NAME *Answer Key*

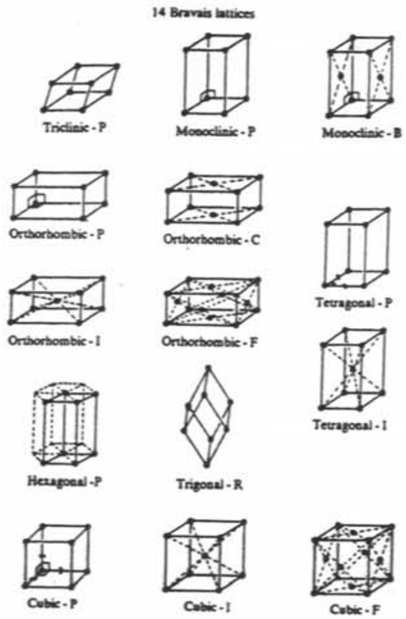
FIRST EXAM

MSE102

Thursday October 7^{th} 2004

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

1. SHORT ANSWER QUESTIONS
   a. Name and sketch four out of the 14 Bravais lattices. Name an example of each. [8]



<u>examples</u> <u>include</u>

Co (hexagonal)
Fe (body centered cubic)
Ni (face centered cubic)
In (tetragonal)

   b. What are the contributions to the interaction energy in a van der Waal's solid? Write out the expression for the interaction and explain each term. [6]

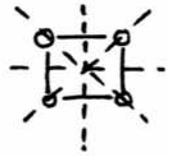
In a van der Waal's solid, there is a balance of an attractive Coulomb interaction between induced dipoles balanced by a repulsive interaction due to the fact that electron distributions from different atoms or molecules do not like to overlap.

$$U_{vdw} = C\left[\underbrace{-\sum_j \left(\frac{\sigma}{p_{ij}R}\right)^6}_{\text{attractive}} + \underbrace{\sum_j \left(\frac{\sigma}{p_{ij}R}\right)^{12}}_{\text{repulsive}}\right]$$

$R \equiv$ nearest neighbor distance ; $r_{ij} \equiv p_{ij}R$ is distance between atom i & j.
$\sigma \equiv$ "size" of repulsive core

c. For a square planar molecule, what are the symmetry operations that take the molecule back into itself? [6]

A square planar molecule has



1 : rotations through 2π

2 : " " π

4 : " " $\frac{\pi}{2}$

m : various reflections about planes shown

$\bar{1} = i$

$\bar{2} = m$!

$\bar{4}$: improper rotations through $\frac{\pi}{2}$

d. For the crystal structure shown to the right, a rare earth ion (black) is surrounded by 8 octahedra composed of a transition metal ion surrounded by oxygen anions. What is the stoichiometry of the material? If the rare earth has a valence of 3+, what does the valence of the transition metal ion have to be?[5]

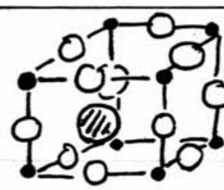
In each unit cell, there are

1. rare earth atom

12 oxygens shared by 4 other cells

• 8 transition metal shared by 8 other cells

$\boxed{RE_1 TM_1 O_3}$



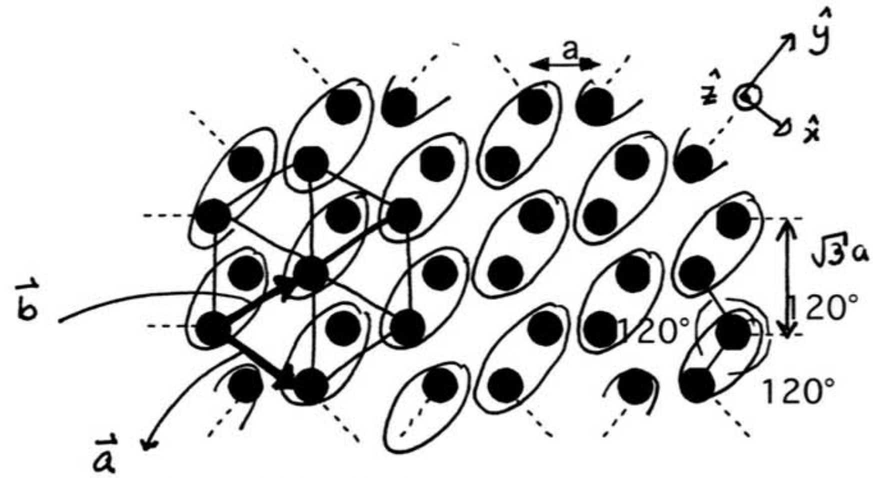
If RE^{3+} and O^{2-}, then for charge neutrality to be true → $\boxed{TM^{3+}}$!

e. What is the relationship between a real space lattice and the corresponding reciprocal lattice? [4]

A set of parallel planes in real space is associated with a reciprocal lattice vector in reciprocal space. The direction of the reciprocal lattice vector corresponds to the normal of the planes in real space. The magnitude of the reciprocal lattice vector is inversely proportional to the spacing of the planes modulo a factor of 2π.

Problem #1.______/29
Problem#2._____/31
Total:_____/~~100~~ 60

2. Consider 3D lattice below composed of atoms of one type. Each atom has three nearest neighbors in the plane of the paper a distance *a* away. Layers of this two dimensional pattern are stacked on top of one another a distance *a* apart.



(a) What is the Bravais lattice of this structure? [2]
(b) What are the primitive translation vectors? [6]
(c) Sketch the unit cell. [4]
(d) What is the basis? [4]
(e) Write down a general expression for a reciprocal lattice vector for this structure. [3]
(f) Sketch and label lengths on the reciprocal lattice. [4]
(g) If atoms of the same type are added to the lattice above so that all atoms have six nearest neighbors in the plane of the paper a distance a away, how does this change the reciprocal lattice? Sketch and label lengths of this new reciprocal lattice. [6]
(h) What are the symmetry elements of this new structure? [2]

(a) Bravais lattice is hexagonal.

(b) Primitive Translation vectors are: $\vec{a} = \sqrt{3}a\hat{x}$, $\vec{b} = \frac{\sqrt{3}}{2}a\hat{x} + \frac{3}{2}a\hat{y}$, $\vec{c} = a\hat{z}$ (see figure above)

(c)

(d) basis is $\{0\ 0\ 0\}$ $\{\frac{a}{2}\ \frac{\sqrt{3}a}{2}\ 0\}$ shown in above diagram

(e) $\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

$$\vec{a}^* = \frac{2\pi}{V}(\underline{b}\times\underline{c}) = \frac{2\pi}{\left(\frac{3\sqrt{3}}{2}a^3\right)}\left(\frac{3}{2}a^2\hat{x} - \frac{\sqrt{3}}{2}a^2\hat{y}\right) = \frac{2\pi}{\sqrt{3}a}\hat{x} - \frac{2\pi}{3a}\hat{y}$$

$$V = \underline{a}\cdot(\underline{b}\times\underline{c}) = \underline{a}\cdot\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ \frac{\sqrt{3}}{2}a & \frac{3}{2}a & 0\\ 0 & 0 & a\end{vmatrix} = \underline{a}\cdot\left(\frac{3}{2}a^2\hat{x} - \frac{\sqrt{3}}{2}a^2\hat{y}\right) = \frac{3\sqrt{3}a^3}{2}$$

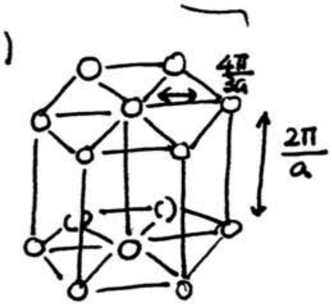
$$\vec{b}^* = \frac{2\pi}{V}(\underline{c}\times\underline{a}) = \frac{2\pi}{V}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ 0 & 0 & a\\ \sqrt{3}a & 0 & 0\end{vmatrix} = \frac{2\pi}{\left(\frac{3\sqrt{3}a^3}{2}\right)}\left(\sqrt{3}a^2\hat{y}\right) = \frac{4\pi}{3a}\hat{y}$$

$$\vec{c}^* = \frac{2\pi}{V}(\underline{a}\times\underline{b}) = \frac{2\pi}{V}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ \sqrt{3}a & 0 & 0\\ \frac{\sqrt{3}}{2}a & \frac{3}{2}a & 0\end{vmatrix} = \frac{3\sqrt{3}}{2}a^2\hat{z}\times\frac{2\pi}{\left(\frac{3\sqrt{3}a^3}{2}\right)} = \frac{2\pi}{a}\hat{z}$$

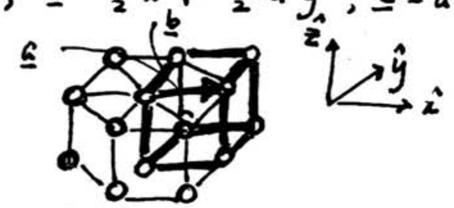
$$\vec{G} = h\left(\frac{2\pi}{\sqrt{3}a}\hat{x} - \frac{2\pi}{3a}\hat{y}\right) + k\,\frac{4\pi}{3a}\hat{y} + l\,\frac{2\pi}{a}\hat{z}$$

where h, k, l are integers!

(f)



(g) If we add an atom to the honeycomb lattice such that each atom has six nearest neighbors a distance a apart. $\longrightarrow$ Bravais lattice is still hexagonal! but with primitive translation vectors : $\underline{a} = a\hat{x}$, $\underline{b} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\,\hat{y}$, $\underline{c} = a\hat{z}$



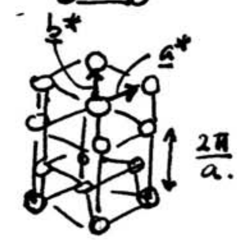
Then the reciprocal lattice vectors are

$$\underline{a}^* = \frac{2\pi}{V}(\underline{b}\times\underline{c}) = \frac{2\pi}{\left(\frac{\sqrt{3}}{2}a^3\right)}\left(\frac{\sqrt{3}}{2}a^2\hat{x} - \frac{a^2}{2}\hat{y}\right)$$

$$= \frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y}$$

$$\underline{b}^* = \frac{2\pi}{V}(\underline{c}\times\underline{a}) = \frac{2\pi}{\left(\frac{\sqrt{3}}{2}a^3\right)}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & a \\ a & 0 & 0 \end{vmatrix} = \frac{4\pi}{\sqrt{3}a}\hat{y}$$

$$\underline{c}^* = \frac{2\pi}{V}(\underline{a}\times\underline{b}) = \frac{2\pi}{\left(\frac{\sqrt{3}}{2}a^3\right)}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a & 0 & 0 \\ \frac{a}{2} & \frac{\sqrt{3}}{2}a & 0 \end{vmatrix} = \frac{2\pi}{a}\hat{z}$$



$$V = \underline{a}\cdot(\underline{b}\times\underline{c})$$

$$= \underline{a}\cdot\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{a}{2} & \frac{\sqrt{3}a}{2} & 0 \\ 0 & 0 & a \end{vmatrix}$$

$$= \underline{a}\cdot\left(\frac{\sqrt{3}}{2}a^2\hat{x} - \frac{a^2}{2}\hat{y}\right)$$

$$= \frac{\sqrt{3}}{2}a^3$$

(h) symmetry elements are those for hexagonal P

$6,\ \bar{6},\ 6/m,\ 622,\ 6mm,\ \bar{6}m2,\ 6/mmm$