NAME Answer Key

FIRST EXAM

MSE102

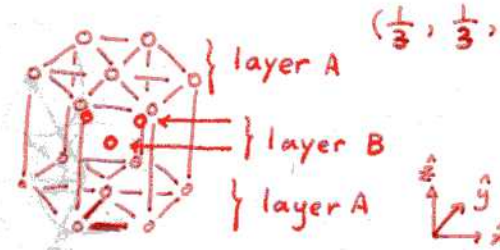
Thursday October 6th 2005

One side of an 8.5x11" sheet and a calculator is allowed. Closed book and notes.

1. SHORT ANSWER QUESTIONS

a. What is the Bravais lattice and basis of hcp Mg?. [6]

hexagonal lattice with a basis of two Mg atoms (one at (0,0,0) and the second at $(\frac{1}{3}, \frac{1}{3}, \frac{1}{2})$)



or if you take the primitive translation vectors to be

$\underline{a}_1' = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$, $\underline{a}_2' = \frac{a}{2}\hat{x} - \frac{a\sqrt{3}}{2}\hat{y}$

$\underline{a}_3' = c\hat{z}$

then basis atoms are at

$(0,0,0)$ $(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$

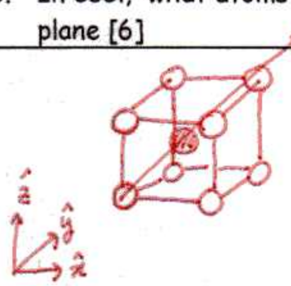
where fractional coordinates are defined as $\vec{r}_j = x_j a\hat{x} + y_j a\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right) + z_j c\hat{z}$

and written (x_j, y_j, z_j)

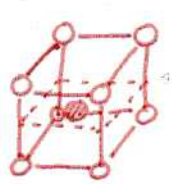
for primitive translation vector

$\underline{a}_1 = a\hat{x}$ $\underline{a}_2 = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$ $\underline{a}_3 = c\hat{z}$

b. In CsCl, what atoms are located along the [1 1 1] direction. Also describe the atoms in the (002) plane [6]

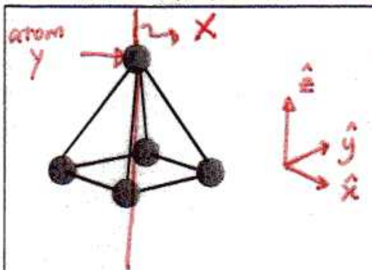


[111] direction contains alternating Cs and Cl atoms



atoms in the (002) plane are just the Cs or just chlorine depending on how you define the unit cell.

c. For a square pyramid molecule, what are the symmetry operations that take the molecule back into itself? List the actual symmetry operators by symbol and explain. [6]



4 : fourfold rotational symmetry around axis X

m : mirror plane in the xz plane that includes atom Y.

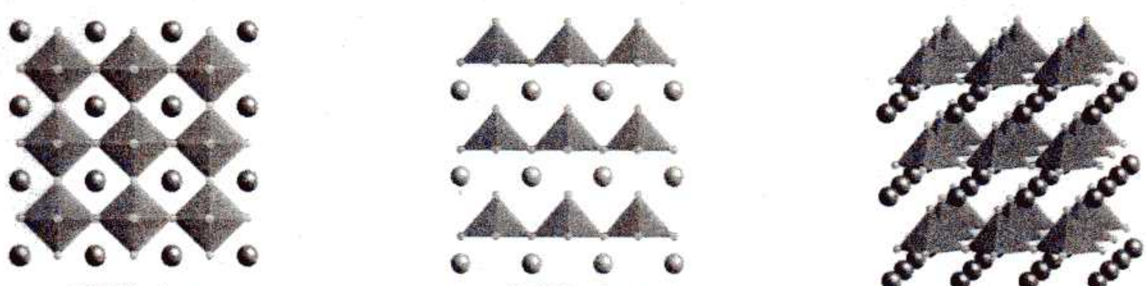
mirror plane in the yz plane that includes atom Y.

mirror plane in the plane parallel to the $\hat{z}$ axis and perpendicularly bisects the $\hat{x}$ and $\hat{y}$ axes

2 : twofold rotational symmetry around axis X

1 : onefold rotational symmetry around axis X

d. For the crystal structure shown to the right, vanadium ions are the electropositive ions and oxygen are the electronegative ions of the square pyramidal polyhedra which are interleaved with the Pb ions. What is the stoichiometry of this material? Explain. [6]



(001) view (100) view

In a unit cell, ① there are 8 Pb atoms shared by 8 other unit cells → 1 Pb

② there is one V atom shared by no other unit cell → 1 V

③ there are 4 O atoms shared by 2 other unit cells → 2 O

④ there is one O atom shared by no other unit cell. → 1 O

⇒ $PbVO_3$

e. What is the relationship between a real space lattice and the corresponding reciprocal lattice? [3]

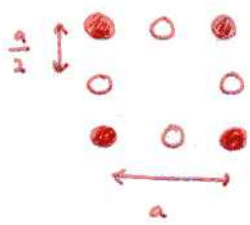
Reciprocal lattice points represent planes in real space. The reciprocal lattice vectors indicate the direction of the surface normal of the plane in real space and the magnitude of the reciprocal lattice vector represents the inverse of the wavelength of the parallel set of real space planes: $|\vec{G}_{hkl}| = \frac{2\pi}{\lambda_{hkl}}$.

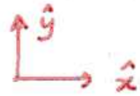
f. Are the reciprocal lattices of a simple cubic lattice (lattice constant ***a*** on a side) with a basis of one atom and a simple cubic lattice (lattice constant ***a*** on a side) with a basis of two atoms, the same or different? Explain. [3]

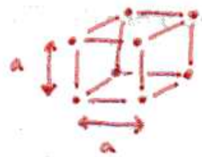
The reciprocal lattices are identical as they represent the planes in real space associated with the real space LATTICE.

Problem #1.______/30
Problem#2._____/30
Total:_____/60

(a) Bravais lattice of the following structure stacked on top of one another a distance a apart is SIMPLE CUBIC







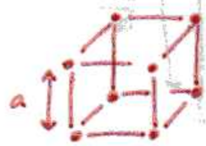
(b) primitive translation vectors are

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

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

$\vec{a}_3 = a\hat{z}$

(c) the unit cell is a simple cubic unit cell - a on a side



(d) basis is made up of three atoms:

one black (0, 0, 0)

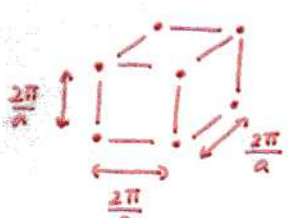
one white ($\frac{1}{2}$, 0, 0)

one white (0, $\frac{1}{2}$, 0)

(e) the general expression for a reciprocal lattice vector: $\vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$ where $\vec{a}_1^*$, $\vec{a}_2^*$ and $\vec{a}_3^*$ are the reciprocal lattice vectors for the simple cubic lattice which are:

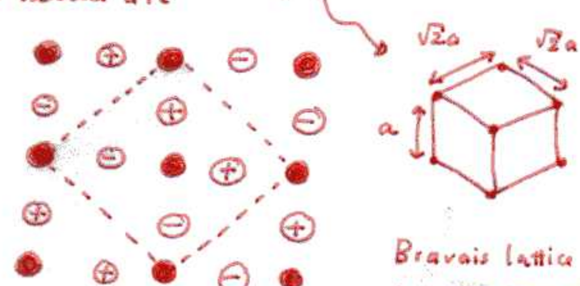
$\vec{a}_1^* = \frac{2\pi}{a}\hat{x}$ $\quad \vec{a}_2^* = \frac{2\pi}{a}\hat{y}$ $\quad \vec{a}_3^* = \frac{2\pi}{a}\hat{z}$

(f)



Reciprocal lattice

(g) If the white atoms are displaced ⊕ and ⊖, the new primitive ~~unit~~ cell and Bravais lattice are



Bravais lattice is ORTHORHOMBIC

(h) The corresponding reciprocal lattice is:

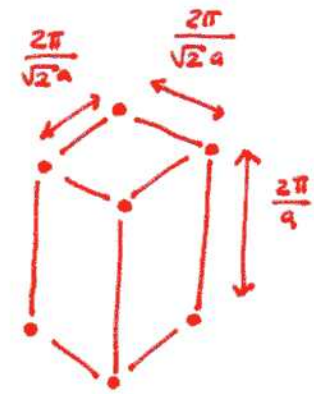
For the orthorhombic lattice, the primitive translation vectors are

$$\vec{a}_1' = \sqrt{2}\,a\,\hat{x}'$$
$$\vec{a}_2' = \sqrt{2}\,a\,\hat{y}'$$
$$\vec{a}_3' = a\,\hat{z}'$$

So the corresponding reciprocal lattice vectors are:

$$\vec{a}_1^* = \frac{2\pi}{\sqrt{2}a}\,\hat{x}'$$
$$\vec{a}_2^* = \frac{2\pi}{\sqrt{2}a}\,\hat{y}'$$
$$\vec{a}_3^* = \frac{2\pi}{a}\,\hat{z}'$$

So the reciprocal lattice is orthorhombic with unit cell



(i) symmetry elements of this new structure is

m , 1 , 2

2 mirror planes