CH3052 Material Science Assignment-1

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CH18B020

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Exercise 1

Part a) Coordination Number

The coordination number of the atoms was found manually by viewing the CIF file on Vesta.

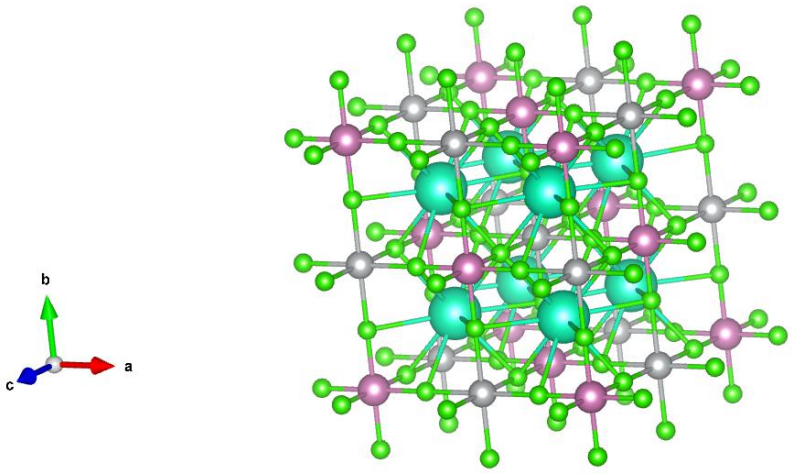

Figure 1: Structure Visualised in Vesta

1. Cs: 12
2. Ag: 6
3. In: 6

Part b) Bond Lengths

The bond lengths were found using the bond length operator and was found to be:

1. Cs-Cl: 3.707 Å
2. Ag-Cl: 2.733 Å
3. In-Cl: 2.507 Å

Part c) Hide bonds greater than 3Å

The Cs-Cl bond were greater than 3Å. Those were removed and the resulting structure is as given below.

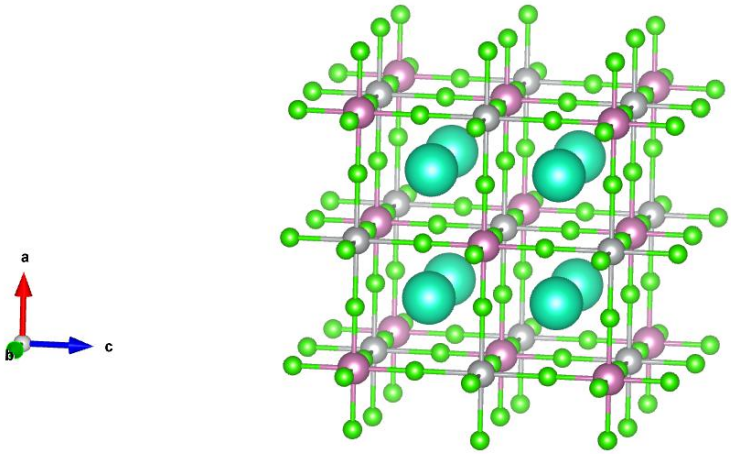

Figure 2: Longer Bonds Removed

Part d) Polyhedral Mode

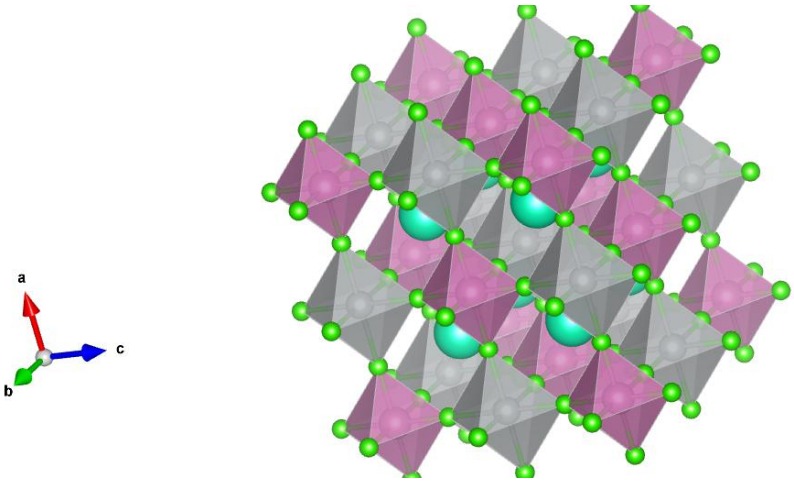

Figure 3: Polyhedral Mode

Purple octahedra are constructed with In (Indium) atom as centre and grey octahedra are constructed with Ag (Silver) atom as centre

Part e) Pore Visualisation

Cs atoms are hidden from the above structure

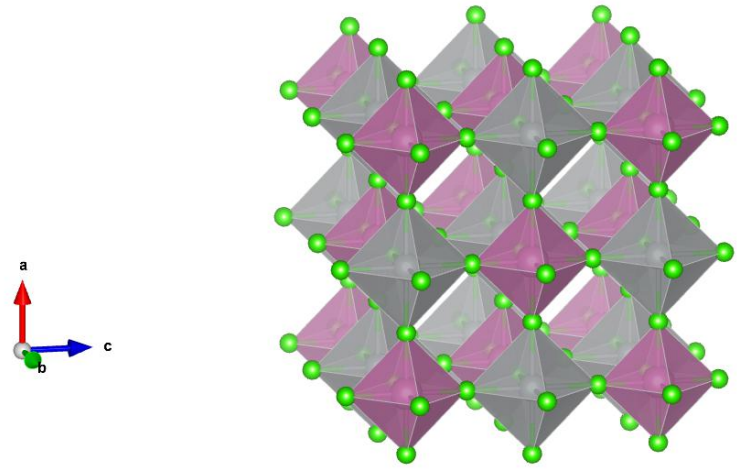

Figure 4: Structure obtained after hiding the Cs atoms

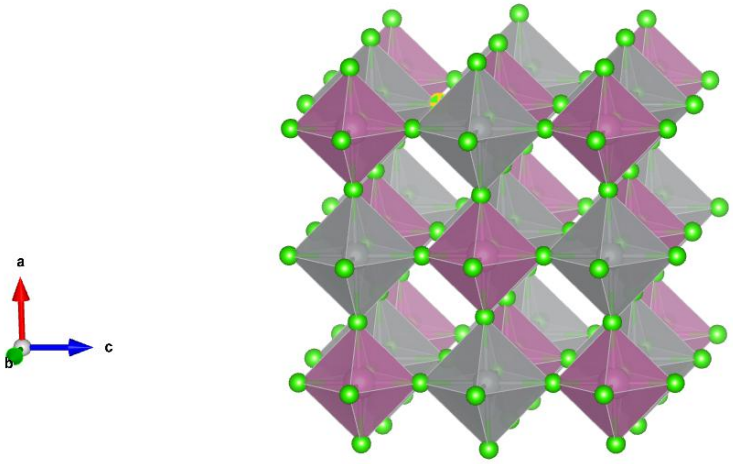

Figure 5: Structure obtained after hiding the Cs atoms; with the narrow pores visible

Part f) Unit Cell & Cation locations

After hiding the bonds and polyhedra we obtain figure 6. These are the coordinates of cations:

1. Locations of **Ag** atoms (**13 atoms** in total displayed; 12 present in **edge centres** and 1 present in **body centre**)
   (a) (10.48059, 0.00000, 5.24030)
   (b) (0.00000, 0.00000, 5.24030)
   (c) (0.00000, 10.48059, 5.24030)
   (d) (10.48059, 10.48059, 5.24030)
   (e) (0.0000, 5.2403, 0.00000)

(f) (0.0000, 5.2403, 10.48059)

(g) (10.48059, 5.24030, 10.48059)

(h) (10.48059, 5.24030, 0.0000)

(i) (5.24030, 0.00000, 10.48059)

(j) (5.24030, 10.48059, 0.0000)

(k) (5.24030, 0.00000, 0.00000)

(l) (5.24030, 10.48059, 10.48059)

(m) (5.24030, 5.24030, 5.24030)

2. Locations of **In** atoms (**16 atoms** in total displayed; 6 present in **face centres** and 8 in **corners**)

(a) (0,0,0)

(b) (10.48059, 0.00000, 0.00000)

(c) (5.24030, 5.24030, 0.00000)

(d) (5.24030, 10.48059, 5.24030)

(e) (10.48059, 5.24030, 5.24030)

(f) (10.48059, 0.00000, 10.48059)

(g) (10.48059, 10.48059, 0.00000)

(h) (10.48059, 10.48059, 10.48059)

(i) (10.48059, 0.00000, 10.48059)

(j) (5.24030, 5.24030, 10.48059)

(k) (0.00000, 0.00000, 10.48059)

(l) (0.00000, 10.48059, 10.48059)

(m) (0.00000, 5.24030, 5.24030)

(n) (0.00000, 10.48059, 0.00000)

(o) (5.24030, 10.48059, 5.24030)

(p) (5.24030, 0.00000, 5.24030)

3. Locations of **Cs** atoms (**8 atoms** in total displayed; All of them present in **tetrahedral voids**)

(a) (2.62015, 2.62015, 2.62015)

(b) (7.86044, 2.62015, 2.62015)

(c) (2.62015, 7.86044, 2.62015)

(d) (2.62015, 2.62015, 7.86044)

(e) (2.62015, 7.86044, 7.86044)

(f) (7.86044, 7.86044, 2.62015)

(g) (7.86044, 2.62015, 7.86044)

(h) (7.86044, 7.86044, 7.86044)

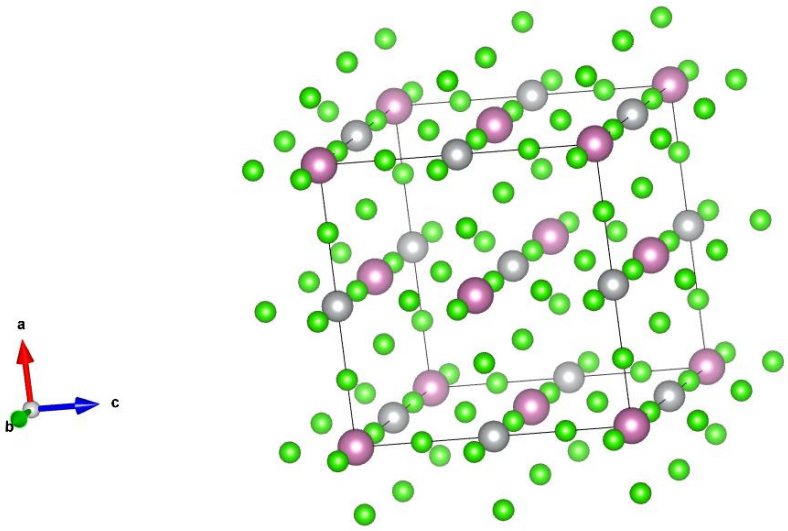

Figure 6: Visualising the unit cell

Effective number of Ag atoms = $12 \cdot \frac{1}{4} + 1 = 4$
Effective number of Cs atoms = $8 \cdot 1 = 8$
Effective number of In atoms = $8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{6} = 4$
Effective number of Cl atoms = $48 \cdot \frac{1}{4} + 12 \cdot \frac{1}{2} = 24$
(48 atoms on edges in the middle of edge centre and corner. 12 atoms on faces in the middle of face centre and an edge centre)

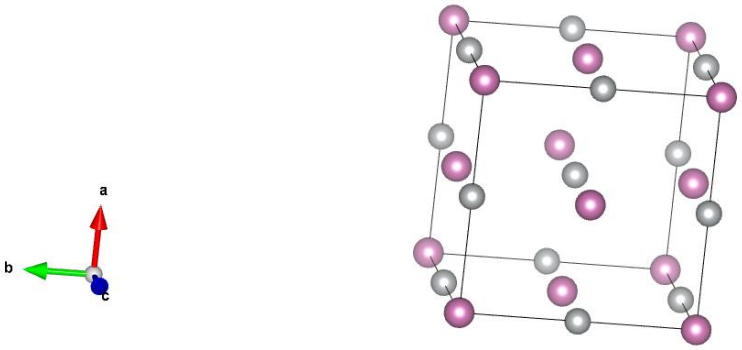

Figure 7: Visualising the unit cell with just the cations

Part g) Miller Planes

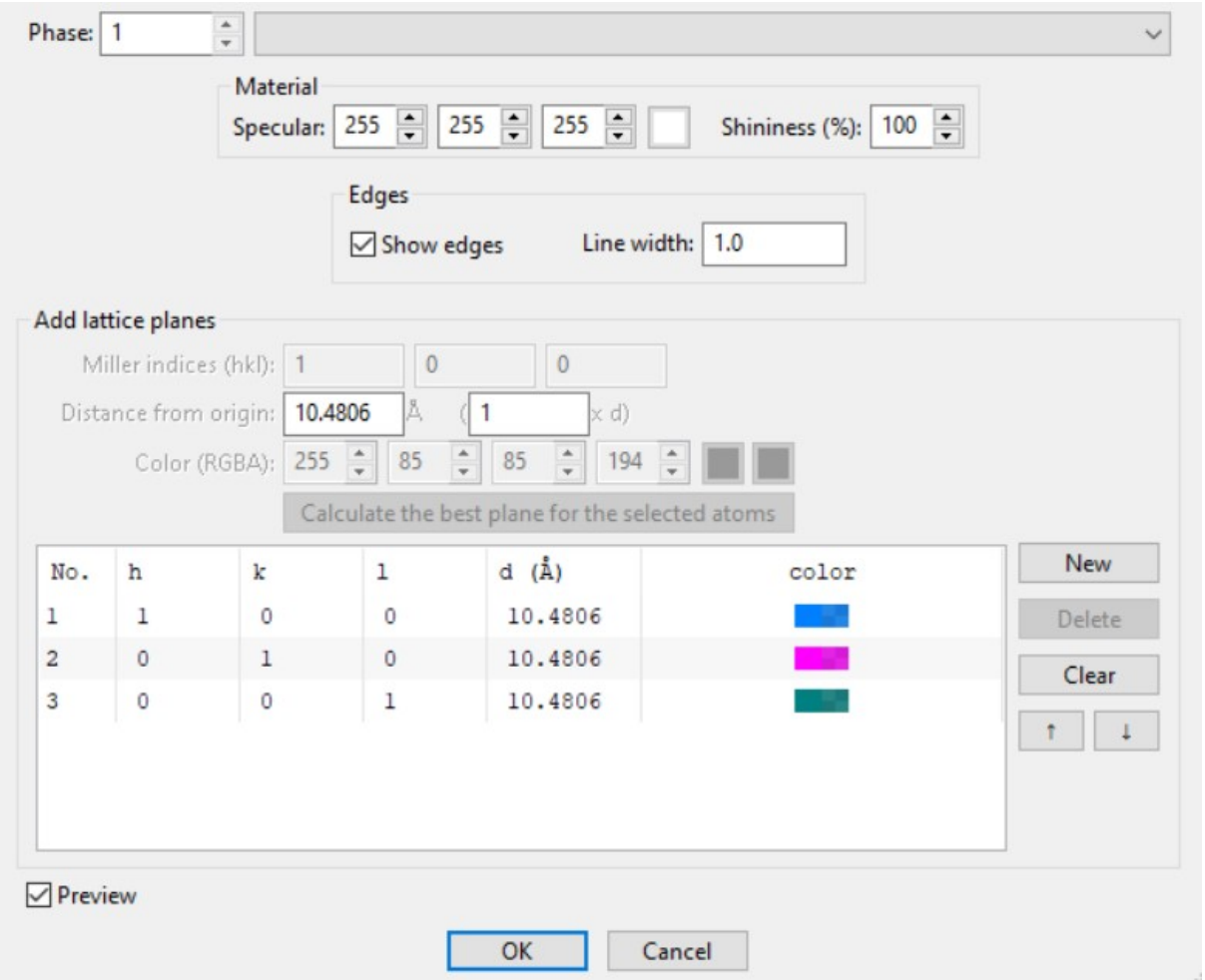

Figure 8: Generating the planes in Vesta

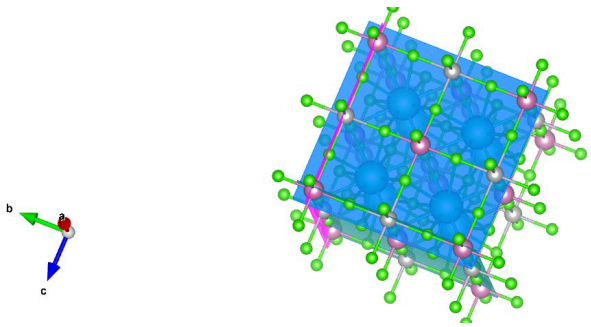

Figure 9: Plane (100)

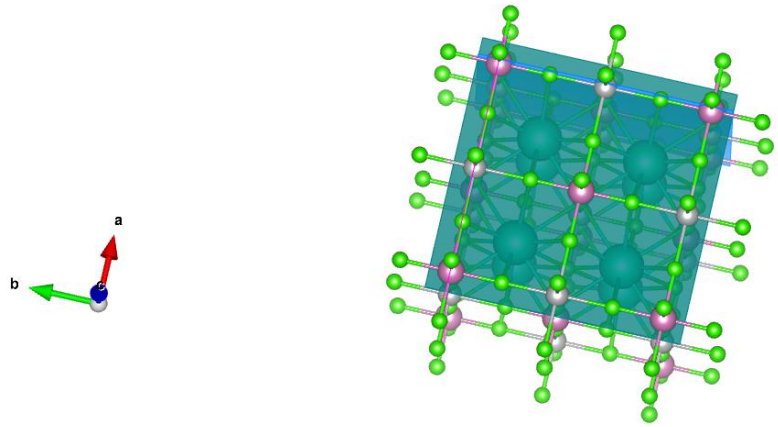

Figure 10: Plane (001)

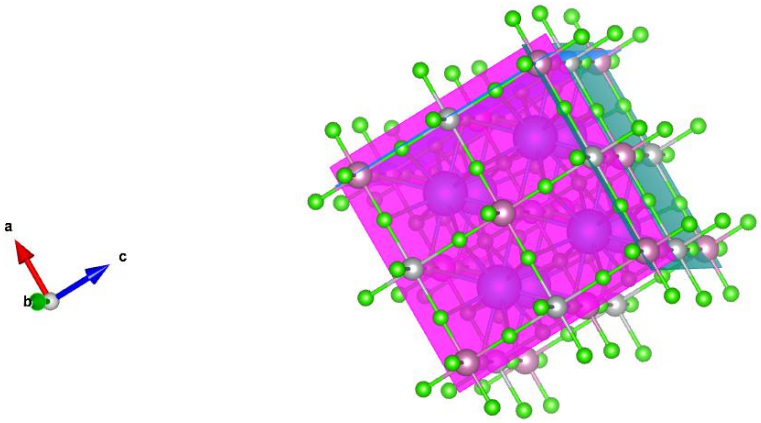

Figure 11: Plane (010)

Yes, all planes have the **same atom composition**: In in corners and centre. Silver in edge centres. Chlorine atoms in between In and Ag parallel to edges. All the planes belong to the **same family**.

Part h) Family of Planes

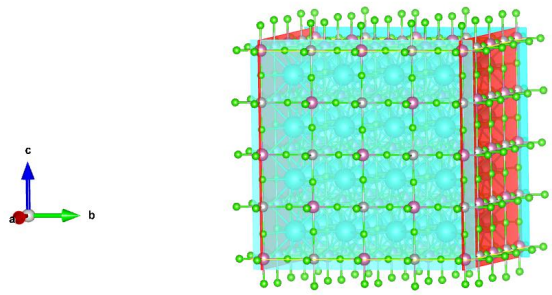

Figure 12: (100) Plane

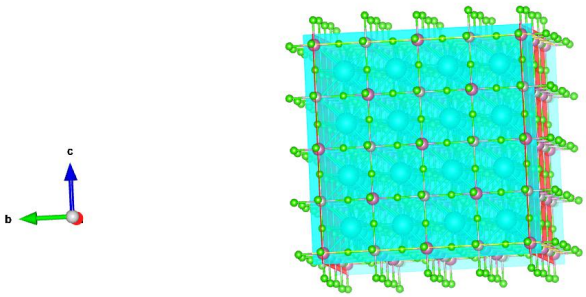

Figure 13: (-100) Plane

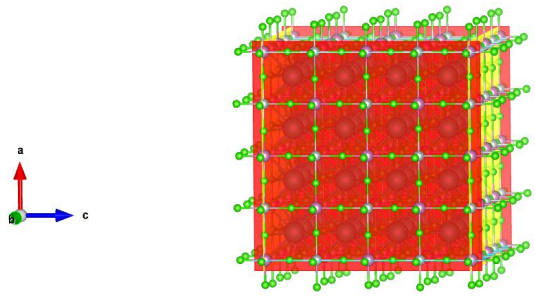

Figure 14: (010) Plane

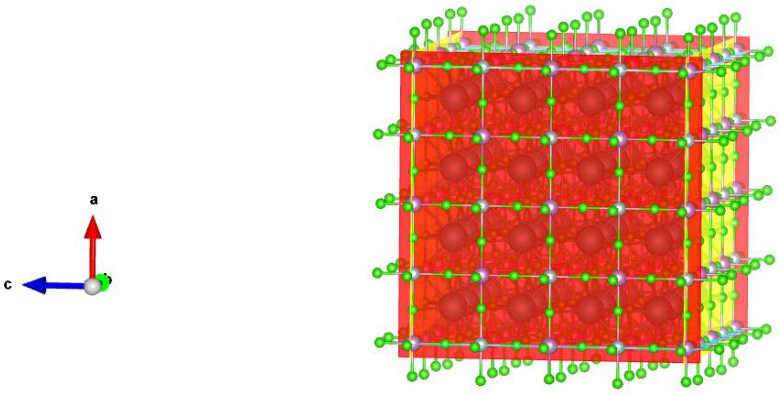

Figure 15: (0 -1 0) Plane

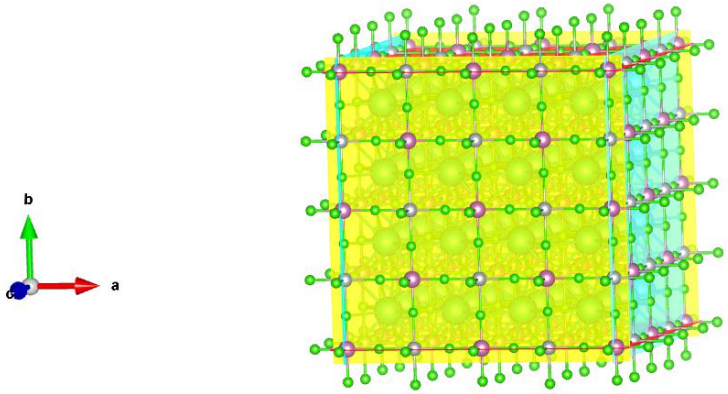

Figure 16: (001) Plane

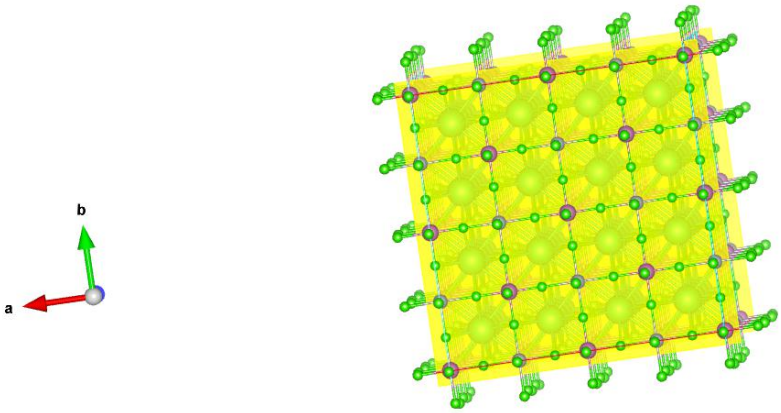

Figure 17: (0 0 -1) Plane

Part i) Comparing (101) and (100) planes

100 Plane (Refer figure 18)
Bond Lengths:

1. In-Cl: 2.507Å
2. Ag-Cl: 2.733Å

Bond Angles:

1. Cl-Ag-Cl: 90°
2. Cl-In-Cl: 90°

101 Plane (Refer figure 19)
Bond Lengths:

1. In-Cl: 2.507Å
2. Ag-Cl: 2.733Å
3. Cs-Cl: 3.7072Å

Bond Angles:

1. Cl-Ag-Cl: 90°
2. Cl-In-Cl: 90°
3. Cl-Cs-Cl: 62.84°

Between the same set of atoms, bond angles and bond lengths remain the same across planes.

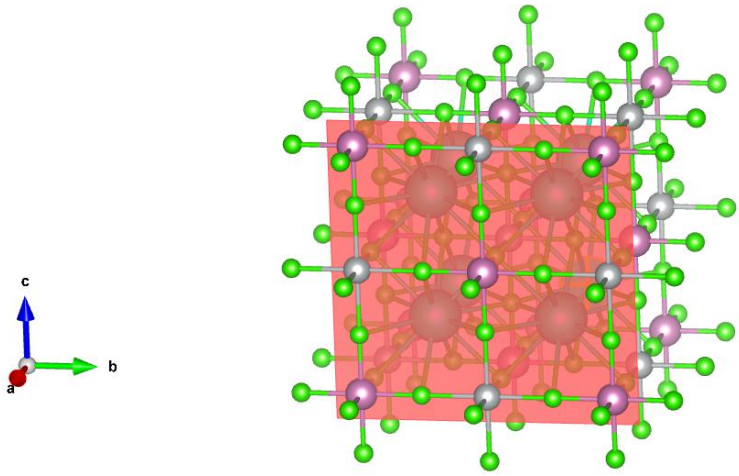

Figure 18: Atoms on 100 Plane

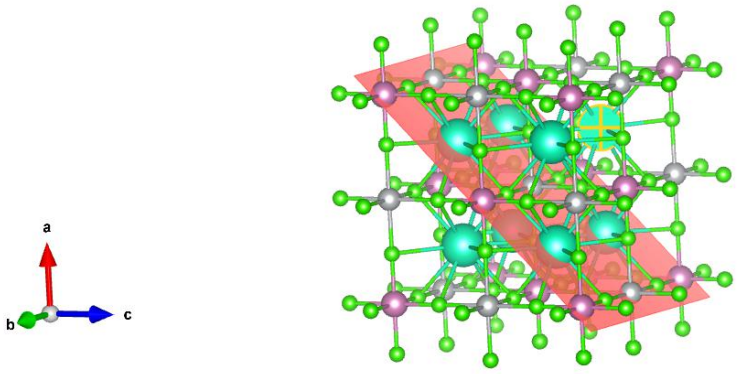

Figure 19: Atoms on 101 Plane

Exercise 2

Part a)

Given below is an extract of the lines mentioning the cell parameters in the CIF file:

```
_cell_length_a    10.480593(54)
_cell_length_b    10.480593(54)
_cell_length_c    10.480593(54)
_cell_angle_alpha  90
_cell_angle_beta   90
_cell_angle_gamma  90
_cell_volume  1151.218(18)
```

From the above lines in the *.CIF* file we find that the parameter values are $a = b = c = 10.4806$Å and $\alpha = \beta = \gamma = 90^{\circ}$
Parameters as shown in Vesta:

Lattice parameters

a	b	c	alpha	beta	gamma
10.48059	10.48059	10.48059	90.0000	90.0000	90.0000

Figure 20: Screenshot of parameters displayed in Vesta

Obviously, since Vesta takes the parameters from the CIF file, the parameters taken in both places match perfectly.