Materials 218/UCSB: Class VI & VII, Part II: More structures: AB_2, A_2B_3, AB_3

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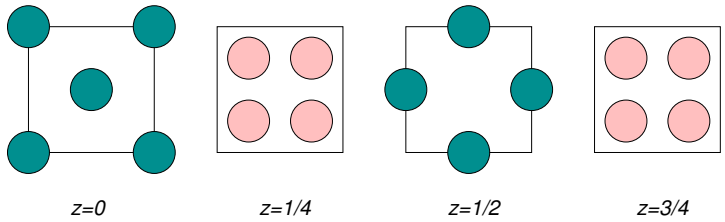
AB_2 structures:

Fluorite CaF_2: SG = $Fm\bar{3}m$ (No. 225) $a = 5.45$ Å

Atom	x	y	z
Ca	0	0	0
F	1/4	1/4	1/4

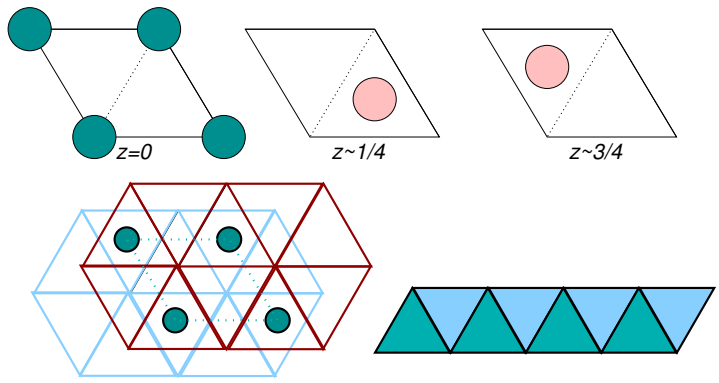


This structure type is also adopted by SrF_2, BaF_2, UO_2, ThO_2, Na_2O (the anti-type), ZrO_2 at high temperatures ...

ZrO_2 can be stabilized in the fluorite structure through doping with Ca^{2+} or Y^{3+} – these are *stabilized* zirconias and have many structural and electrochemical applications.

CdI_2: SG = $P\bar{3}m1$ (No. 164) $a = 4.24$ Å $c = 6.84$ Å

Atom	x	y	z
Cd	0	0	0
I	2/3	1/3	~ 0.25

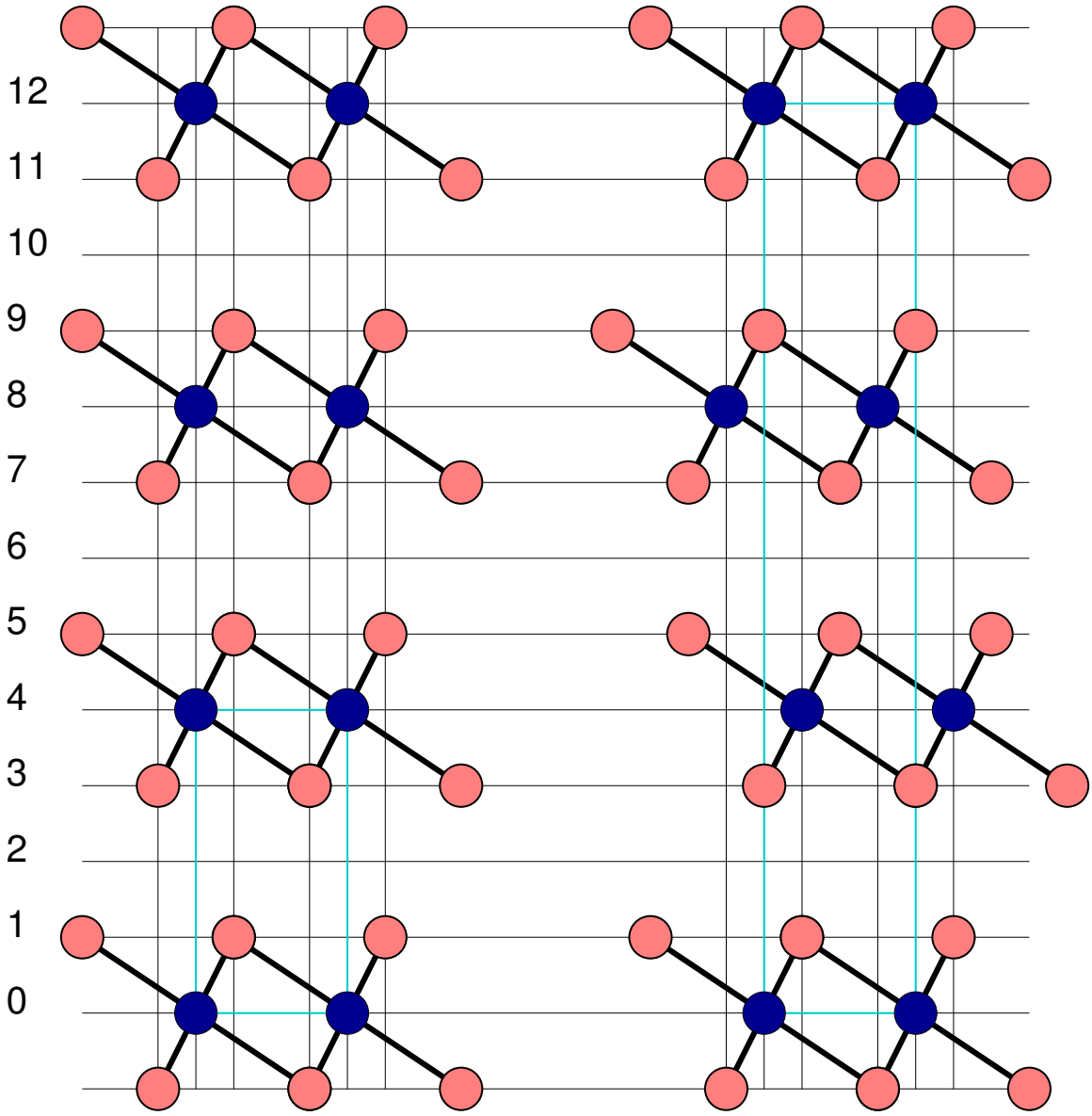


This structure type is also adopted by PbI_2, $MgCl_2$, $FeCl_2$, ZnI_2, $Cd(OH)_2$, $Mg(OH)_2$, TaS_2, NbS_2 ...

$CdCl_2$: SG = $R\bar{3}m$ (No. 166) $a = 3.85$ Å $c = 17.46$ Å

Atom	x	y	z
Cd	0	0	0
Cl	2/3	1/3	$\sim 1/12$

The $CdCl_2$ structure is to the CdI_2 structure what ABCABC stacking is to ABAB stacking:

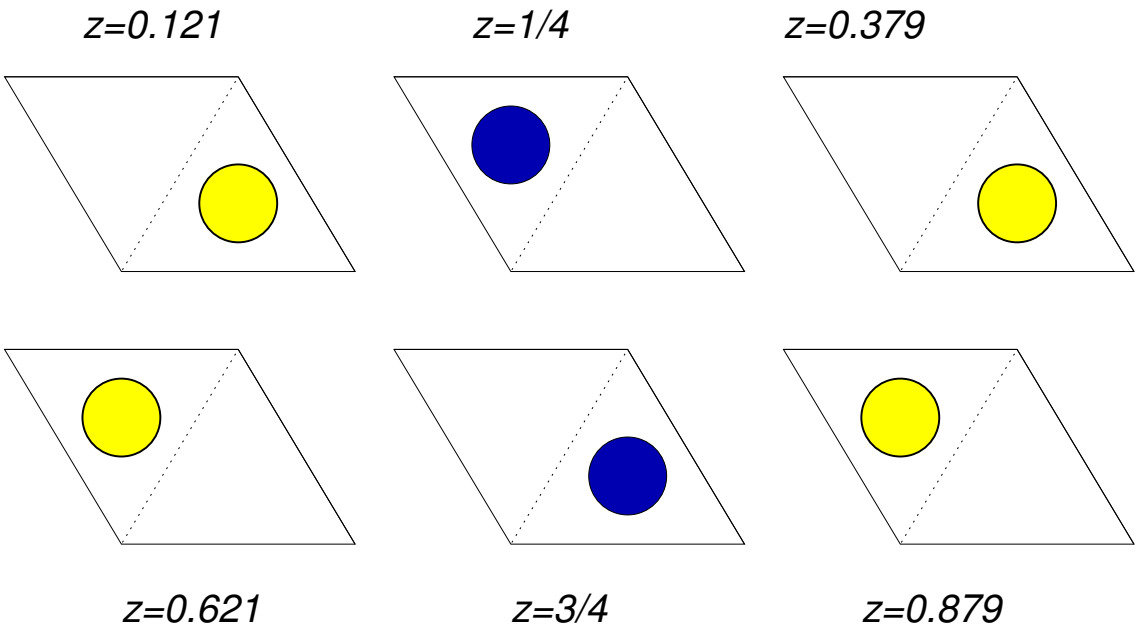


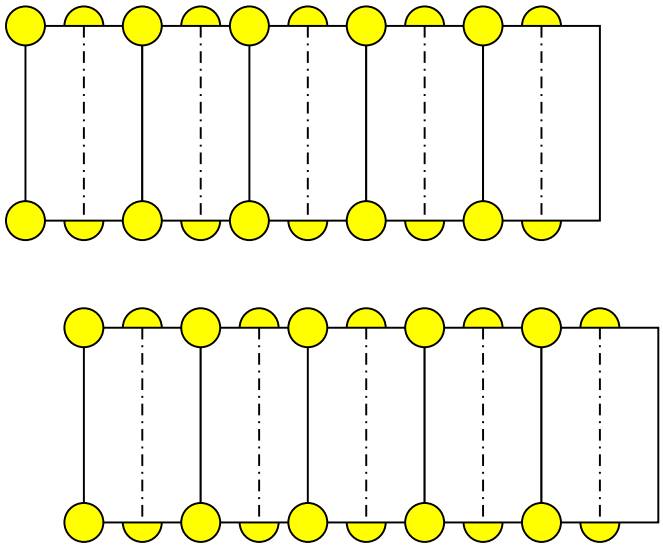
On the left is the structure of CdI_2 projected down the b axis and on the right is the structure of $CdCl_2$. The cyan-colored box marks the unit cell.

MoS_2: SG = $P6_3/mmc$ (No. 194) a = 3.160 Å c = 12.294 Å

Atom	x	y	z
Mo	1/3	2/3	1/4
S	1/3	2/3	0.621

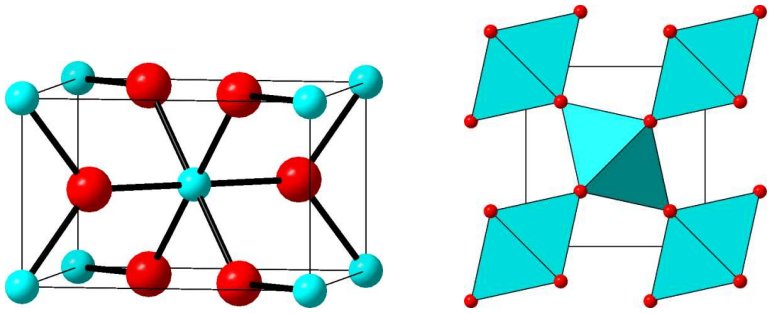
Unlike the CdI_2 structrure where the cations are octahedral, in MoS_2, the cations are in the centers of trigonal prisms formed by the S.





Rutile TiO_2: SG = $P4_2/mnm$ (No. 136) $a = 4.592$ Å $c = 2.959$ Å

Atom	x	y	z
Ti	0	0	0
O	0.3051	0.3051	0

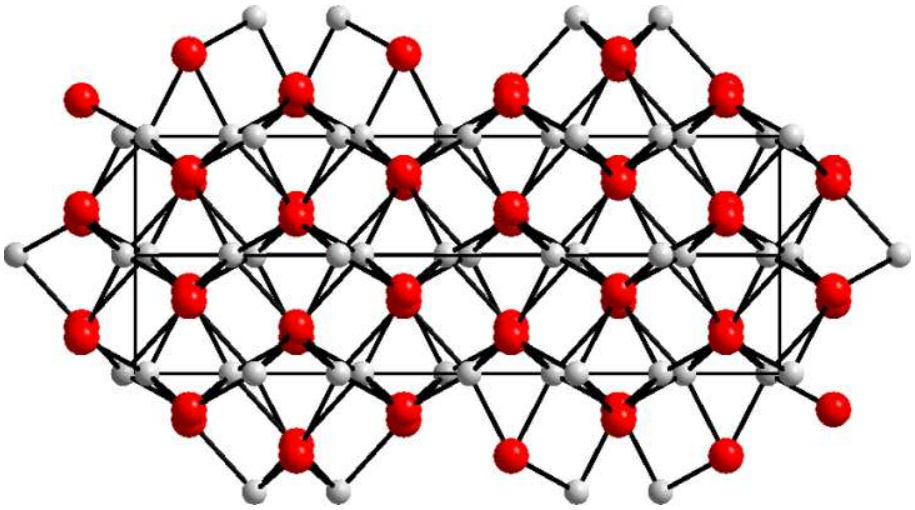


Left: The rutile structure showing the TiO_6 octahedron within a single unit cell.

Right: The rutile structure showing many TiO_6 octahedra sharing corners. The view is down the c axis. This is also the structure of CrO_2, MoO_2, RuO_2 ...

Al_2O_3: SG = $R\bar{3}c$ (No. 167) $a = 4.759$ Å $c = 12.992$ Å

Atom	x	y	z
Al	0	0	0.35217
O	0.30168	0	1/4



The corundum structure with the c axis going from left to right. Red spheres are O and grey are Al.

ReO_3: SG = $Pm\bar{3}m$ (No. 221) $a = 3.754$ Å

Atom	x	y	z
Re	0	0	0
O	1/2	0	0