AB_3 Compounds

1) Perovskite Type → 3 Dimensional (ReO3)
2) TlI_3 → 1 Dimensional
3) $ZrSe_3$ type → 2 Dimensional and variants
4) $AlCl_3$ Type → 2 Dimensional structure

Less Common

1) MoO_3 Type
2) $Ba(MnS_3)$ Type
3) $NdTe_3$
4) $CoAs_3$

ReO_3 perovskite Type-Cubic

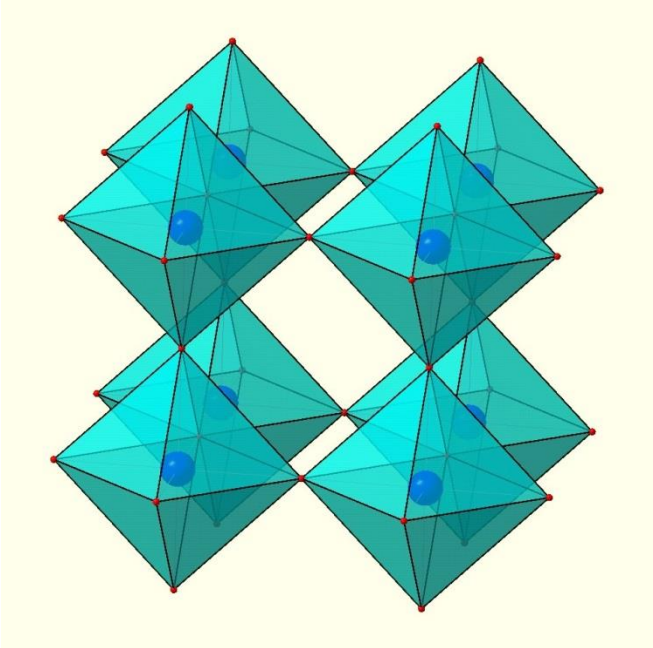
Examples

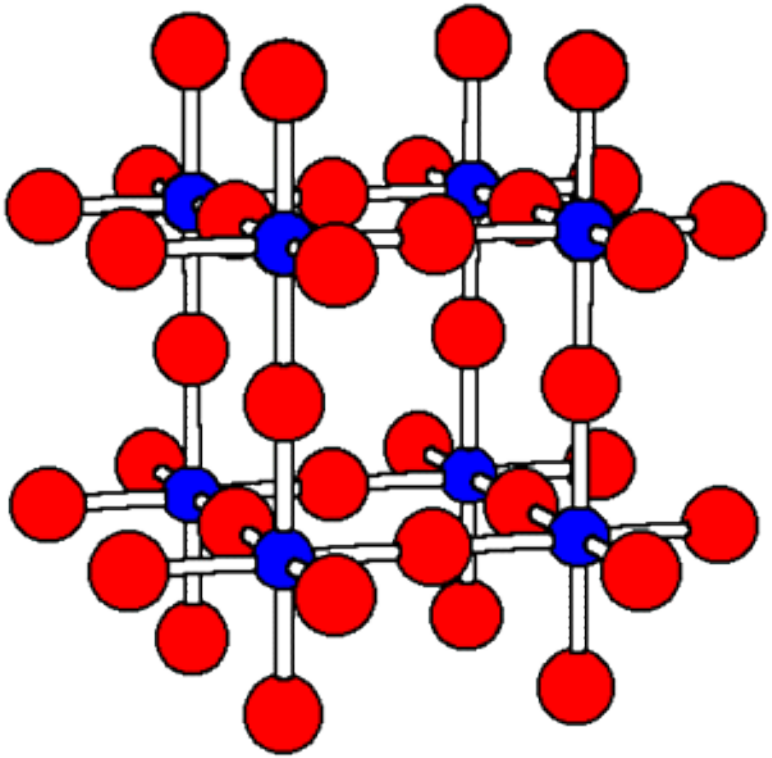
WO3 VF3 TiOF2

FeF3 MoOF2

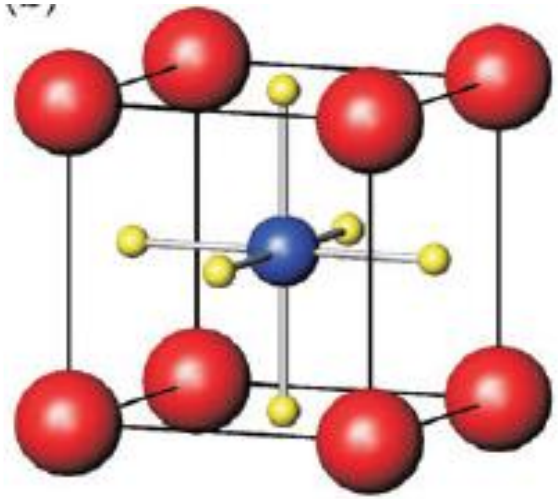
Li3N

Cu3N





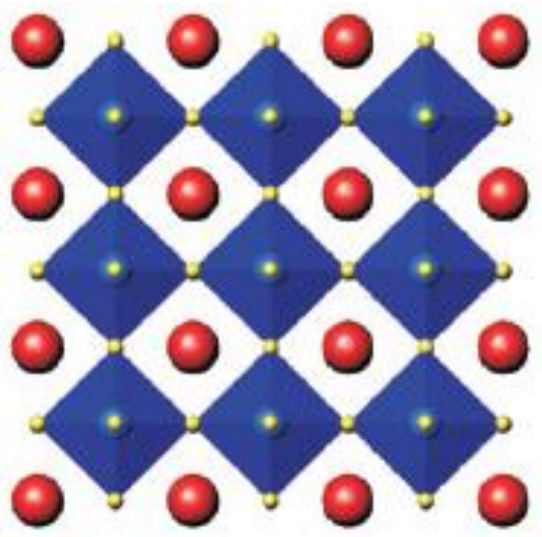
Filled perovskite



A^{2+}

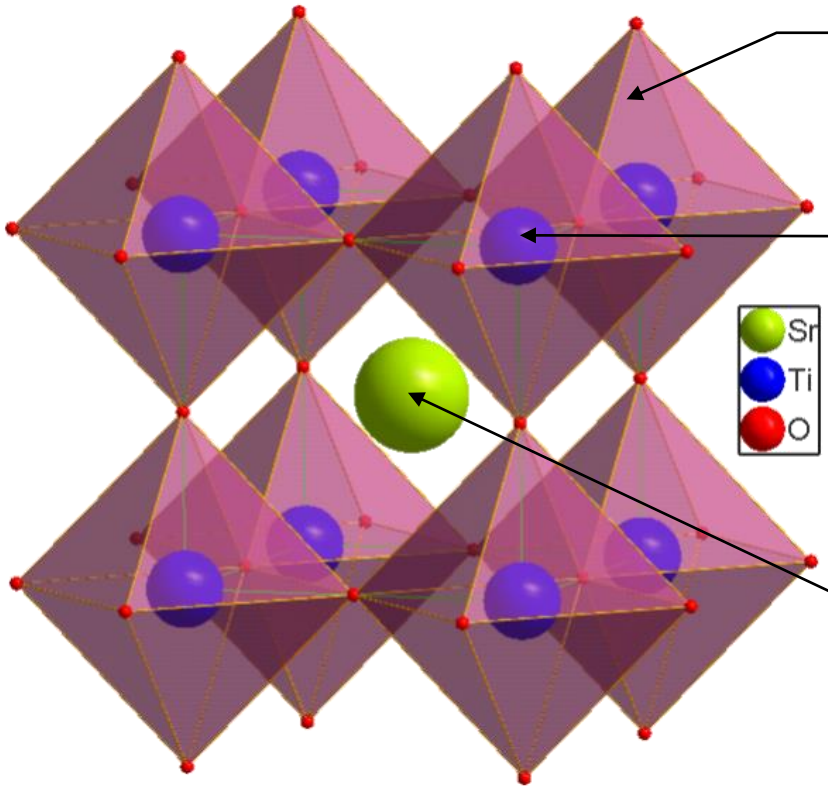
B^{4+}

O^{2-}



Cubic perovskite $SrTiO_3$

$Pm\bar{3}m$

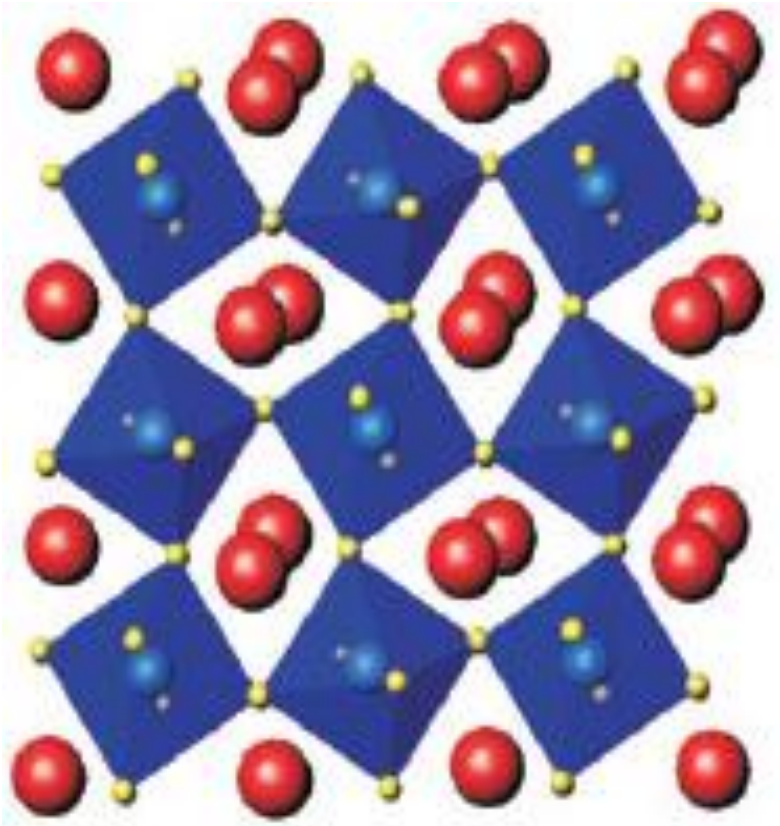


Oxygen
Octaedra

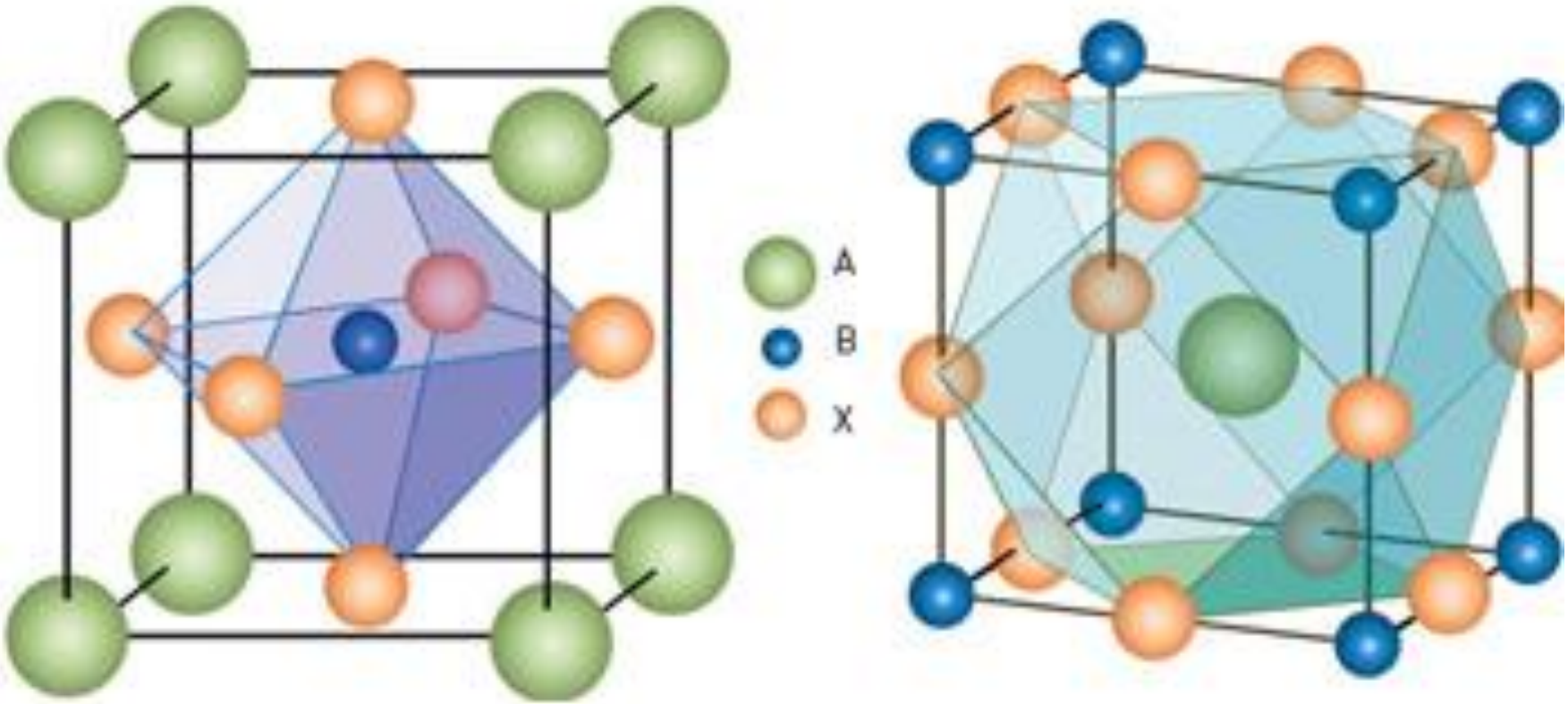
Octaedral site B cations :
Nb, Ta, Ti, Zr, Fe, Mn, ….

Dodecaedral site A cations :
K, Na, Ca, Sr, Ba, Pb, Bi, Y, La, …

Distorted perovskite structure ($CaTiO_3$)



Perovskite



Cubic perovskite $SrTiO_3$

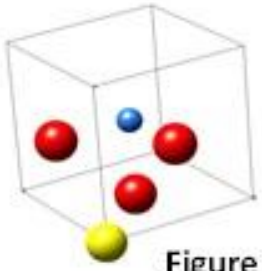


Figure 2.

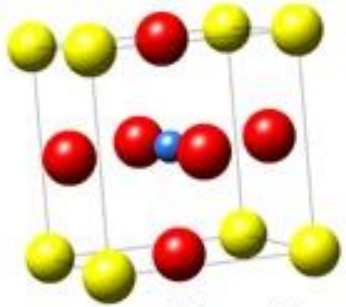


Figure 3.

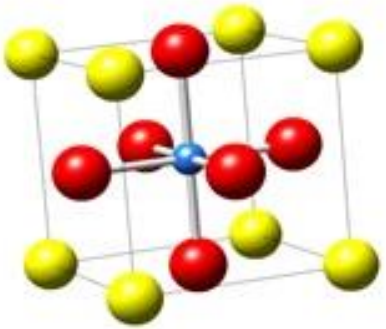


Figure 4.

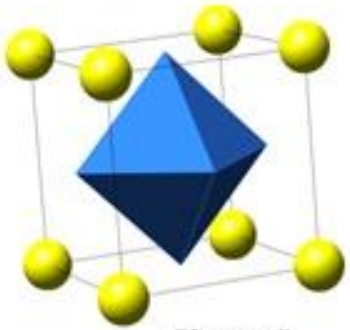


Figure 5.

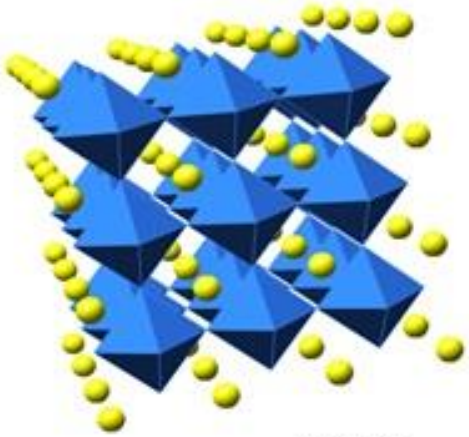


Figure 6.

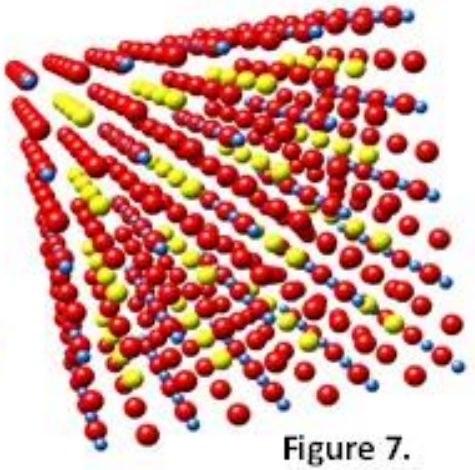


Figure 7.

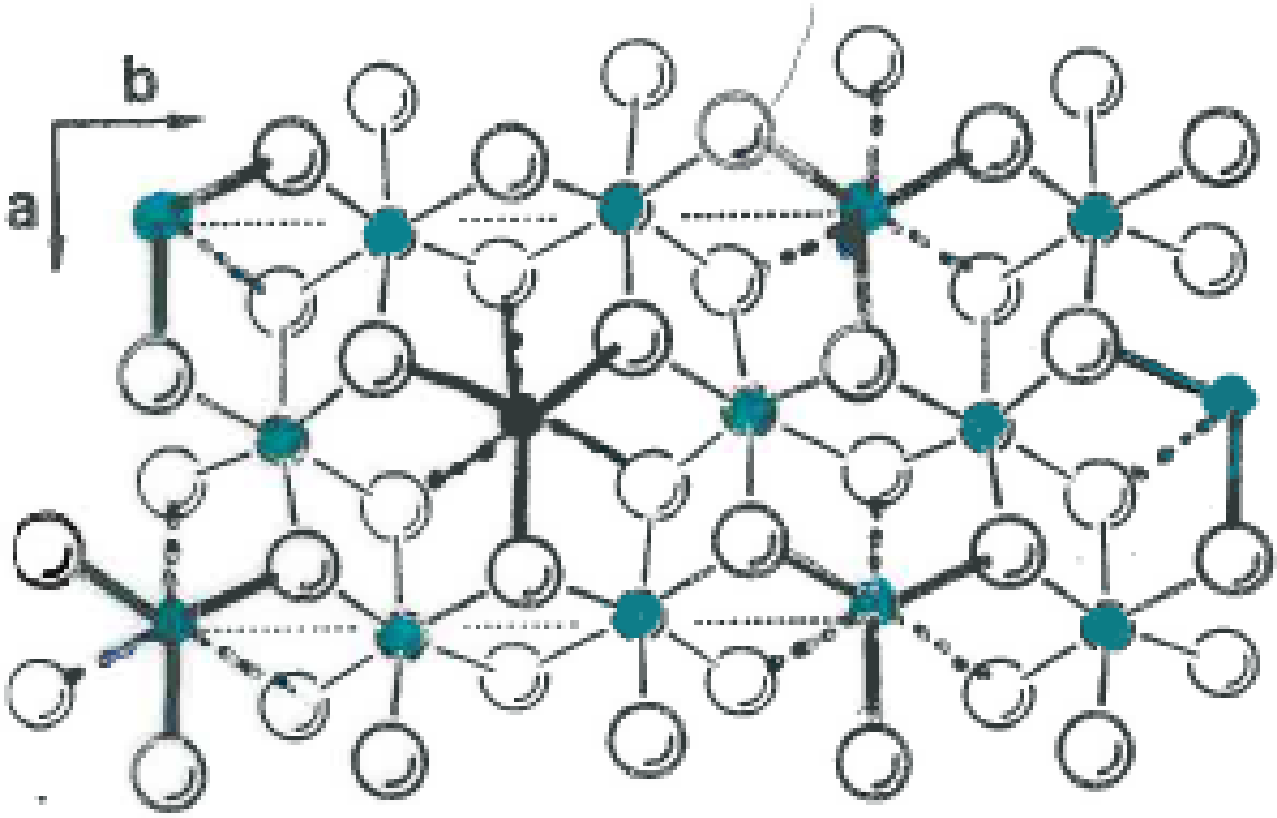
$AlCl_3$ Type

Defect CdCl2 type

Cd3Cl6

Cd2 □ Cl6

AlCl3



$FeCl_3$, $Al(OH)_3$,$GaCl_3$ $CrCl_3$

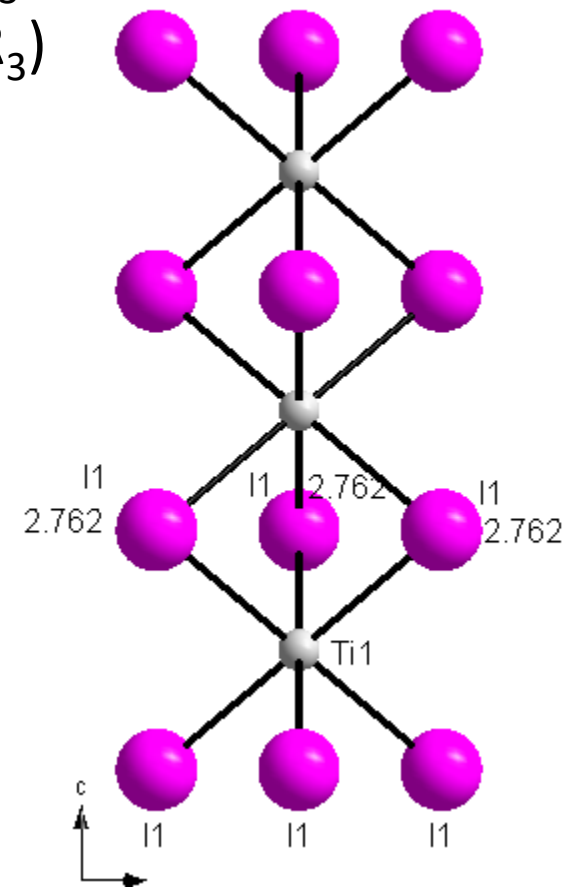
TiI_3 Type

One Dimensional chains

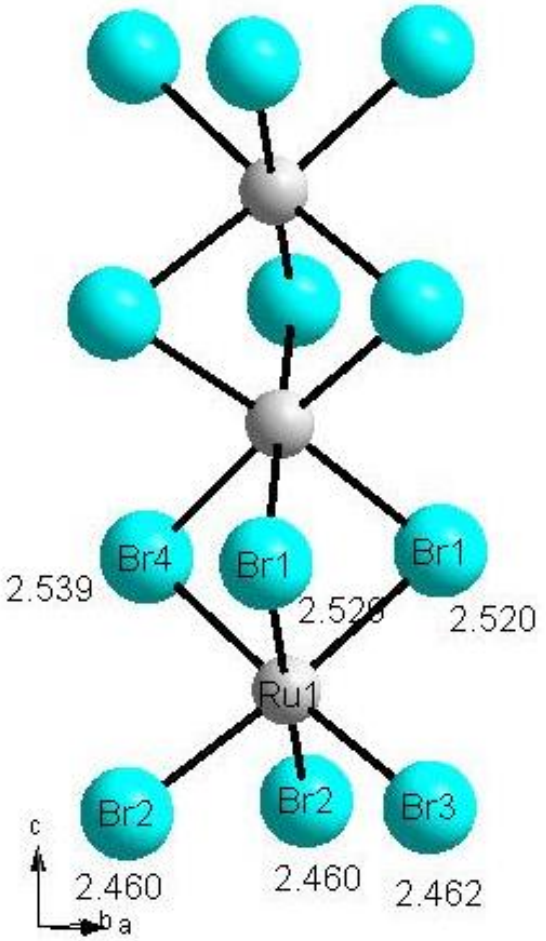
$CsNiCl_3$

$Mo(SR_3)$

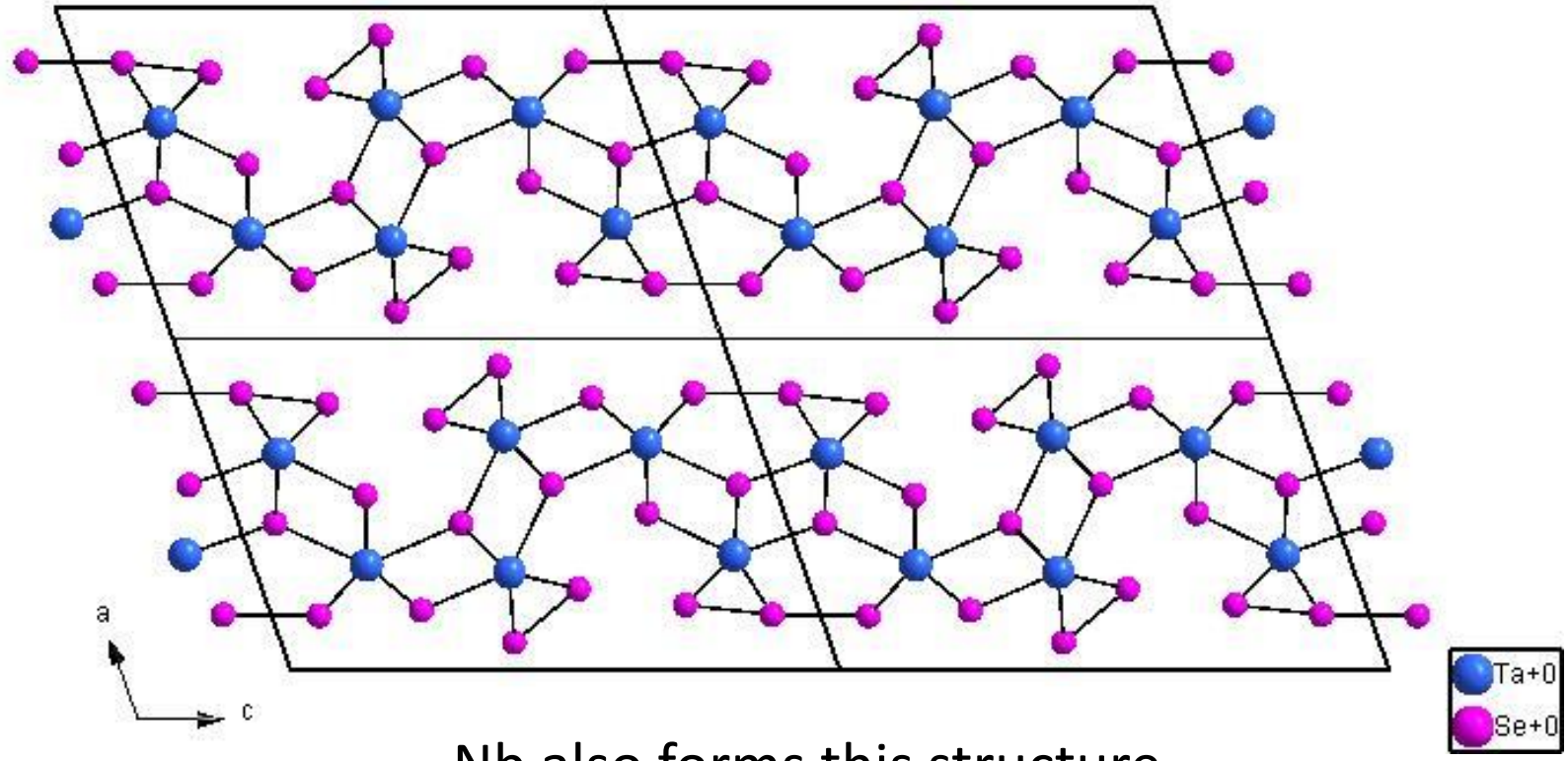
MoI_3



$RuBr_3$ Dostorted TiI_3



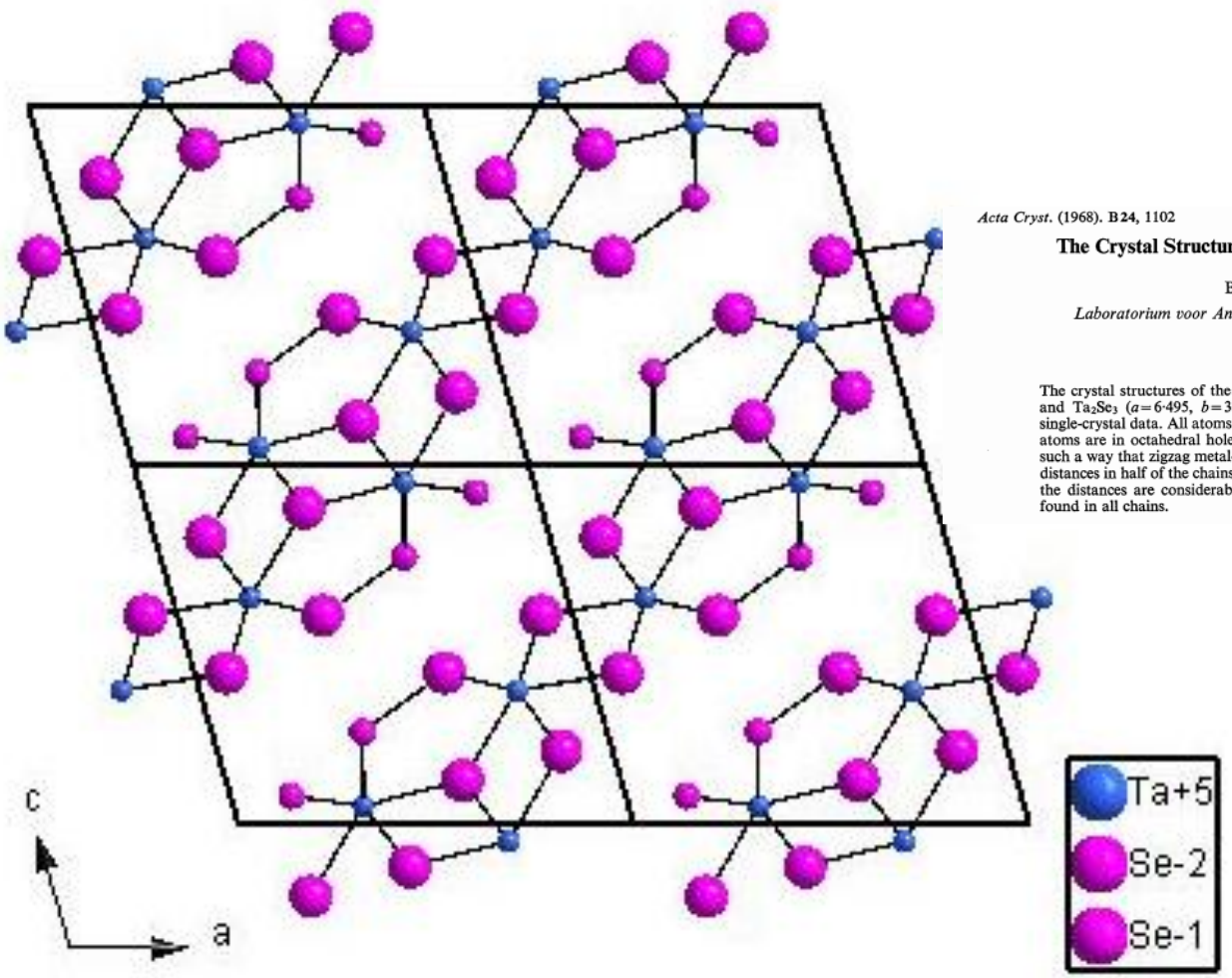
$TaSe_3$ and TaS_3_P21/m



Nb also forms this structure

Journal of Solid State Chemistry (1982), 41, 315-322

$TaSe_3\_P2_1$



Acta Cryst. (1968). B24, 1102

The Crystal Structures of Niobium(III) Selenide and Tantalum(III) Selenide

BY F. KADIJK, R. HUISMAN AND F. JELLINEK

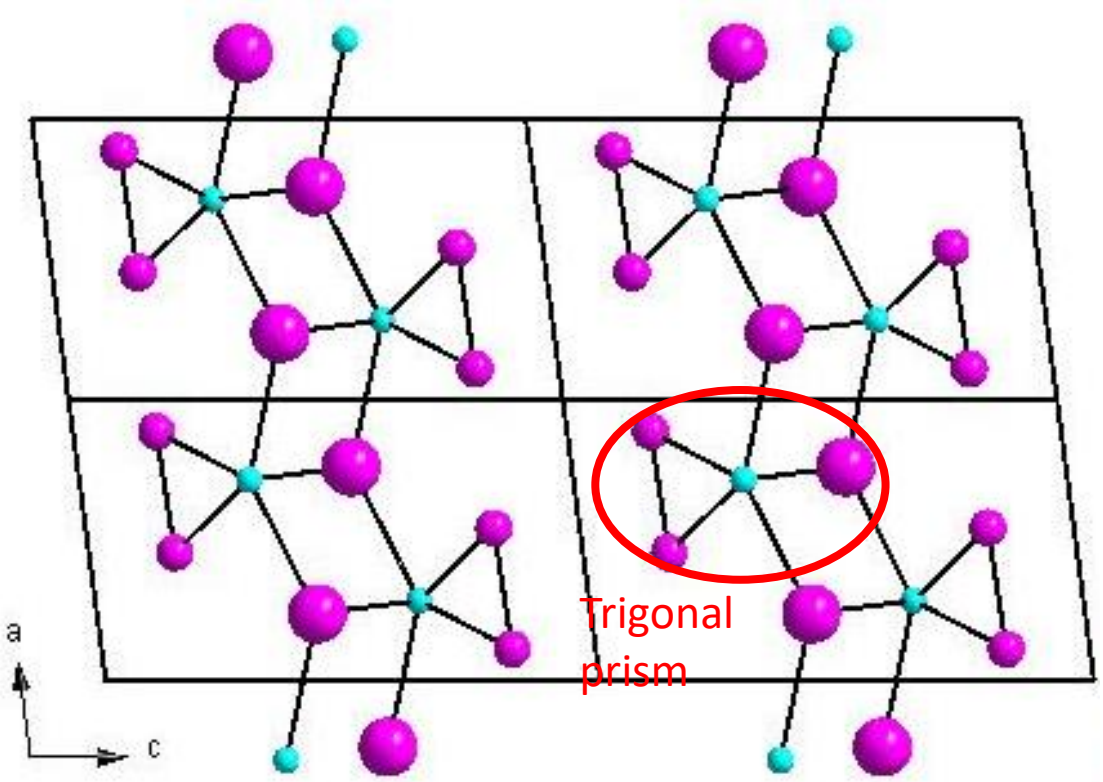
Laboratorium voor Anorganische Chemie, Rijksuniversiteit Groningen, The Netherlands

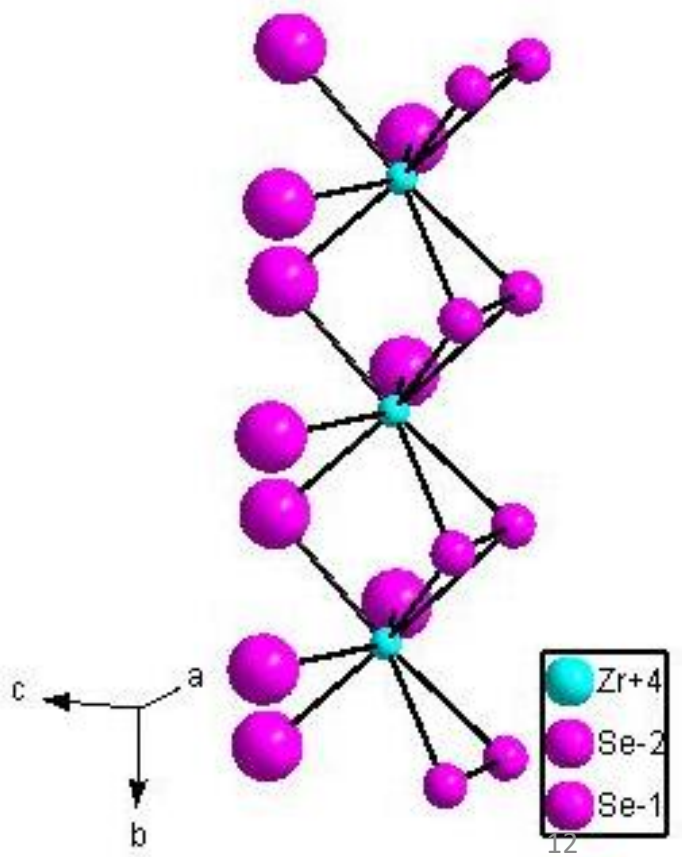
(*Received* 28 *July* 1967)

The crystal structures of the monoclinic phases Nb_2Se_3 ($a = 6{\cdot}503$, $b = 3{\cdot}434$, $c = 9{\cdot}215$ Å; $\beta = 103{\cdot}39°$) and Ta_2Se_3 ($a = 6{\cdot}495$, $b = 3{\cdot}408$, $c = 9{\cdot}206$ Å; $\beta = 103{\cdot}63°$) have been determined and refined from single-crystal data. All atoms are in the special position $2(e)$: $\pm(x\,\frac{1}{4}\,z)$ of space group $P2_1/m$. The metal atoms are in octahedral holes of a *chh* close packing of selenium, but the structures are deformed in such a way that zigzag metal–metal chains are formed. These chains are of two kinds; the metal–metal distances in half of the chains are comparable to those in the pure metals, in the other half of the chains the distances are considerably longer. In the isotypic phase Mo_2S_3 short metal–metal distances are found in all chains.

Acta Chemica Scandinavica (1-27,1973-42,1988), (1965), 19, 701-710

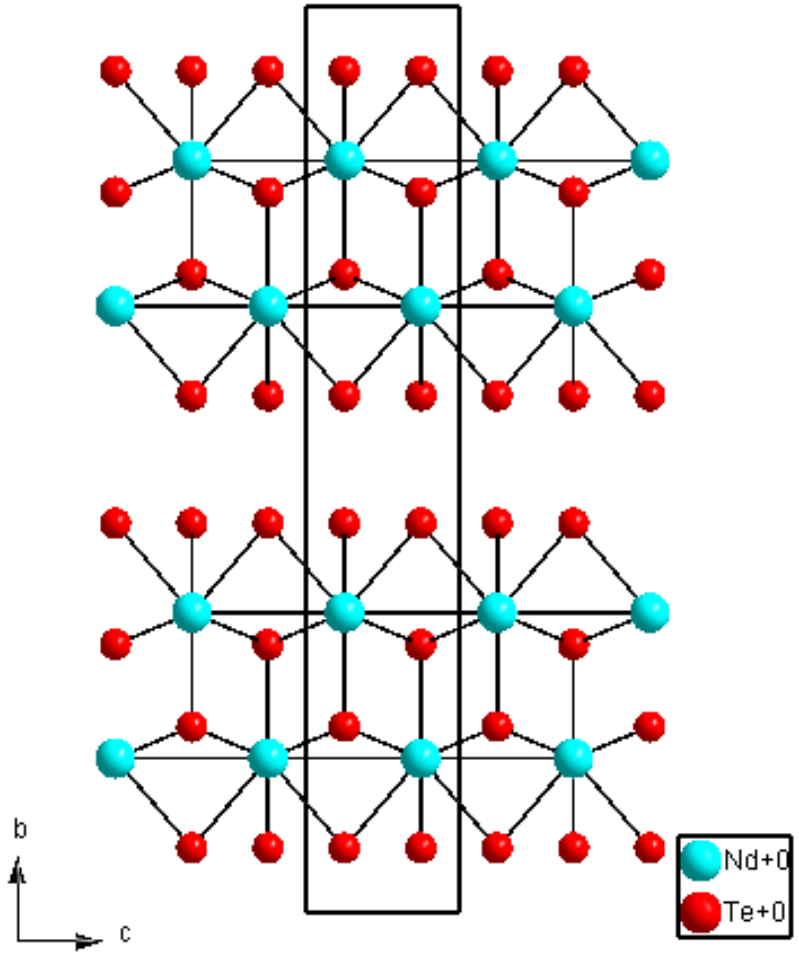
$ZrSe_3$ and Variants

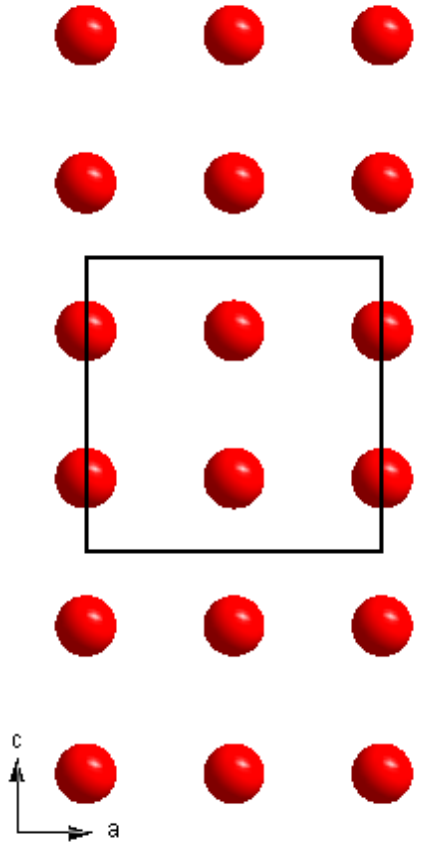




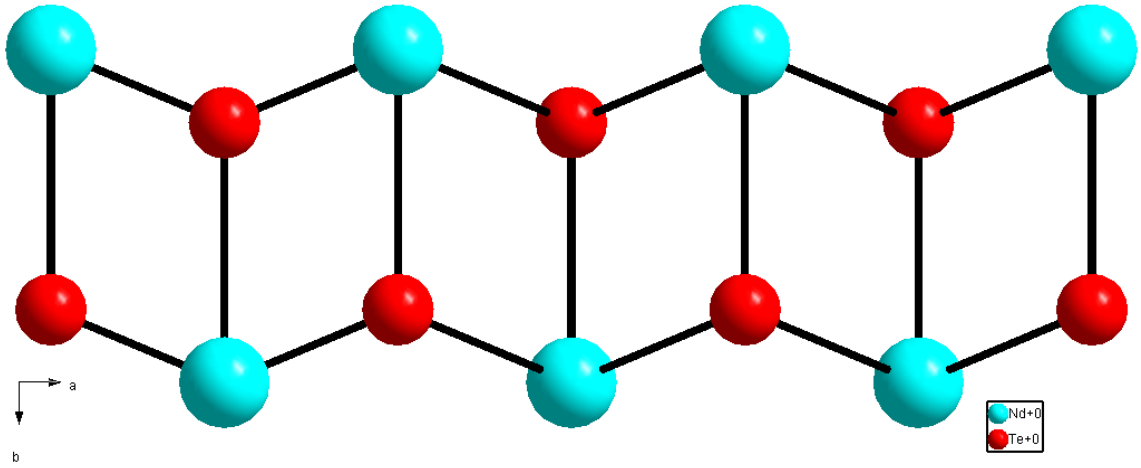
TiS3, ZrS3, HfS3
US3,NpS3,
USe3, NpSe3
UTe3, ThTe3

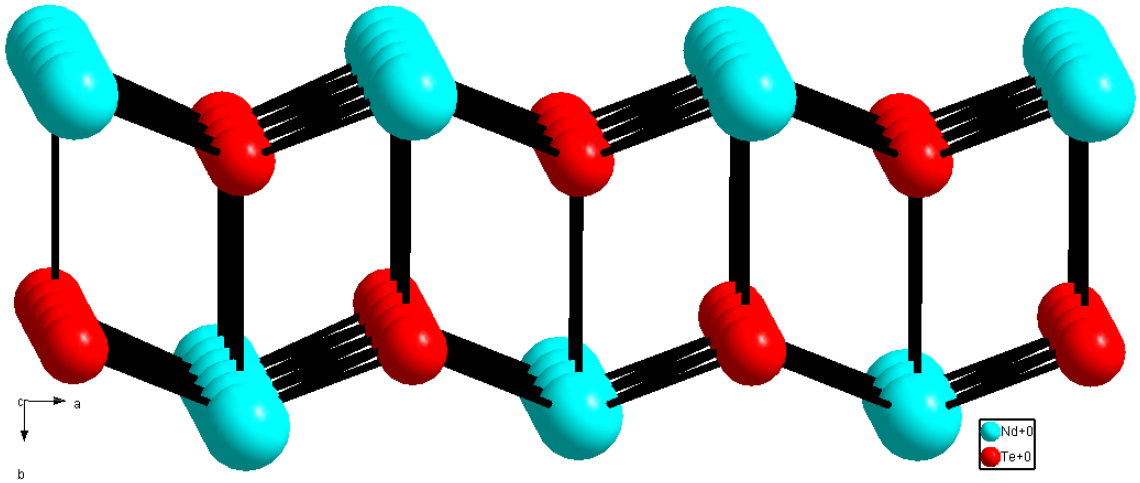
$NdTe_3$

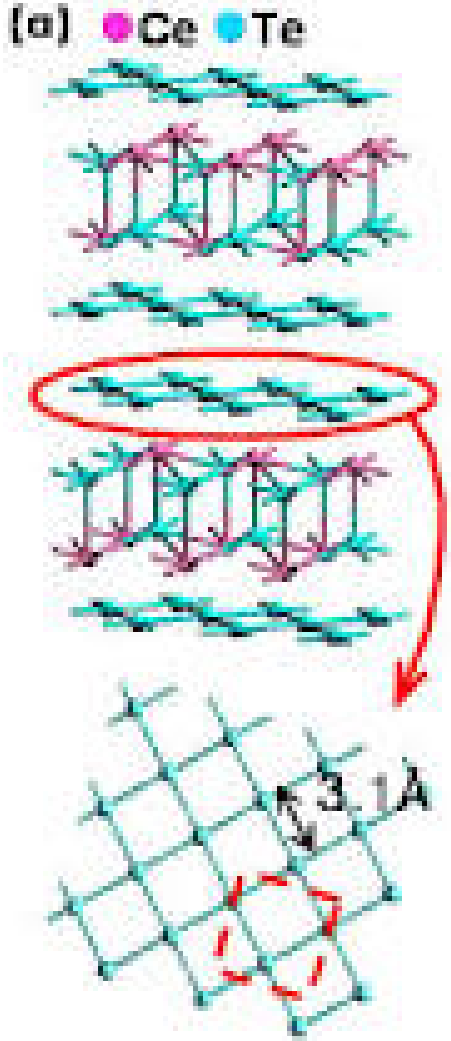




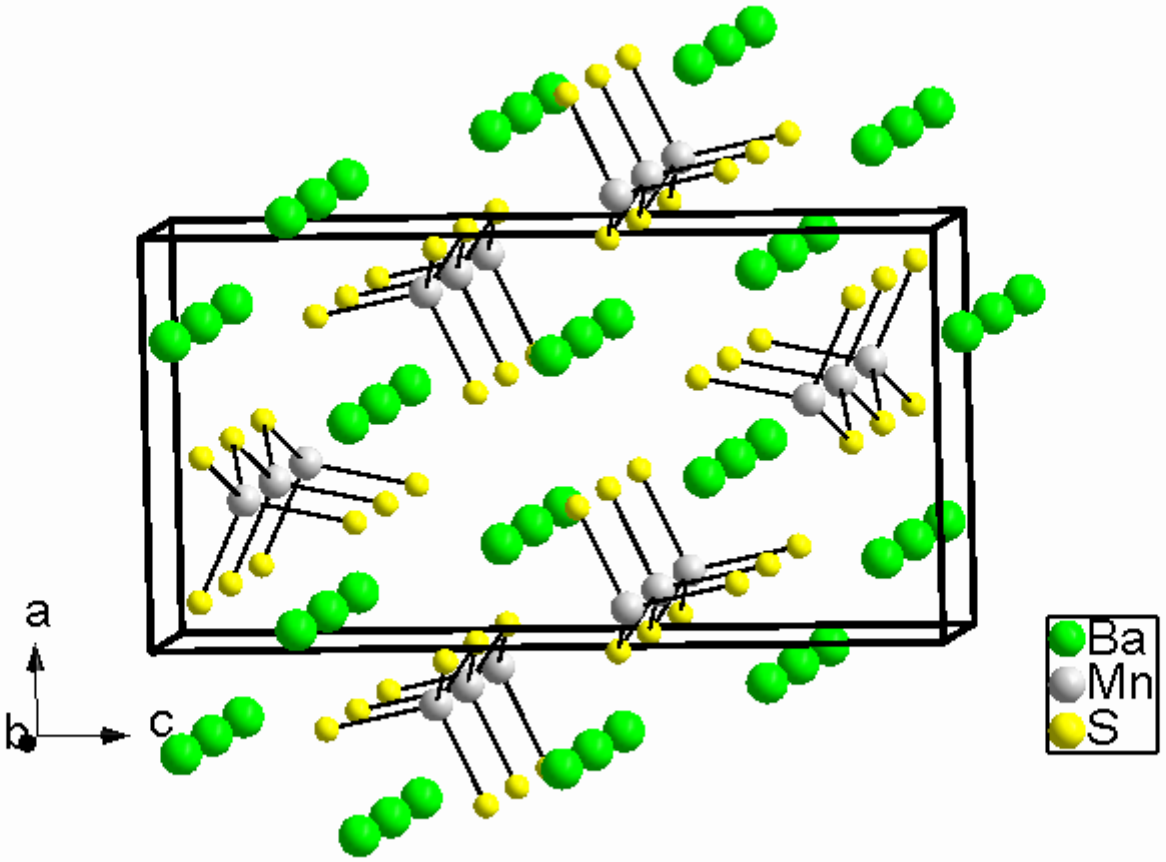
$NdTe_3$



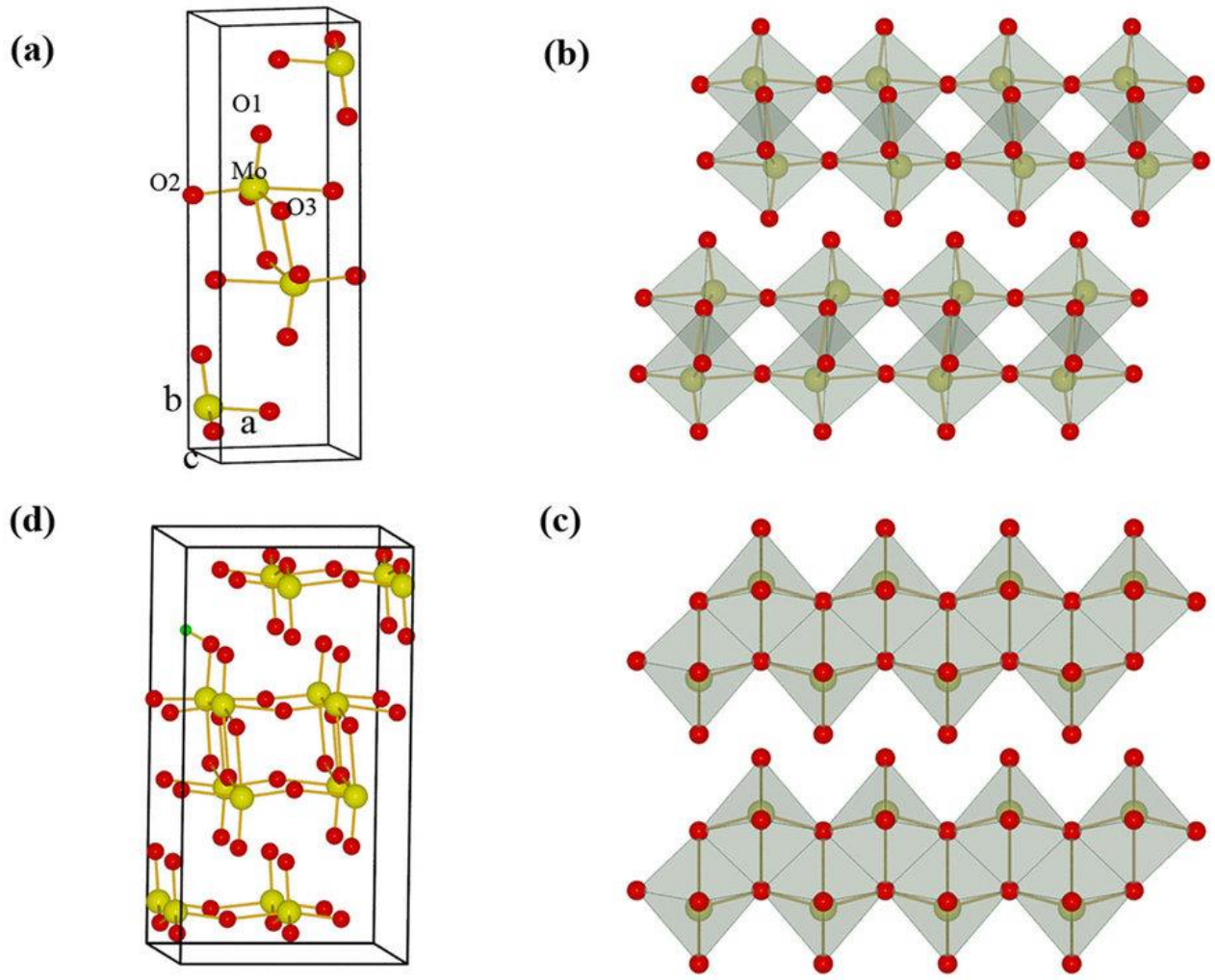




Ba_2MnS_3



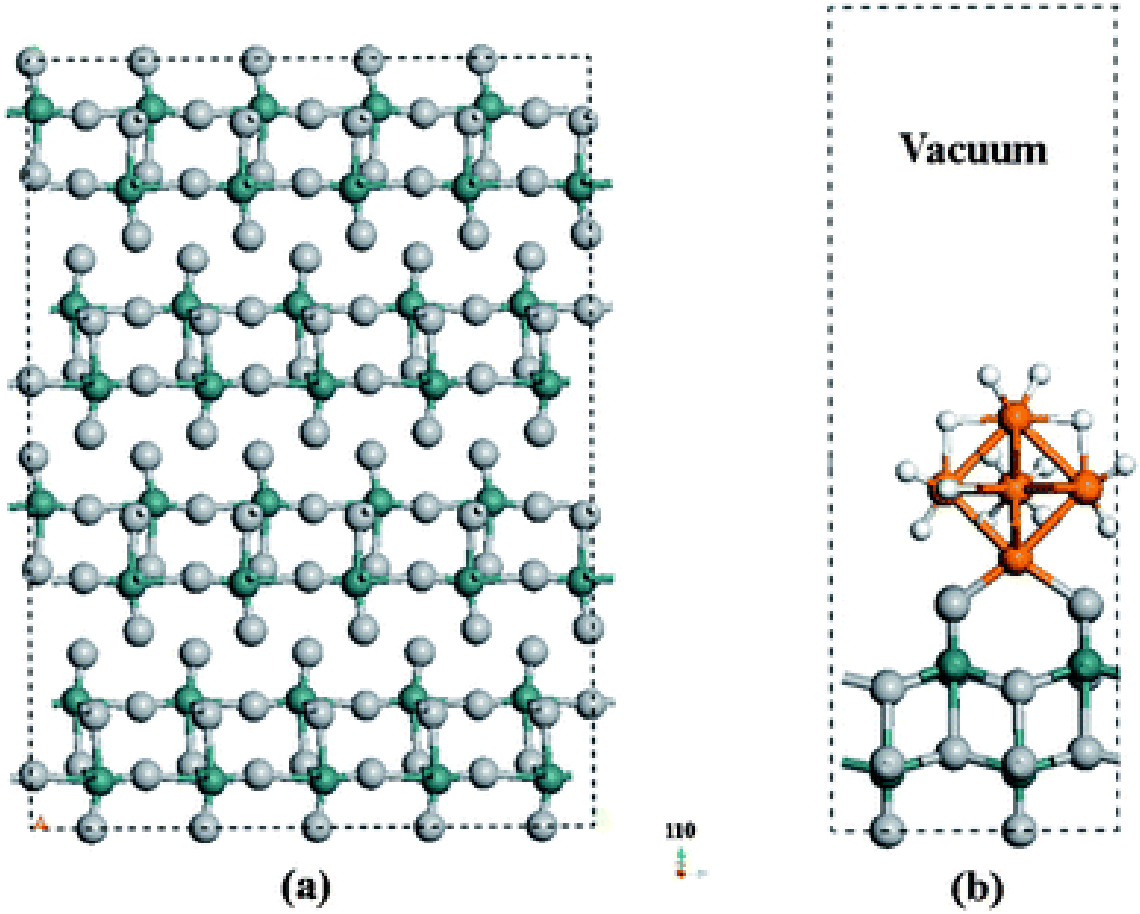
MoO_3 type



Unique structure found in no other compound. Layered.

Shows interesting intercalation/ion-insertion chemistry

MoO_3 type

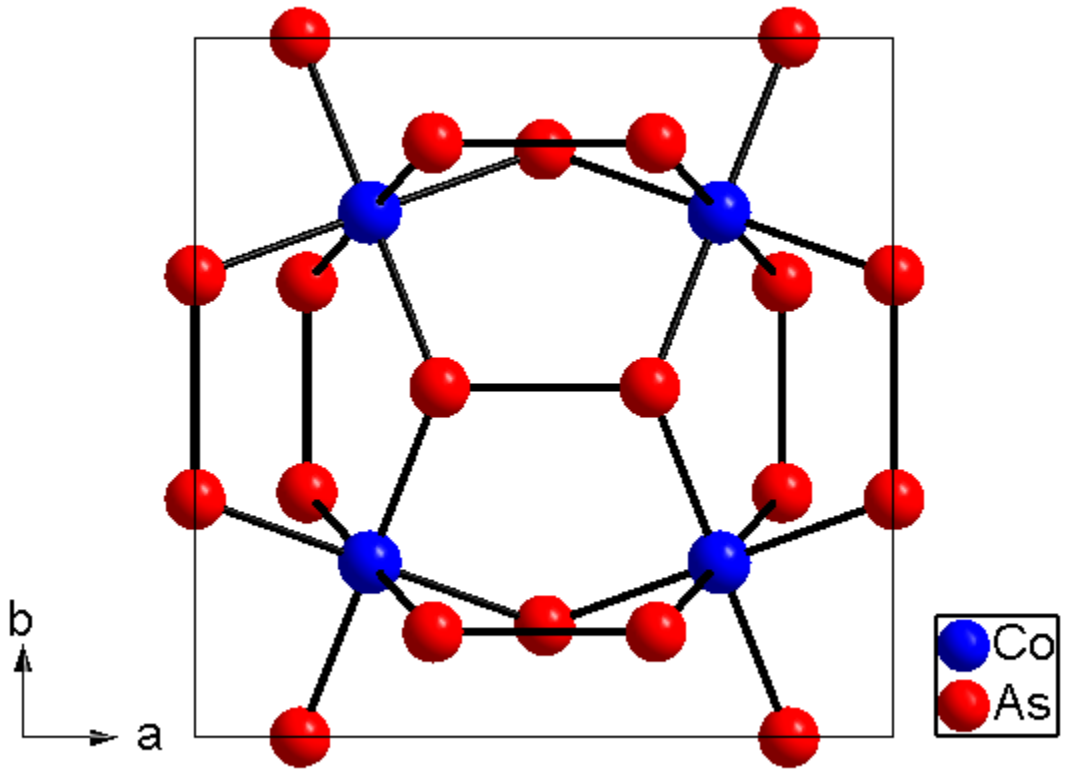


The MoO_3 structure

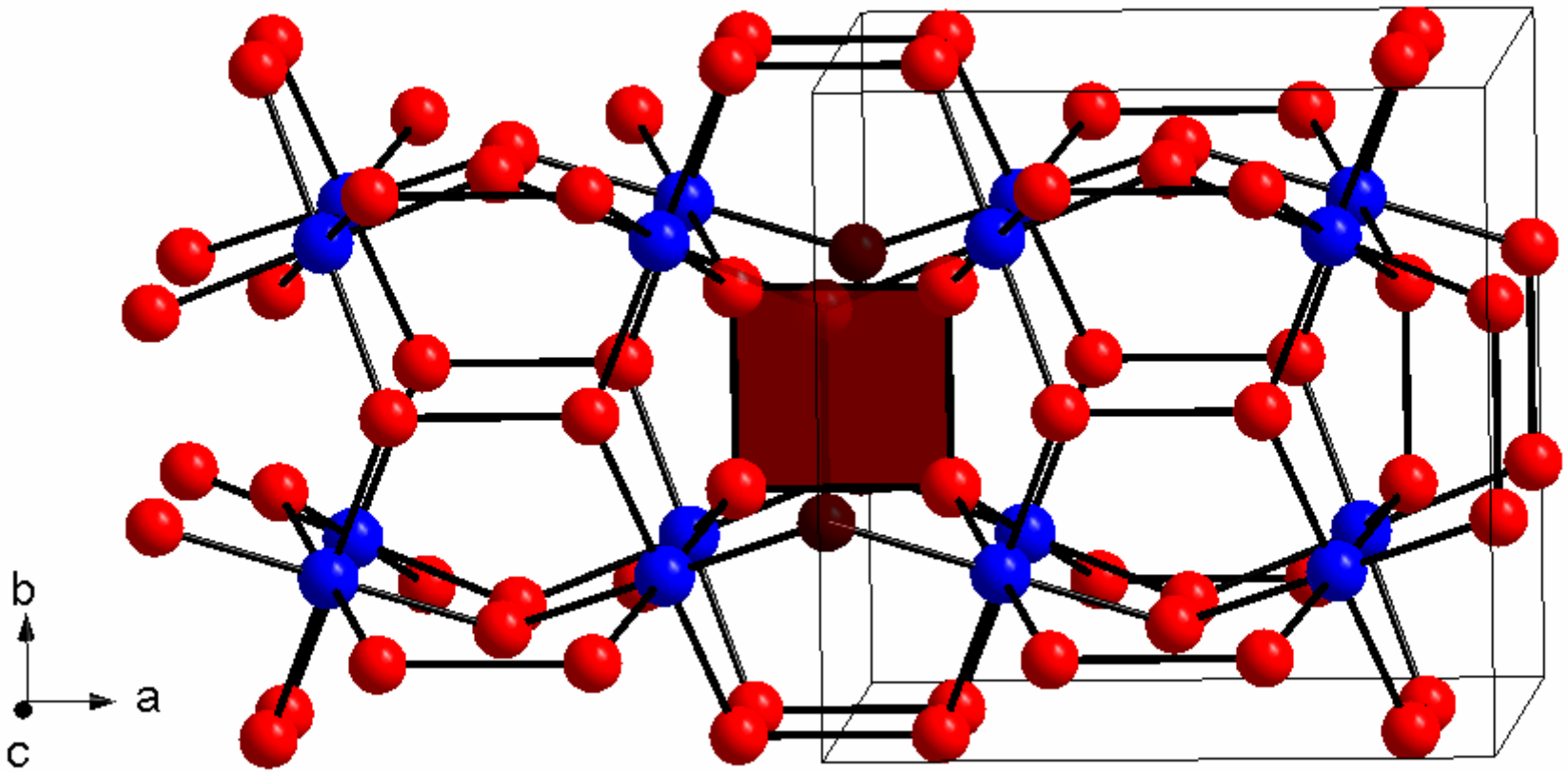
Unique structure found in no other compound. Layered.

Shows interesting intercalation/ion-insertion chemistry

$CoAs_3$ Skutterudite

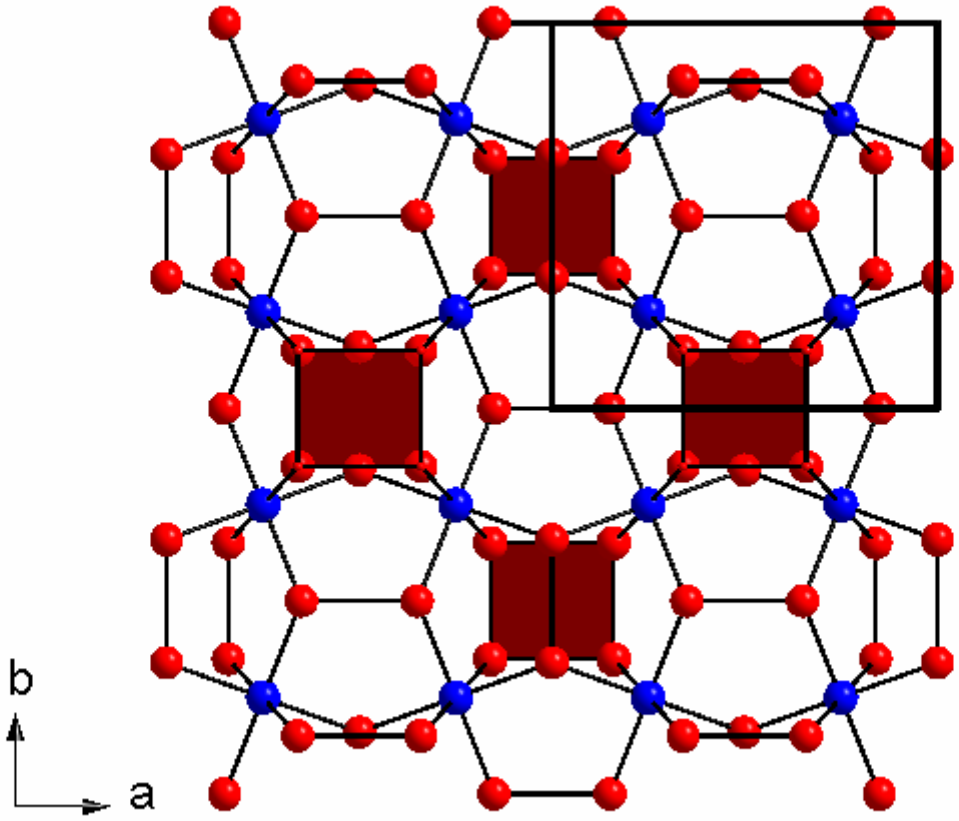


$CoAs_3$ Skutterudite

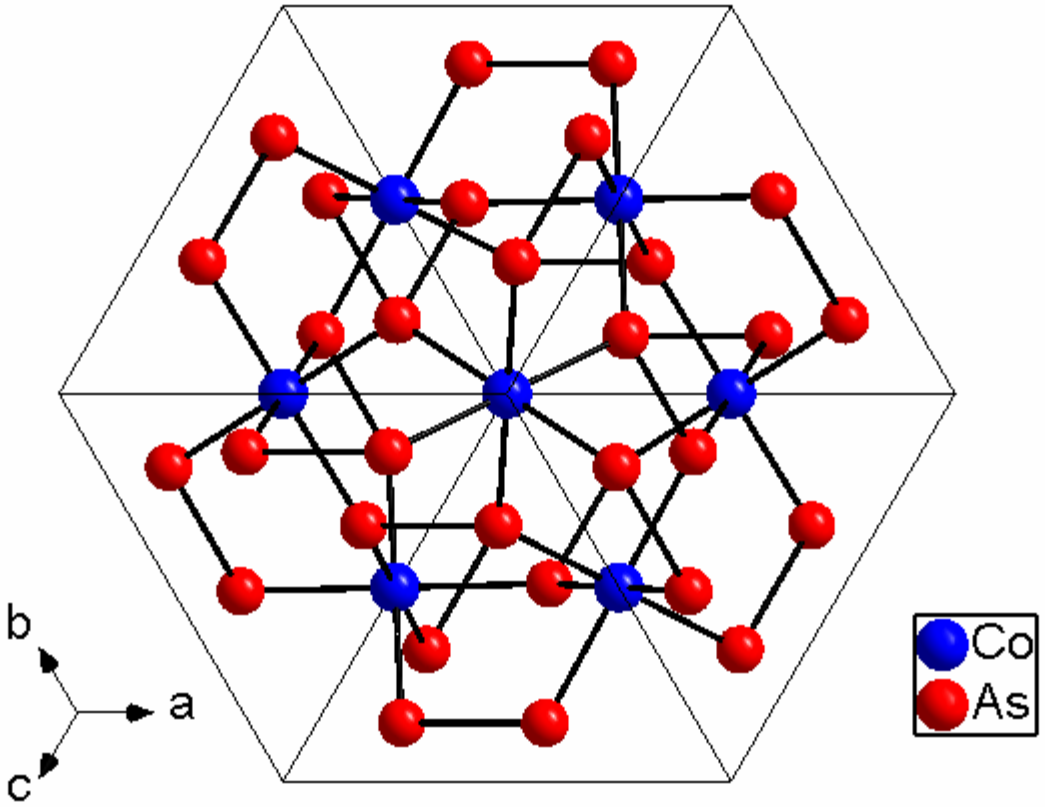


AsS_4 squares

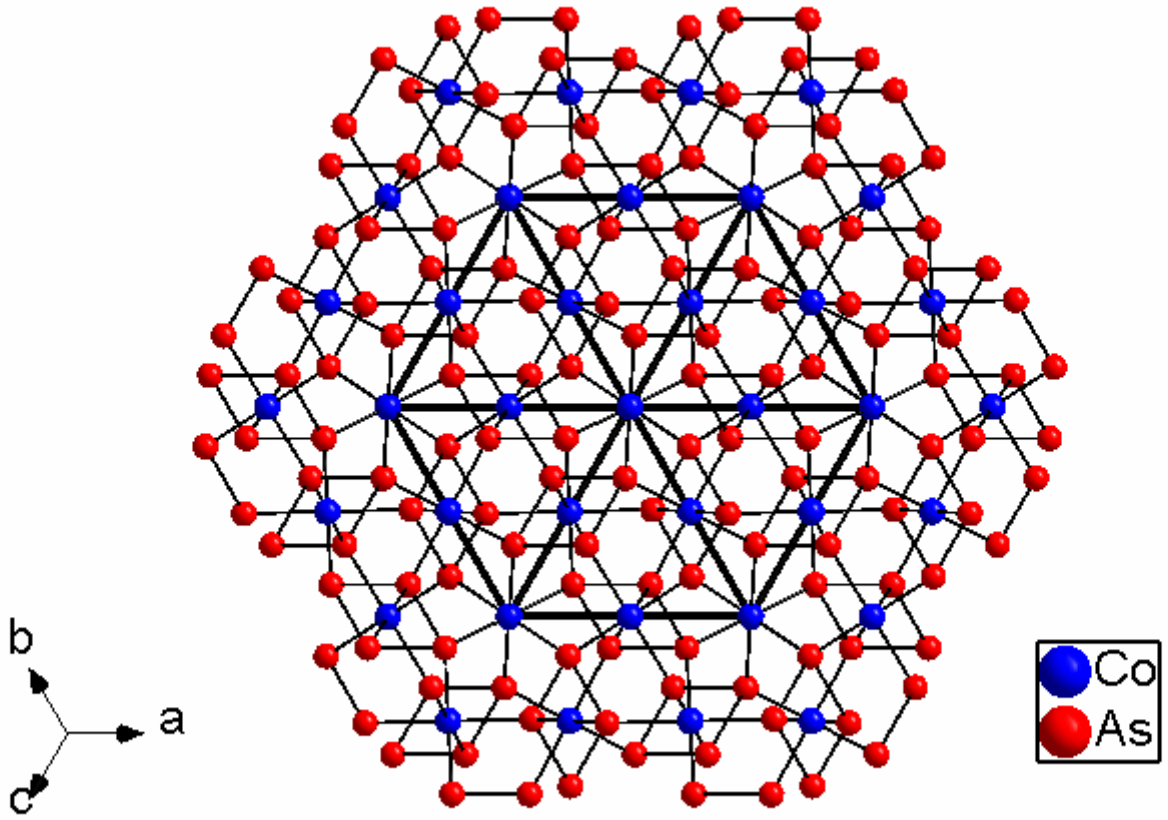
$CoAs_3$ Skutterudite



$CoAs_3$ Skutterudite

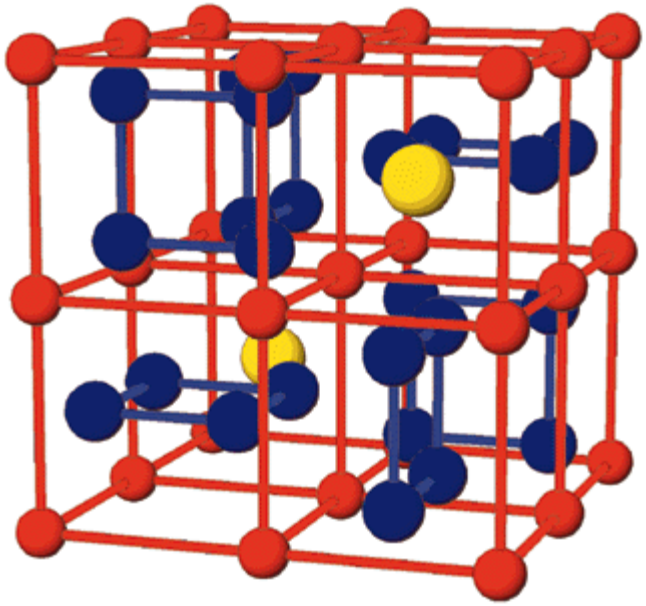


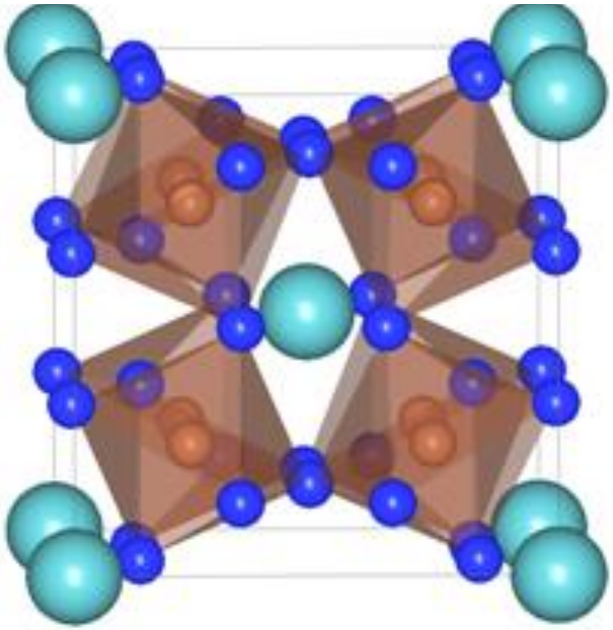
$CoAs_3$ Skutterudite

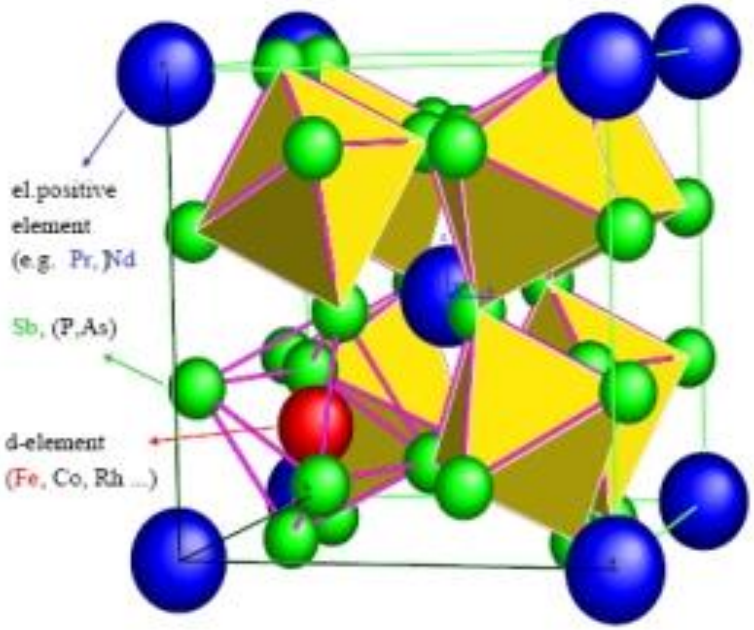


Filled Skutterudite

$LaFe_4Sb_{12}$







Disordered Perovskite

Skutterudite, $CoAs_3$

	STRUCTURE TYPE	SPACE GROUP	SPACE GROUP NUMBER
cI32	As_3Co	$Im\bar{3}$	204

REFERENCE
I. Oftedal
1928 66 P517 ZEITSCHRIFT FUER KRISTALLOGRAPHIE, KRISTALLGEOM., KRISTALLPHYS., KRISTALLCHEM

a = 0.8197 b = c = [nm]
ALPHA = BETA = GAMMA = [DEGREE]
ORIGIN AT $m\bar{3}$
ATOMIC POSITIONS :

ATOMS	WYCKOFF NOTATION	SYMMETRY	x	y	z	OCCUPANCY
As	24(g)	m	0.0	0.350	0.150	1.00
Co	8(c)	$\bar{3}$	0.25	0.25	0.25	1.00

As_3Co	As-Co-Ni	As_3Ir
As_3Rh	$Co_2Ge_3S_3$	$Co_2Ge_3Se_3$
Co-Ni-Sb	CoP_3	$CoSb_3$
$FeNiSb_6$	$Ge_3Ir_2S_3$	$Ge_3Ir_2Se_3$
$Ge_3Rh_2S_3$	IrP_3	$IrSb_3$
$Ir_2S_3Sn_3$	NiP_3	P_3Pd
P_3Rh		

	STRUCTURE TYPE	SPACE GROUP	SPACE GROUP NUMBER
cI32	Ca_3Hg	$I\bar{4}3m$	217

REFERENCE
M. Puselj et al.
1978 51 P75 CROATICA CHEMICA ACTA