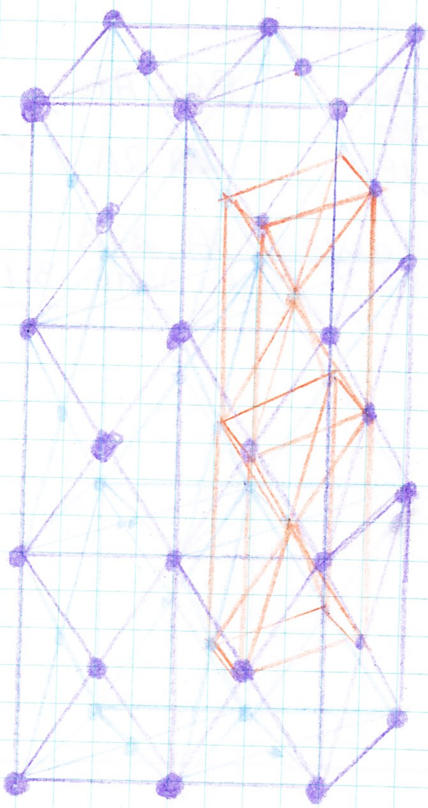
95.545 Stimets 26/30 Sept. 11, 2009 Meg Noah

1) In the tetragonal crystal system there are two allowed lattice centerings, namely the primitive (P) and the body-centered (I). Consider a face-centered (F) tetragonal lattice.

a) Show that the lattice is equivalent to P or I.

FCC below in purple is equivalent to BCC below in orange.



8 8 8

b) Assuming the FCC lattice has lattice constants $\vec{a}$ and $\vec{c}$, what are the equivalent in BCC?

$\vec{c}_{FCC} = \vec{c}_{BCC}$ $\quad \frac{\sqrt{2}}{2}\vec{a}_{FCC} = \vec{a}_{BCC}$

c) Why does not the same equivalence hold in Cubic crystal systems?

There is no way to define a face centered cubic lattice with the BCC system. The center point of the BCC generates both the 8 points of the simple crystal or primative component and the center points of the faces in the x-y plane. These are not both integral values of a side of a cube.

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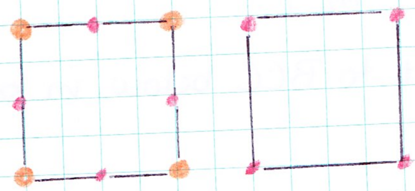
2.) Show the representations of the following crystal structures in the cubic system as a set of stacked layers using square lattices e, f, g, h.

$Pm\bar{3}m$ (#221)

α ReO_3



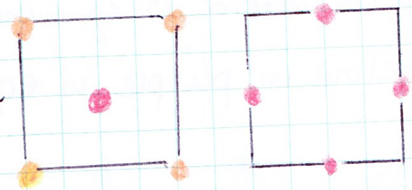
A~~e~~Bfa
1αRe, 2O
1A, 2B's

Be ✓
1O
1B

2 layers 1A, 3B
fits αReO_3 ratio 1:3

$Pm\bar{3}m$ (#221)

Cu_3Au



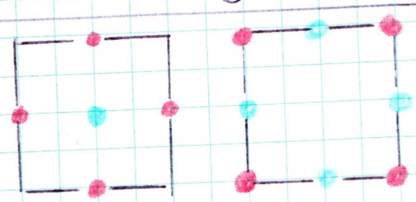
~~BenBea~~
AenBe
1A, 1B

~~Bfa~~ Afa
~~2B~~ 2A ✓

2 layers 3A, ~~2~~1B
fits Cu_3Au ratio 3:1

NbO

$Pm\bar{3}m$
(#221)



Aen Bfa
2B 1A

~~AeBf~~
Afa Be
1B 2A

2 layers 3B, 3A
fits ratio NbO 1:1

$Fm\bar{3}m$ (#225)

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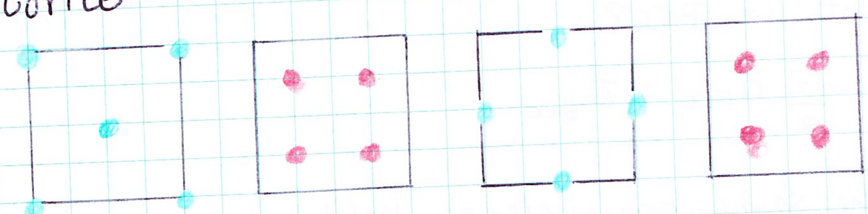
CaF_2 Fluorite

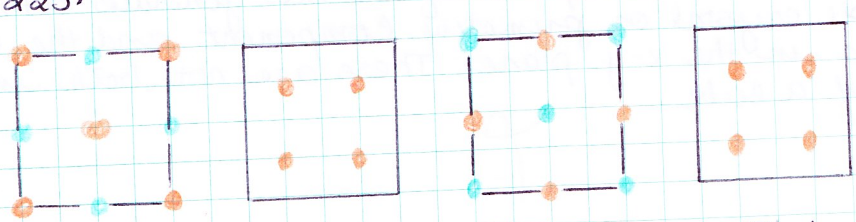


Af, 2A's   Bhd, 4B's   Afa, 2A's   Bhd, 4B's

4 layers
4A's
8B's
fits 1:2 ratio ✓

$Fm\bar{3}m$ (#225)

AlF_3



AfA Bf
2A's, 2B's

Bhd
4B's

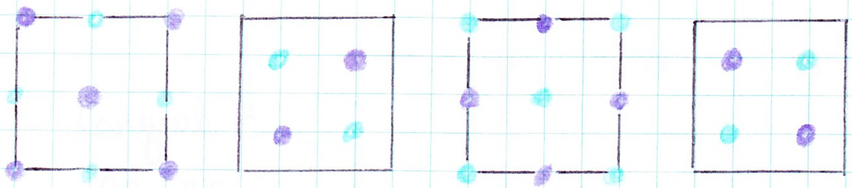
Af, Bfa
2As 2Bs

Bhd
4Bs

4 layers
4As, 12Bs
fits 1:3 ratio

2.) continued...

Fd$\bar{3}$m NaTl (#227)



Af Bfa	Afd$_1$ Bfd$_2$	Afa Bf	Afd$_2$ Bfd$_1$
2A, 2B	2A, 2B	2A, 2B	2A, 2B

4 layers

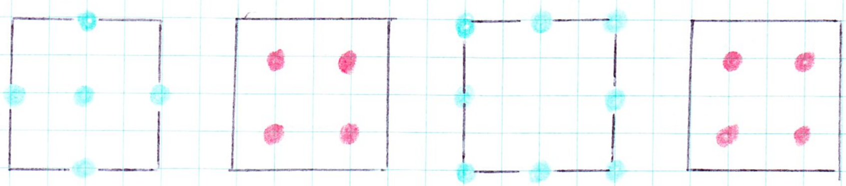
8A, 8B

ratio 1:1

works for NaTl

Im$\bar{3}$m Pt_3O_4

(#229)



4 layers

~~Aga~~ Agn	Bhd	Ag	Bhd
3A	4B	3A	4B

3.) Consider the PtS structure ($P4_2/mmc$) (#131)

Primitive Vectors

$\vec{A}_1 = a\hat{x}$

$\vec{A}_2 = a\hat{y}$

$\vec{A}_3 = c\hat{z}$

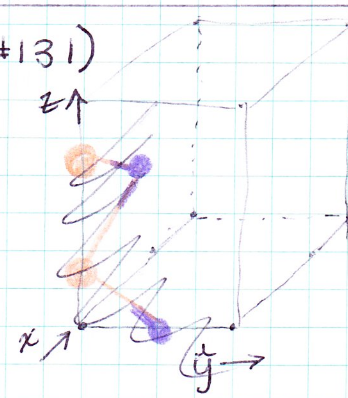
Basis Vectors

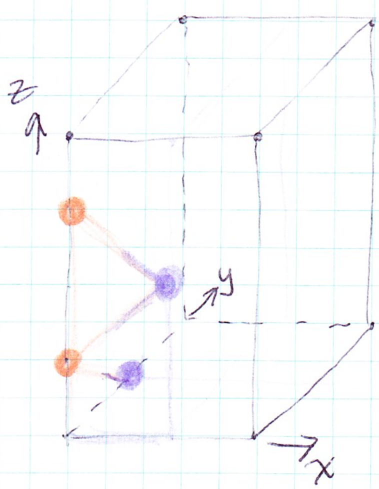
$\vec{B}_1 = \frac{1}{2}a\hat{y}$ Pt

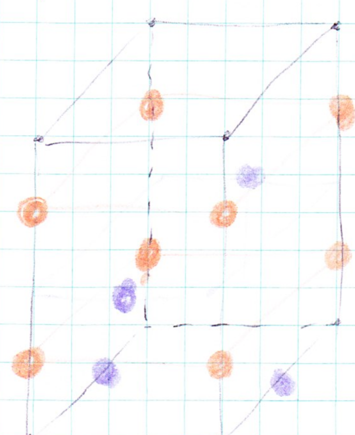
$\vec{B}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{z}$ Pt

$\vec{B}_3 = \frac{1}{4}\hat{z}$ S

$\vec{B}_4 = \frac{3}{4}\hat{z}$ S



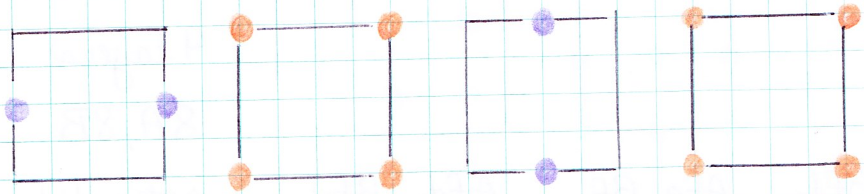




unit cell
2S and 2Pt

4-fold symmetry

Pt S Stacked Layers



A ~~B~~ea$_2$	Be	A ~~B~~ea$_1$	Be
1A	1B	1A ~~2B~~	1B

4 layers

2A, 2B

ratio 1:1 PtS

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