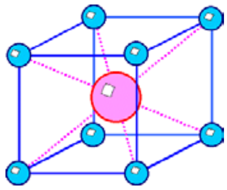
## Answer for Homework II (Crystal structure)

Calculate the theoretical density of the compounds containing these following crystal structure;

1) Caesium Chloride structure (e.g. CsCl)



Crystal structure details;

1) Primitive cubic lattice type of $Cl^-$ ions (blue) with $Cs^+$ ion (Pink) sits in the middle
2) Containing one atom of Cs (in the middle) and one atom of Cl (corner sharing so 1/8 x 8 = 1).
3) Unit cell parameters

   a=b=c= 4.123 Å

   $\alpha=\beta=\gamma= 90^\circ$ from [http://www.ilpi.com/inorganic/structures/cscl/]
4) Atomic number of Cs = 132.91 g/mole and Cl = 35.45 g/mole

**Calculation:**

Mass of unit cell = mass of one atom of Cs +mass of one atom of Cl

$$= \left(\frac{1 \times 132.91}{6.02 \times 10^{23}}\right) + \left(\frac{1 \times 35.45}{6.02 \times 10^{23}}\right)$$

$= 2.80 \times 10^{-22}$ g

Volume of cubic (primitive) unit cell = (length of unit cell $)^3$ → get the length from reference

$= (4.123)^3$ Å$^3$

$= 70.09$ Å$^3$

Unit conversion to cm $= 70.09\ \text{Å}^3 \times \frac{10^{-24}\ \text{cm}^3}{1\ \text{Å}^3}$ (as 1 Å$^3$=1x$10^{-24}$ cm$^3$)

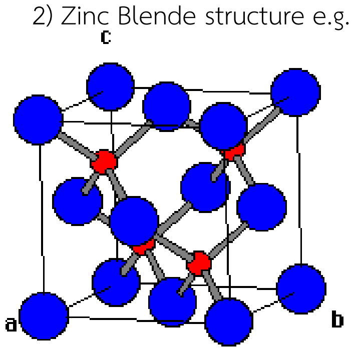
$= 7.009 \times 10^{-23}$ cm$^3$

Thus, density = mass / volume

$$= \frac{2.80 \times 10^{-22}\, g}{7.009 \times 10^{-23}\, cm}$$

**= 3.99 g/cm$^3$** ANS

2) Zinc Blende structure e.g. ZnS compound




Crystal structure details;

1) Face-centred cubic lattice type of $S^{2-}$ ions (blue) with $Zn^{2+}$ ion sits in the hole

2) Containing 4 atoms of Zn all inside the unit cell and 4 atoms of S (fcc packing so **1/8 x 8** (corner) **+1/2 x 6** (face of the box)**= 4**).

3) Unit cell parameters

a=b=c= 5.41 Å

$\alpha=\beta=\gamma= 90^{\circ}$ from [http://www.ilpi.com/inorganic/structures/zincblende/index.html]

4) Atomic number of Zn = 65.38 g/mole and S = 32.06 g/mole

**Calculation:**

Mass of unit cell = mass of 4 atoms of Zn +mass of 4 atoms of S

$$= \left(\frac{4 \times 65.38}{6.02 \times 10^{23}}\right) + \left(\frac{4 \times 32.06}{6.02 \times 10^{23}}\right)$$

$= 6.47 \times 10^{-22}$ g

Volume of cubic (primitive) unit cell = (length of unit cell $)^3$ → get the length from reference

$= (5.41)^3$ Å$^3$

$= 158.3$ Å$^3$

Unit conversion to cm

$$= 158.3\ \text{Å}^3 \times \frac{10^{-24}\ \text{cm}^3}{1\ \text{Å}^3}$$

(as 1 Å$^3$=1x10$^{-24}$ cm$^3$)

$= 1.583 \times 10^{-22}$ cm$^3$

Thus, density = mass / volume

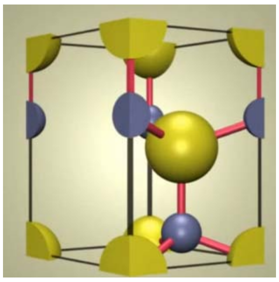
$$= \frac{6.47 \times 10^{-22}\ g}{1.583 \times 10^{-22}\ cm}$$

**= 4.09 g/cm$^3$ ANS**

3) ZnS (Wurtzite)

Method 1

http://www.youtube.com/watch?v=U7rvS7kdEu0



Crystal structure details;

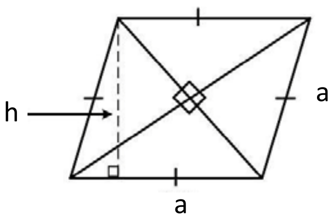
1) Containing 2 atoms of Zn in purple (one insides the unit cell and another one shared to other 4 boxes (1/4 x 4), and 2 atoms of S in yellow (one insides the unit cell and another one is at corner shared location (1/8 x 8)

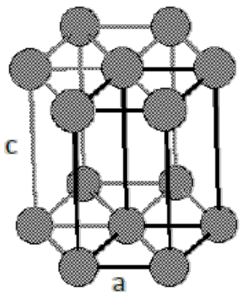
2) Unit cell parameters

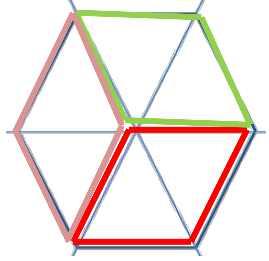
a=b= 382 pm = 3.82 Å  c = 626 pm = 6.26 Å

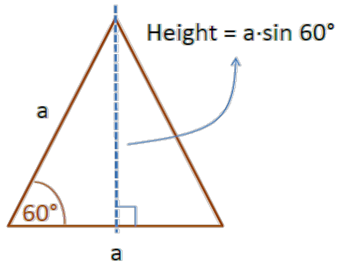
$\alpha=\beta= 90^{\circ}$ and $\gamma=120^{\circ}$ from [http://www.kayelaby.npl.co.uk/chemistry/3_7/3_7_7.html]

3) Atomic number of Zn = 65.38 g/mole and S = 32.06 g/mole






Calculation:

Mass of unit cell = mass of 2 atoms of Zn +mass of 2 atoms of S

$$= \left(\frac{2 \times 65.38}{6.02 \times 10^{23}}\right) + \left(\frac{2 \times 32.06}{6.02 \times 10^{23}}\right)$$

$= 3.24 \times 10^{-22}$ g

Volume of cubic (primitive) unit cell = (area of the red parallelogram) x (height; c)

= (3.82 x (3.82 x sin 60°) x (6.26) Å$^3$

= 79.1 Å$^3$

Unit conversion to cm

$$= 79.1\ \text{Å}^3 \times \frac{10^{-24}\ \text{cm}^3}{1\ \text{Å}^3}$$

(as 1 Å$^3$=1x10$^{-24}$ cm$^3$)

$= 7.91 \times 10^{-23}$ cm$^3$

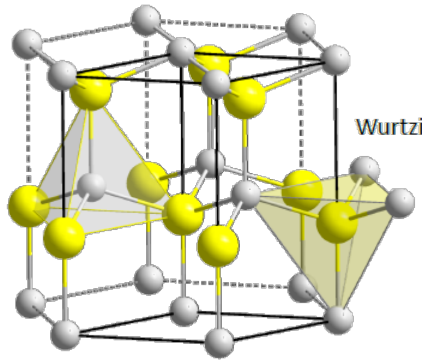
Thus, density = mass / volume

$$= \frac{3.24 \times 10^{-22}\ g}{7.91 \times 10^{-23}\ cm}$$

**= 4.10 g/cm$^3$** ANS

## Method 2

If you consider as hexagonal structure, which includes 3 boxes (from method 1), number of atoms inside and volume of the unit cell need to be reconsidered.




1) number of atoms (3 x number of each atoms in one box)

So there will be 6 atoms of Zn and 6 atoms of S.

2) Volume = hexagonal shape area x height of unit cell.

3) hexagonal shape area includes 6 triangles

**Calculation:**

Mass of unit cell = mass of 6 atoms of Zn +mass of 6 atoms of S

$$= \left(\frac{6 \times 65.38}{6.02 \times 10^{23}}\right) + \left(\frac{6 \times 32.06}{6.02 \times 10^{23}}\right)$$

$= 9.72 \times 10^{-22}$ g

Volume of cubic (primitive) unit cell = (area of the base) x (height; c)

$= (6 \times \frac{1}{2} \times 3.82 \times (3.82 \times \sin 60°) \times (6.26)$ Å$^3$

$= 237$ Å$^3$

Unit conversion to cm $= 237$ Å$^3$ | $10^{-24}$ cm$^3$ / 1 Å$^3$ (as 1 Å$^3$=1x10$^{-24}$ cm$^3$)

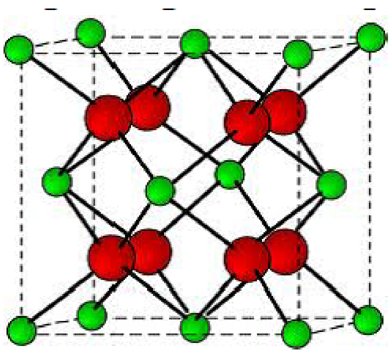
$= 2.37 \times 10^{-22}$ cm$^3$

Thus, density = mass / volume

$$= \frac{9.72 \times 10^{-22}\, g}{2.37 \times 10^{-22}\, cm}$$

**= 4.10 g/cm$^3$ ANS**

4) Fluorite structure ($CaF_2$)



Crystal structure details;

1) Face-centred cubic lattice type of $Ca^{2+}$ ions (Green) with $F^-$ (red) ions sit in the tetrahedral holes

2) Containing 8 atoms of F all inside the unit cell and 4 atoms of Ca (fcc packing so 1/8 x 8 (corner) +1/2 x 6 (face of the box)= 4).

3) Unit cell parameters

a=b=c= 545 pm = 5.45 Å

$\alpha=\beta=\gamma= 90^\circ$ from [http://www.kayelaby.npl.co.uk/chemistry/3_7/3_7_7.html]

4) Atomic number of Ca = 40.078 g/mole and F = 18.998 g/mole

**Calculation:**

Mass of unit cell = mass of 4 atoms of Ca +mass of 8 atom of F

$$= \left(\frac{4 \times 40.078}{6.02 \times 10^{23}}\right) + \left(\frac{8 \times 18.998}{6.02 \times 10^{23}}\right)$$

$= 5.1876 \times 10^{-22}$ g

Volume of cubic (primitive) unit cell = (length of unit cell $)^3$ → get the length from reference

$= (5.45)^3$ Å$^3$

$= 162$ Å$^3$

Unit conversion to cm

$$= 162 \text{ Å}^3 \times \frac{10^{-24}\ \text{cm}^3}{1\ \text{Å}^3}$$

(as 1 Å$^3$=1x$10^{-24}$ cm$^3$)

$= 1.62 \times 10^{-22}$ cm$^3$

Thus, density = mass / volume

$$= \frac{5.1876 \times 10^{-22}\, g}{1.62 \times 10^{-22}\, cm}$$

= 3.20 g/cm$^3$ ANS