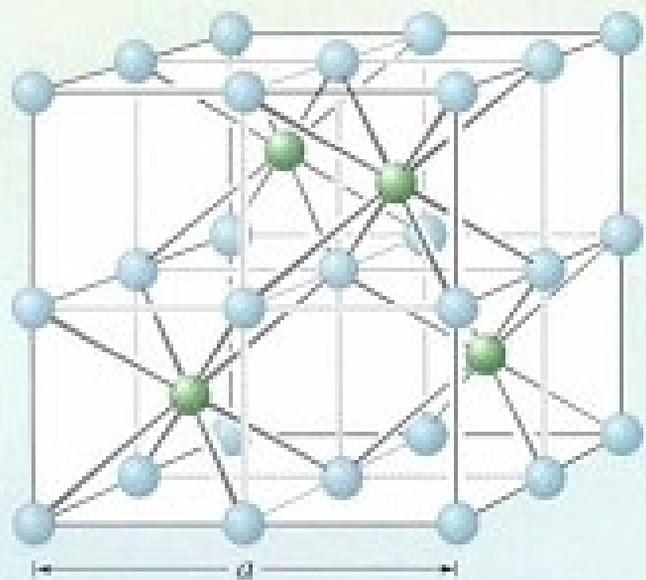




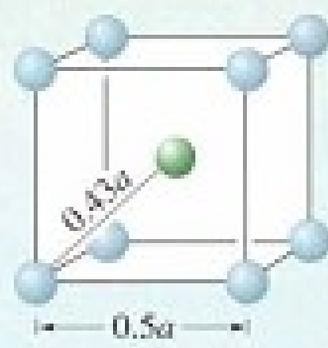
(b)



(c)

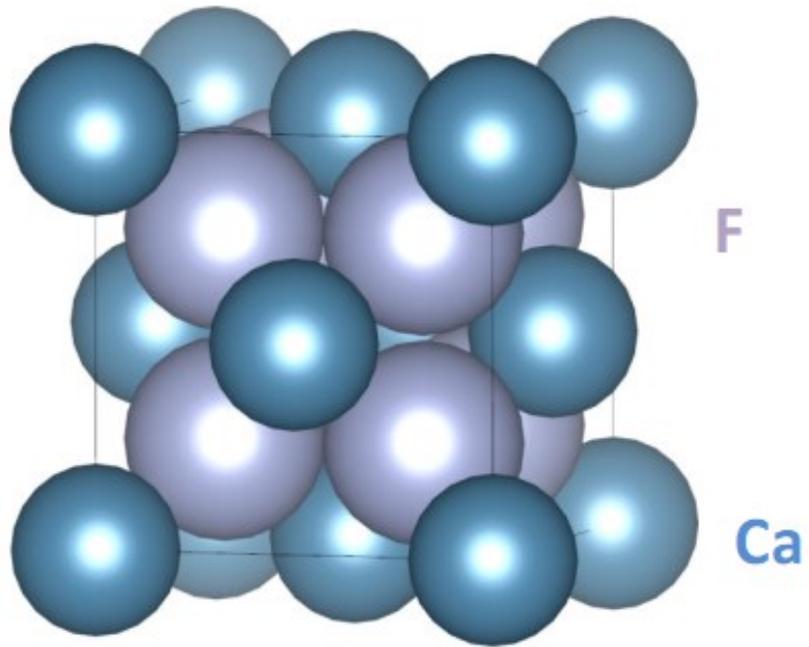


(d)

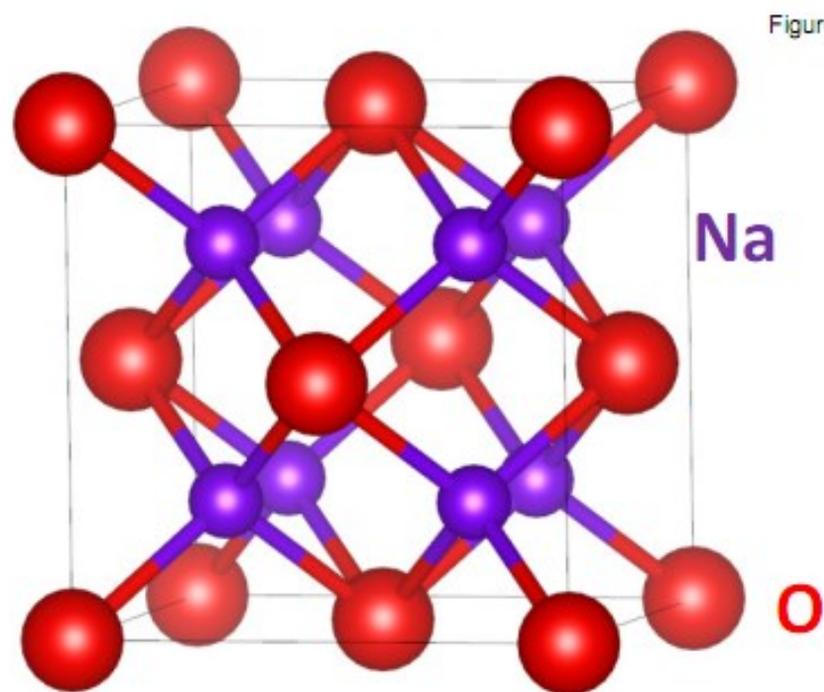


(e)



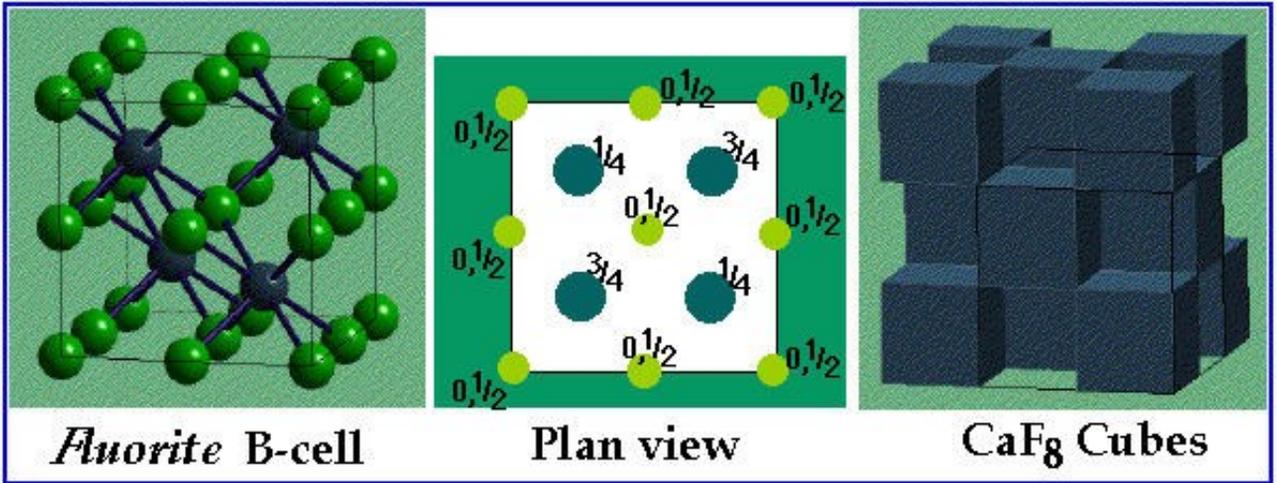


CaF_2 (*fluorite*)



Na_2O (*antifluorite*)

Celda tipo B de la fluorita



La estructura de fluorita la adoptan los fluoruros de cationes divalentes grandes, SrCl_2 , BaCl_2 y los óxidos de cationes tetravalentes grandes (Zr, Hf, Ce, Th, U).

La antifluorita la adoptan los óxidos y calcogenuros de metales alcalinos

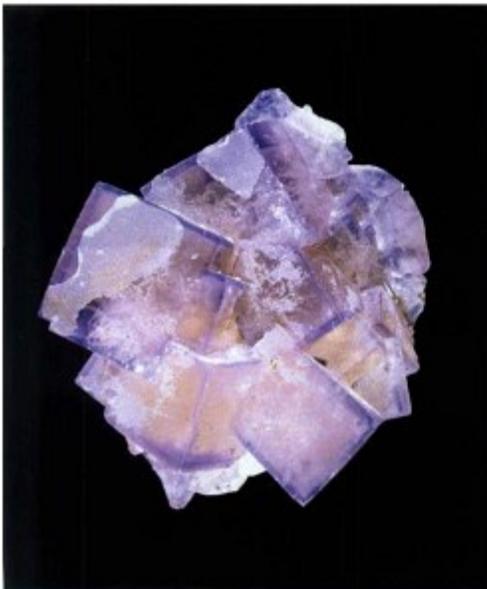
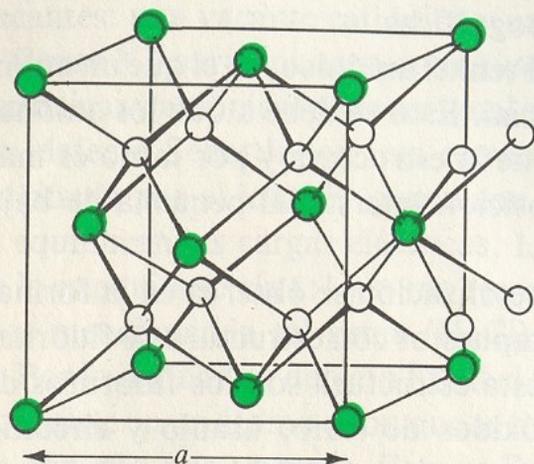


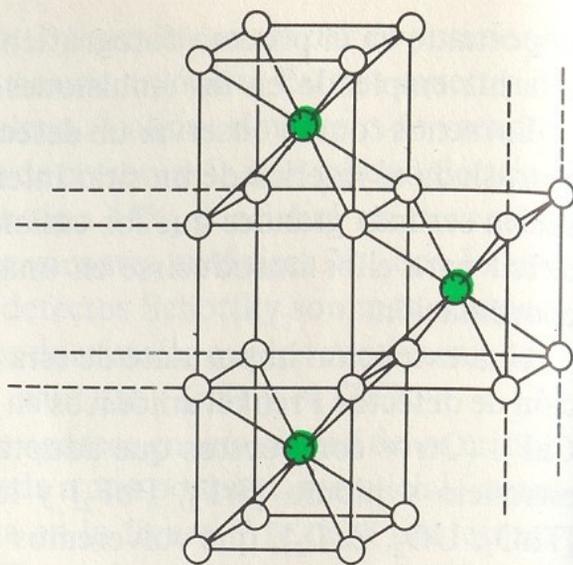
Figure 4.12 The mineral Blue John, which has the fluorite structure; the name is a corruption of the French *bleu-jaune*, which describes the main colours in the mineral.



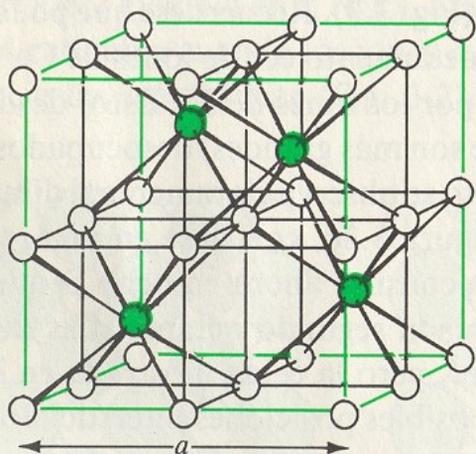
Figure 4.13 A vase made from Blue John.



(a)

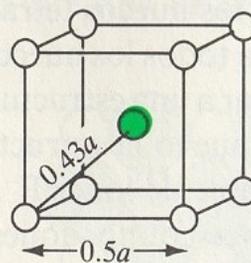


(b)



(c)

● Cation ○ Anion



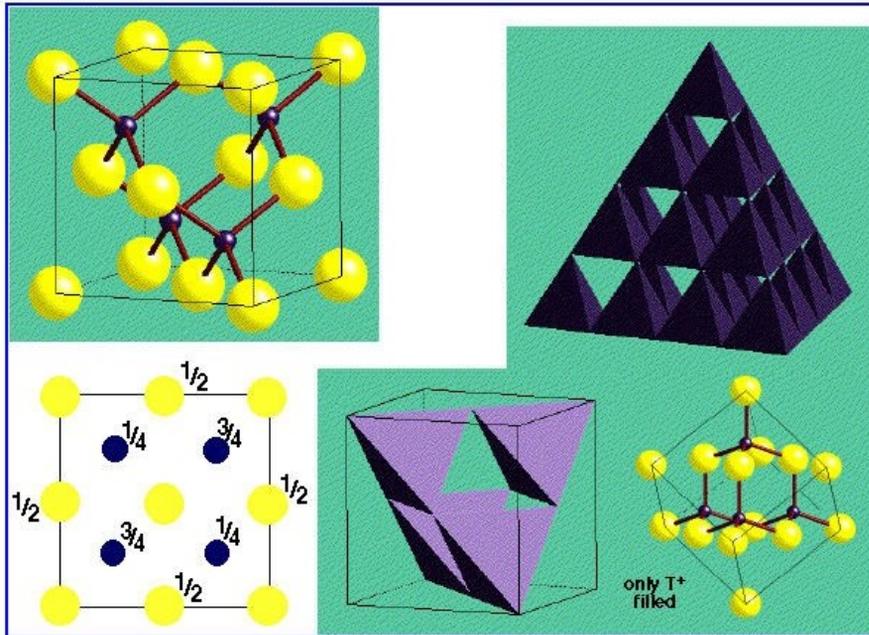
(d)

Figura 3.3 Estructura cristalina de la fluorita, MX_2 . (a) Celda unitaria como empaquetamiento ecc de cationes. (b) y (c) La misma estructura redibujada como una red cúbica simple de aniones. En la figura (c) la celda unitaria se marca con un trazo coloreado. (d) Dimensiones de la celda.

Table 1.10 *Some compounds with fluorite or antiferite structure, a/Å*

Fluorite structure				Antiferite structure			
CaF ₂	5.4626	PbO ₂	5.349	Li ₂ O	4.6114	K ₂ O	6.449
SrF ₂	5.800	CeO ₂	5.4110	Li ₂ S	5.710	K ₂ S	7.406
SrCl ₂	6.9767	PrO ₂	5.392	Li ₂ Se	6.002	K ₂ Se	7.692
BaF ₂	6.2001	ThO ₂	5.600	Li ₂ Te	6.517	K ₂ Te	8.168
CdF ₂	5.3895	UO ₂	5.372	Na ₂ O	5.55	Rb ₂ O	6.74
β-PbF ₂	5.940	NpO ₂	5.4334	Na ₂ S	6.539	Rb ₂ S	7.65

Blenda de zinc



- Arreglo CCP de S^{2-} con iones Zn^{2+} en la mitad de los huecos tetraédricos (solo T^+ o T^- llenos)
- Tipo de malla FCC
- $Z=4$, 4 unidades de ZnS por unidad de celda
- Motivo S^{2-} en $(0,0,0)$ Zn^{2+} en $(1/4,1/4,1/4)$
- Coordinación 4:4 (tetraédrica)
- Los sitios de cationes y aniones son topológicamente idénticos

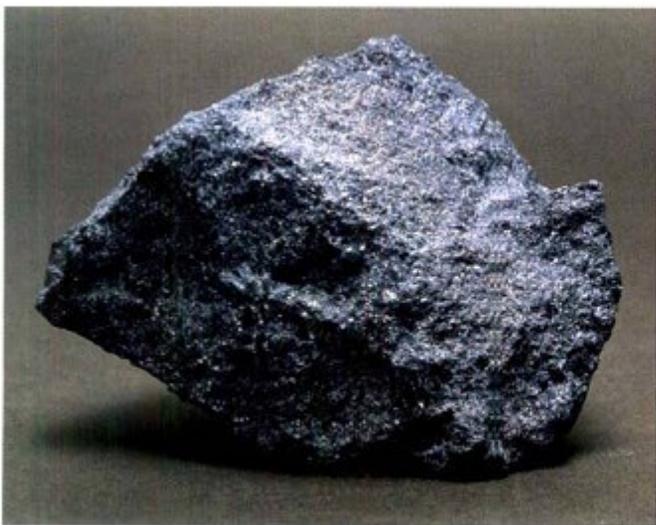


Figure 4.9 Crystals of sphalerite (Black Jack).

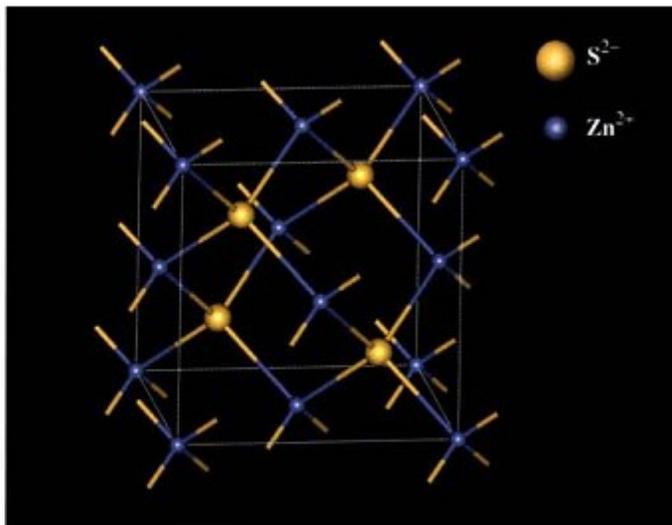
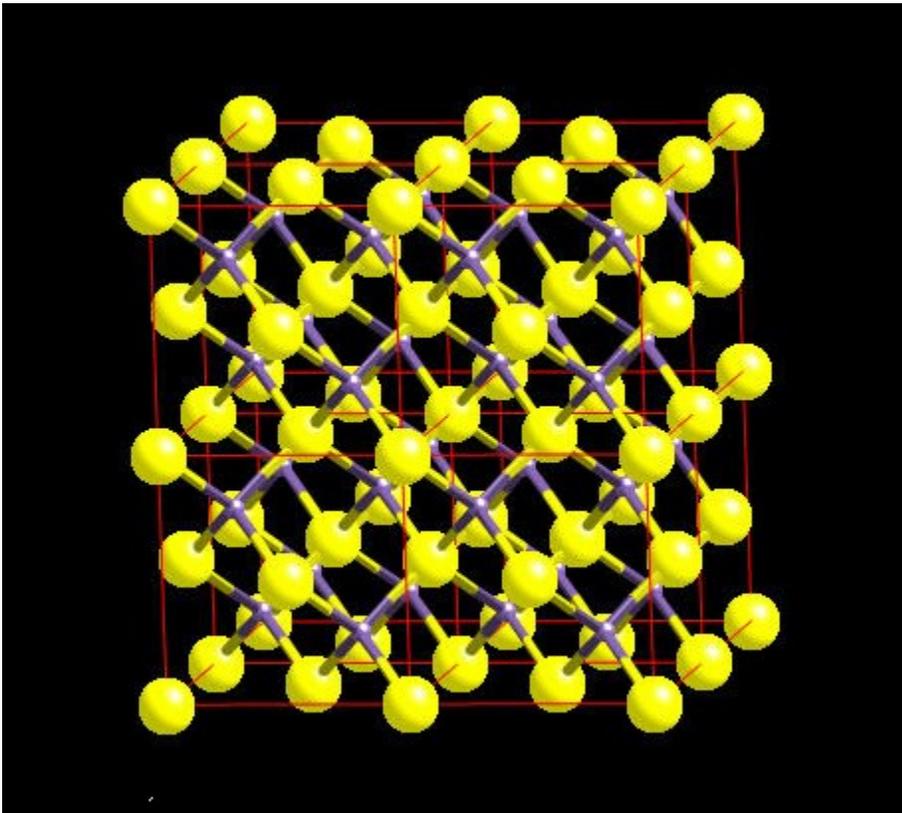
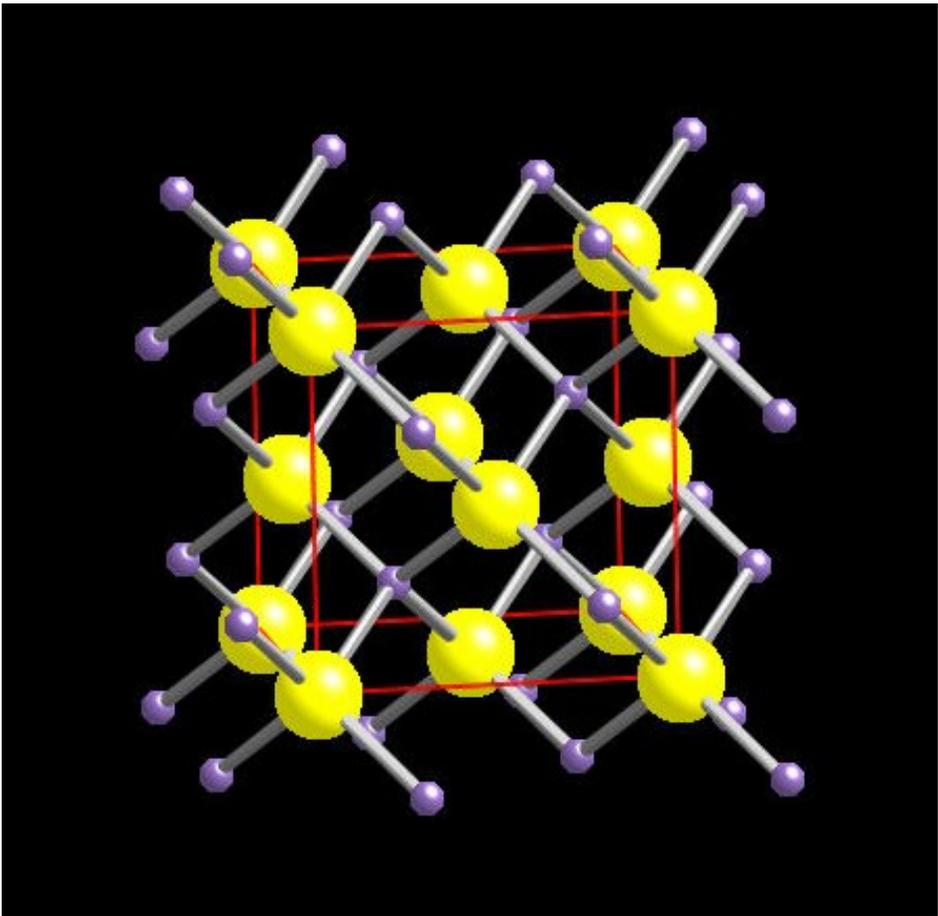
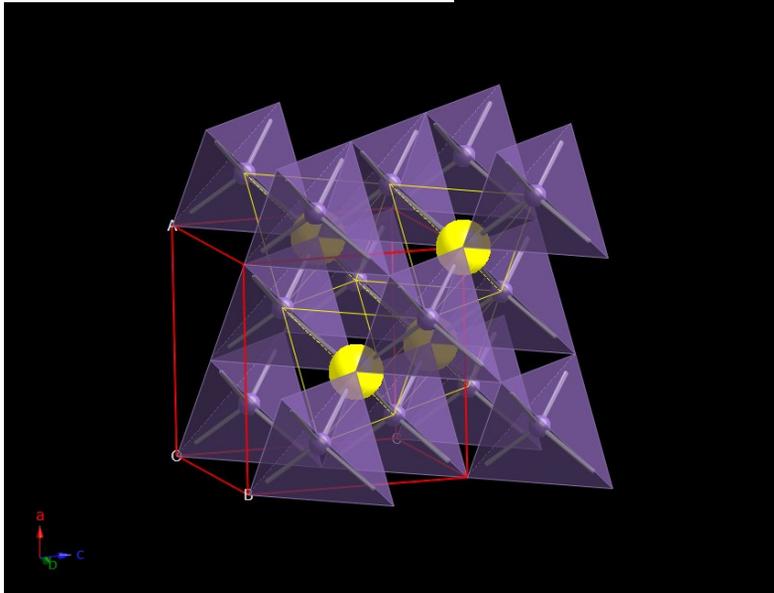
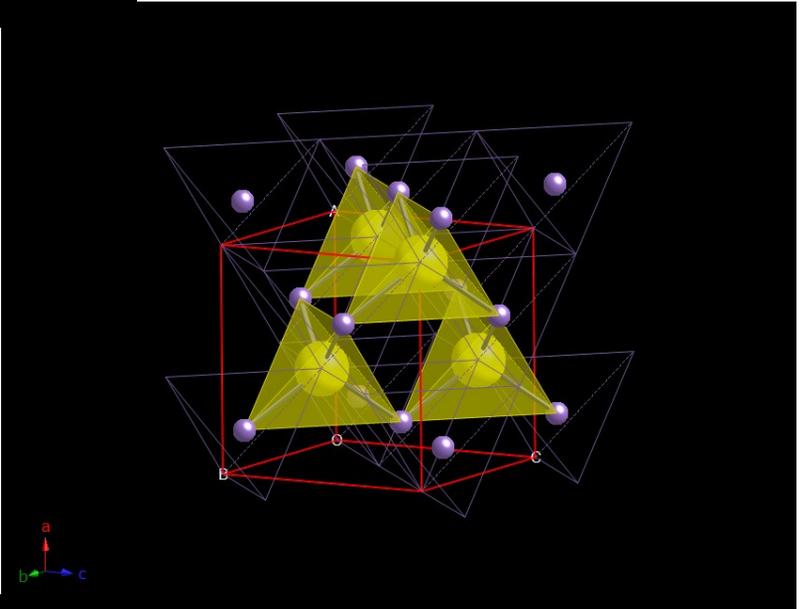
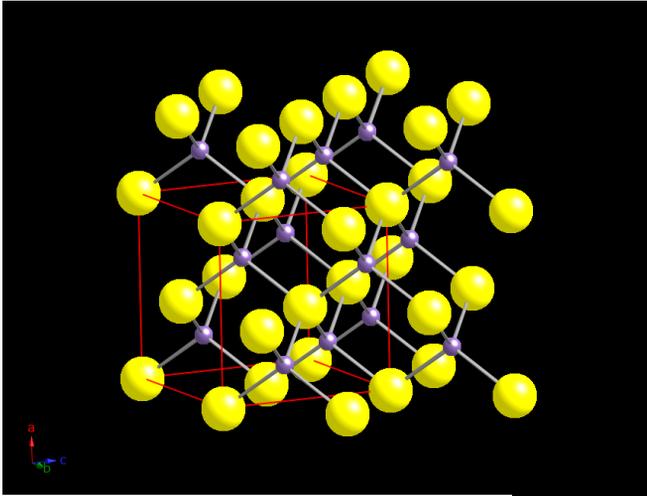
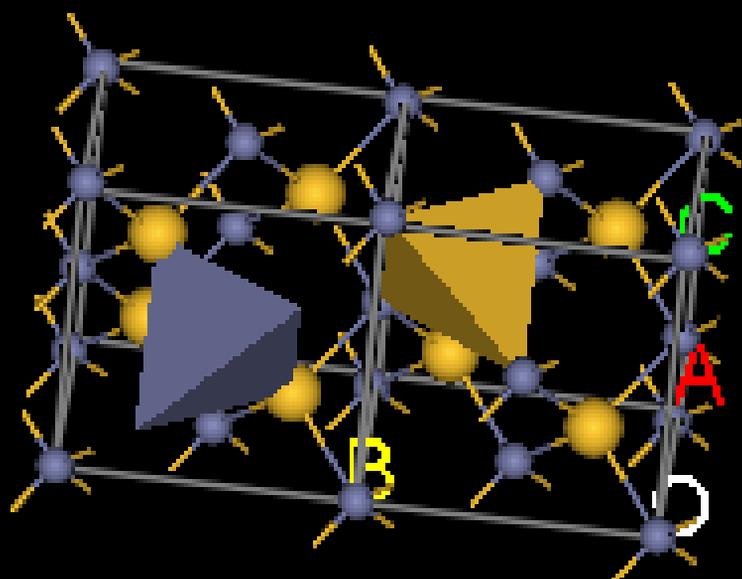
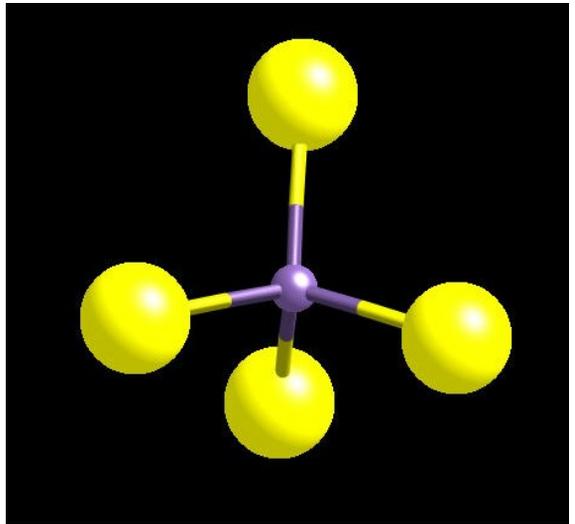
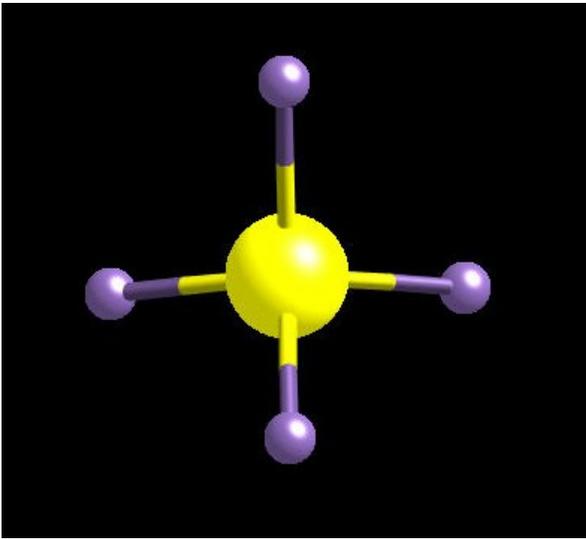
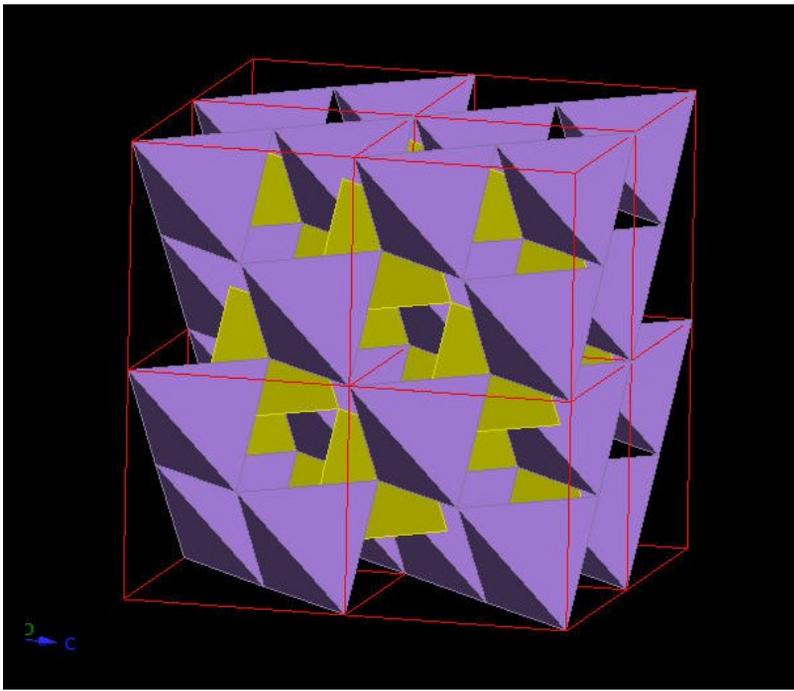


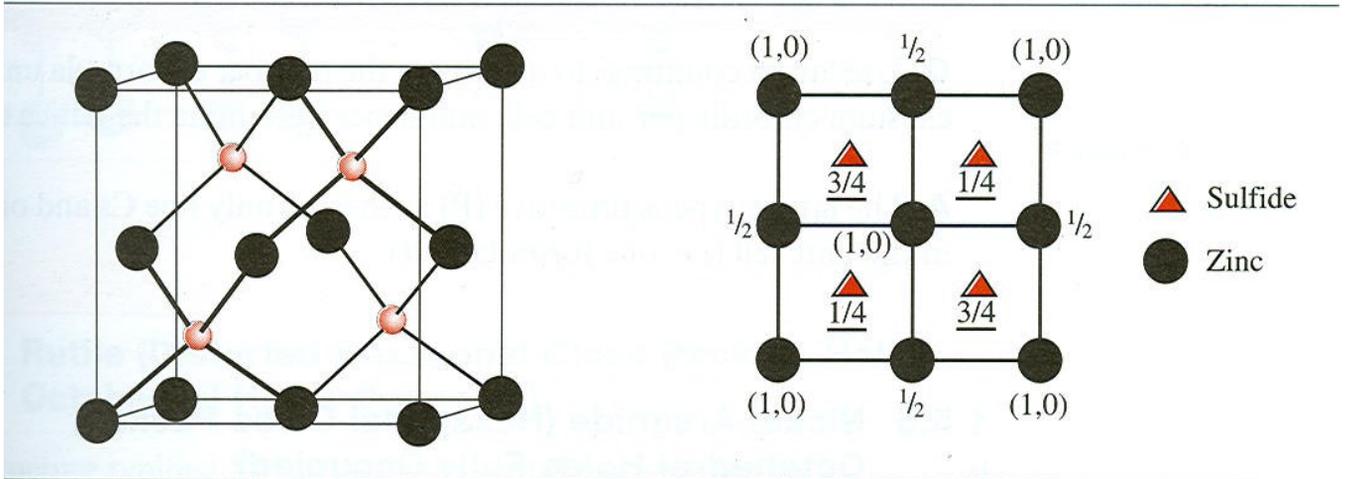
Figure 4.10 Unit cell of zinc blende.



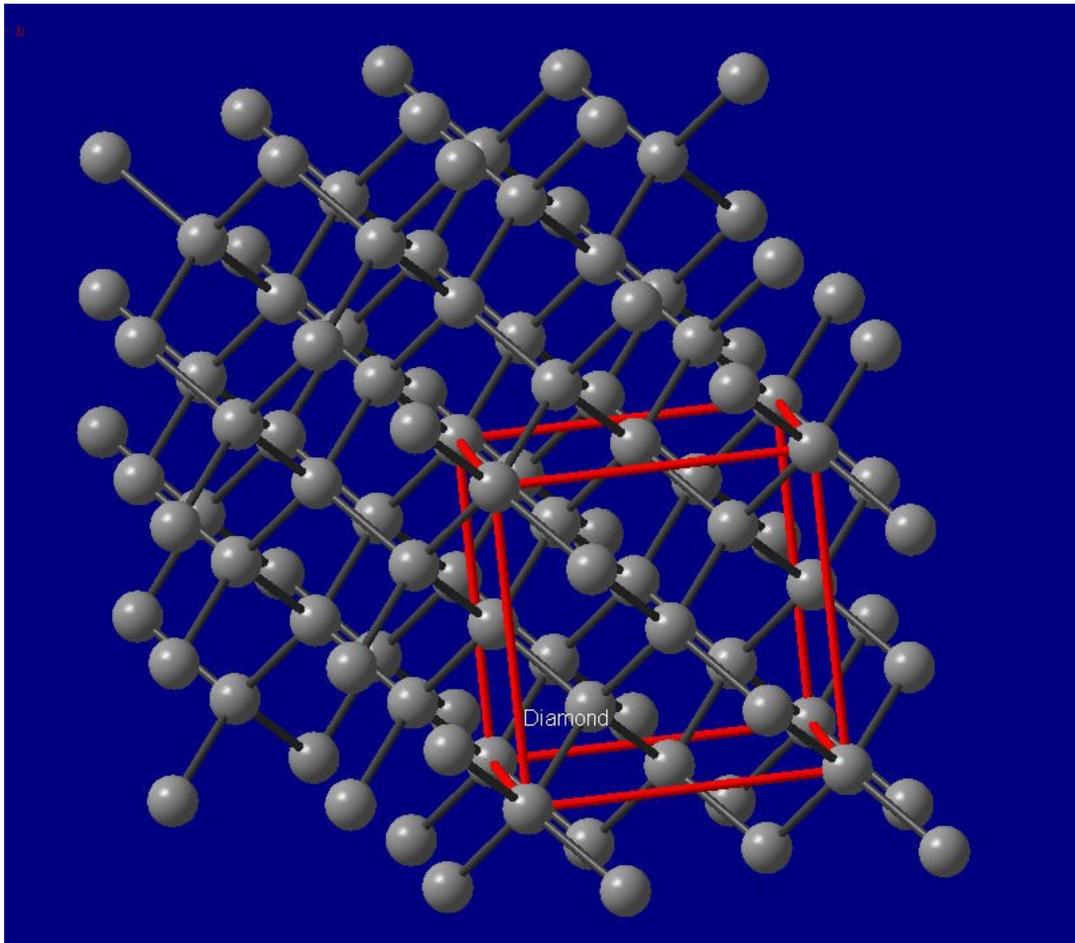






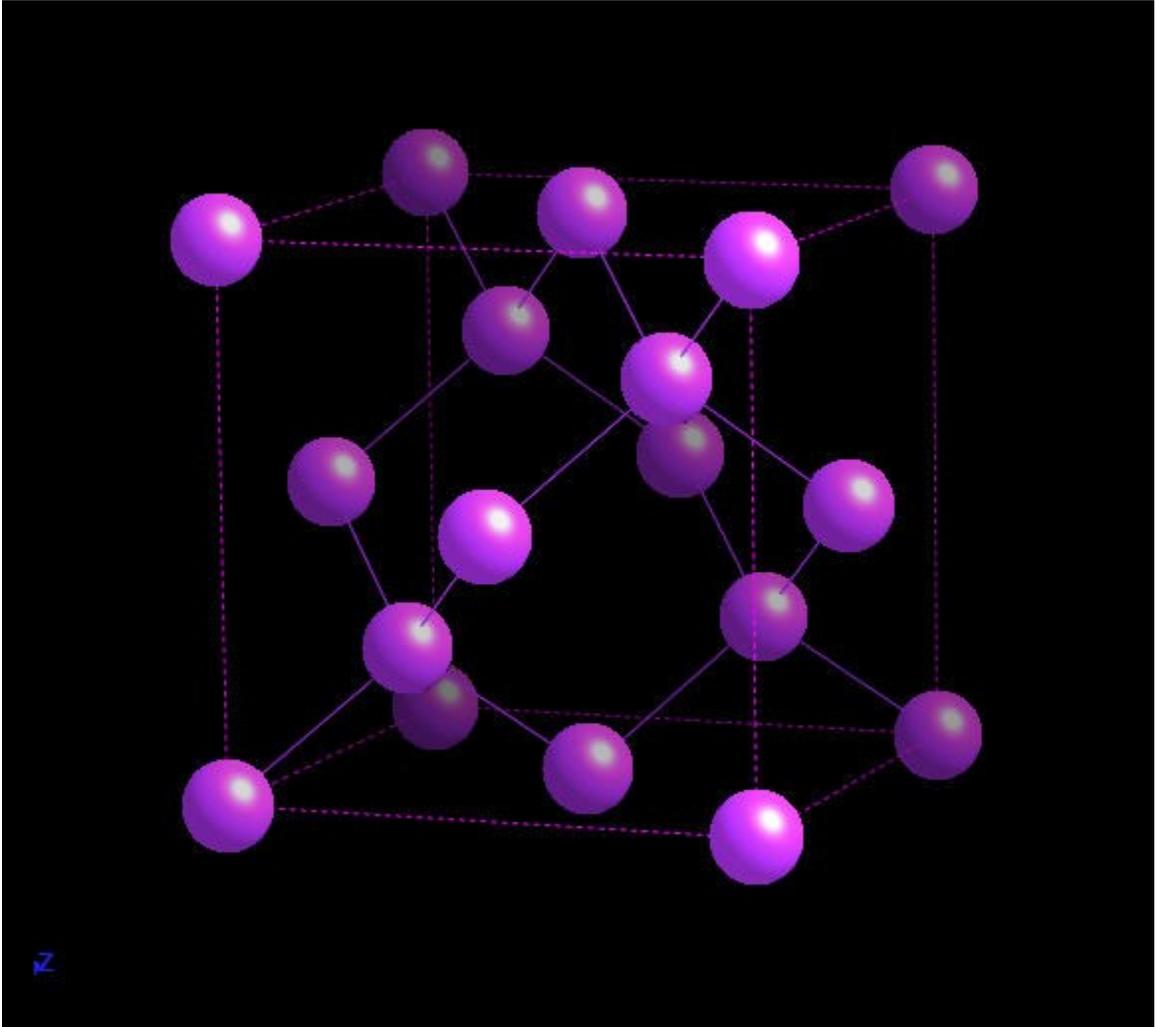


Estructura de blenda de Zinc



Estructura de Diamante

Estructura basada en blenda de zinc

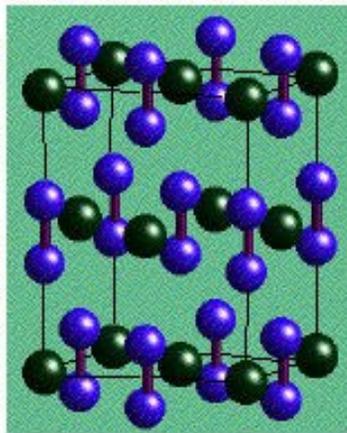
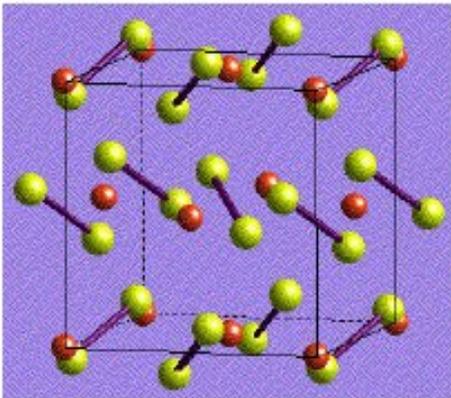


Estructura de diamante, Si, Ge

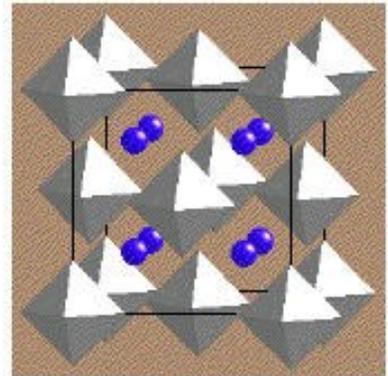
La estructura de **blenda de Zinc** la adoptan los cationes polarizables Cu^+ , Ag^+ , Cd^{2+} , Ga^{3+} y los aniones, también polarizables, I^- , S^{2-} , P^{3-} .

Compuestos típicos de esta estructura: $\text{Cu}(\text{F}, \text{Cl}, \text{Br}, \text{I})$, AgI , $\text{Zn}(\text{S}, \text{Se}, \text{Te})$, $\text{Ga}(\text{P}, \text{As})$, $\text{Hg}(\text{S}, \text{Se}, \text{Te})$.

NaCl Variants



CaF₂ Variant

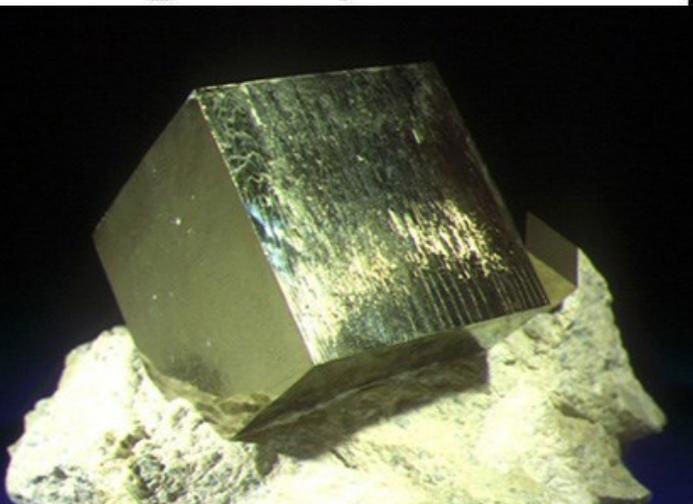


FeS₂

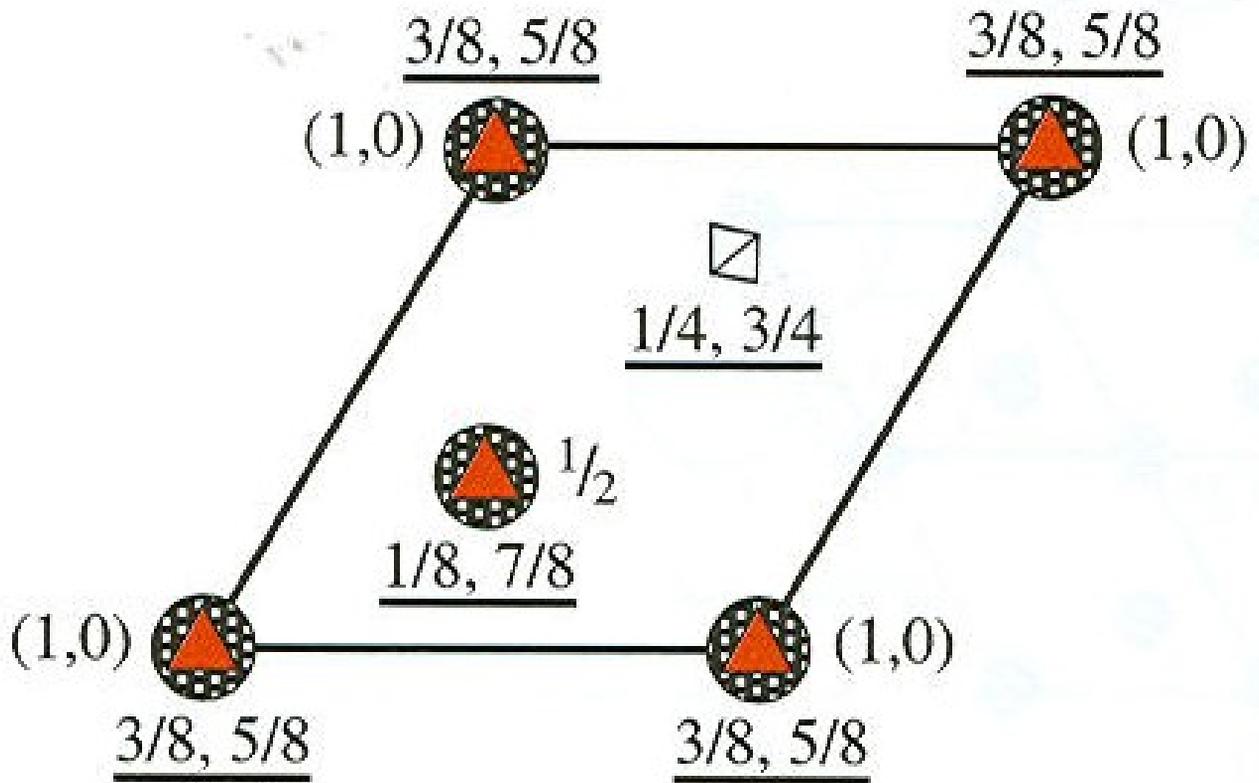
Pyrite

SrO₂

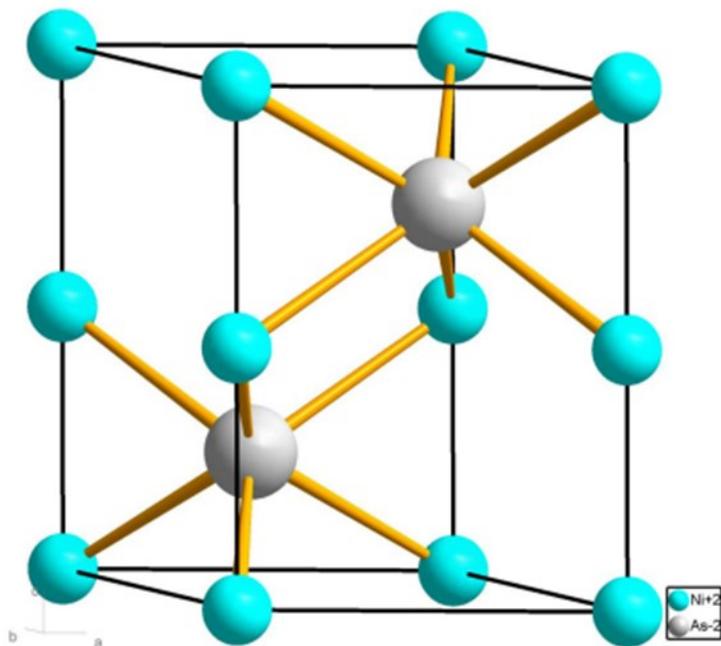
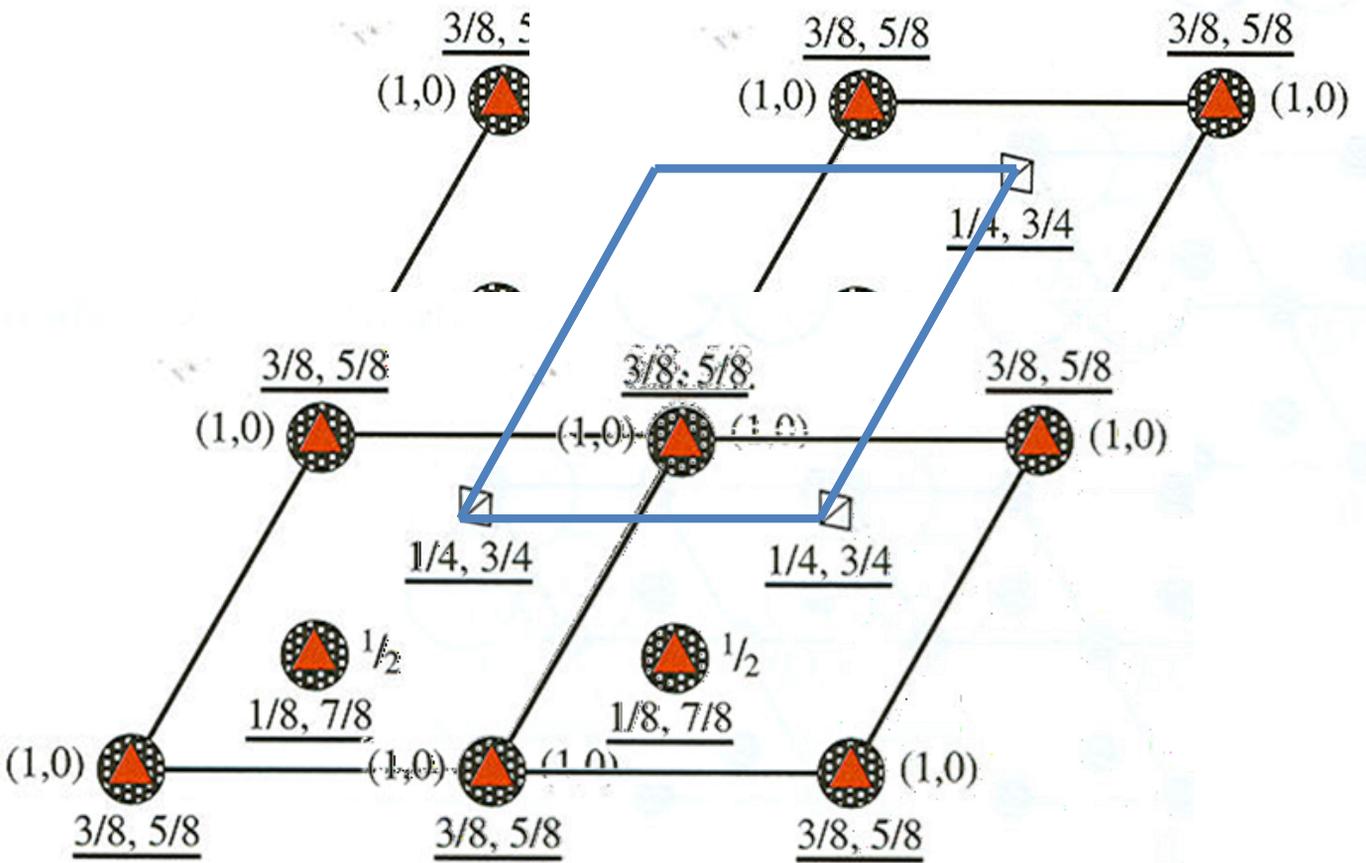
K₂PtCl₆



Huecos octaédricos y tetraédricos de celda hexagonal compacta HCP

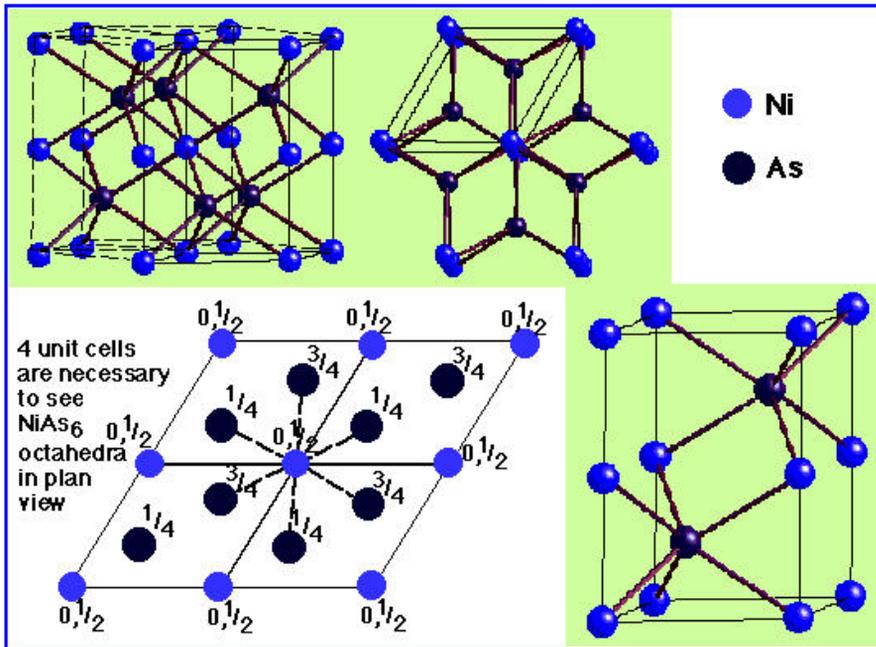


- ◇ Octahedral hole
(positions – underlined numbers)
- Atoms or ions
- ▲ Tetrahedral hole
(positions – underlined)



ESTRUCTURAS DERIVADAS DEL EMPACAMIENTO HEXAGONAL COMPACTO, HCP.

Estructura de arseniuro de níquel



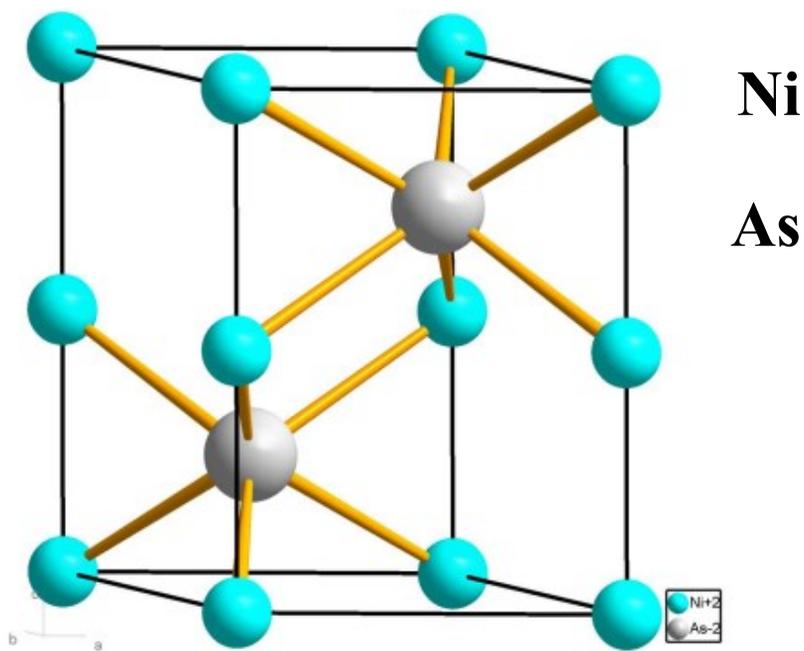
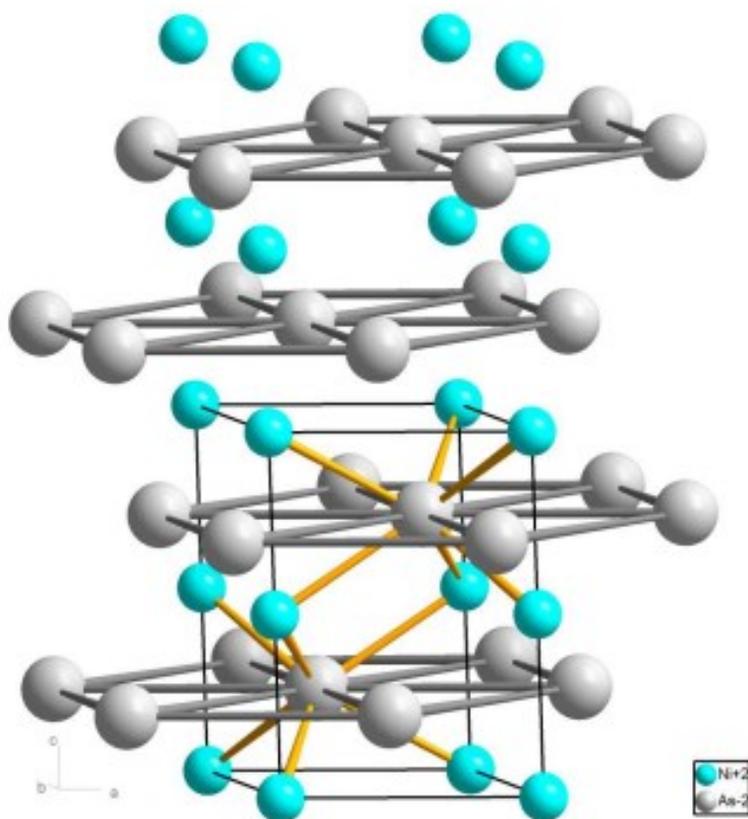
Arreglo hexagonal compacto de As con Ni en todos los huecos octaédricos

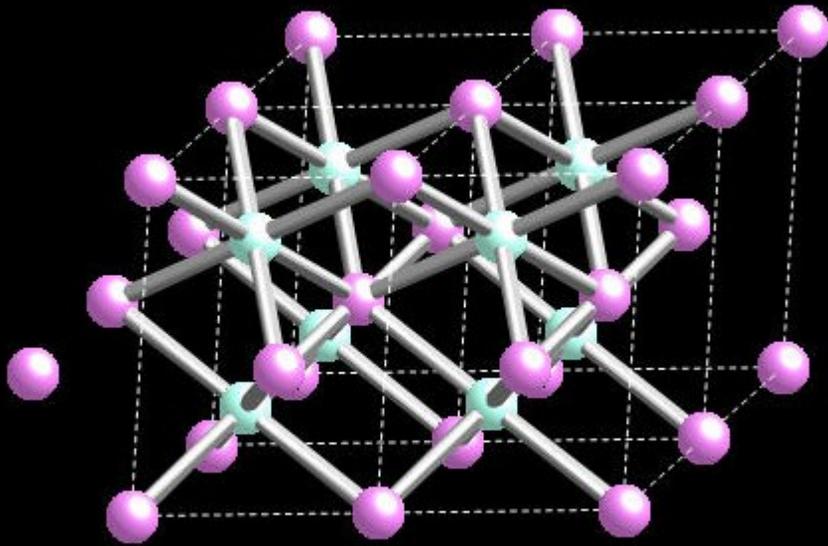
Malla: hexagonal P $a=b$, $c=8/3 a$ Å

Motivo: 2 Ni en $(0,0,0)$ y $(0,0,1/2)$ 2 As en $(2/3, 1/3, 1/4)$ y $(1/3, 2/3, 3/4)$

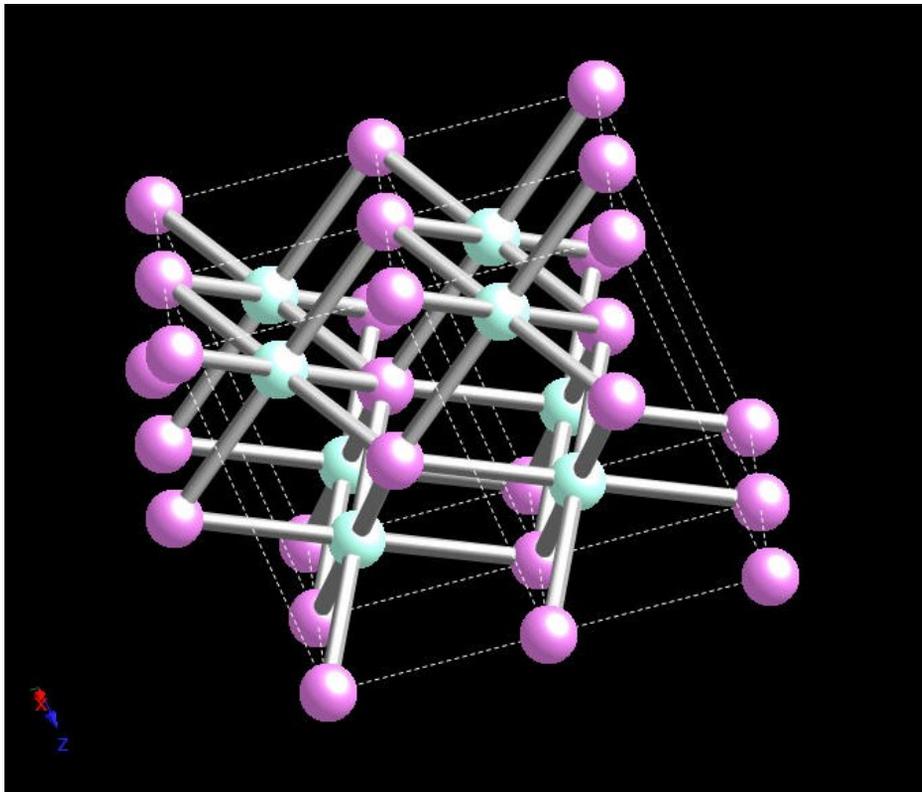
2 unidades de NiAs por celda unitaria

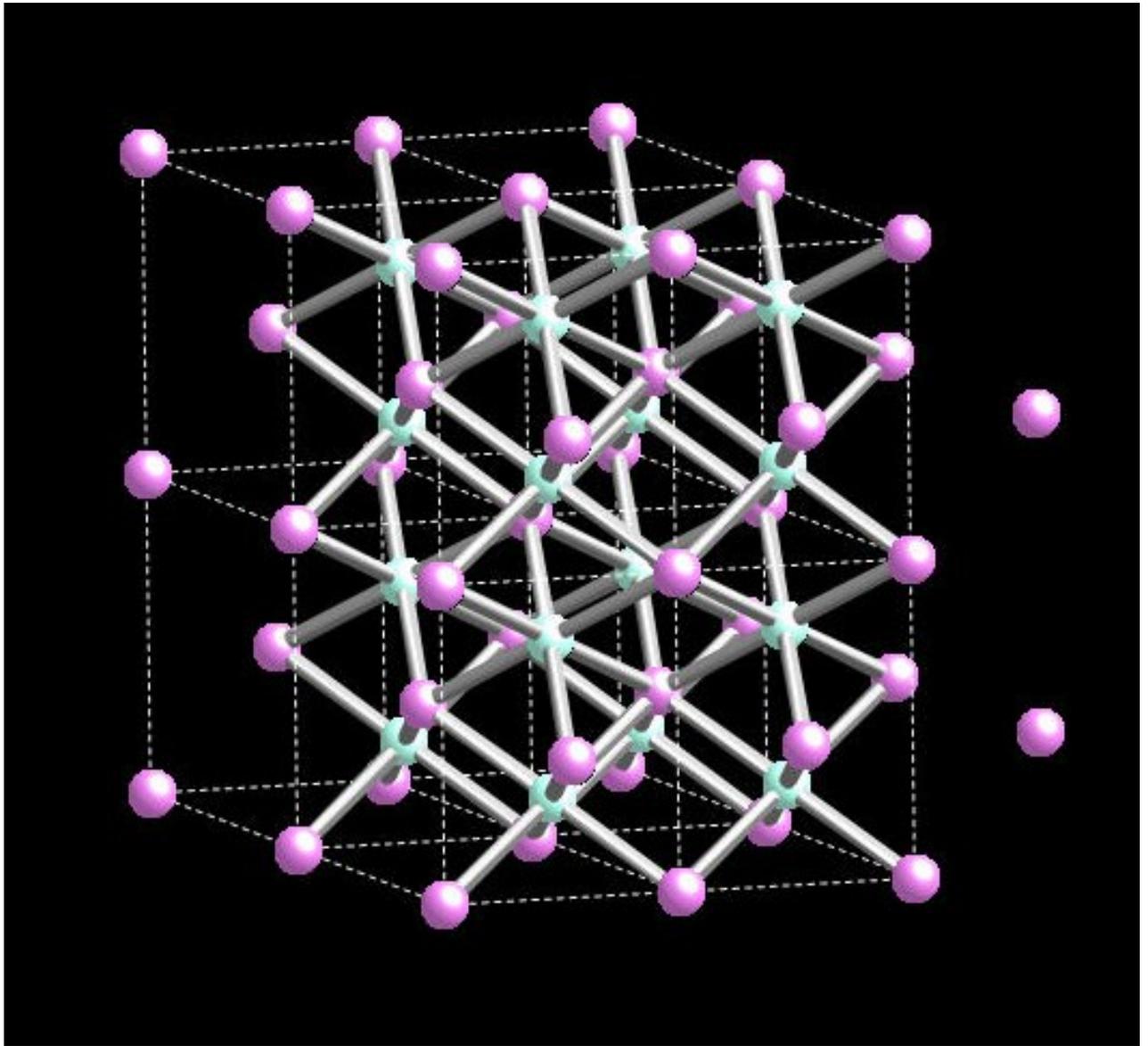
Coordinación 6 para Ni (octaédrica) y 6 para As (prisma triangular).

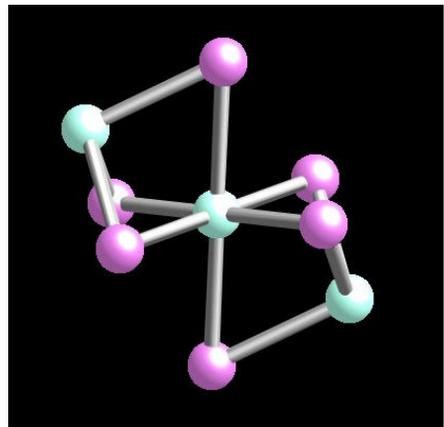
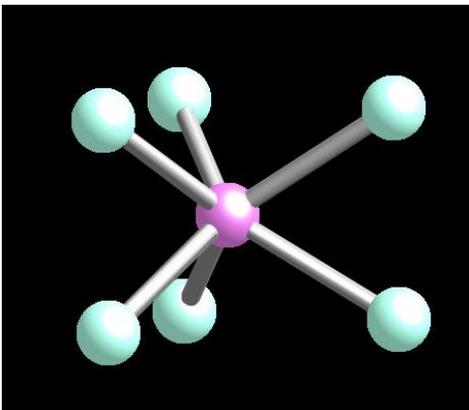
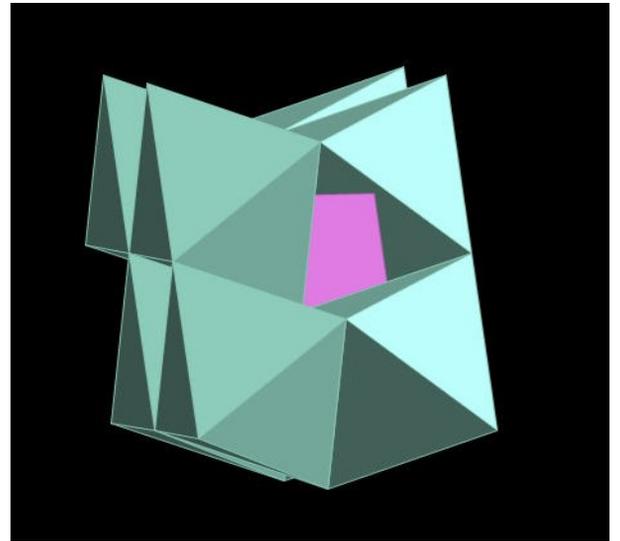
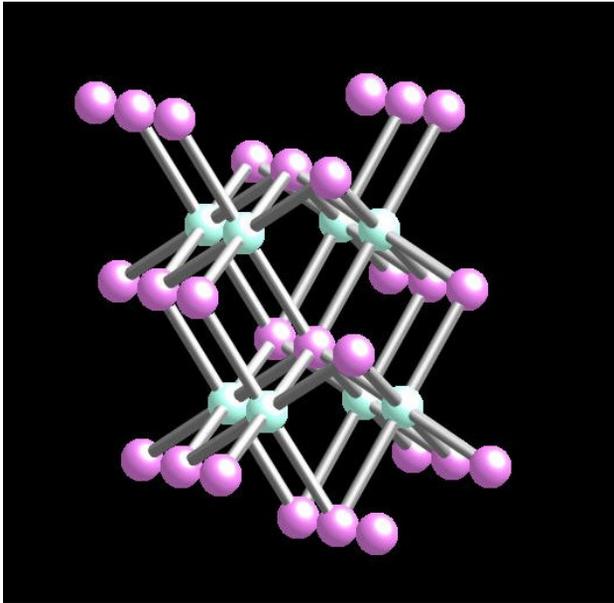
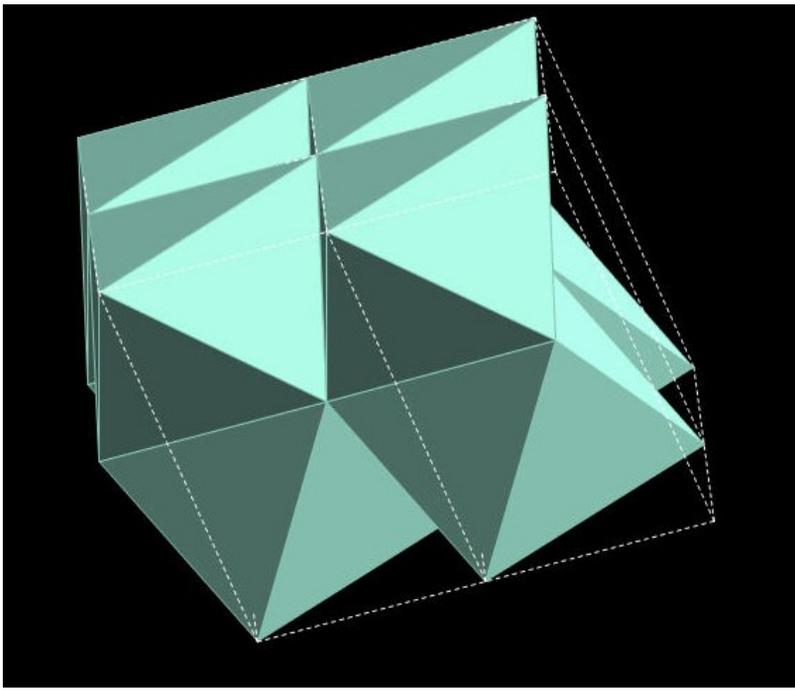


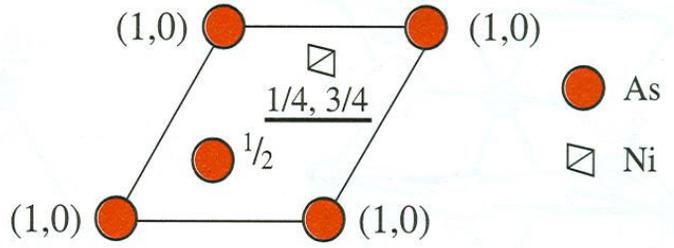
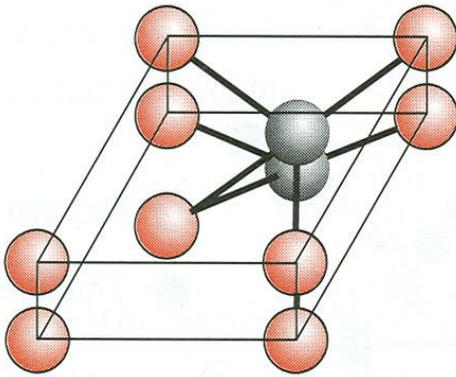


Estructura de NiAs

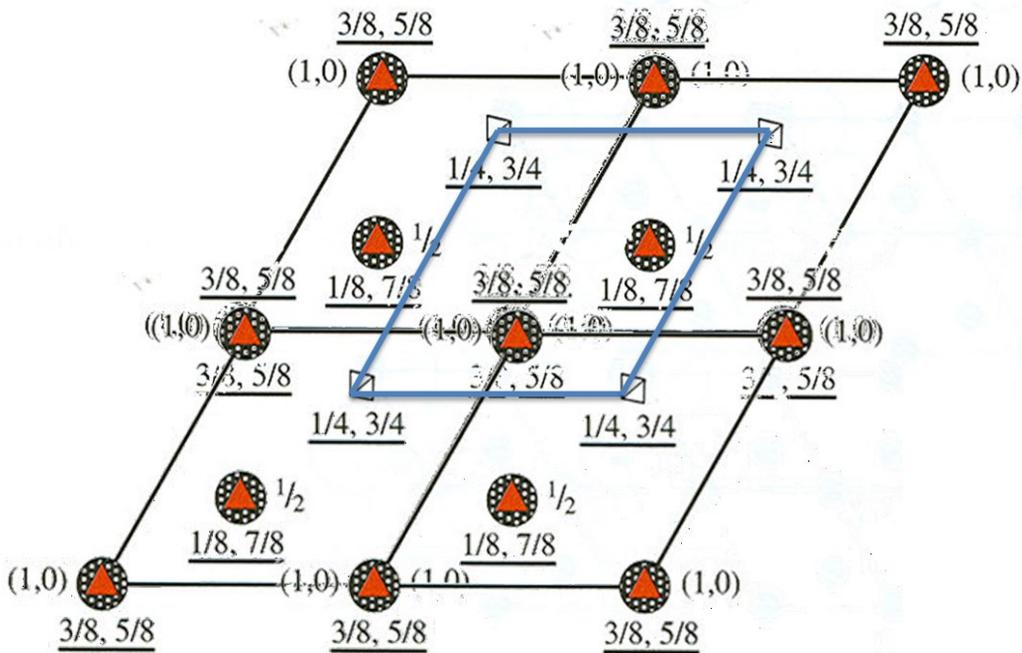








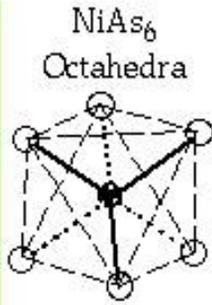
Estructura de Arseniuro de Níquel



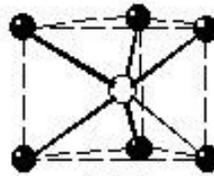
“Coordinación 6 para Ni (octaédrica) y 6 para As (prisma triangular).”



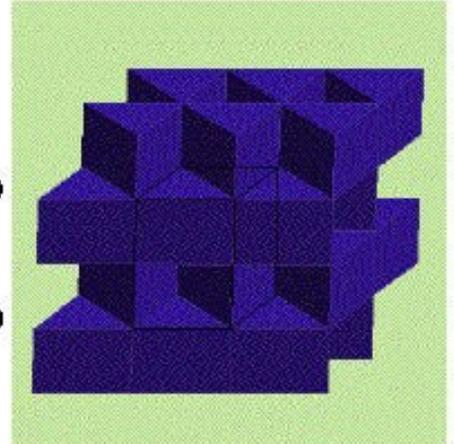
NiAs₆ Octahedra



NiAs₆
Octahedra



AsNi₆
Trigonal
Prisms



AsNi₆ Trigonal Prisms

La estructura de arseniuro de níquel la adoptan los metales de transición con calcógenos: Ti(S,Se,Te); Cr(S,Se,Te,Sb); Ni(S,Se,Te,As,Sb,Sn)

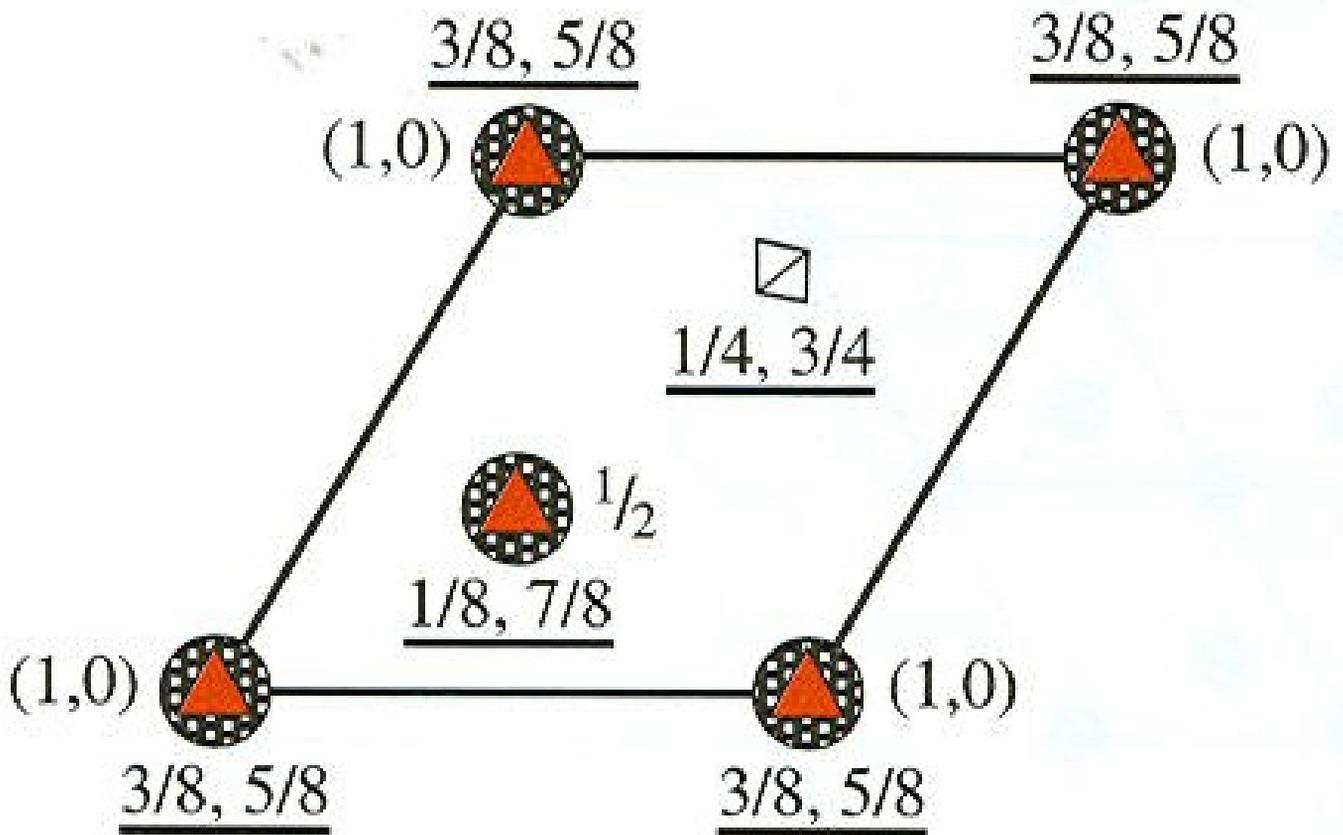
Table 1.13 *Some compounds with the NiAs structure*

Compound	$a/\text{\AA}$	$c/\text{\AA}$	c/a	Compound	$a/\text{\AA}$	$c/\text{\AA}$	c/a
NiS	3.4392	5.3484	1.555	CoS	3.367	5.160	1.533
NiAs	3.602	5.009	1.391	CoSe	3.6294	5.3006	1.460
NiSb	3.94	5.14	1.305	CoTe	3.886	5.360	1.379
NiSe	3.6613	5.3562	1.463	CoSb	3.866	5.188	1.342
NiSn	4.048	5.123	1.266	CrSe	3.684	6.019	1.634
NiTe	3.957	5.354	1.353	CrTe	3.981	6.211	1.560
FeS	3.438	5.880	1.710	CrSb	4.108	5.440	1.324
FeSe	3.637	5.958	1.638	MnTe	4.1429	6.7031	1.618
FeTe	3.800	5.651	1.487	MnAs	3.710	5.691	1.534
FeSb	4.06	5.13	1.264	MnSb	4.120	5.784	1.404
δ' -NbN [†]	2.968	5.549	1.870	MnBi	4.30	6.12	1.423
PtB [†]	3.358	4.058	1.208	PtSb	4.130	5.472	1.325
PtSn	4.103	5.428	1.323	PtBi	4.315	5.490	1.272

[†]Anti-NiAs structure.

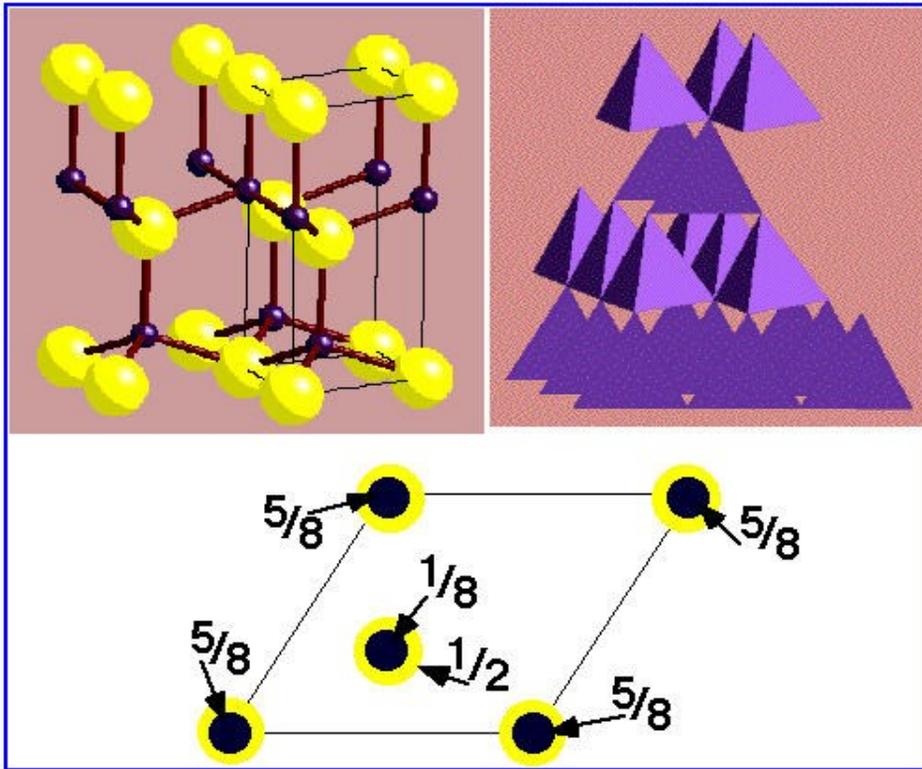
Ref: West p. 46-47

ESTRUCTURA DE WURTZITA:



- ◇ Octahedral hole
(positions – underlined numbers)
- Atoms or ions
- ▲ Tetrahedral hole
(positions – underlined)

ESTRUCTURA DE WURTZITA:



Arreglo hexagonal compacto de S²⁻ con Zn²⁺ en la mitad de los huecos tetraédricos (T⁺ o T⁻ llenos)

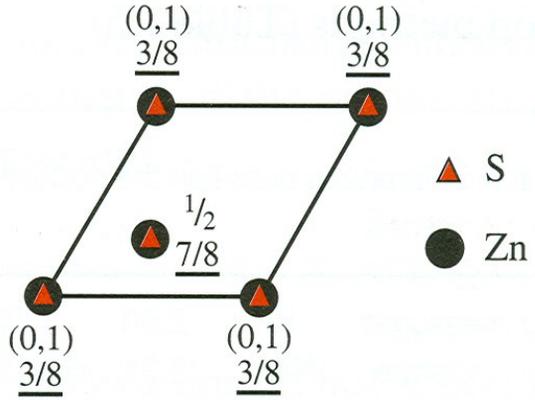
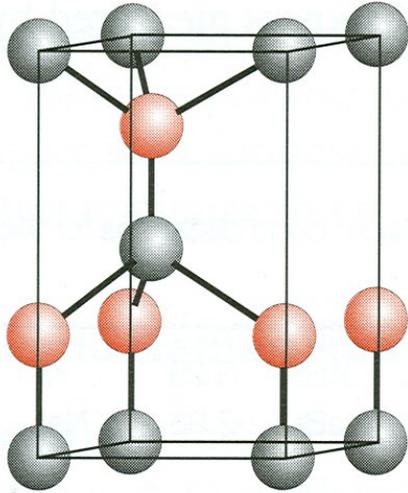
hcp;

Malla hexagonal , $a=b$, $c=(8/3)^{1/2} a$

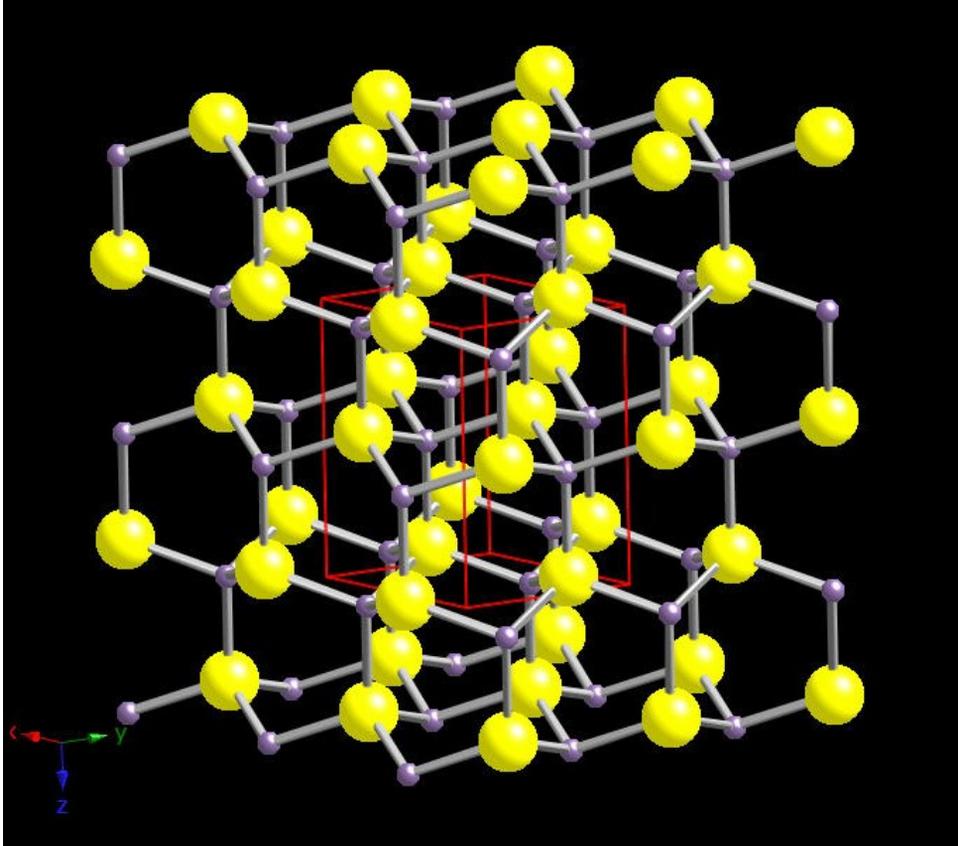
Motivos: 2S en (0,0,0) y (2/3, 1/3, 1/2) y 2 Zn en (2/3,1/3, 1/8) y (0,0,5/8)

2 unidades de ZnS en la celda unitaria

Coordinación 4:4 (tetraédrica)

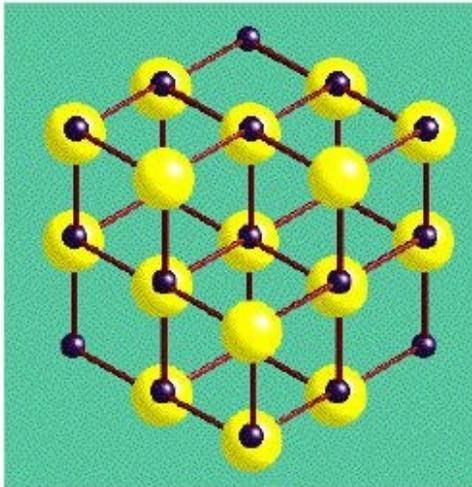


Estructura de Wurtzita

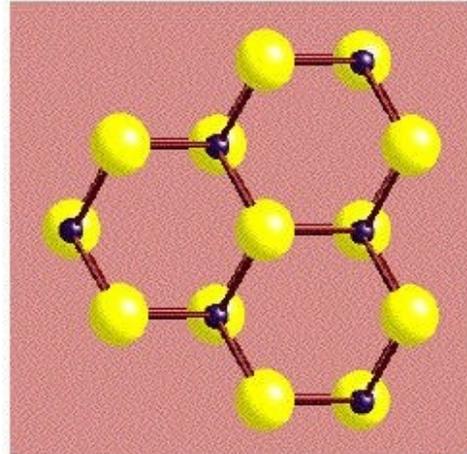


Comparaciones entre blenda de Zn y wurtzita

Vista en un plano

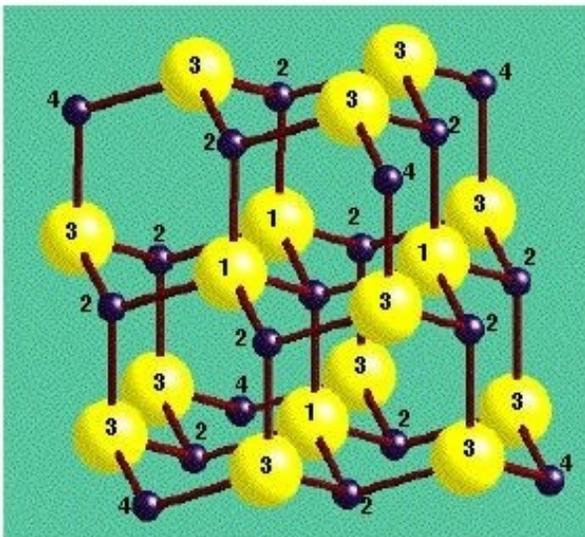


Zinc Blende
CCP ABC repeat

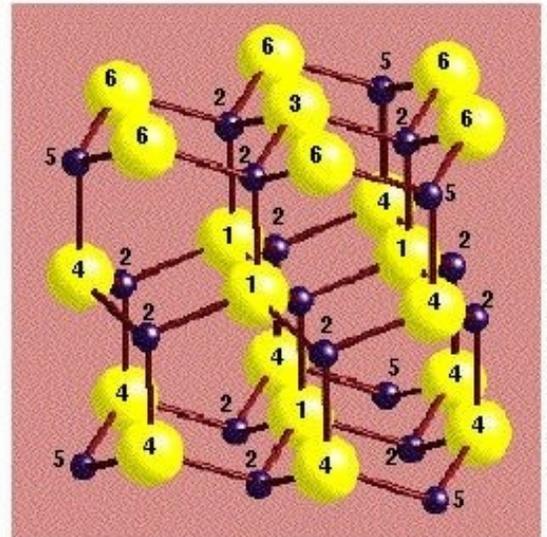


Wurtzite
HCP AB repeat

COORDINATION ENVIRONMENTS



Zinc Blende



Wurtzite

4 Nearest Neighbours (*Tetrahedral*)
12 Next-Nearest Neighbours

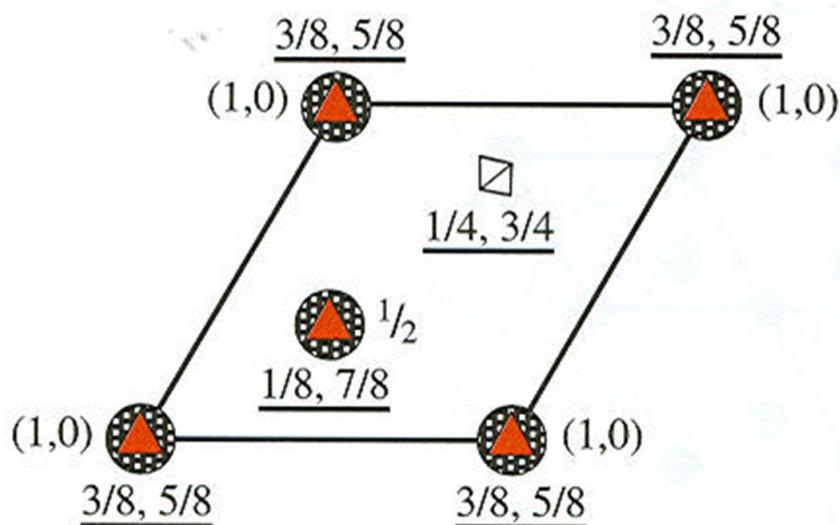
Cubic

Anti-Cubic

Table 1.12 Some compounds with the wurtzite structure

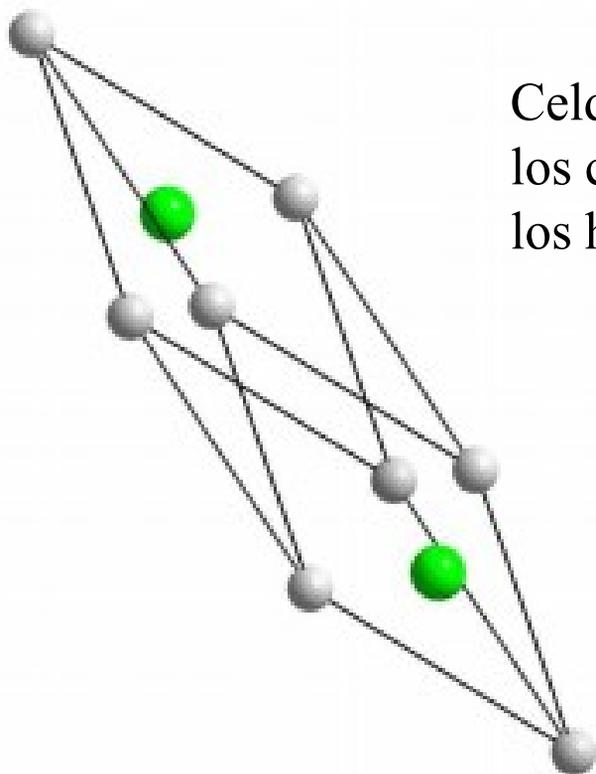
Compound	$a/\text{Å}$	$c/\text{Å}$	u	c/a	Compound	$a/\text{Å}$	$c/\text{Å}$	u	c/a
ZnO	3.2495	5.2069	0.345	1.602	AgI	4.580	7.494		1.636
ZnS	3.811	6.234		1.636	AlN	3.111	4.978	0.385	1.600
ZnSe	3.98	6.53		1.641	GaN	3.180	5.166		1.625
ZnTe	4.27	6.99		1.637	InN	3.533	5.693		1.611
BeO	2.698	4.380	0.378	1.623	TaN	3.05	4.94		1.620
CdS	4.1348	6.7490		1.632	NH ₄ F	4.39	7.02	0.365	1.600
CdSe	4.30	7.02		1.633	SiC	3.076	5.048		1.641
MnS	3.976	6.432		1.618	MnSe	4.12	6.72		1.631

BeO, ZnO, NH₄F also adopt this structure type.

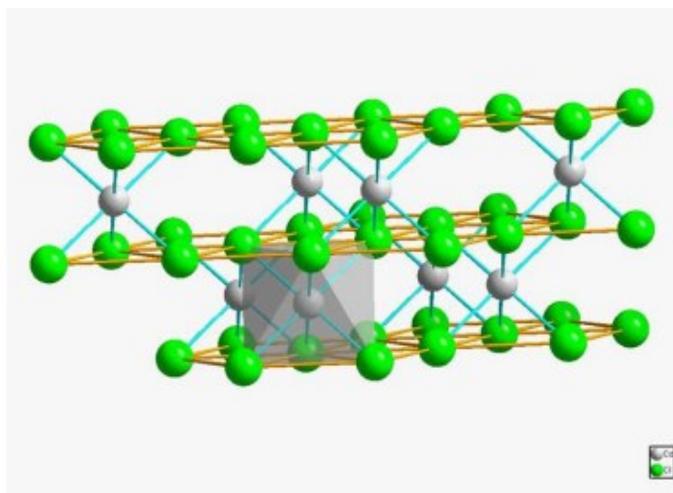
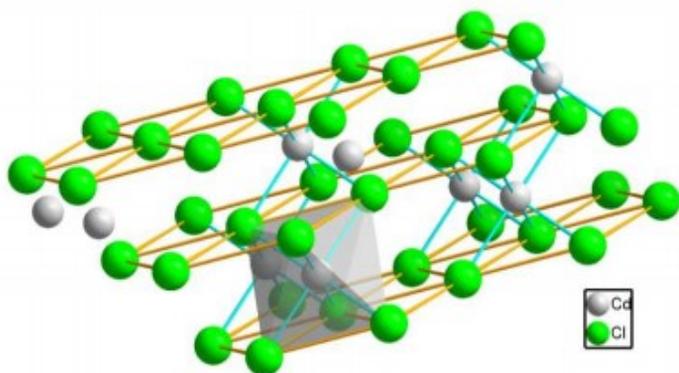


- ◇ Octahedral hole
(positions – underlined numbers)
- Atoms or ions
- ▲ Tetrahedral hole
(positions – underlined)

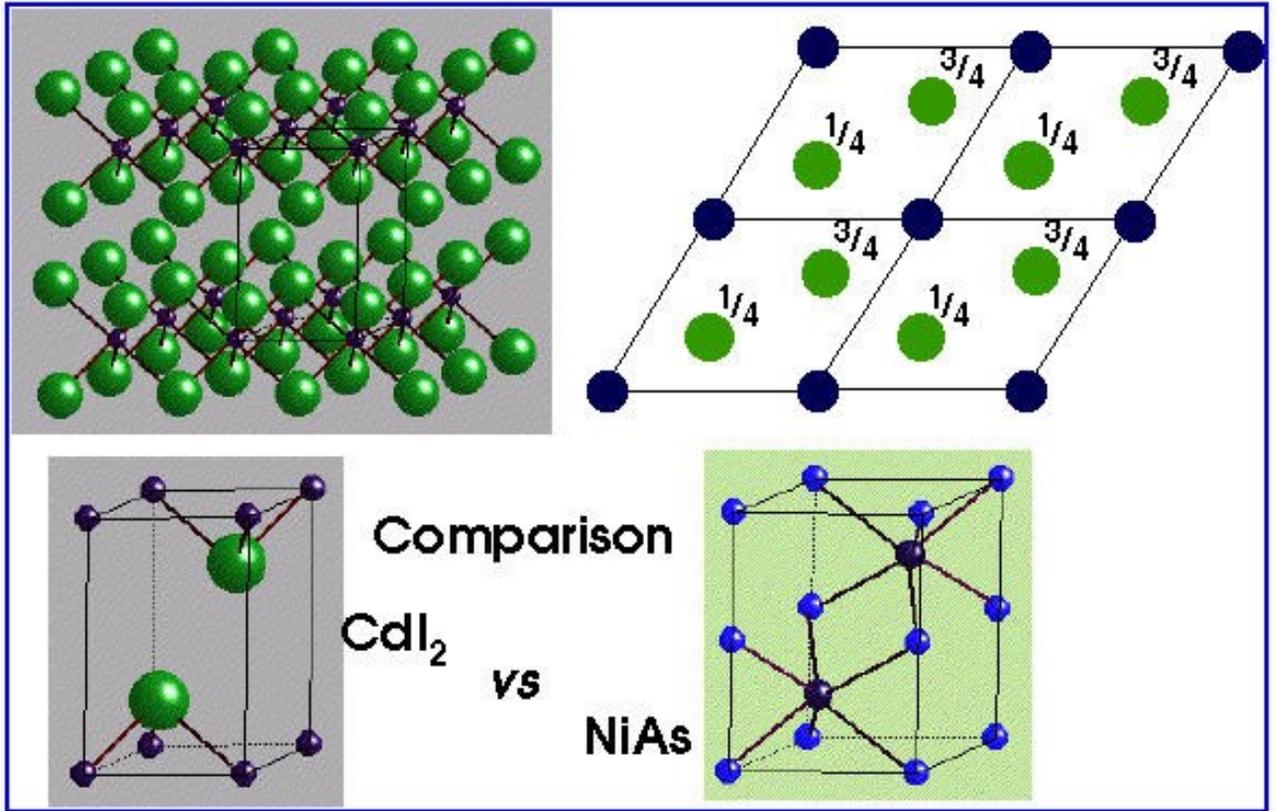
Celda de cloruro de Cd



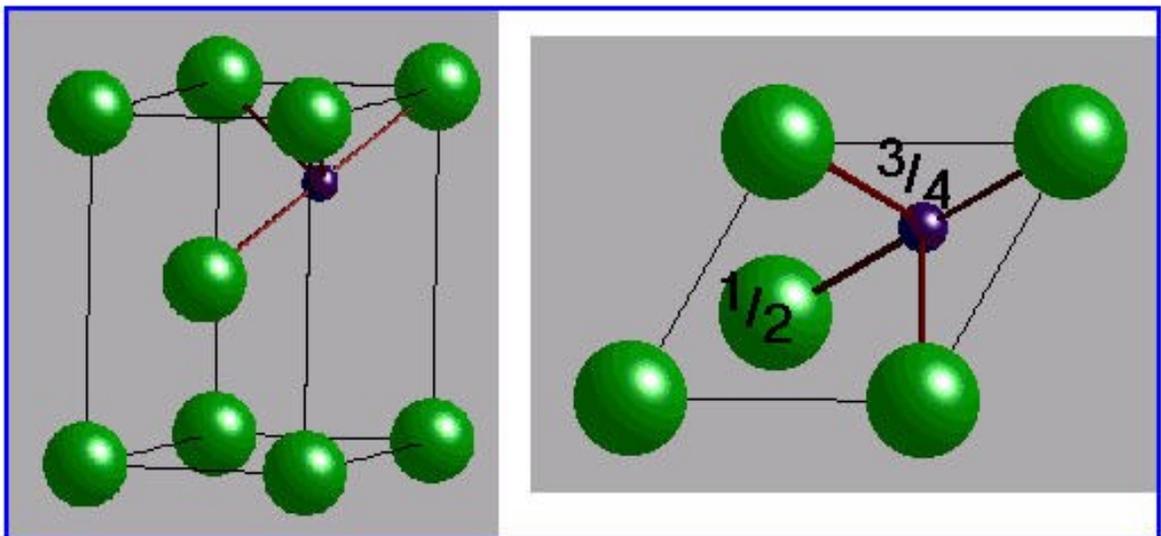
Celda del tipo hcp de aniones, con los cationes ocupando la mitad de los huecos octaédricos

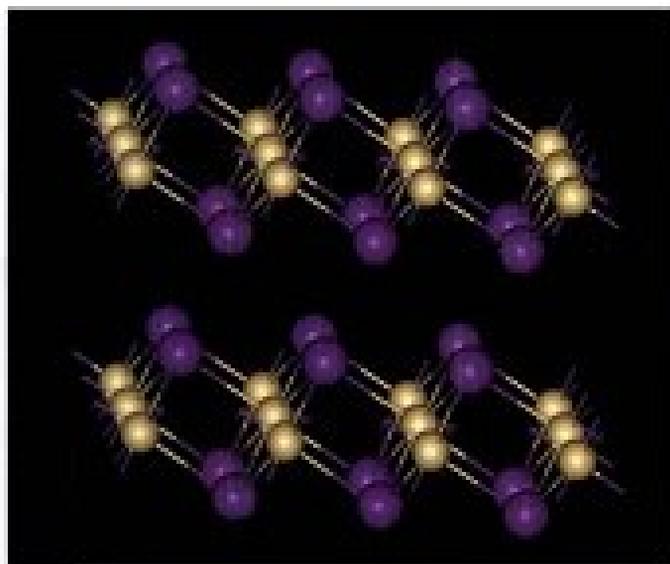


ESTRUCTURA DEL YODURO DE CADMIO

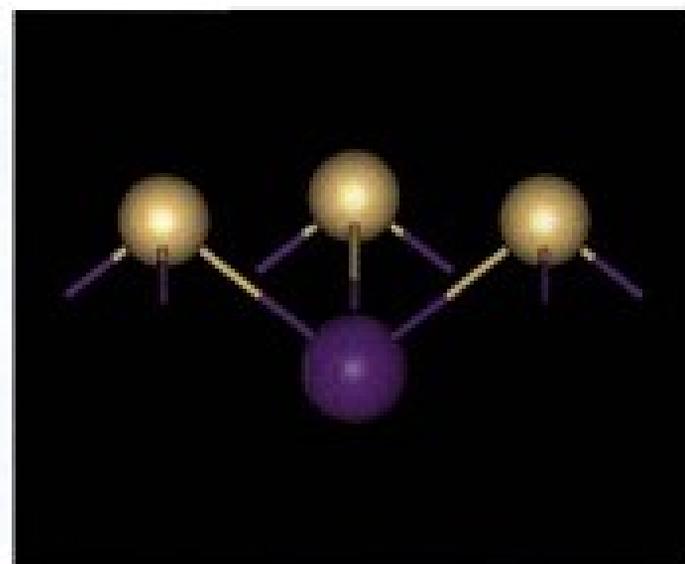


Arreglo de yoduros en HCP con Cd en huecos octaédricos de capas alternadas (la mitad de los huecos octaédricos)

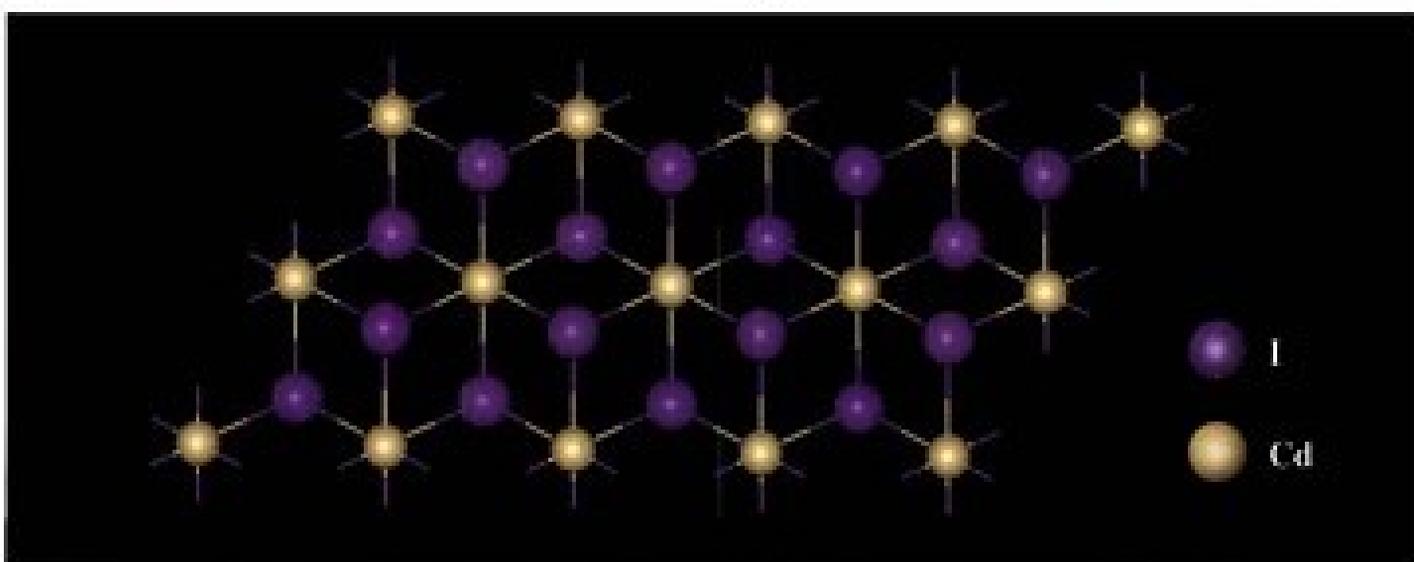




(a)



(c)



(b)

Malla hexagonal P

Motivo: Cd en (0,0,0); 2I en $(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$ y $(\frac{1}{3}, \frac{3}{2}, \frac{3}{4})$

Z=1, una unidad de CdI₂ por celda unitaria

Coordinación 6 para Cd (octaédrica) y 3 para I (piramidal)

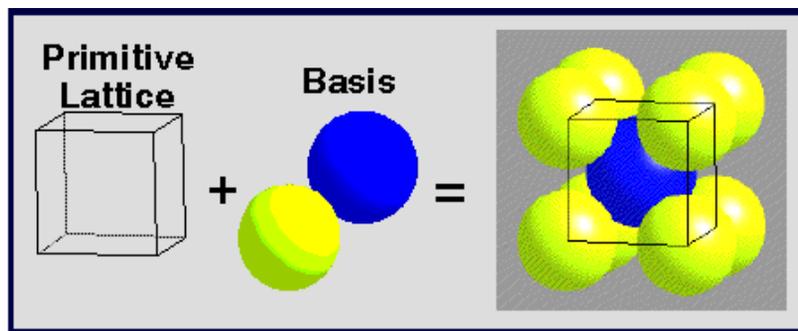
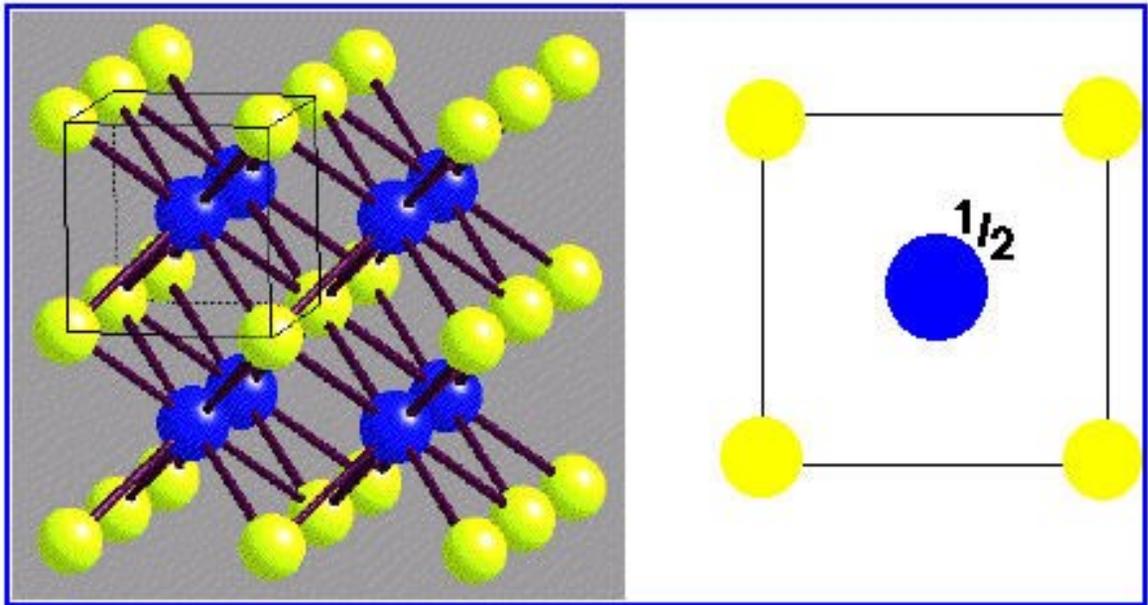
La estructura de CdI₂ la adoptan los yoduros de cationes medianamente polarizables; Los bromuros y cloruros de cationes fuertemente polarizables como PbI₂, FeBr₂, VCl₂

También la adoptan los hidróxidos de muchos cationes divalentes (Mg, Ni)(OH)₂

También dicalcogenuros de muchos cationes tetravalente como TiS₂, SrSe₂, CoTe₂.

ESTRUCTURAS NO COMPACTAS

CLORURO DE CESIO



Malla cubica P

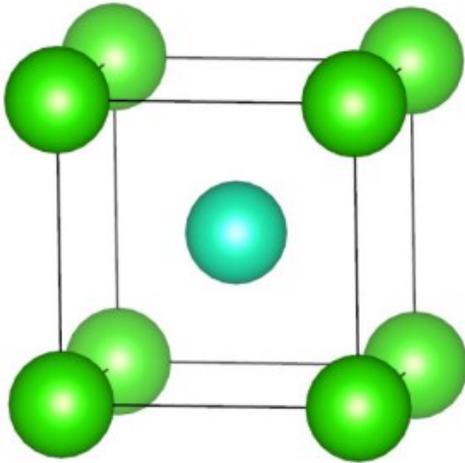
Motivo: Cl en (0,0,0) y Cl en (1/2,1/2,1/2)

Z=1, 1 unidad de CsCl por celda unitaria

Coordinacion 8:8 (cubica)

Adoptada por cloruros, bromuros y yoduros de cationes de gran tamaño

Estructura tipo CsCl

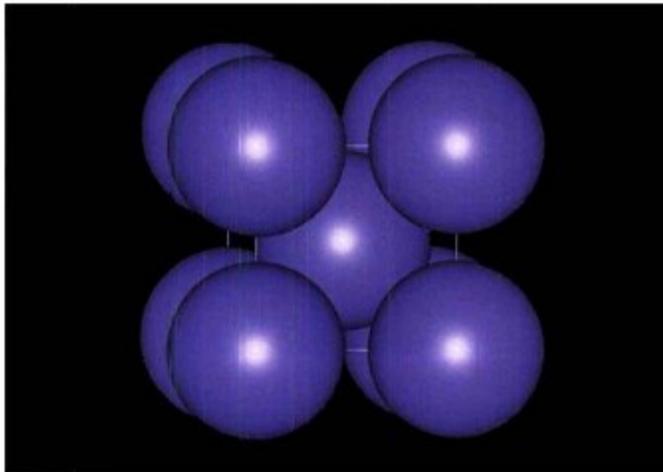


La celda es cúbica P con motivo en 0,0,0 y en $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ Con aniones y cationes totalmente intercambiables

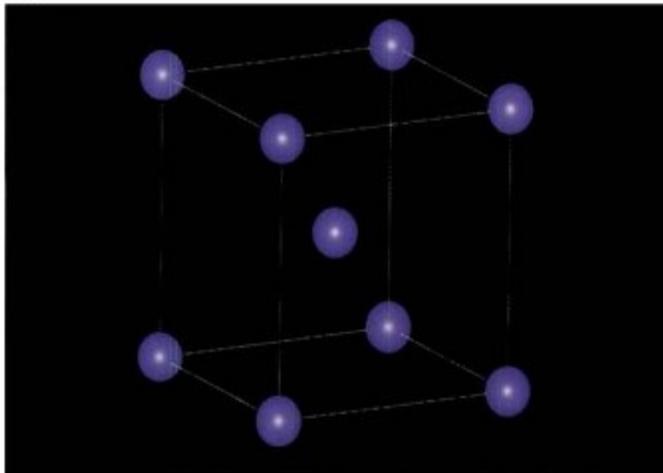
Table 1.14 Some compounds with the CsCl structure

Compound	$a/\text{Å}$	Compound	$a/\text{Å}$	Compound	$a/\text{Å}$	Compound	$a/\text{Å}$
CsCl	4.123	NH ₄ Br	4.0594	CuPd	2.988	AlNi	2.881
CsBr	4.286	TlCl	3.8340	AuMg	3.259	LiHg	3.287
CsI	4.5667	TlBr	3.97	AuZn	3.19	MgSr	3.900
CsCN	4.25	TlI	4.198	AgZn	3.156		
NH ₄ Cl	3.8756	CuZn	2.945	LiAg	3.168		

Estructuras BCC

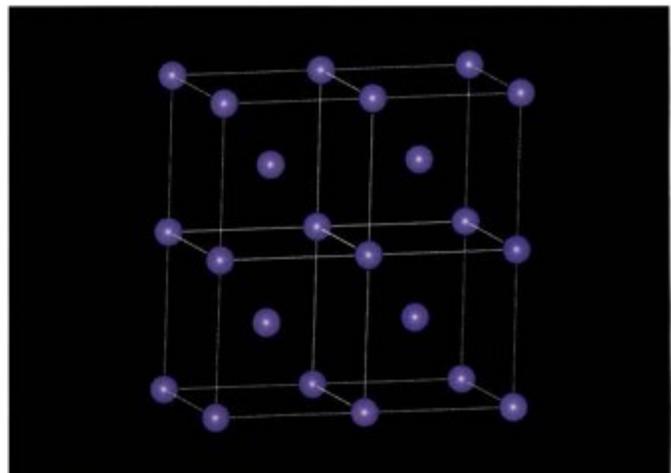


(a)

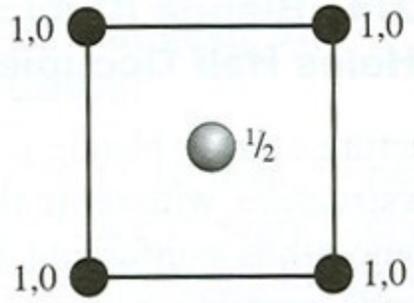
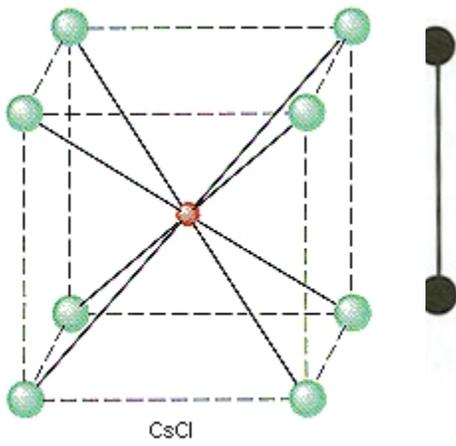


(b)

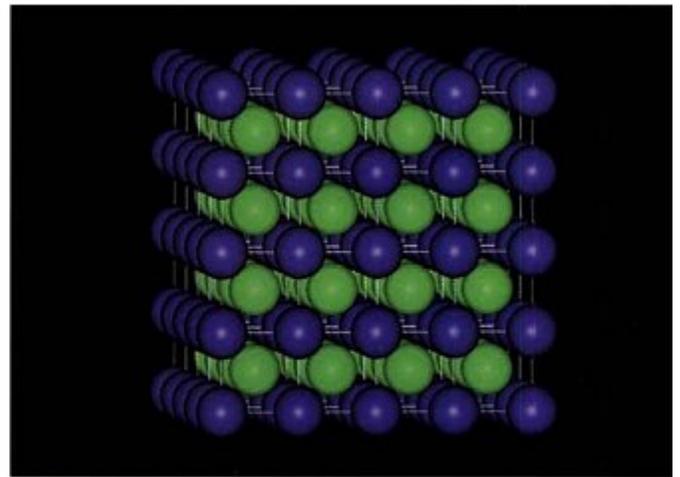
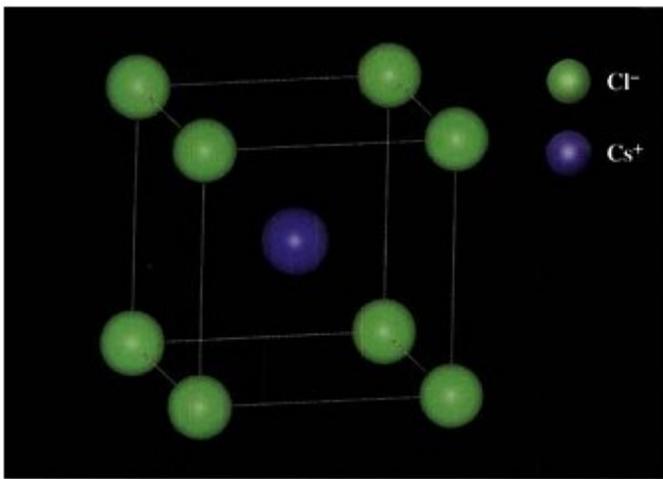
Figure 2.14 A body-centred cubic array, as adopted by sodium, potassium, etc.: (a) one cube, space-filling representation; (b) one cube, ball-and-stick model; (c) four cubes, ball-and-stick model. 



(c)



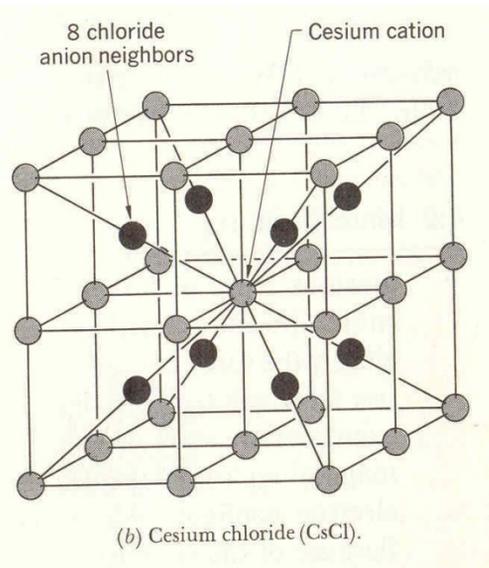
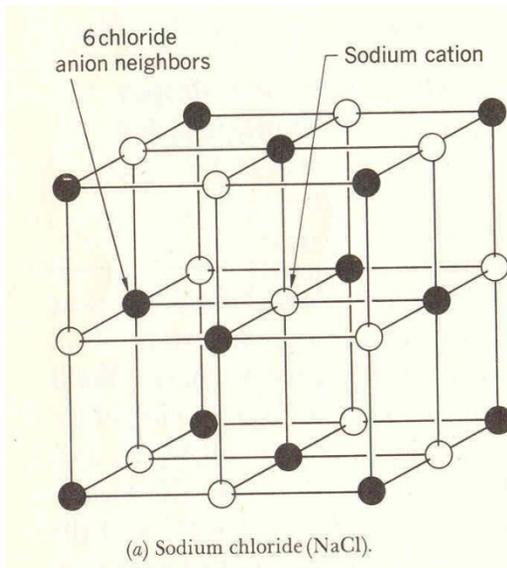
Estructura de Cloruro de Cesio



(a)

(b)

Figure 4.1 (a) The unit cell of caesium chloride, CsCl; (b) the extended CsCl structure, based on an alternative unit cell. 



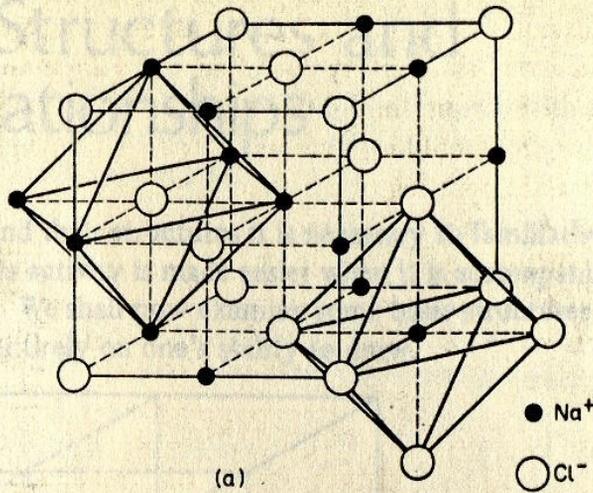


Fig. 36a The sodium chloride structure 6:6 co-ordination

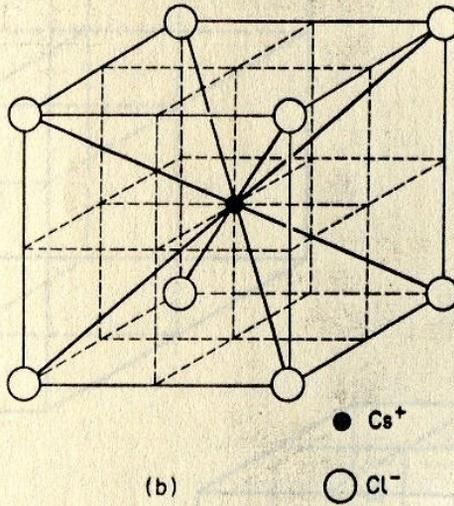


Fig. 36b The caesium chloride structure 8:8 co-ordination

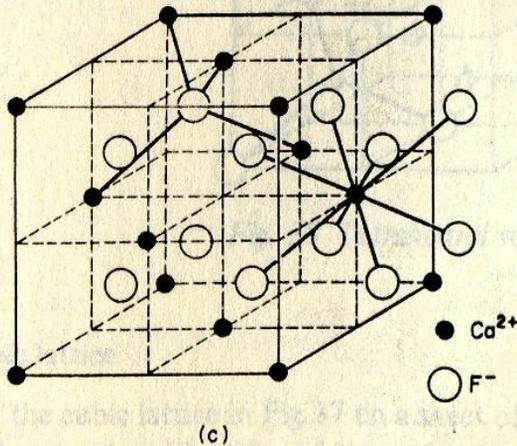
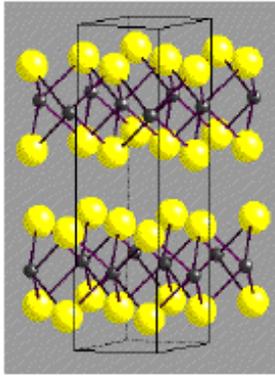
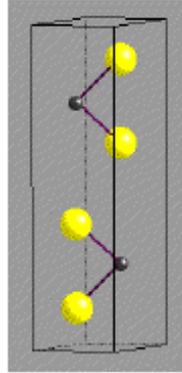
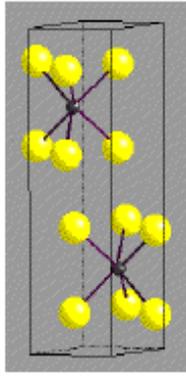


Fig. 36c The fluorite structure 8:4 co-ordination

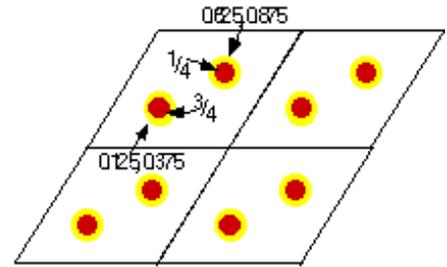
La molibdenita, MoS



Clinographic Views



Unit Cell



Plan View

Hay capas hexagonales de átomos de S que no están empacadas en 3D

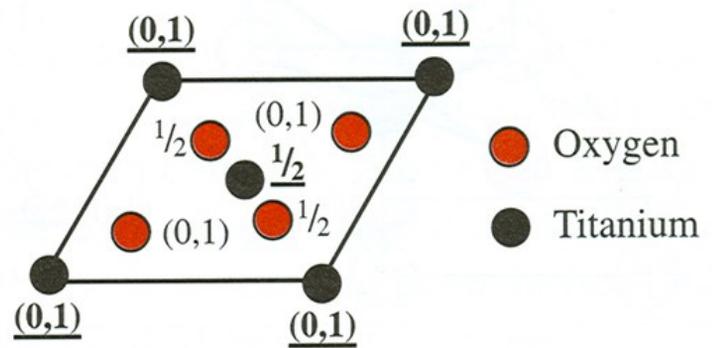
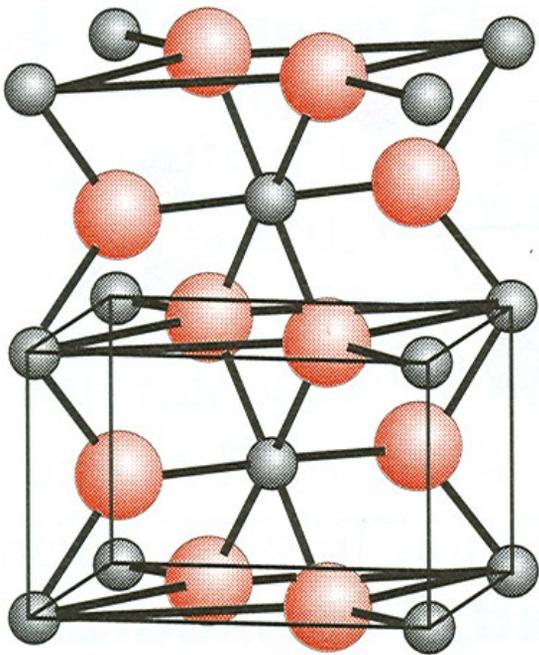
Malla: hexagonal –P

Motivo: 2 Mo en $(2/3, 1/3, 3/8)$ y $(1/3, 2/3, 1/4)$;

4I en $(2/3, 1/3, 1/8)$, $(2/3, 1/3, 3/8)$, $((1/3, 2/3, 5/8)$, $(1/3, 2/3, 7/8)$

2 Unidades de MoS₂ en la celda unitaria

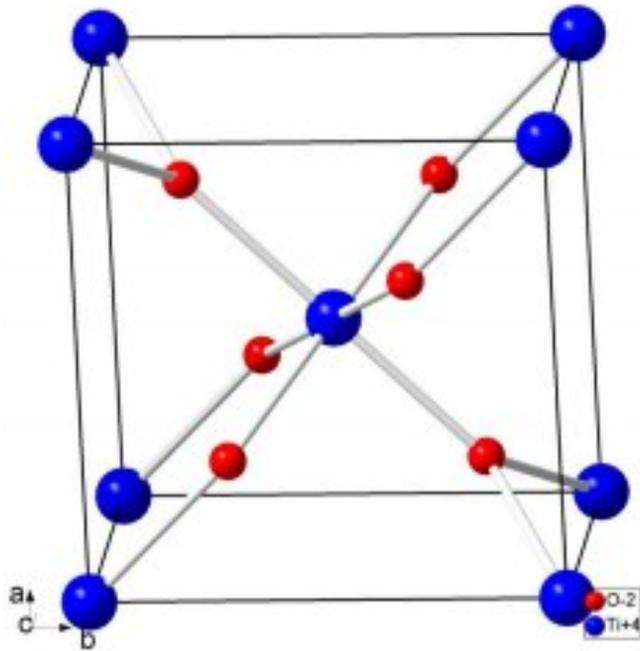
Coordinación de 6 para Mo (trigonal prismática) y para S es de 3 (base piramidal).



Estructura hexagonal compacta distorsionada de rutilo (TiO_2)

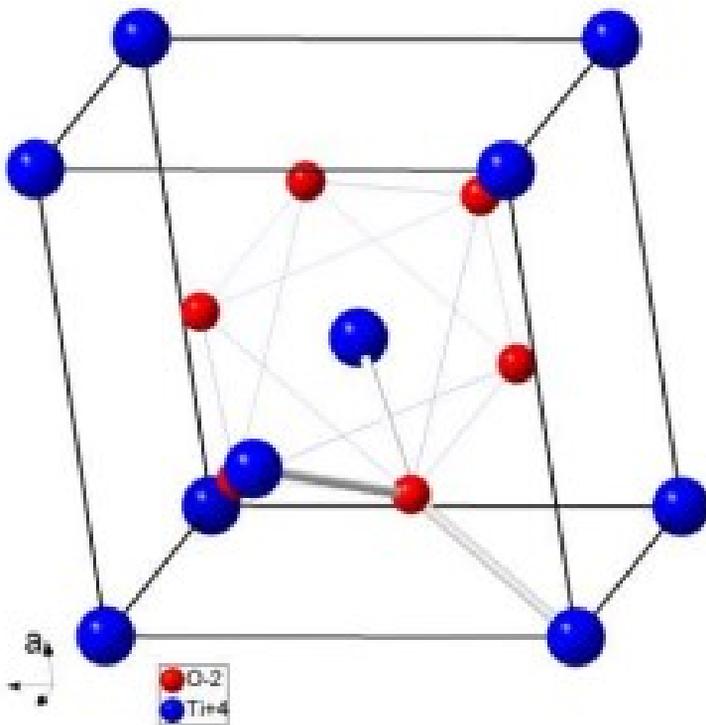


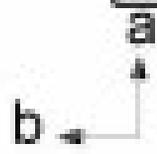
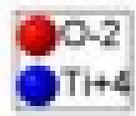
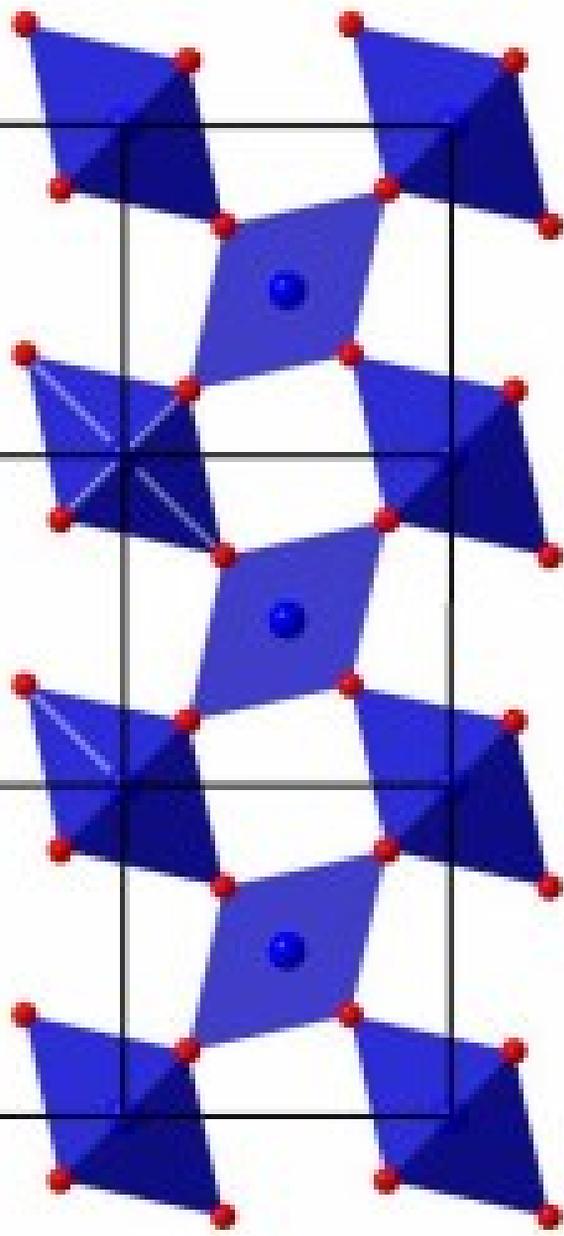
Estructura del Rutilo

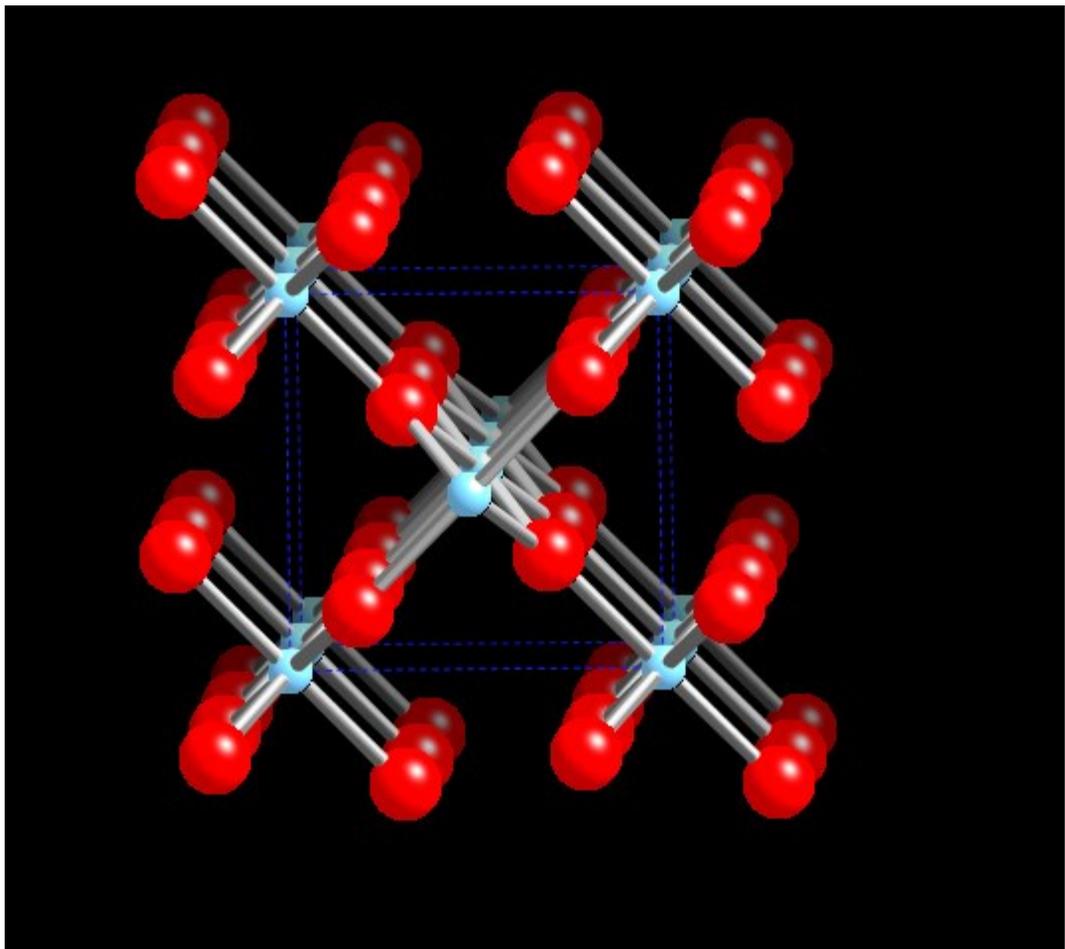


Celda tetragonal no empacada.

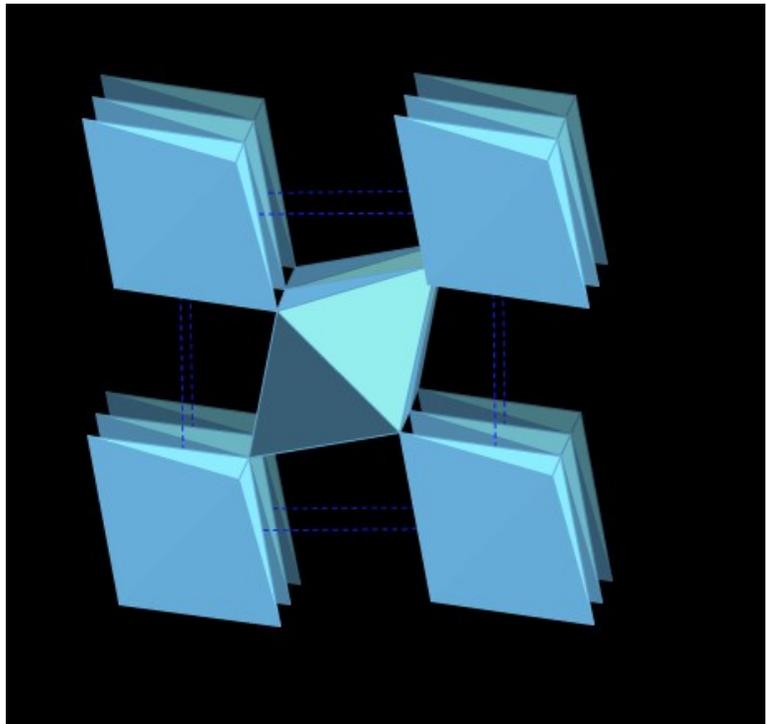
Cada Ti está rodeado por 6 oxígenos y cada oxígeno está rodeado por tres titanios en un plano que hacen las esquinas de un triángulo casi equilátero.







Dos Rutilos



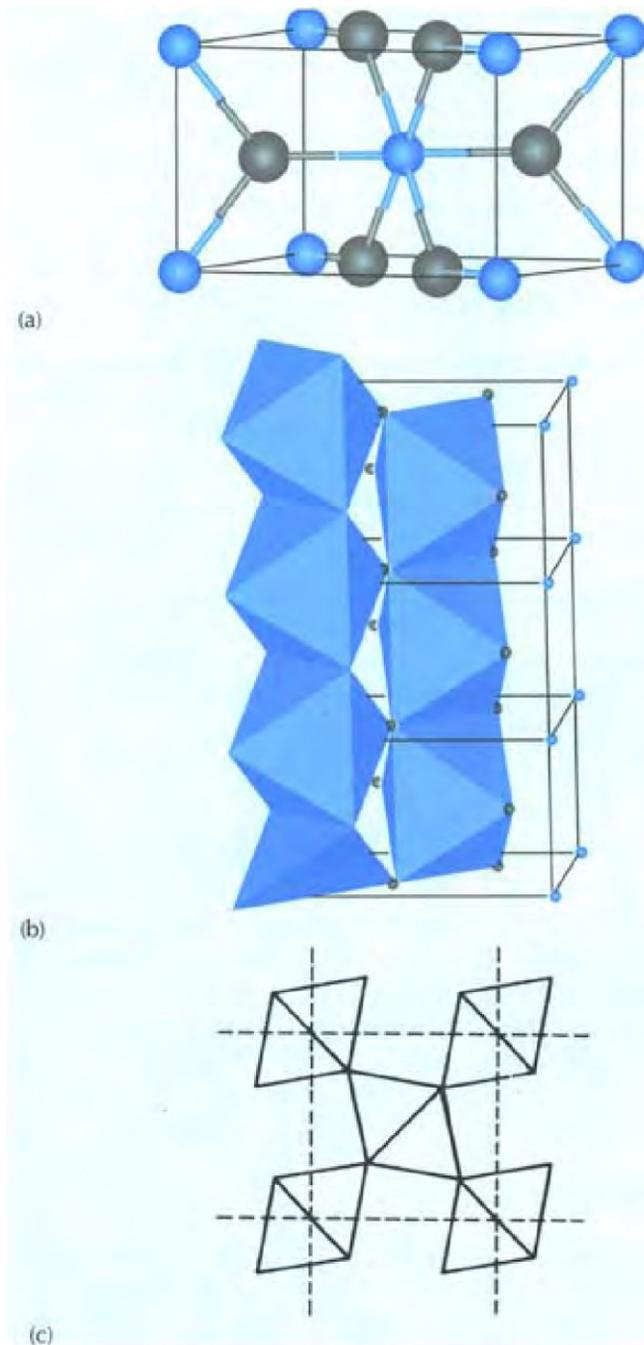
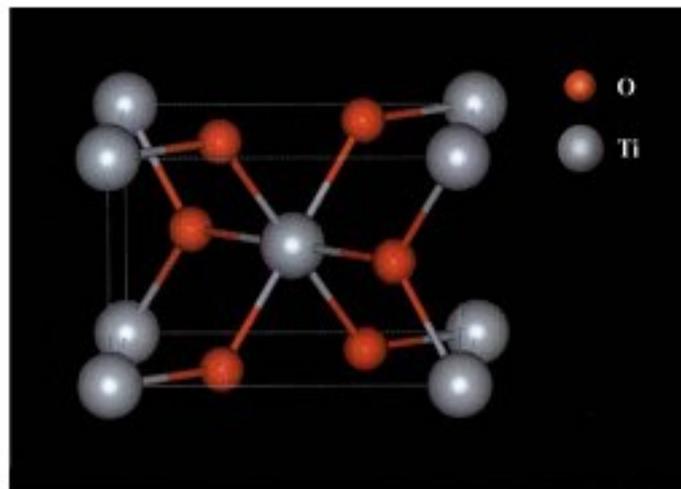
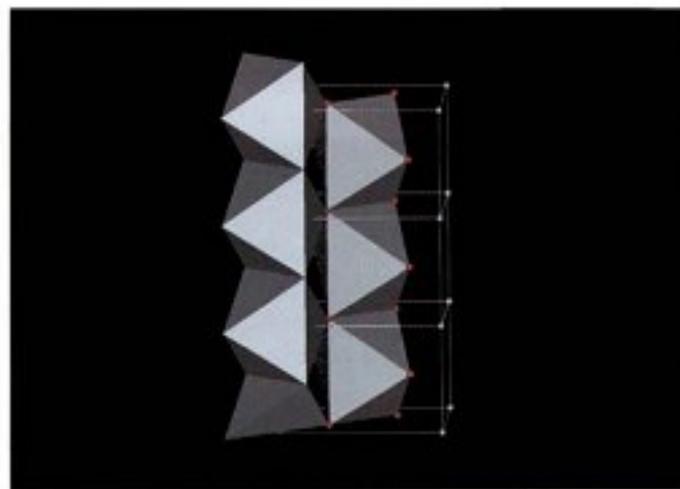


FIGURE 1.41 The crystal structure of rutile, TiO_2 . (a) Unit cell, (b) parts of two chains of linked $[TiO_6]$ octahedra, and (c) projection of structure on base

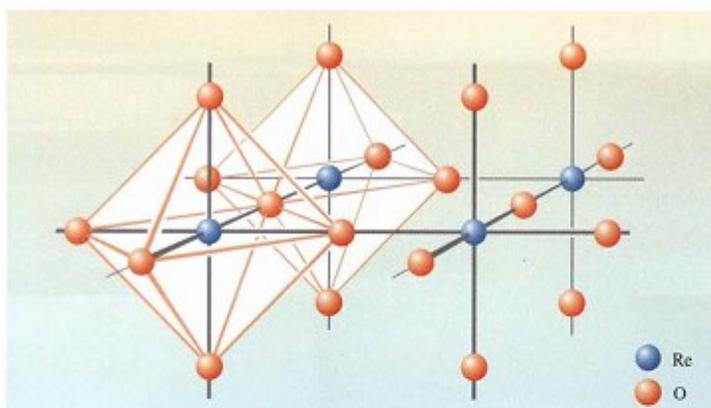
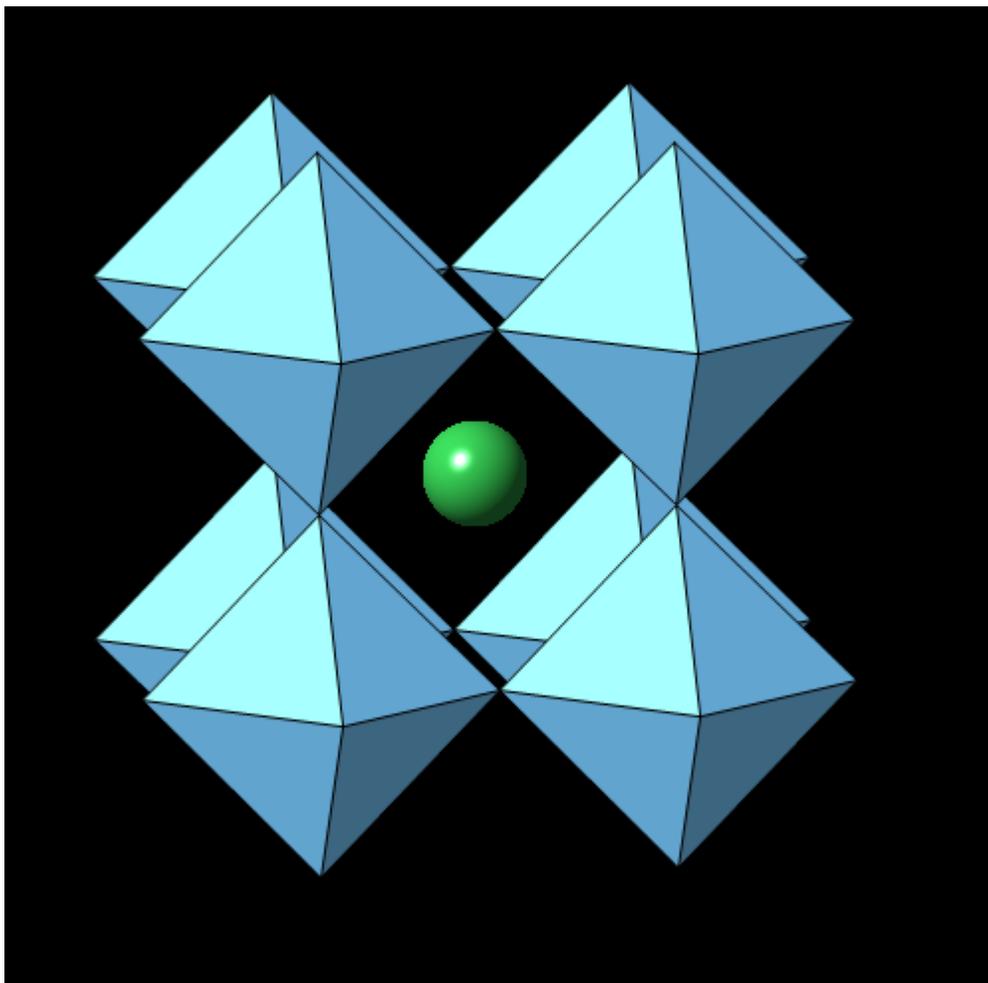


(a)

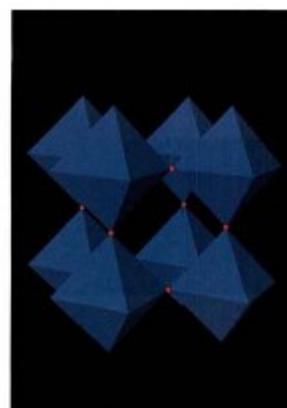


(b)

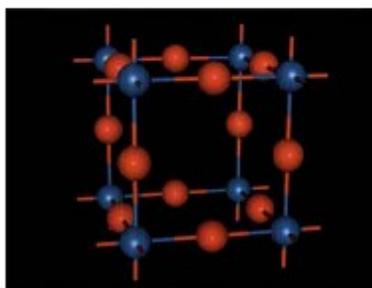
Figure 4.16 The crystal structure of rutile, TiO₂: (a) a unit cell; (b) parts of two columns of TiO₆ octahedra. 



(a)



(b)



(c)

Figure 4.18 Part of the ReO_3 structure, showing linking of ReO_6 octahedra through their corners: (a) part of a single layer; (b) part of two layers, showing linked octahedra; (c) a unit cell. □

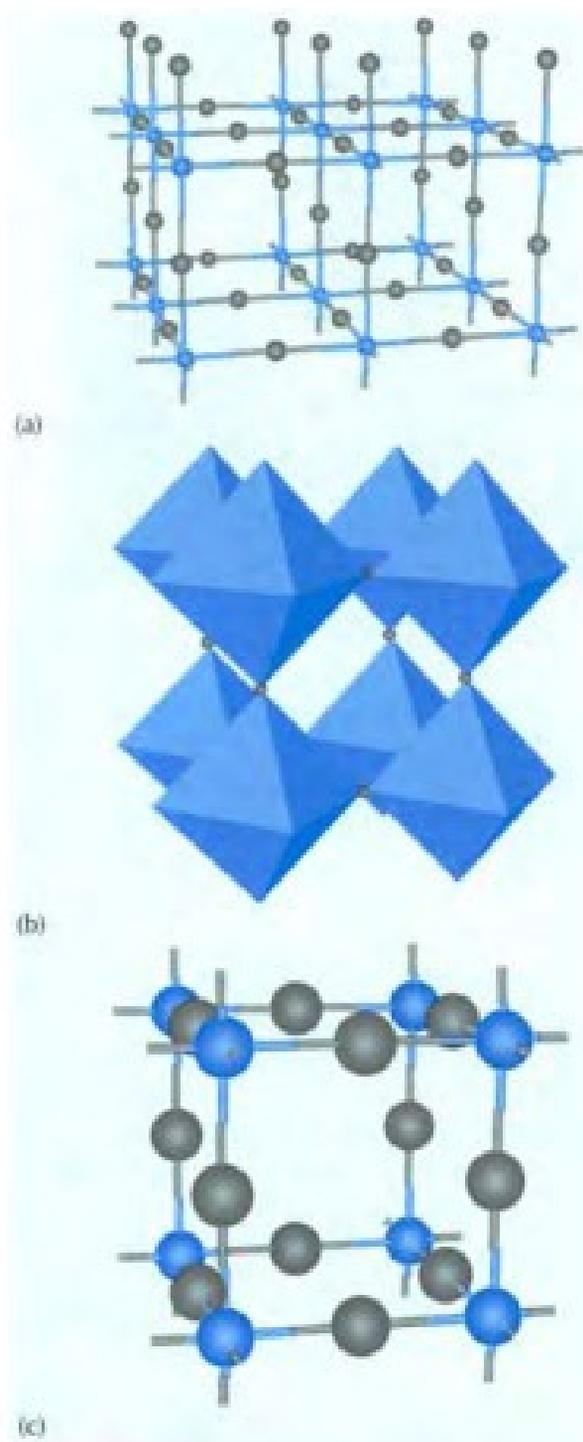
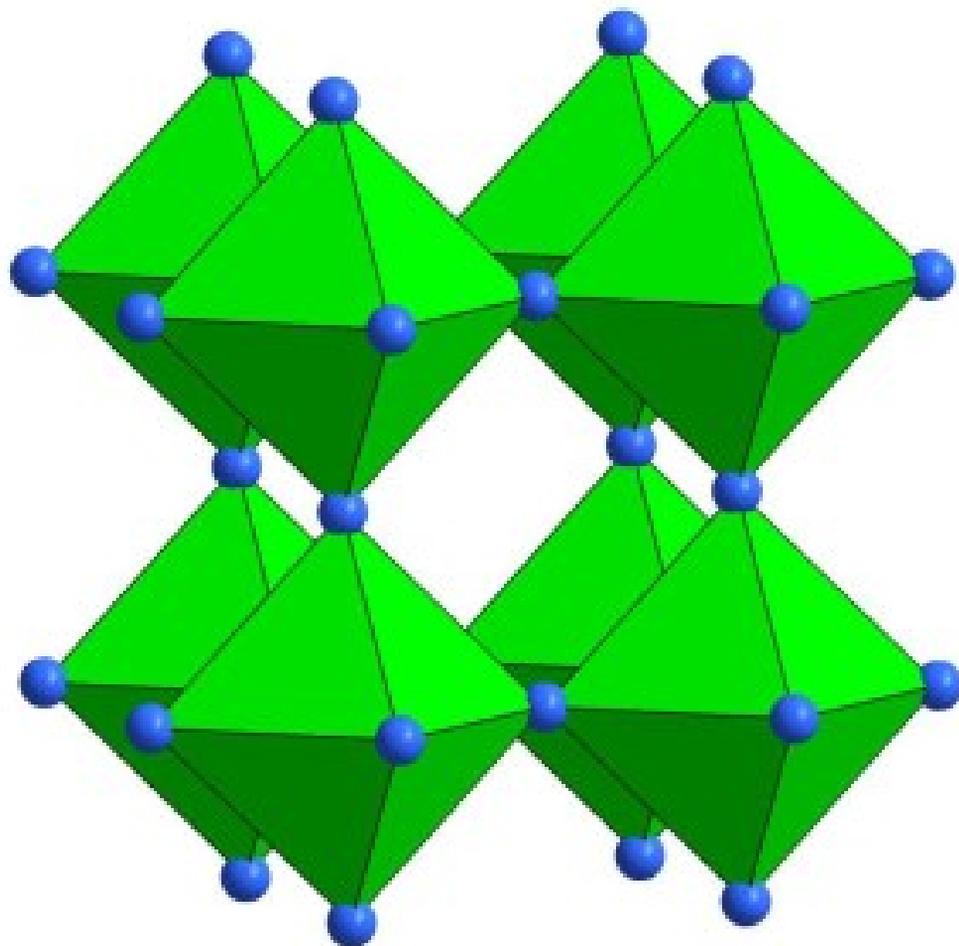
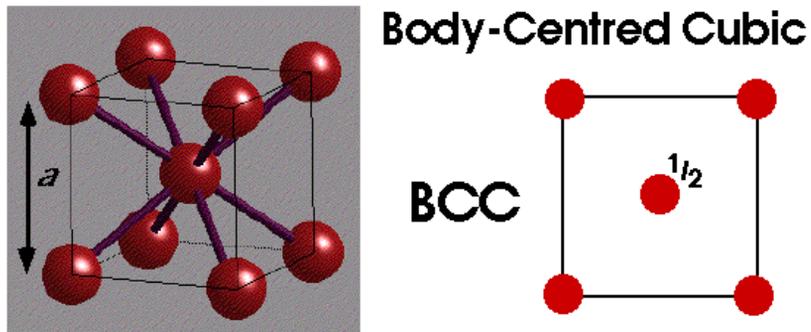


FIGURE 1.42 (a) Part of the ReO_3 structure, (b) ReO_3 structure showing the linking of $[\text{ReO}_6]$ octahedra, and



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68 % del espacio esta ocupado (f de e)

Los números de coordinación son:

8 vecinos colocados a $0.87 a$

hay 6 más colocados a $1a$ (segundos vecinos)

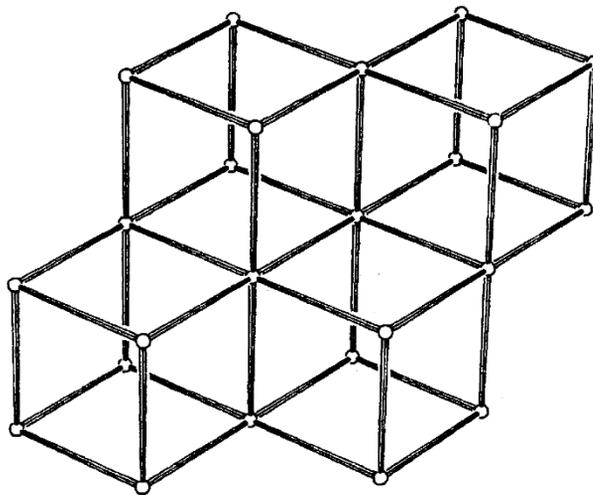


Fig. 12. The simple cubic structure of α -Polonium

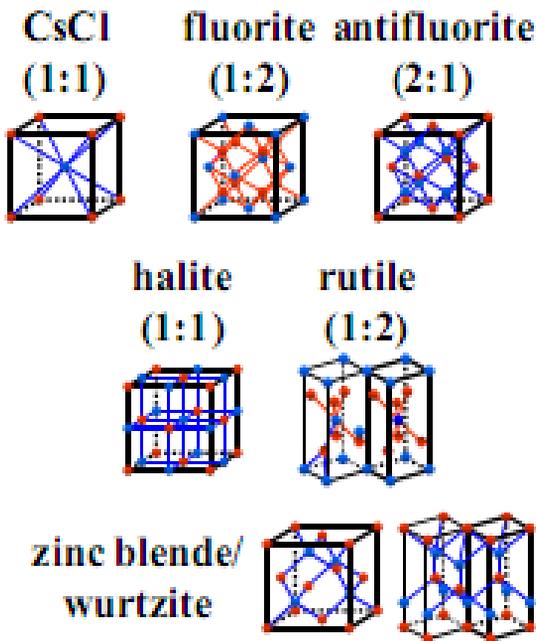
Interatomic distances in some simple structures

Table 1.11 Calculation of interatomic distances in some simple structures

Structure type	Distance	Number of such distances	Magnitude of distance in terms of unit cell dimensions
Rock salt (cubic)	Na-Cl	6	$a/2 = 0.5a$
	Cl-Cl	12	$a/\sqrt{2} = 0.707a$
	Na-Na	12	$a/\sqrt{2} = 0.707a$
Zinc blende (cubic)	Zn-S	4	$a\sqrt{3}/4 = 0.433a$
	Zn-Zn	12	$a/\sqrt{2} = 0.707a$
	S-S	12	$a/\sqrt{2} = 0.707a$
Fluorite (cubic)	Ca-F	4 or 8	$a\sqrt{3}/4 = 0.433a$
	Ca-Ca	12	$a/\sqrt{2} = 0.707a$
	F-F	6	$a/2 = 0.5a$
Wurtzite ^a (hexagonal)	Zn-S	4	$a\sqrt{3}/8 = 0.612a = 3c/8 = 0.375c$
	Zn-Zn	12	$a = 0.612c$
	S-S	12	$a = 0.612c$
Nickel arsenide ^a (hexagonal)	Ni-As	6	$a/\sqrt{2} = 0.707a = 0.433c$
	As-As	12	$a = 0.612c$
	Ni-Ni	2	$c/2 = 0.5c = 0.816a$
	Ni-Ni	6	$a = 0.612c$
Caesium chloride (cubic)	Cs-Cl	8	$a\sqrt{3}/2 = 0.866a$
	Cs-Cs	6	a
	Cl-Cl	6	a
Cadmium iodide (hexagonal)	Cd-I	6	$a/\sqrt{2} = 0.707a = 0.433c$
	I-I	12	$a = 0.612c$
	Cd-Cd	6	$a = 0.612c$

^aThese formulae do not necessarily apply when c/a is different from the ideal value of 1.633.

Radius Ratio



If lattice type unknown:

$$U_0 = \frac{120,200vZ^+Z^-}{r_0} \left(1 - \frac{34.5}{r_0} \right)$$

v # of ions per "molecule"

