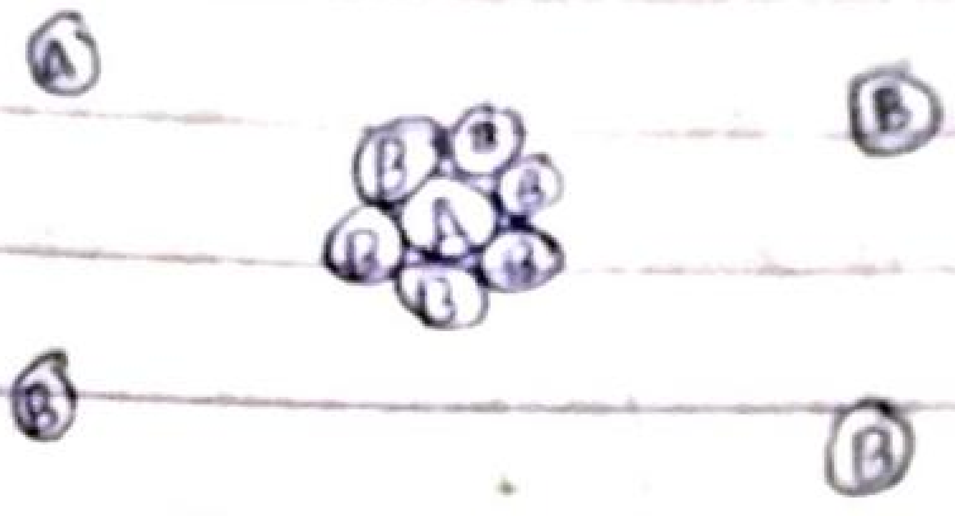
T. D. C. Part I ; Chem. (Hons.)

Unit III Paper II (Gr. A) Phy. Chem.

Factors for determination of crystal str...

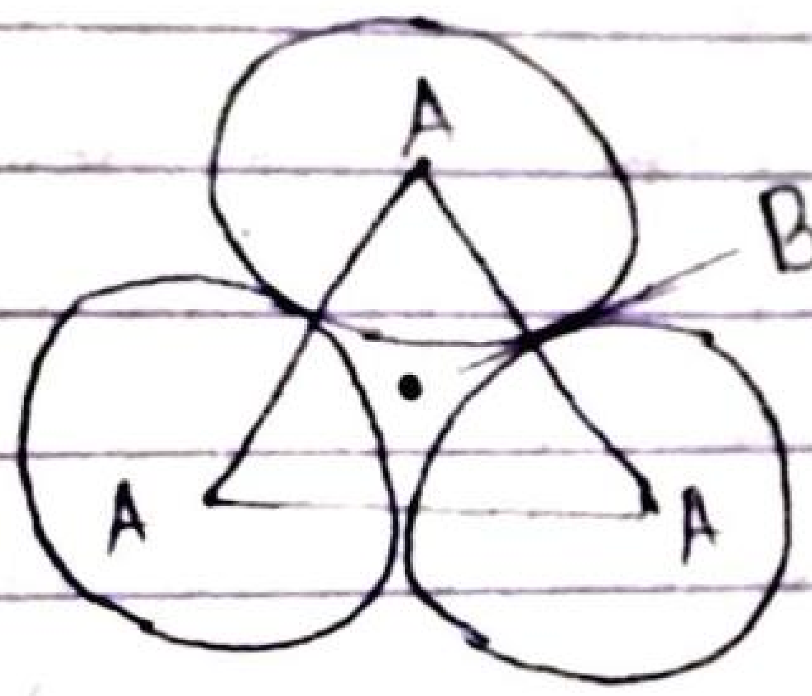
① Co-ordination number :→

It is no. of closest unit to a particular unit. e.g for the arrangement.



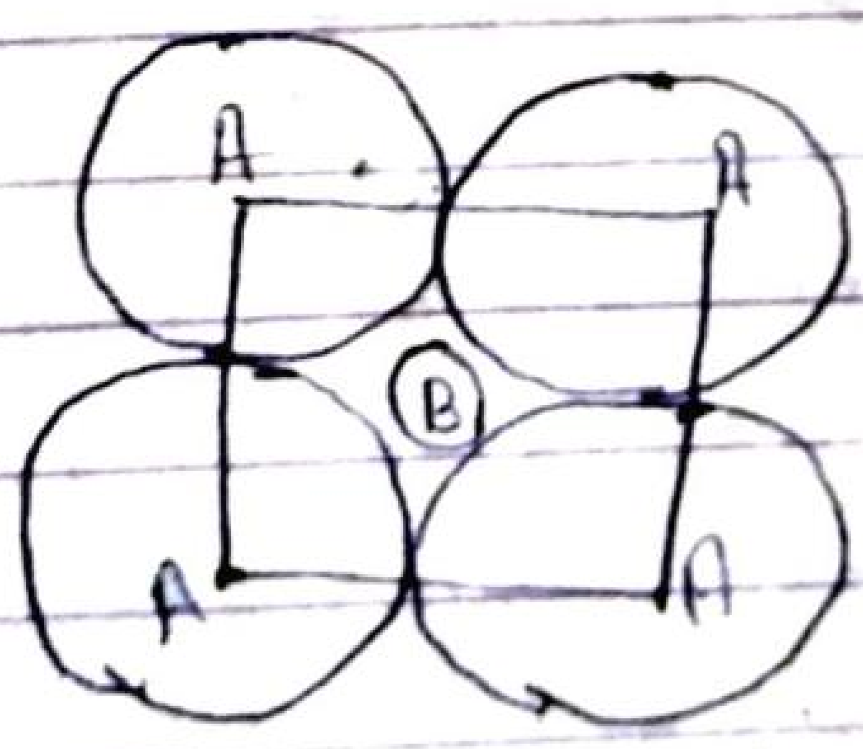
There is six B closest to A and hence co-ordination no. of A = 6

In triangular structure



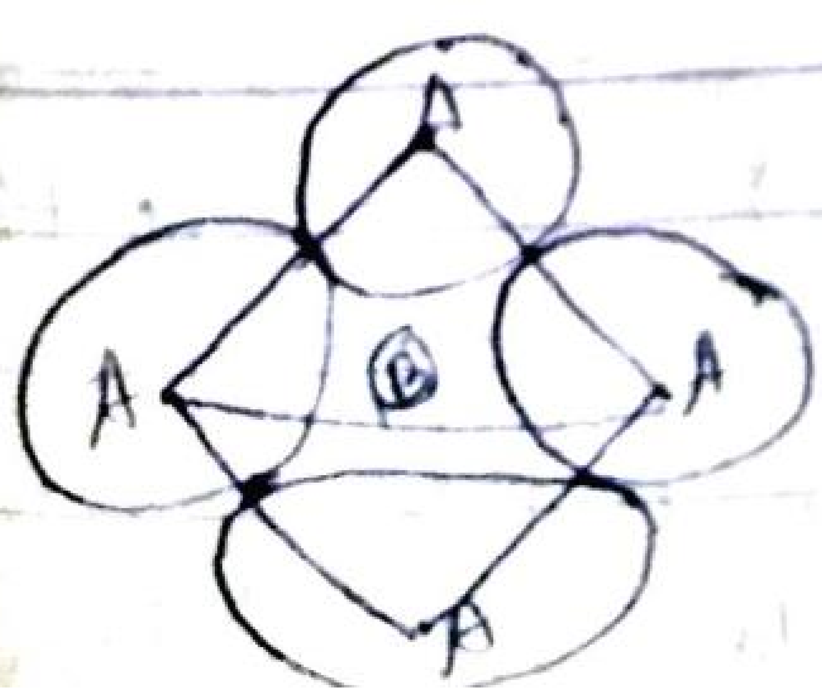
3 'A' occupy the corner of triangle and one B occupies the interstice formed by them Hence C.N of B = 3 and structure is hence trigonal.

For square planar :→



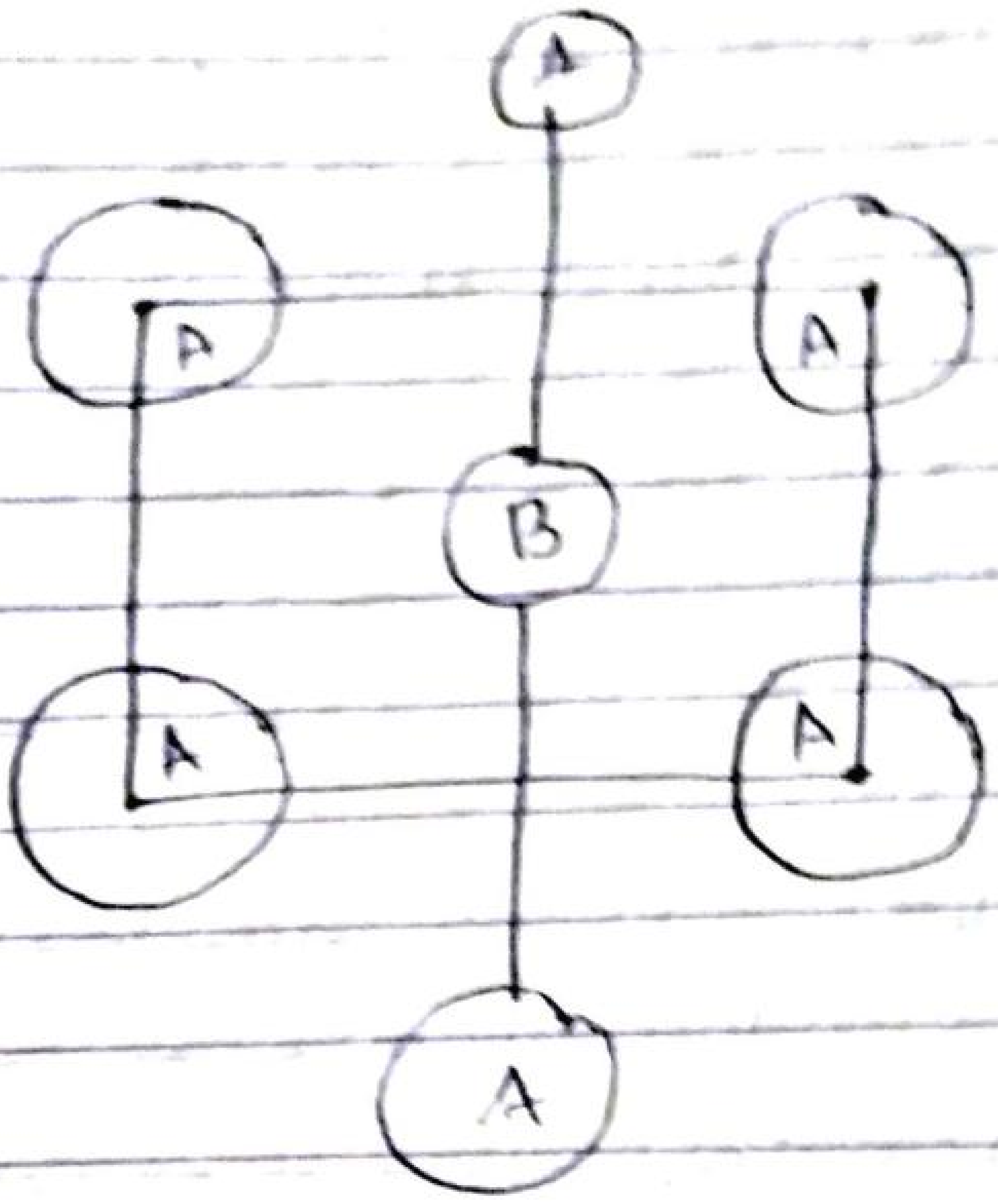
C.N of B = 4

For Tetrahedral Structure :→



A occupies the corner of a tetrahedron and B is placed in tetrahedral hole. Thus C.N of B = 4.

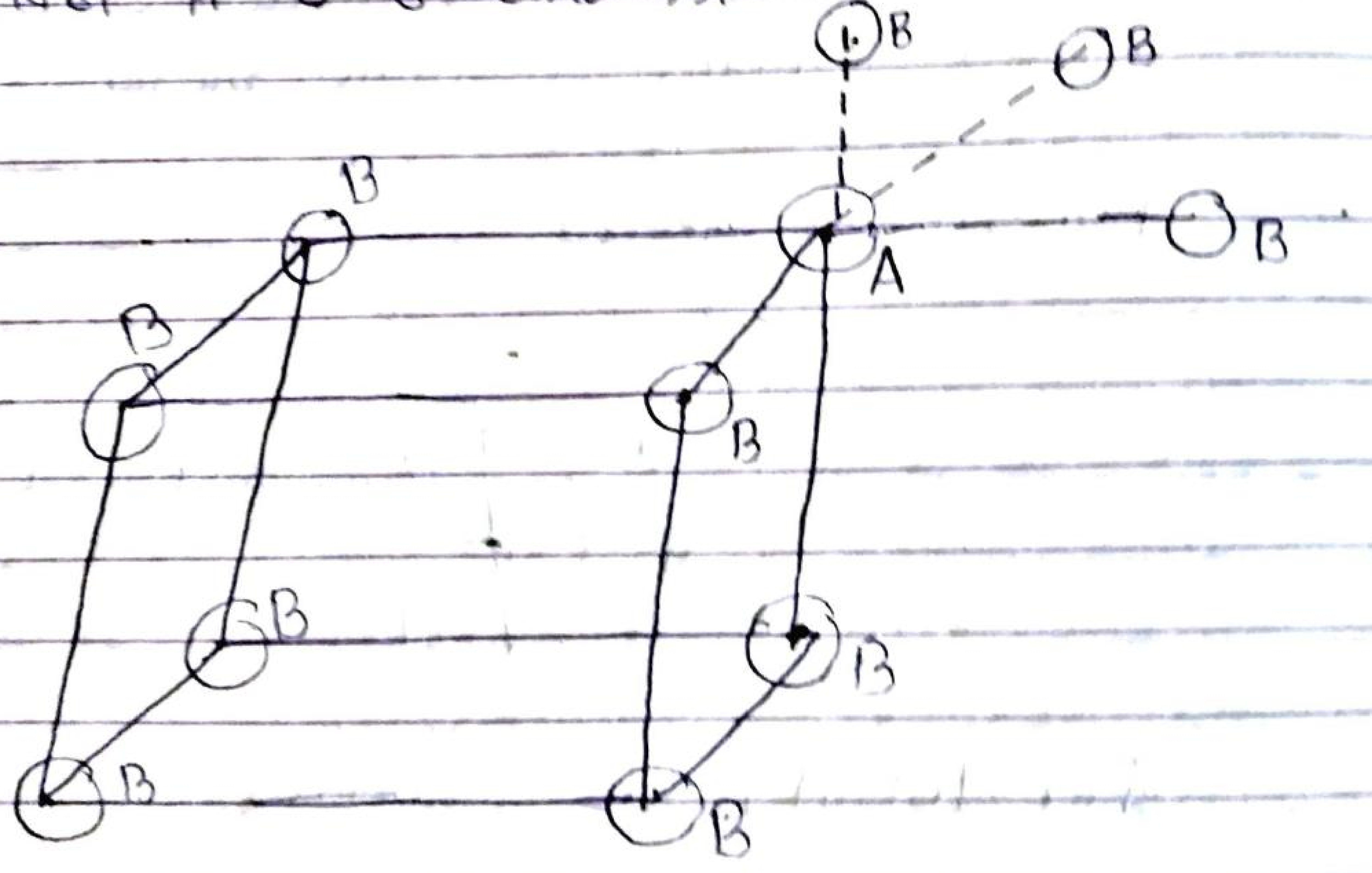
For Octahydral structure :→



B occupies this Octahydral str. and its C.N = 6

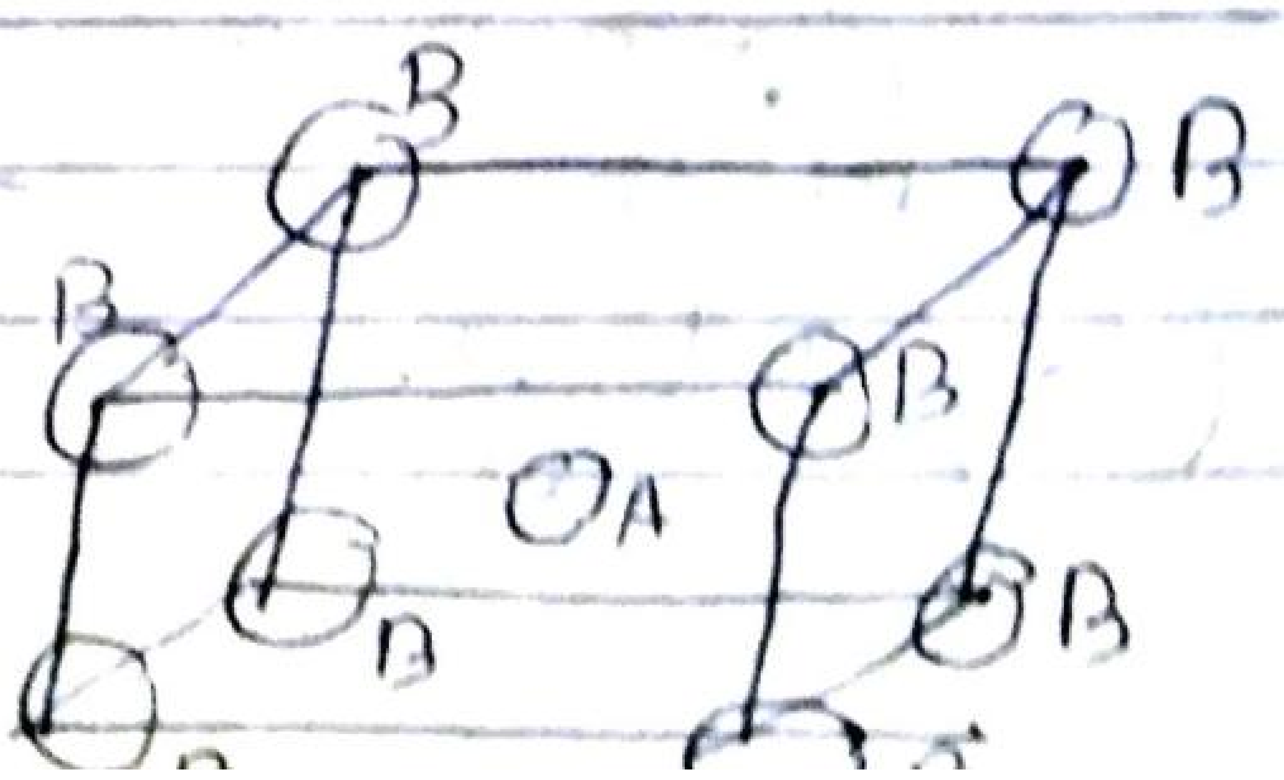
For a simple cubic :→

There are six B units arround A along the sides. other at face diagonals and body diagonals are farther than B. hence C.N of A is 6 and str. is octahydral.



For B.C.C. Structure

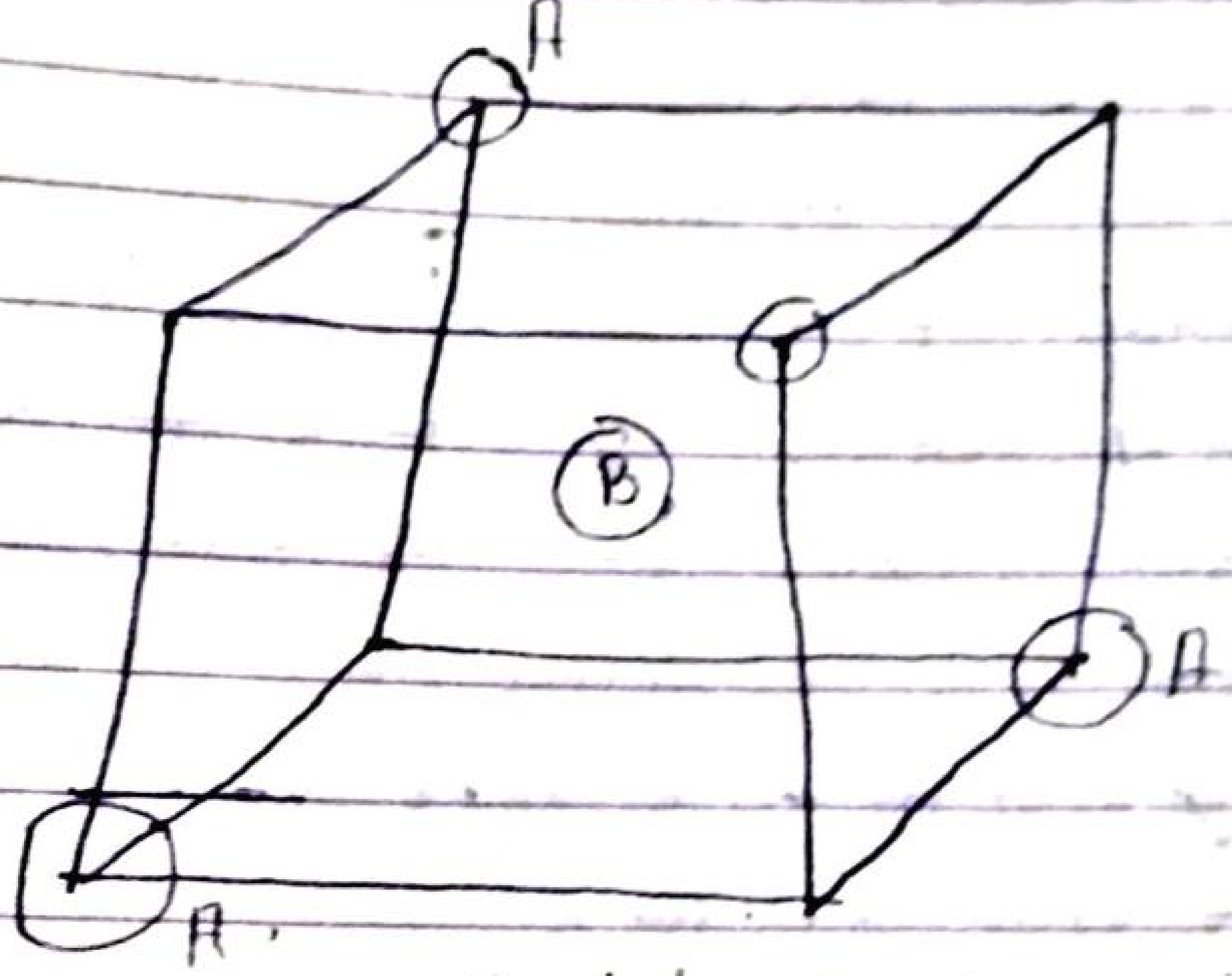
C.N of A = 8



For F.C.C str. units of face centre are the nearest to A. There are 3 such in an units cell. Since 8 cubes meet at a points. A is comman to 8 cubes. Thus A has $8 \times 3 = 24$ close units.

But each unit lying on a face centre is comman to 2 cubes and thus is counted twice. Hence C.N of $A = \frac{8 \times 3}{2} = 12$.

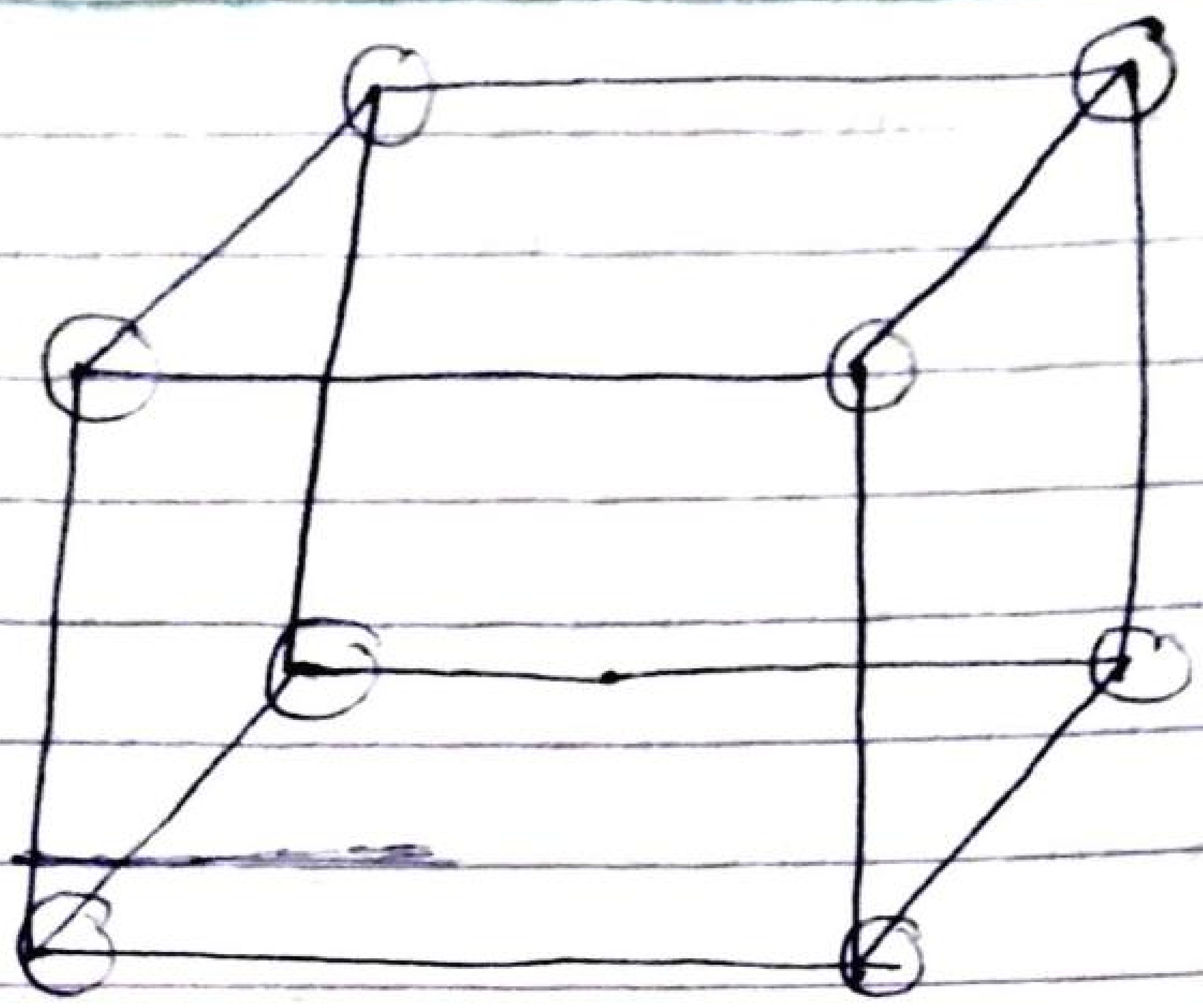
For td. stre.



A td. is formed when units occupy alternate corners of a cubic and the body centre and thus the units A lying in tetrahydral hole has C.N = 4.

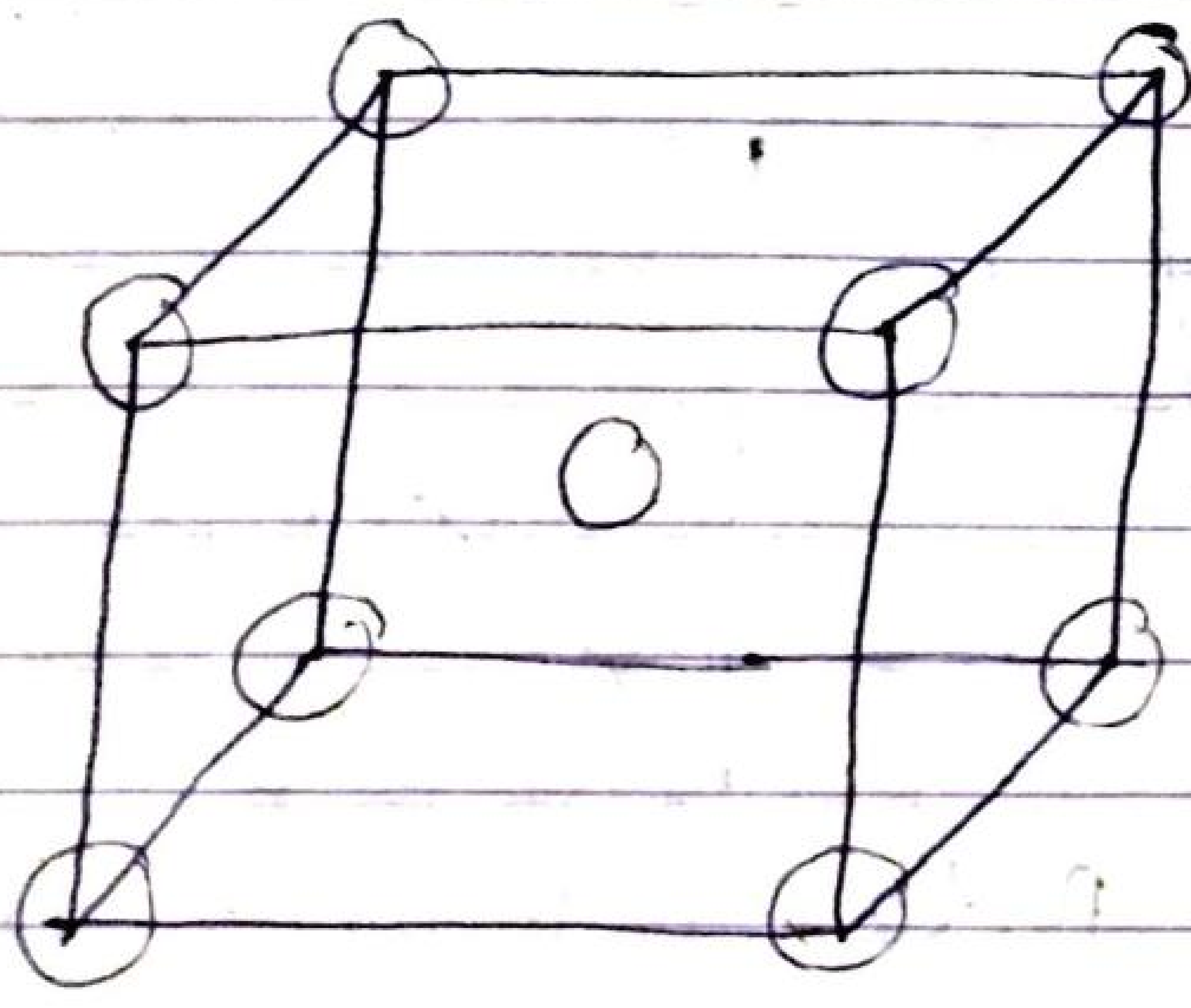
Effective number of units :→

It is the no. of full units (atoms or ions or molecules) present in an unit cell and is denoted by n. In a simple cubic units occupy the lattice points at the corners. Since 8 cubes meet at a point in a lattice, only $\frac{1}{8}$ of an unit is present in an unit cell.



$n = 8\times\frac{1}{8} = 1$

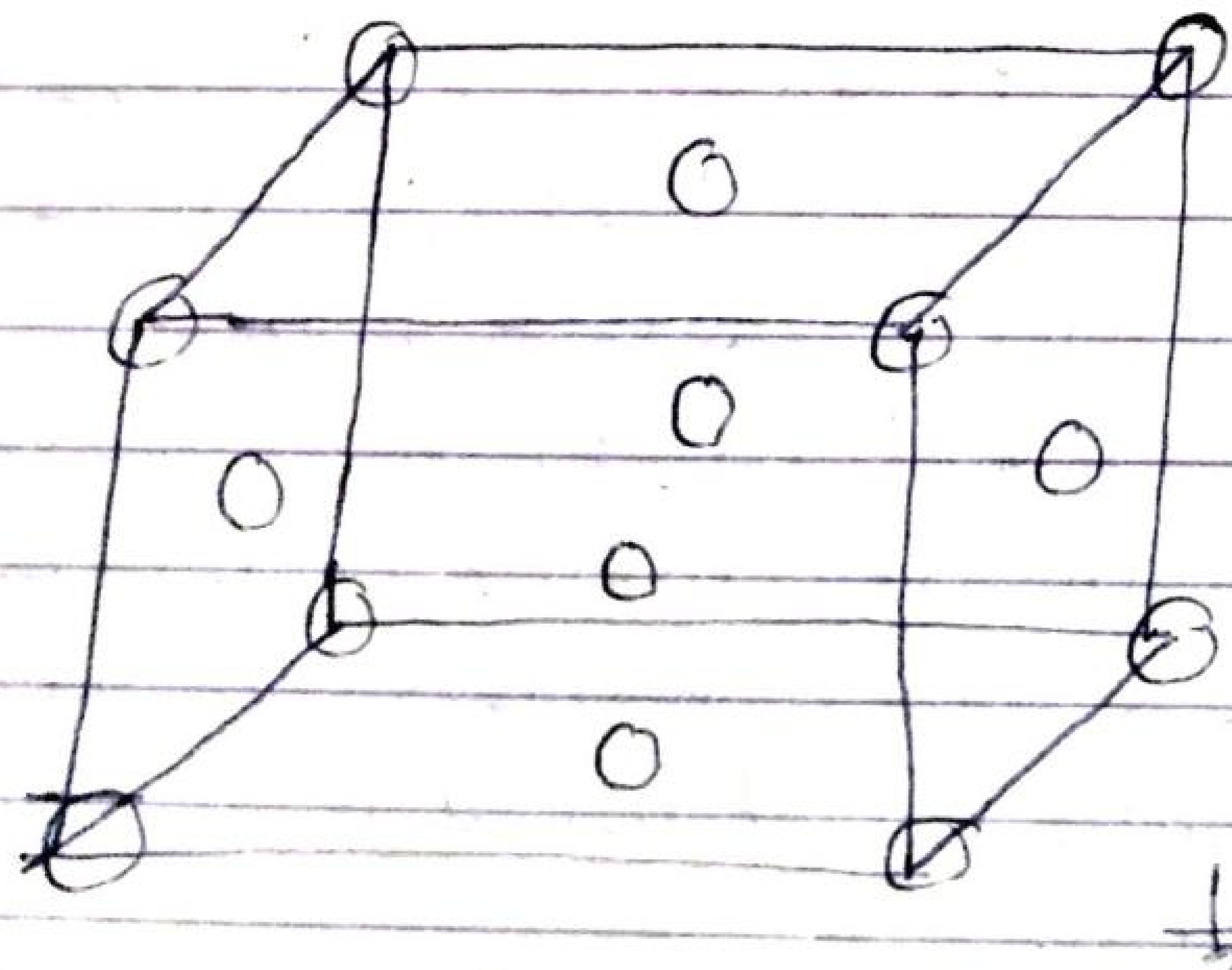
In B.C.C :→



8 units at the corner contribute $\frac{1}{8}$ each and one at the centre is compeletly inside the unit cell and contibute one and hence

$n = 8\times\frac{1}{8} + 1 = 2.$

In F.C.C →.



Since 8 cubes meet at a point $\frac{1}{8}$ of each unit is present in an unit cell and since two cubes meet at a face $\frac{1}{2}$ of each unit is present in the unit cell. There are 8 units at the 8 corners and 6 units at the six faces.

So, that $n = 8\times\frac{1}{8} + 6\times\frac{1}{2} = 1+3 = 4.$