Assignment 1

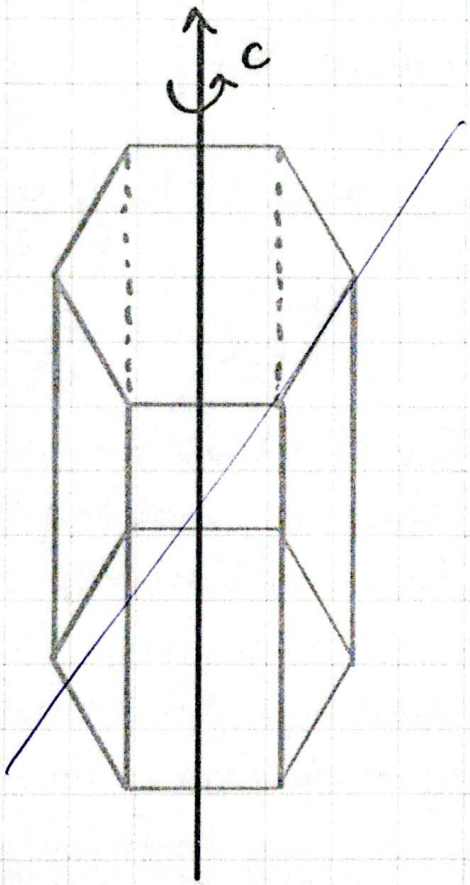
22 Feb 2026 Sabieh

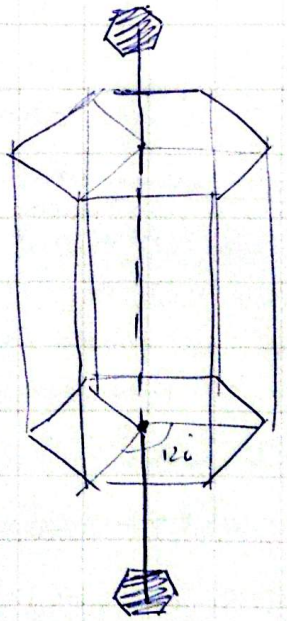
Solution

{ Q7 canceled due to a typo. Will give again - HW3. }

Question 1:-

Lies along the c-axis through the center of hexagon.



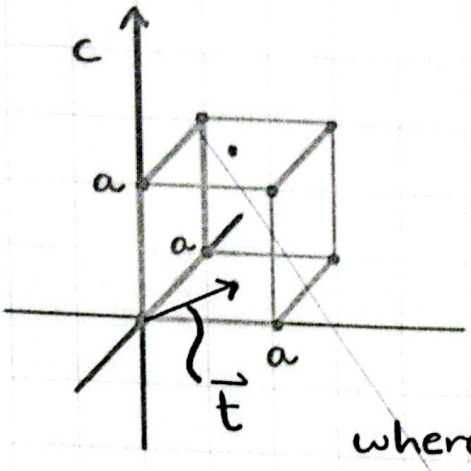


I have stacked three hexagonal unit cells side-by-side

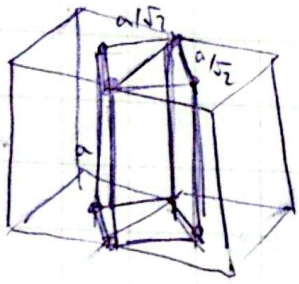
The 6-fold axis, 6 =  is along the intersectional line ∥ [0,0,1] of these three cells.

Question 2:-

a)



where $\vec{t} = \left(\frac{1}{2}, \frac{1}{2}, 0\right)$



C-centering a cubic unit cell creates a primitive tetragonal cell, which has lower symmetry. Two sides of this tetragonal cell have length $a/\sqrt{2}$ and one side has a. Lower symmetry cannot be preferred over higher symmetry. The tetragonal

and $|\vec{t}| = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2}$

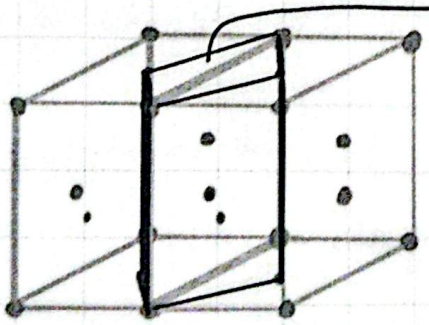
$= \frac{a}{\sqrt{2}} < a$

The shortest translation is less than a, making this cube not the smallest repeating unit cell.

Such a lattice can always be transformed into a primitive lattice by redefining the unit cell.

primitive cell is shown by thick lines in the diagram above.

b)

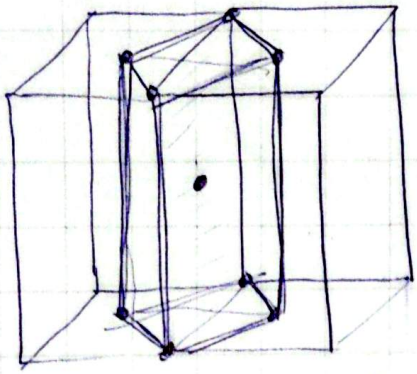


An F-centered tetragonal lattice can be reduced to a smaller, body-centered tetragonal lattice

Incorrect

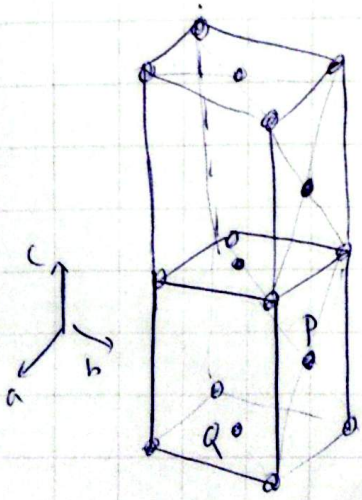
(a) Centering only two faces of a cubic unit cell would no longer maintain the 3-fold axis of symmetry that a cubic lattice has.

(b)



Face centring a tet. unit cell converts this into an I-centred tet. unit cell, which is already a distinct Bravais lattice. Hence F-centring tetragonal does not create any unique centring not already included. See the thick-lined I tetragonal in the accompanying diagram.

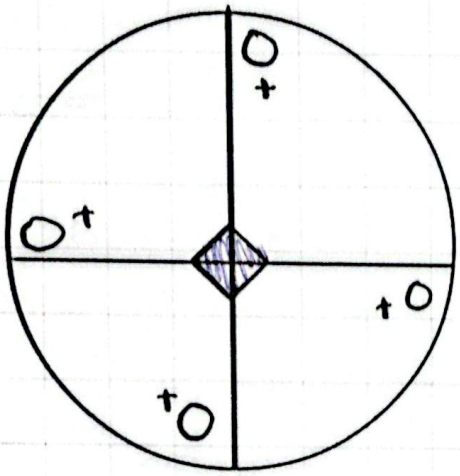
(c)



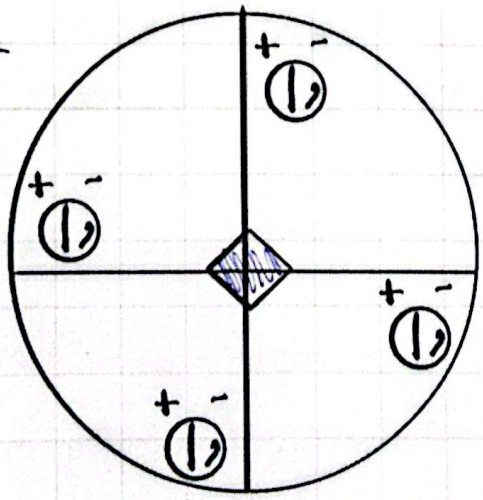
Here we have centred the C and B faces of a cubic u.c. You will notice that P and Q have different environments. For example, P has a neighbouring lattice point at a translation $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ whereas Q does not have a lattice point at such a displacement. Hence, centring two faces only renders the arrangement useless, it is no longer a lattice!

Question 3:-

a) $C_4 \equiv 4$

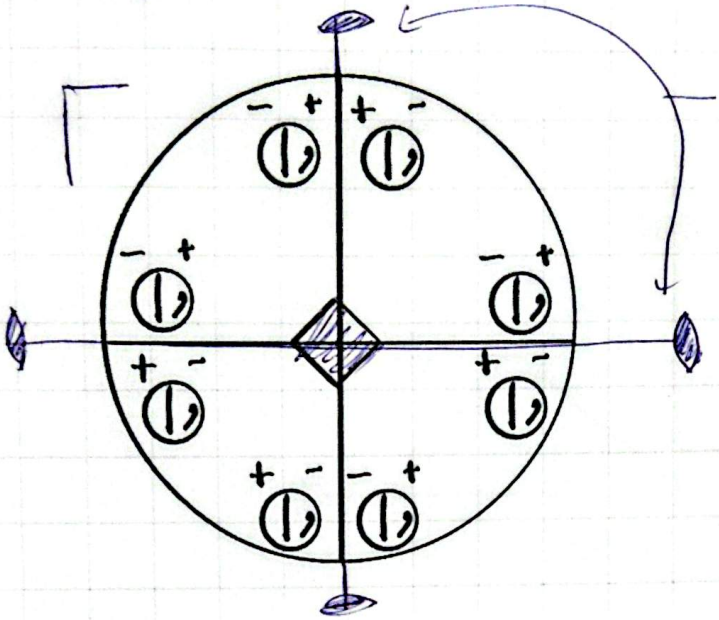


$C_{4h} \equiv 4/m$



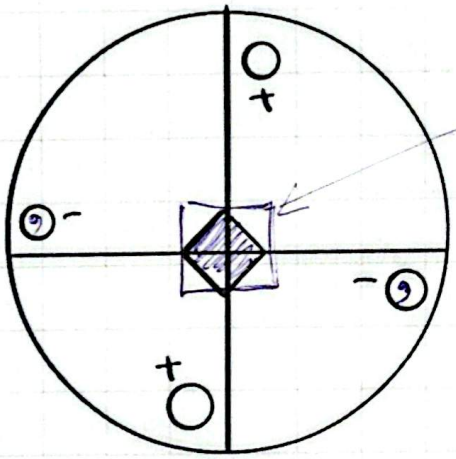
Shows the perpendicular mirror plane.

$D_{4h} \equiv 4/mmm$

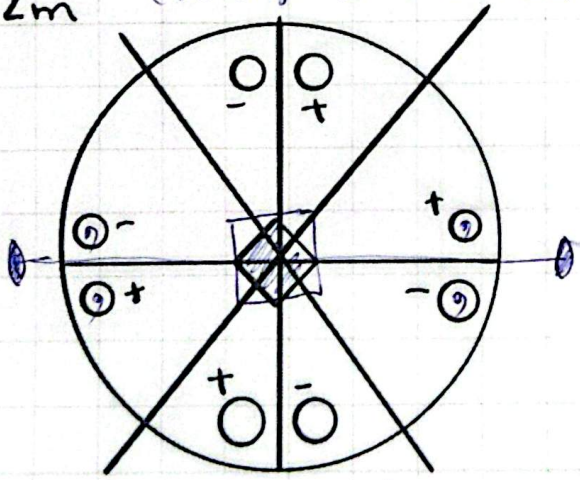


b)

$\bar{4}$



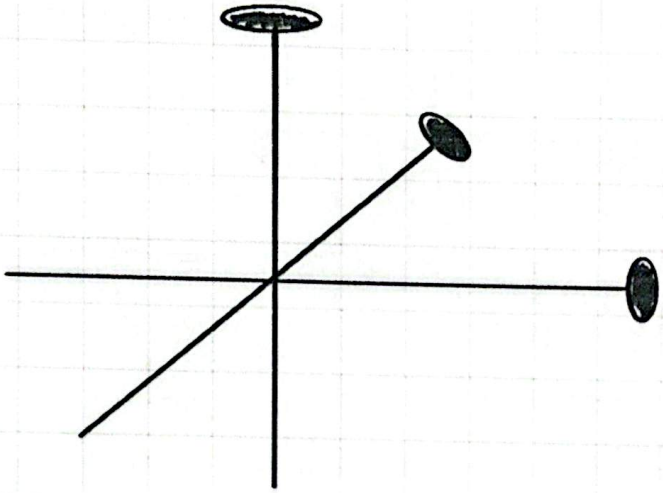
$D_{2d} \equiv \bar{4}2m$ (belongs to the tetragonal class)



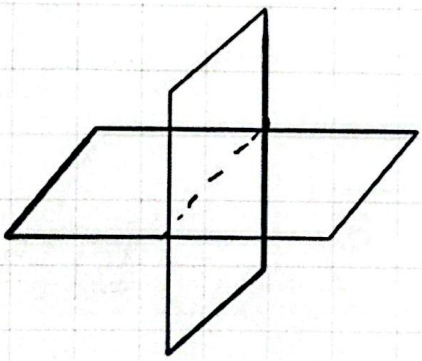
Check to unpack the point group symbol $\bar{4}2m$ which includes a $\bar{4}$ axis along c, 2 fold axis along a (a b) and a diagonal mirror plane m.

Question 4:-

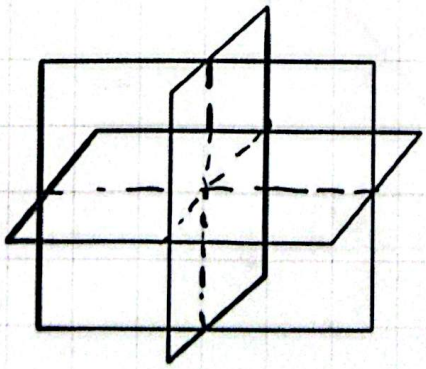
222:-



mm:-



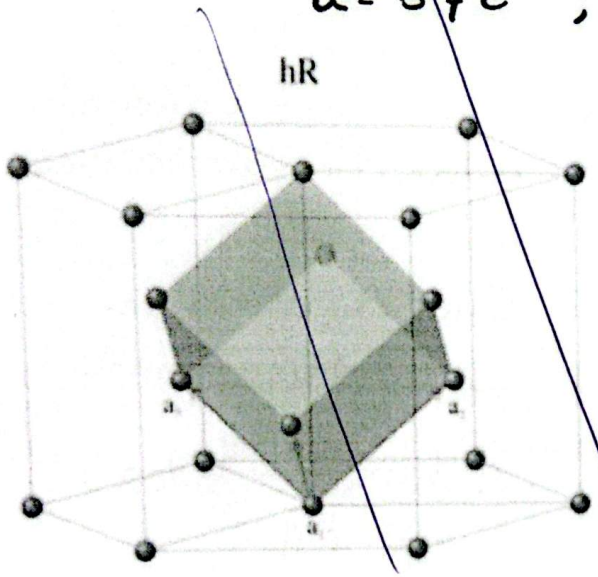
mmm:-



Question 5:-

For the hexagonal unit cell:

$a = b \neq c$; $\gamma = 120°$



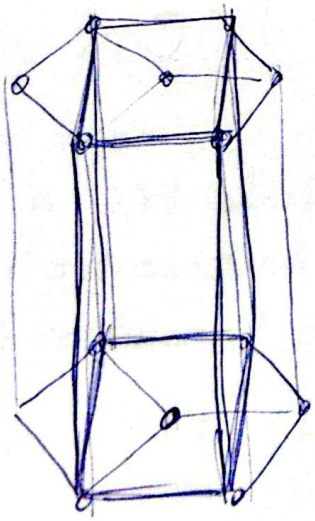
This rhombohedral lattice can also be described using the same hexagonal axes stated above.

Its cell dimensions are:-

$a = b = c$;

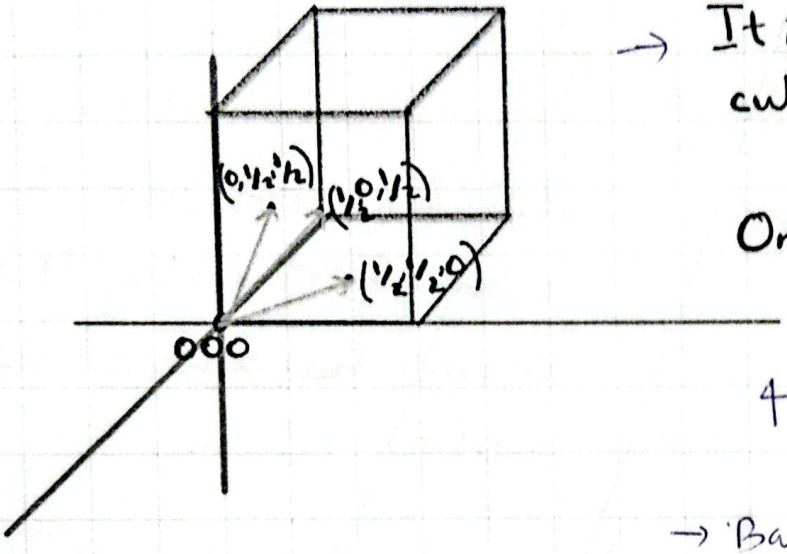
$\alpha = \beta = \gamma \neq \pi/2$

The diagram shows a hexagonal system with three unit cells drawn side by side. Accidentially $a = b = c$. It can be seen that this generates a C-centred orthorhombic Bravais lattice. This is shown in thicker lines in this diagram.



Question 6:-

a) Au:-



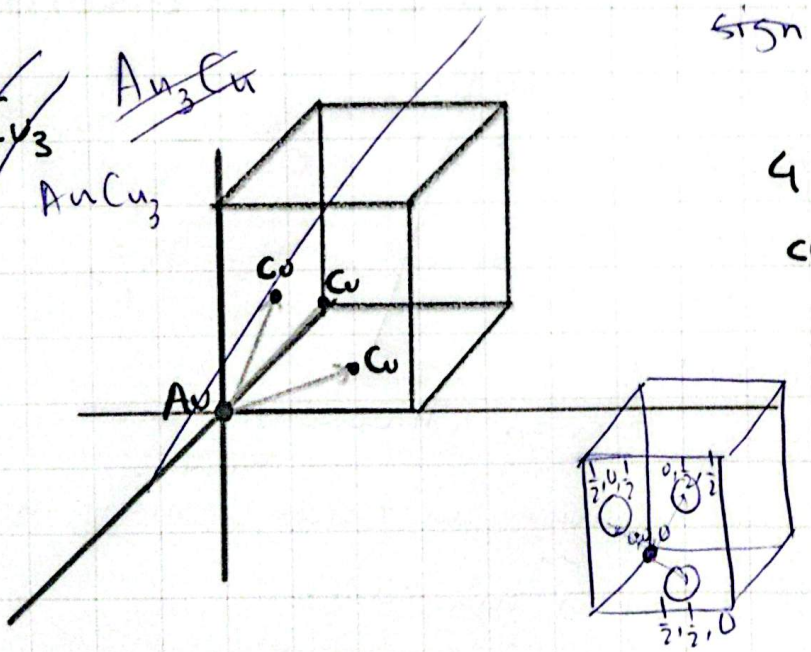
→ It is a face-centered cubic Bravais lattice

One Au atom per lattice point

4 lattice points per unit cell.

→ Basis / Motif is one single Au atom.

b) ~~AuCu$_3$~~ ~~Au$_3$Cu~~ AuCu$_3$



4 atoms per primitive cubic cell
(1 Au + 3 Cu)

• Au
○ Cu

Even though this Bravais lattice looks FCC, a translation from corner to the face-centre is from Au → Cu atoms. Therefore, such a translation is not symmetric.

$\frac{\vec{a}}{2}+\frac{\vec{c}}{2}$, $\frac{\vec{a}}{2}+\frac{\vec{b}}{2}$, $\frac{\vec{b}}{2}+\frac{\vec{c}}{2}$.

This Bravais lattice is simply a primitive cubic one.
The basis is 1 Au and 3 Cu atoms displaced with translation vectors