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Assignment - 4

Solution - 1

* Lattice Point ⇒ It is the position in the unit cell or in a crystal where the probability of finding an atom is the highest.

* Bravais Lattice ⇒ When the discrete points are atoms, ions or polymer strings of solid matter, the Bravais lattice concept is used formally define a crystalline arrangement and its frontiers.

* Primitive cell :- The smallest possible unit cell of a lattice, have lattice points at each of its eight vertices only.

* Coordination number :- The number of atoms or ions immediately surrounding a central atom in a complex or crystal.

* Atomic Packing fraction :- It is the percentage of total space filled by the particles

$$ATF = \frac{\text{Volume occupied by all spheres in unit cell}}{\text{Total volume}} \times 100$$

* Simple Cubic :

$a = 2r.$

No. of spheres per unit cell $= \frac{1}{8} \times 8 = 1.$

Atomic Packing Fraction $= \dfrac{\frac{4}{3}\pi r^3}{8r^3} = 0.524.$

$\therefore$ Percentage of ATF = 52.4 %.

* BCC :-

No. of Spheres = 2

$a = \dfrac{4r}{\sqrt{3}}.$

Atomic Packing fraction $= \dfrac{2 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} \times 100$

$= \dfrac{2 \times \frac{4}{3}\pi}{\frac{16}{\cancel{3}}} \times 100$

$= \dfrac{\pi}{2} \times 100 = 68\%$

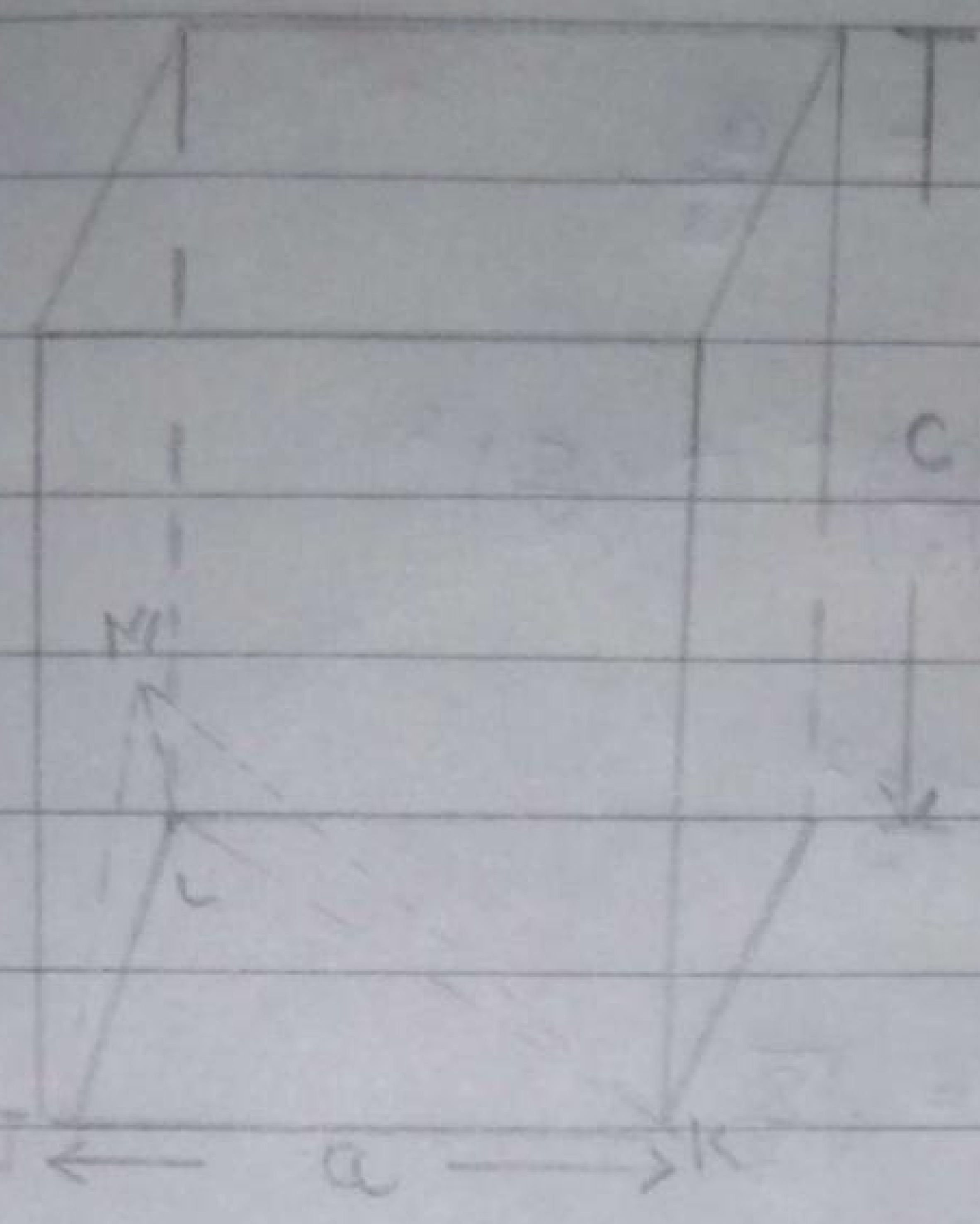
* FCC :

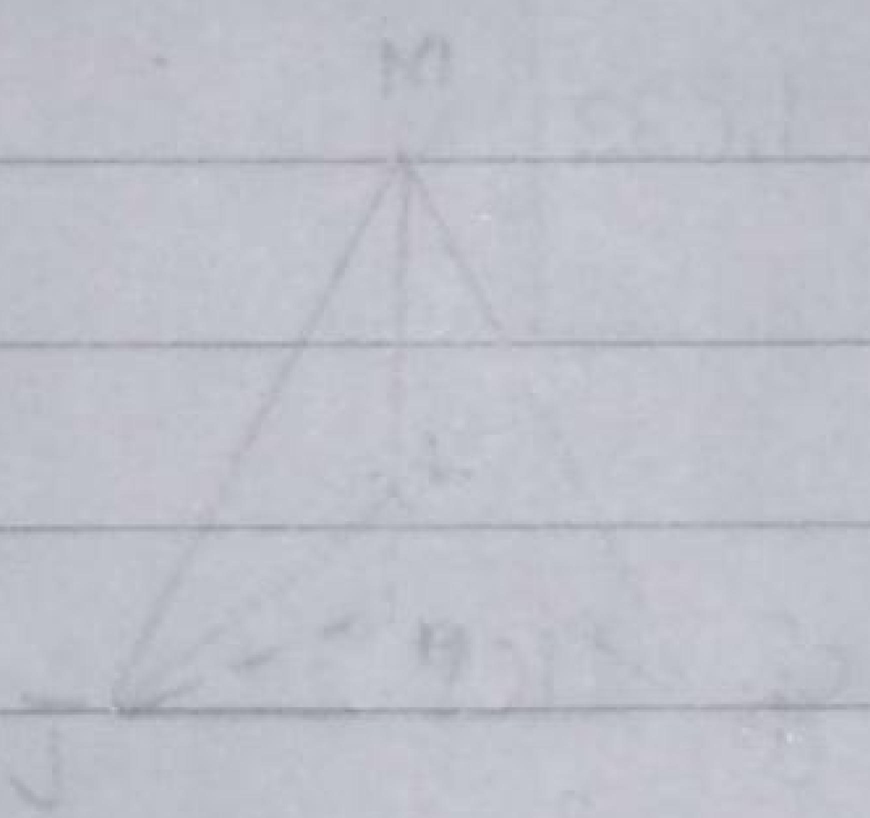
No. of Spheres = 4

$a = \dfrac{4}{\sqrt{2}} r$

$ATF = \dfrac{4 \times \frac{4}{3}\pi r^3 \times 2}{4 \times 4 \cdot r^{\cancel{3}}} = 74\%$

Solution-2



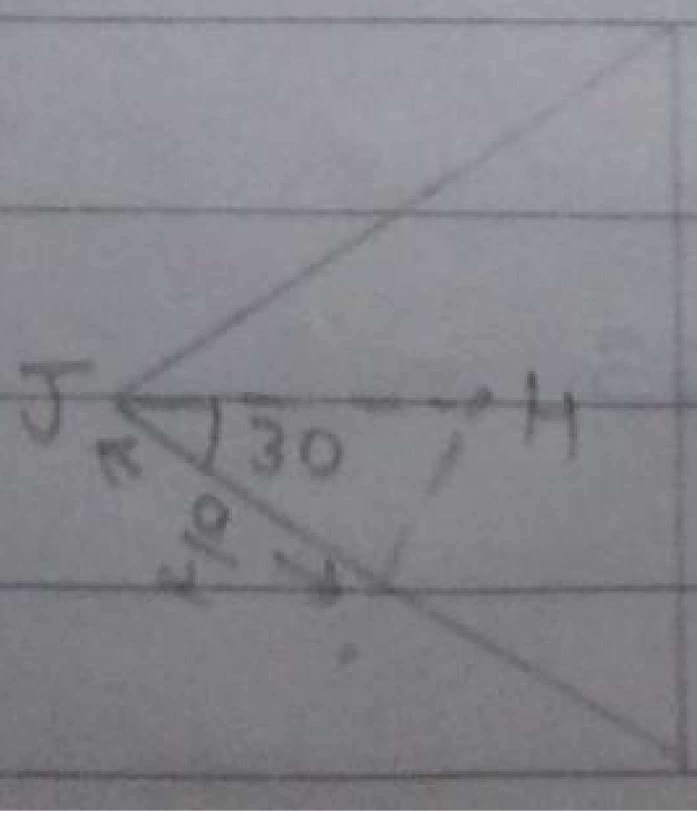


$\overline{MH} = \frac{c}{2}$

$\overline{JM} = \overline{JK} = 2R = a$

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$$

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$



$$\cos 30^\circ = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}$$

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

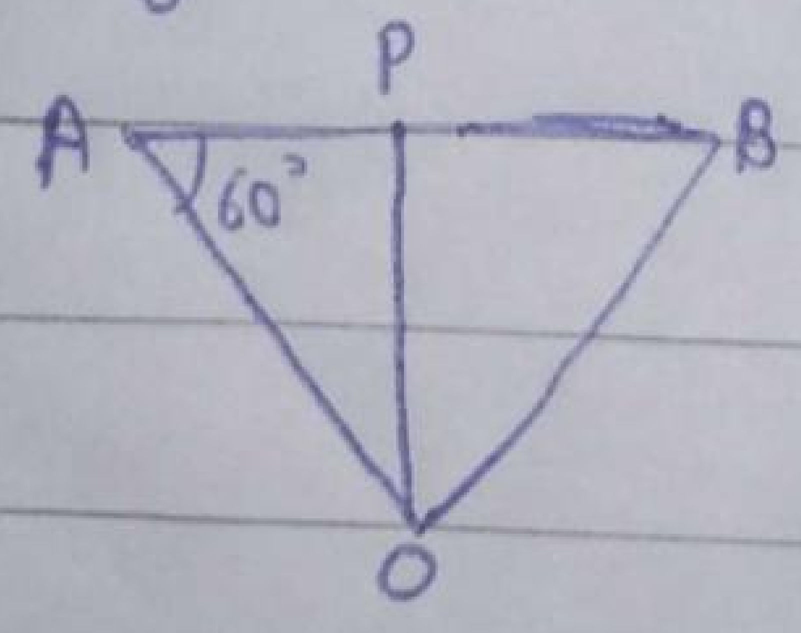
$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$$

$$a^2 = \frac{a^2}{3} + \frac{c^2}{2}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}}$$

$$\boxed{\frac{c}{a} = 1.633}$$

Packing Efficiency of HCP :-



Area of $\Delta OAB = 0.5 \times AB \times OP$

$$= \frac{1}{2} \times a \times a \sin 60^\circ = \frac{\sqrt{3}}{4} a^2$$

Area of Basal plane $= 6 \times \frac{\sqrt{3}}{4} a^2 = \frac{3\sqrt{3}}{2} a^2$

$$a = 2R.$$

$$\frac{c}{a} = 1.63$$

$c = 1.63a = 3.26R$

Unit cell volume

$$V_c = c \times \text{base area}.$$

$$= 3.26R \times 10.392R^2 = 33.878R^3$$

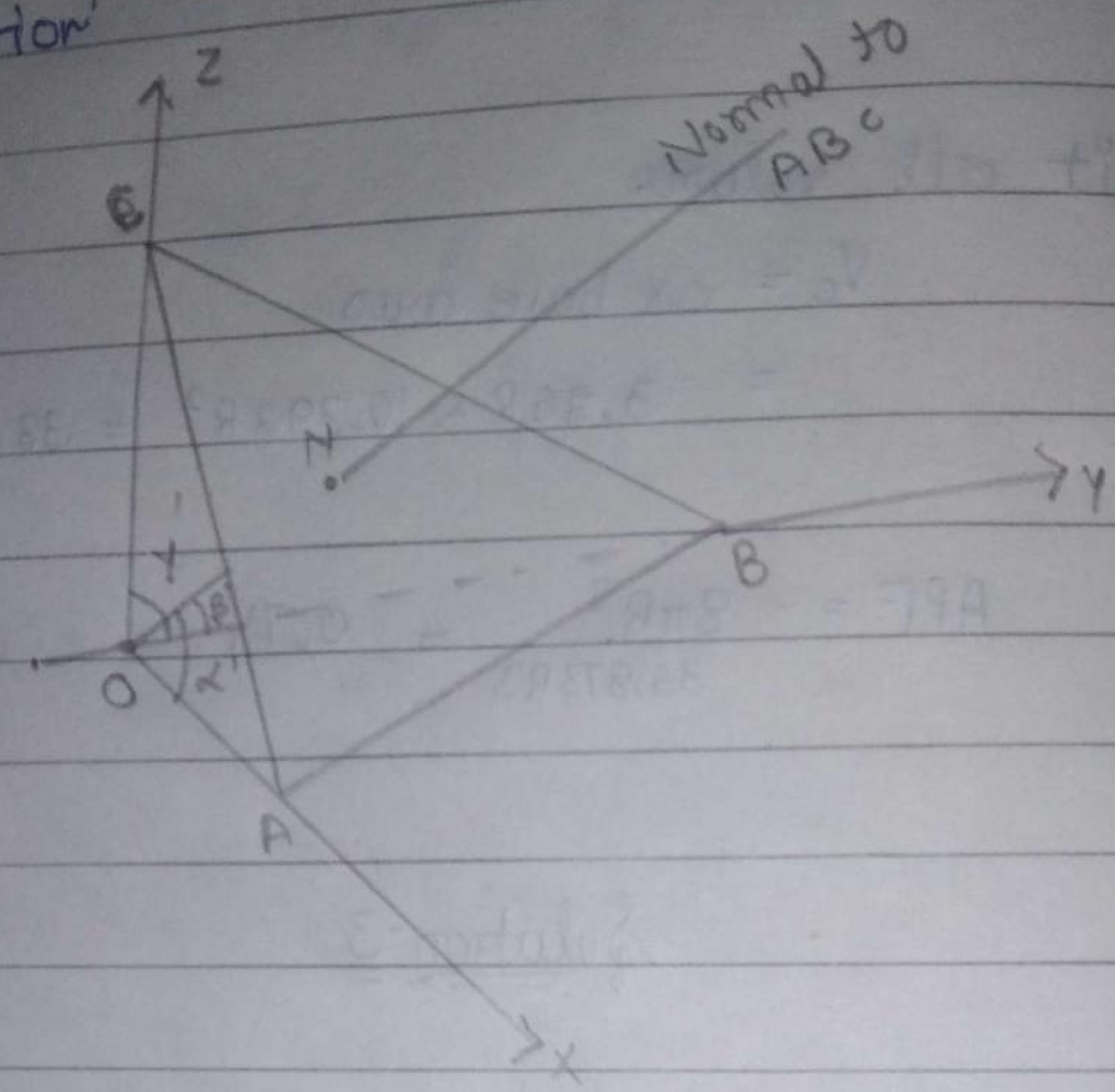
$$APF = \frac{8\pi R^3}{33.873R^3} = 0.74.$$

Solution-3

Miller indices form a notation system in crystallography for planes in Bravais lattices. In particular, a family of lattice planes is determined by three integers h, k and l.

Miller indices are determined by intersection of plane with the axes. The reciprocal of these intercepts are computed and fractions are cleared to give h,k and l.

Derivation:



$OA = a/h$

$OB = a/k$

$OC = a/l$

$\cos\alpha' = \frac{dh}{a}$

$\cos\beta' = \frac{dk}{a}$

$\cos\gamma' = \frac{dl}{a}$

$ON = (x^2+y^2+z^2)^{1/2}$

$d = (d^2\cos^2\alpha' + d^2\cos^2\beta' + \cos^2\gamma')^{1/2}$

$\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1$

For orthogonal co-ordinates

Substituting the valus.

$$\left(\frac{d}{OA}\right)^2 + \left(\frac{d}{OB}\right)^2 + \left(\frac{d}{OC}\right)^2 = 1.$$

$$\left(\frac{dh}{a}\right)^2 + \left(\frac{dK}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

$$\frac{d^2}{a^2}(h^2 + K^2 + l^2) = 1$$

$$\boxed{d_{hKl} = \frac{a}{\sqrt{h^2 + K^2 + l^2}}}$$