

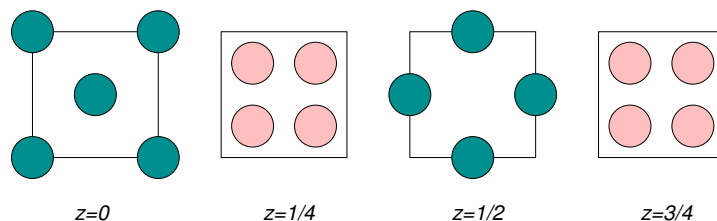
More crystals structures:

Ram Seshadri (seshadri@mrl.ucsb.edu)

AB₂ structures:

Fluorite CaF₂: SG = $Fm\bar{3}m$ (No. 225) $a = 5.45 \text{ \AA}$

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

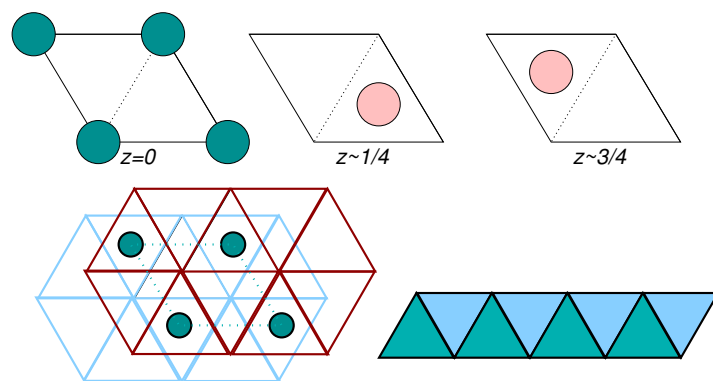


This structure type is also adopted by SrF₂, BaF₂, UO₂, ThO₂, Na₂O (the anti-type), ZrO₂ at high temperatures ...

ZrO₂ can be stabilized in the fluorite structure through doping with Ca²⁺ or Y³⁺ – these are *stabilized zirconias* and have many structural and electrochemical applications.

CdI₂: SG = $P\bar{3}m1$ (No. 164) $a = 4.24 \text{ \AA}$ $c = 6.84 \text{ \AA}$

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

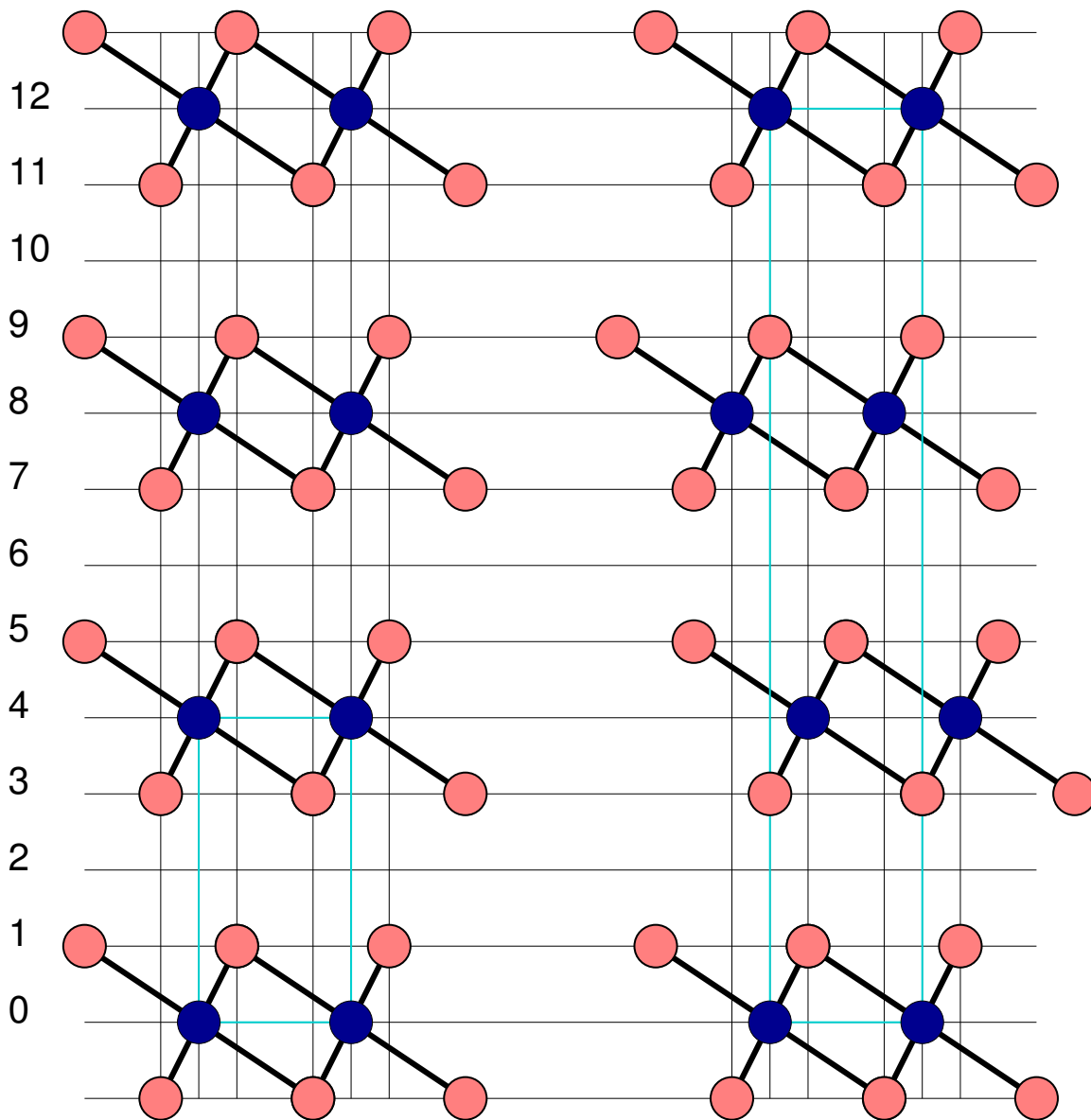


This structure type is also adopted by PbI₂, MgCl₂, FeCl₂, ZnI₂, Cd(OH)₂, Mg(OH)₂, TaS₂, NbS₂ ...

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

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:

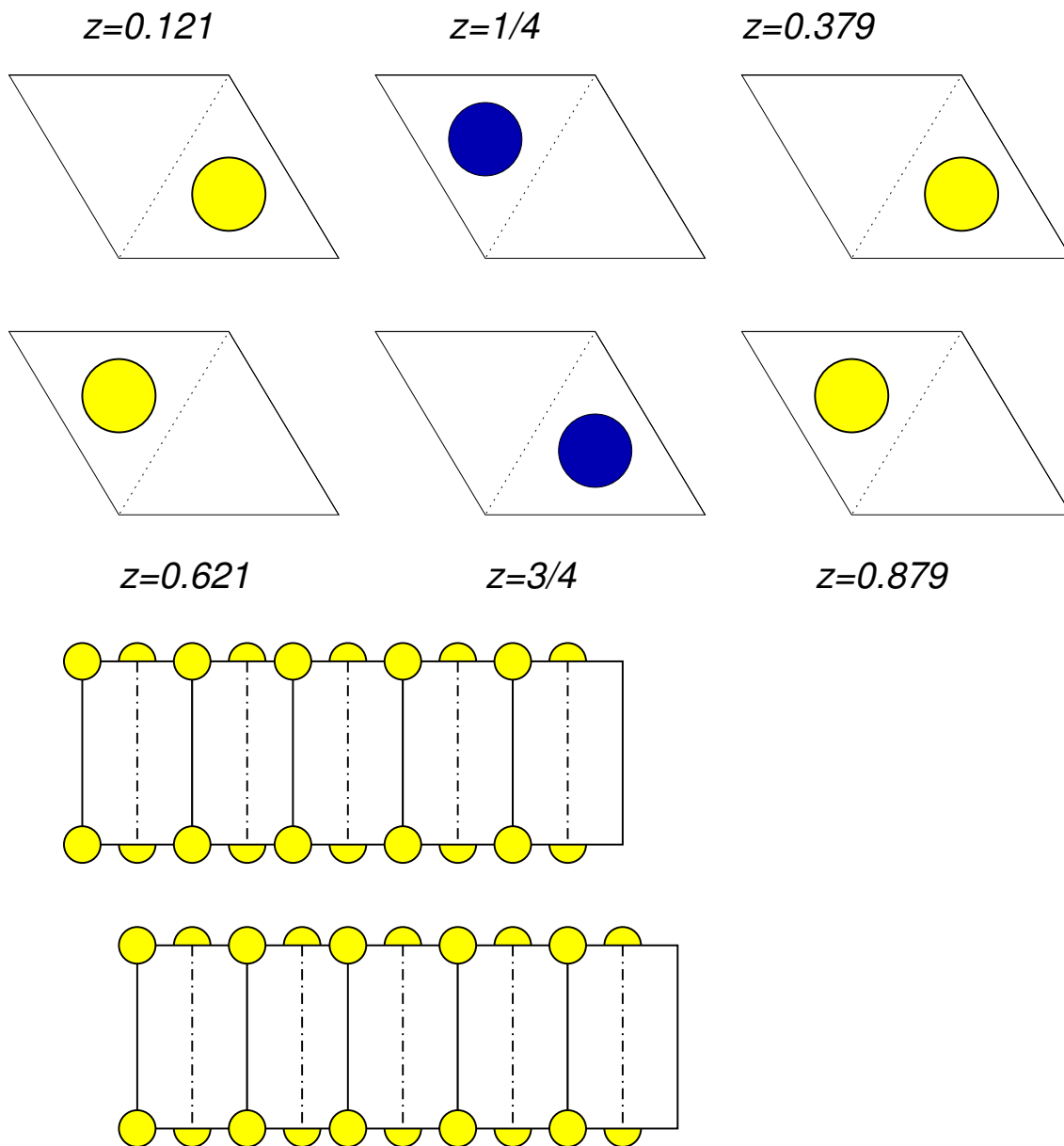


On the left is the structure of CdI_2 projected down the b axis and on the right is the structure of CdCl_2 . The cyan-colored box marks the unit cell.

MoS₂: SG = $P6_3/mmc$ (No. 194) $a = 3.160 \text{ \AA}$ $c = 12.294 \text{ \AA}$

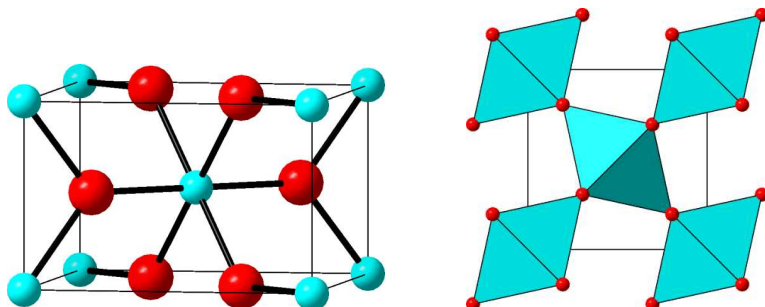
Atom	x	y	z
Mo	1/3	2/3	1/4
S	1/3	2/3	0.621

Unlike the CdI₂ structure where the cations are octahedral, in MoS₂, the cations are in the centers of trigonal prisms formed by the S.



Rutile TiO_2 : SG = $P4_2/mnm$ (No. 136) $a = 4.592 \text{ \AA}$ $c = 2.959 \text{ \AA}$

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

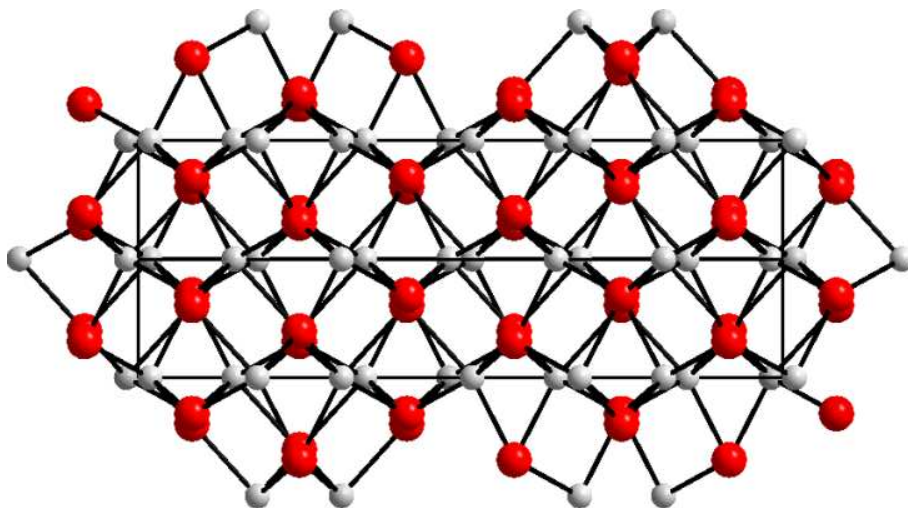


Left: The rutile structure showing the TiO_6 octahedron within a single unit cell.

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 , $\text{RuO}_2 \dots$

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

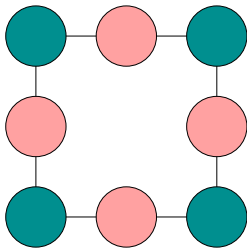
Atom	x	y	z
Al	0	0	0.35217
O	0.30168	0	1/4



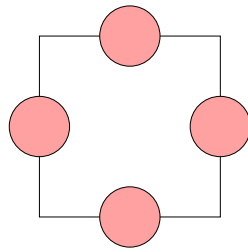
The corundum structure with the c axis going from left to right. Red spheres are O and grey are Al.

ReO₃: SG = $Pm\bar{3}m$ (No. 221) $a = 3.754 \text{ \AA}$

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



$z=0$



$z=1/2$