

# **WORKSHEET**

## **PRACTICAL-1**

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**COURSE:** MED201

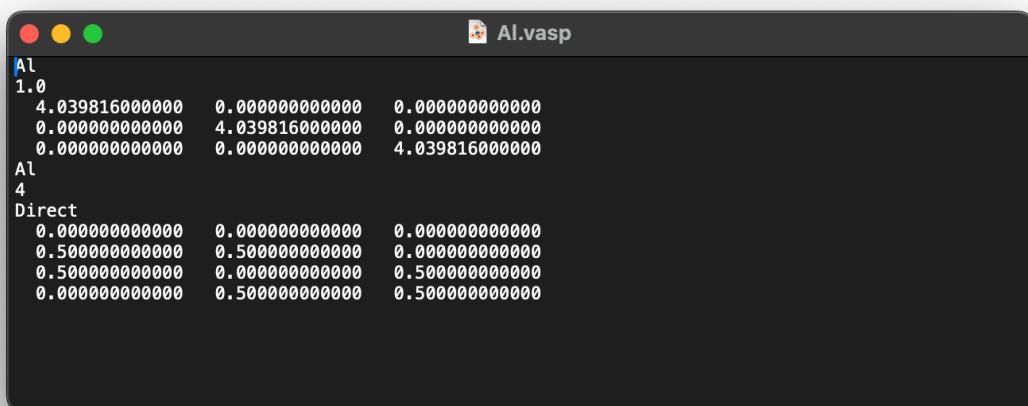
**BATCH:** PA

**STREAM:** BTech CSE

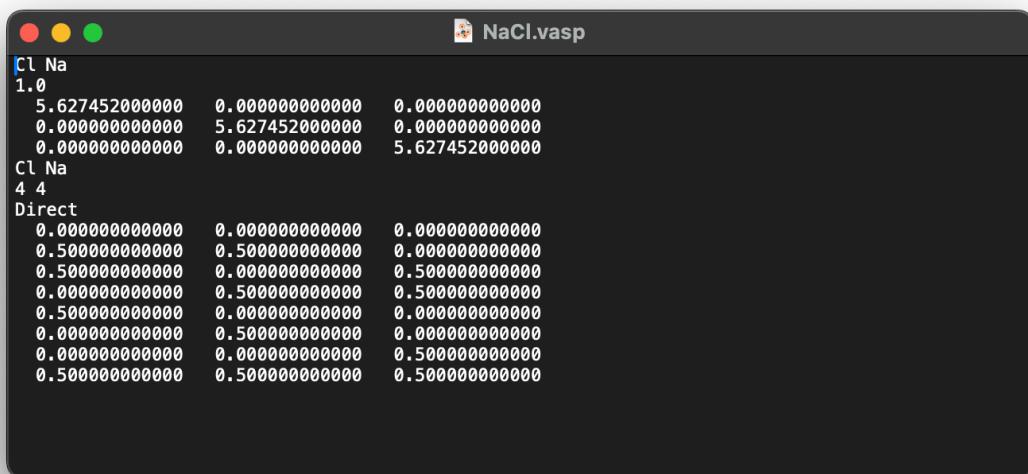
Open the Al.vasp and NaCl.vasp files in VESTA application to solve the problems.

### **ANSWER 1**

To find the lattice parameters of Al and NaCl, open the .vasp file in a text editor.



```
Al
1.0
 4.039816000000  0.000000000000  0.000000000000
 0.000000000000  4.039816000000  0.000000000000
 0.000000000000  0.000000000000  4.039816000000
Al
4
Direct
 0.000000000000  0.000000000000  0.000000000000
 0.500000000000  0.500000000000  0.000000000000
 0.500000000000  0.000000000000  0.500000000000
 0.000000000000  0.500000000000  0.500000000000
```



```
Cl Na
1.0
 5.627452000000  0.000000000000  0.000000000000
 0.000000000000  5.627452000000  0.000000000000
 0.000000000000  0.000000000000  5.627452000000
Cl Na
4 4
Direct
 0.000000000000  0.000000000000  0.000000000000
 0.500000000000  0.500000000000  0.000000000000
 0.500000000000  0.000000000000  0.500000000000
 0.000000000000  0.500000000000  0.500000000000
 0.500000000000  0.000000000000  0.000000000000
 0.000000000000  0.500000000000  0.000000000000
 0.000000000000  0.000000000000  0.500000000000
 0.500000000000  0.500000000000  0.500000000000
```

We get the following results:

| For Al                      | For NaCl                    |
|-----------------------------|-----------------------------|
| $a = 4.0398160 \text{ \AA}$ | $a = 5.6274520 \text{ \AA}$ |
| $b = 4.0398160 \text{ \AA}$ | $b = 5.6274520 \text{ \AA}$ |

|                 |                 |
|-----------------|-----------------|
| c = 4.0398160 Å | c = 5.6274520 Å |
|-----------------|-----------------|

Then to find angles we open the files in VESTA and go to summary tab.

```

Al
Space Group: P 1 (#1-1)
a = 4.03982 Å α = 90.0000°
b = 4.03982 Å β = 90.0000°
c = 4.03982 Å γ = 90.0000°
V = 65.9303 Å^3

Cl Na
Space Group: P 1 (#1-1)
a = 5.62745 Å α = 90.0000°
b = 5.62745 Å β = 90.0000°
c = 5.62745 Å γ = 90.0000°
V = 178.2114 Å^3

```

**Output      Summary**

We get the following results:

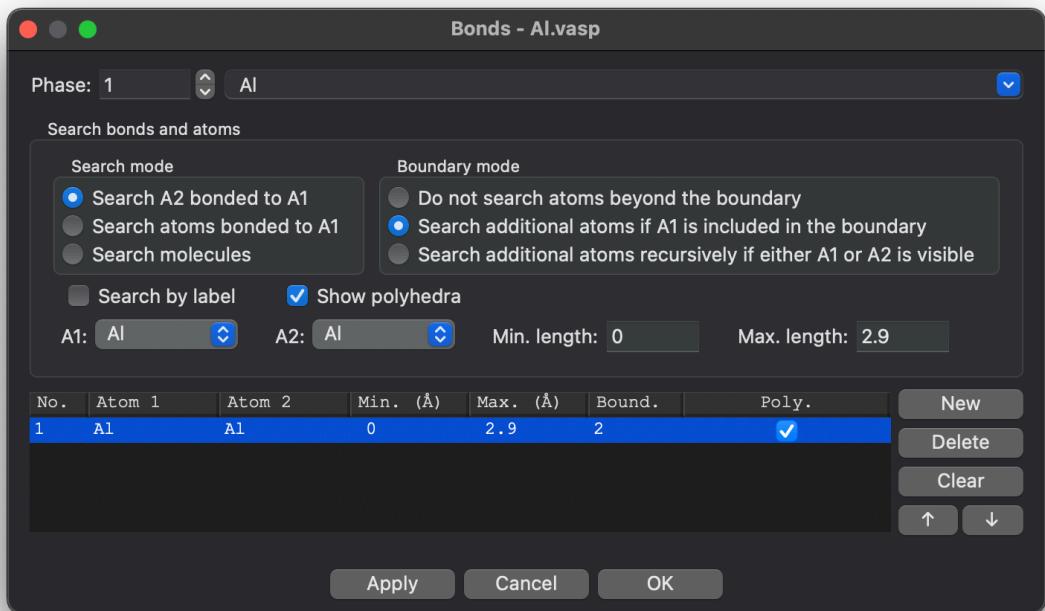
| For Al  | For NaCl |
|---------|----------|
| α = 90° | α = 90°  |
| β = 90° | β = 90°  |
| γ = 90° | γ = 90°  |

## Answer 2

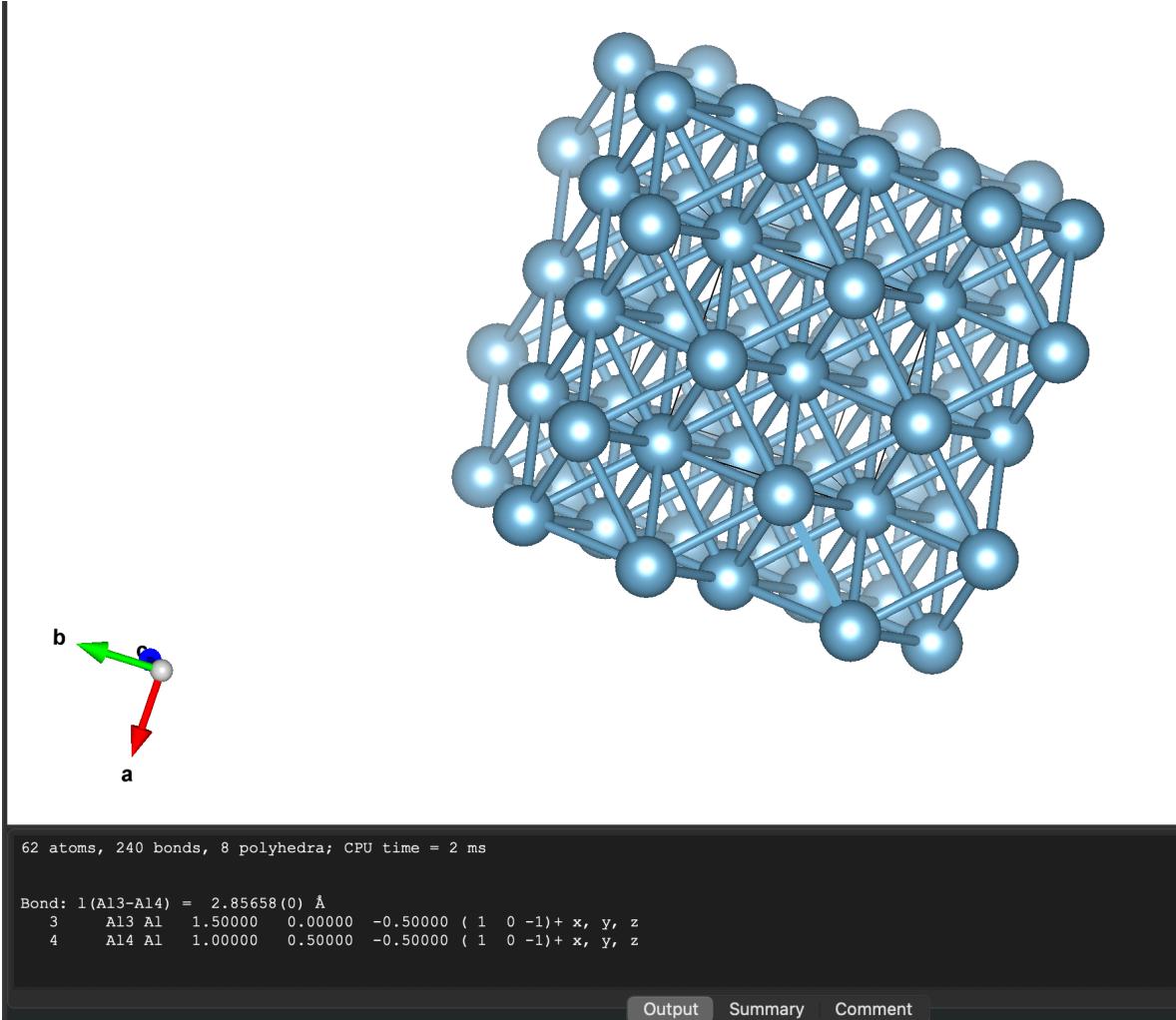
After importing the structure in Vesta, go to Edit>Bonds and add a new bond to see bond line structures as follows:

### **For Al:**

Set the max length as 2.9 and the structure underneath appears.



Click on one of the bonds to obtain information about it as shown.

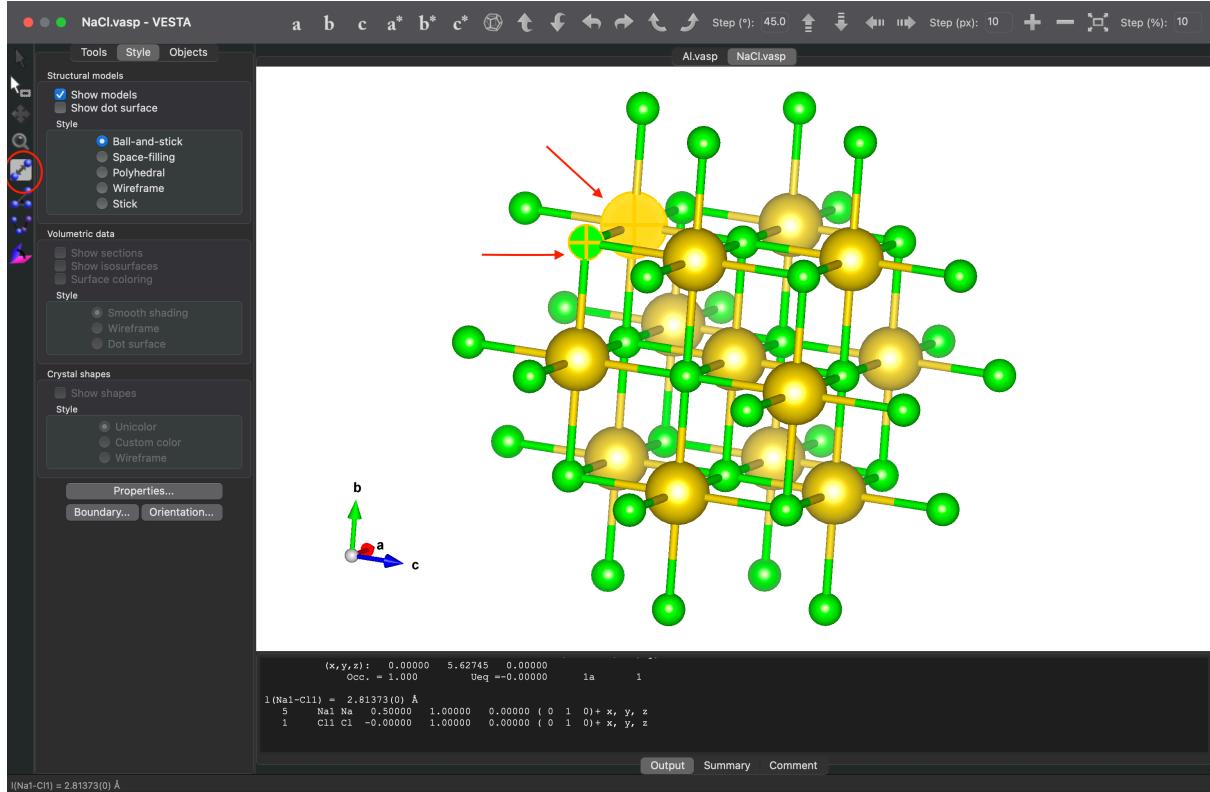


From this, we conclude:

**Inter atomic distance of Al-Al is 2.85658 Å.**

**For NaCl:**

We click on 2 atoms options in the corner (circled below) and then we click on an Na atom and a Cl atom (as pointed by arrows in the below screenshot) to obtain interatomic distance of Na-Cl.

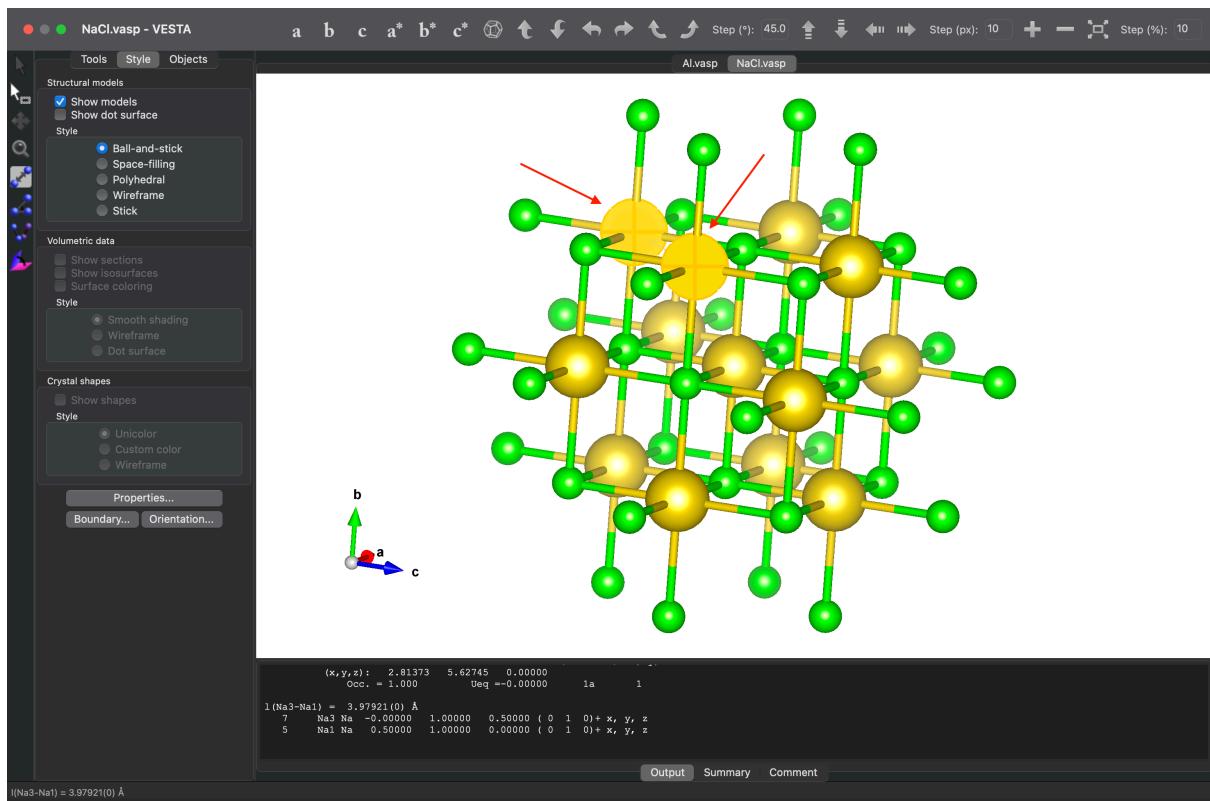


From this, we conclude:

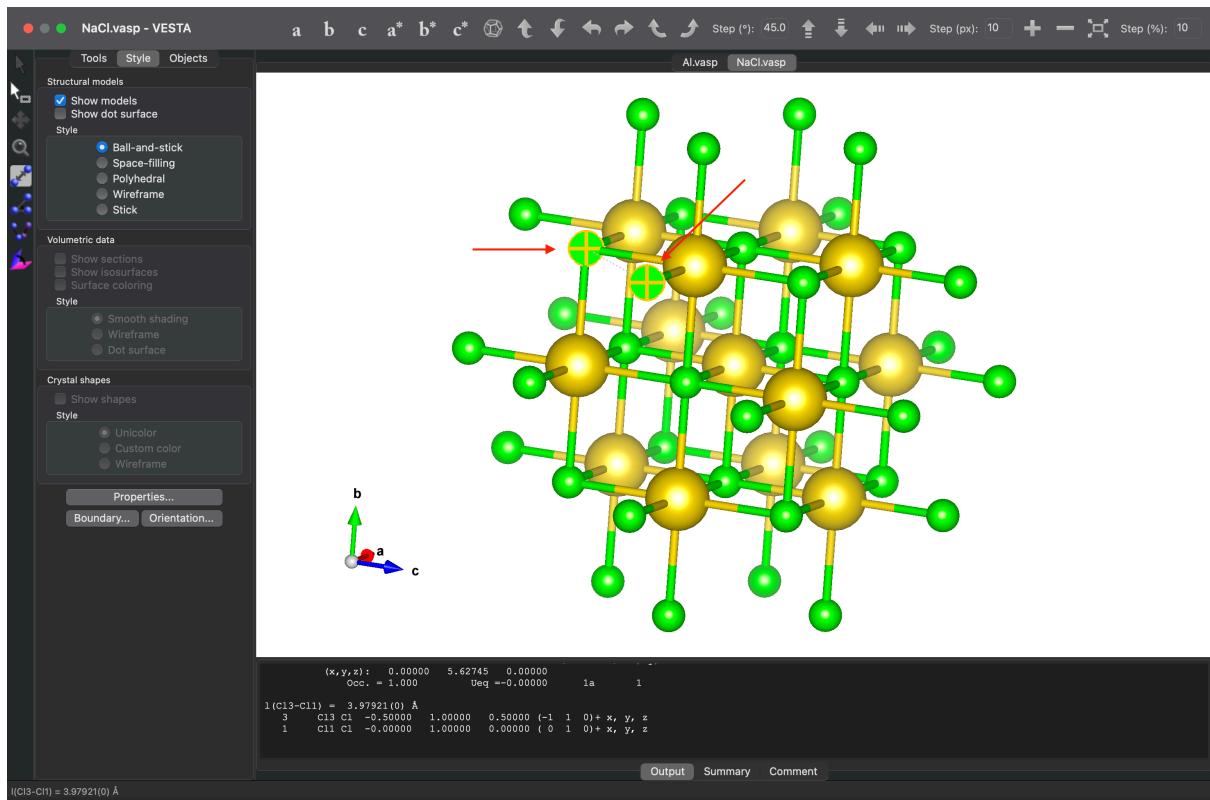
**Inter atomic distance of Na-Cl is 2.81373 Å.**

We repeat the same steps to find inter-atomic distances of Na-Na and Cl-Cl.

(Atoms taken are marked by arrows)



From this, we conclude:  
**Inter atomic distance of Na-Na is 3.979210 Å.**



From this, we conclude:

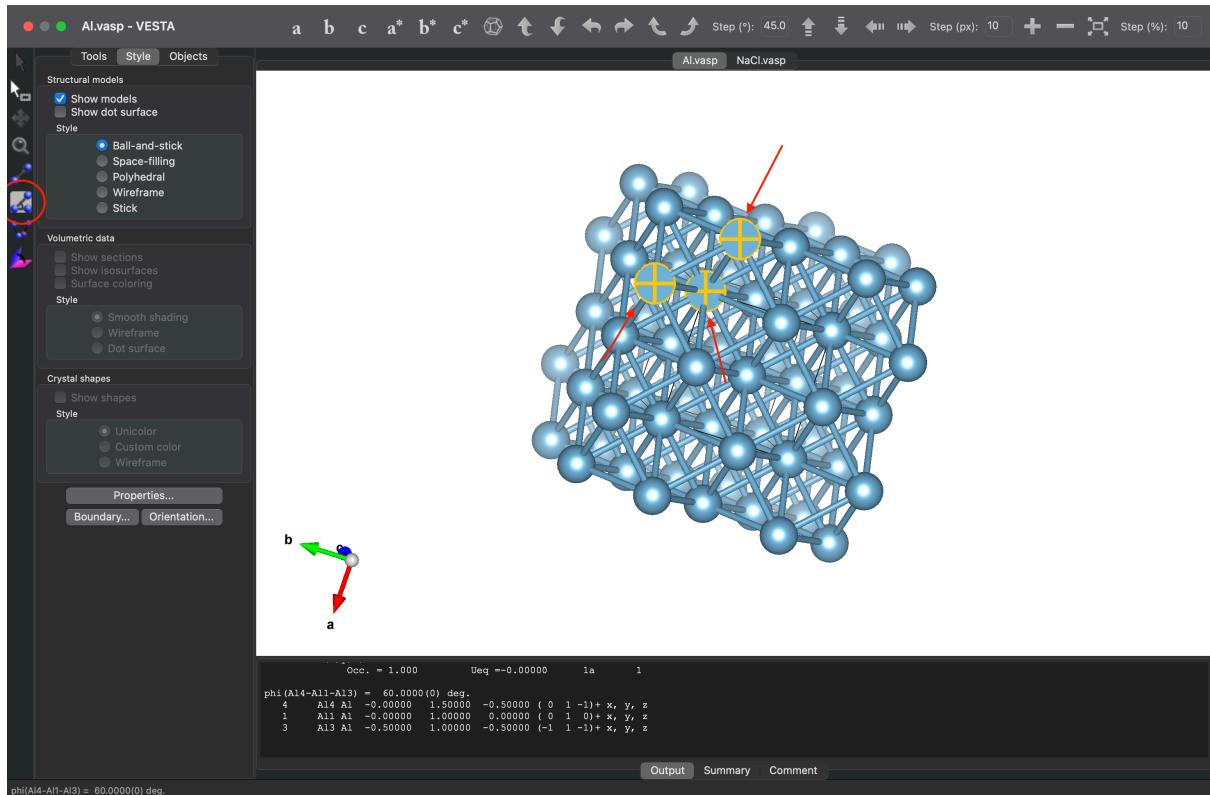
Inter atomic distance of Cl-Cl is 3.979210 Å.

### Answer 3

Now we find the angles between atoms.

We click on 3 atoms options in the corner (circled below) and then we click on 3 atoms (as pointed by arrows in the below screenshot) to obtain angle between them.

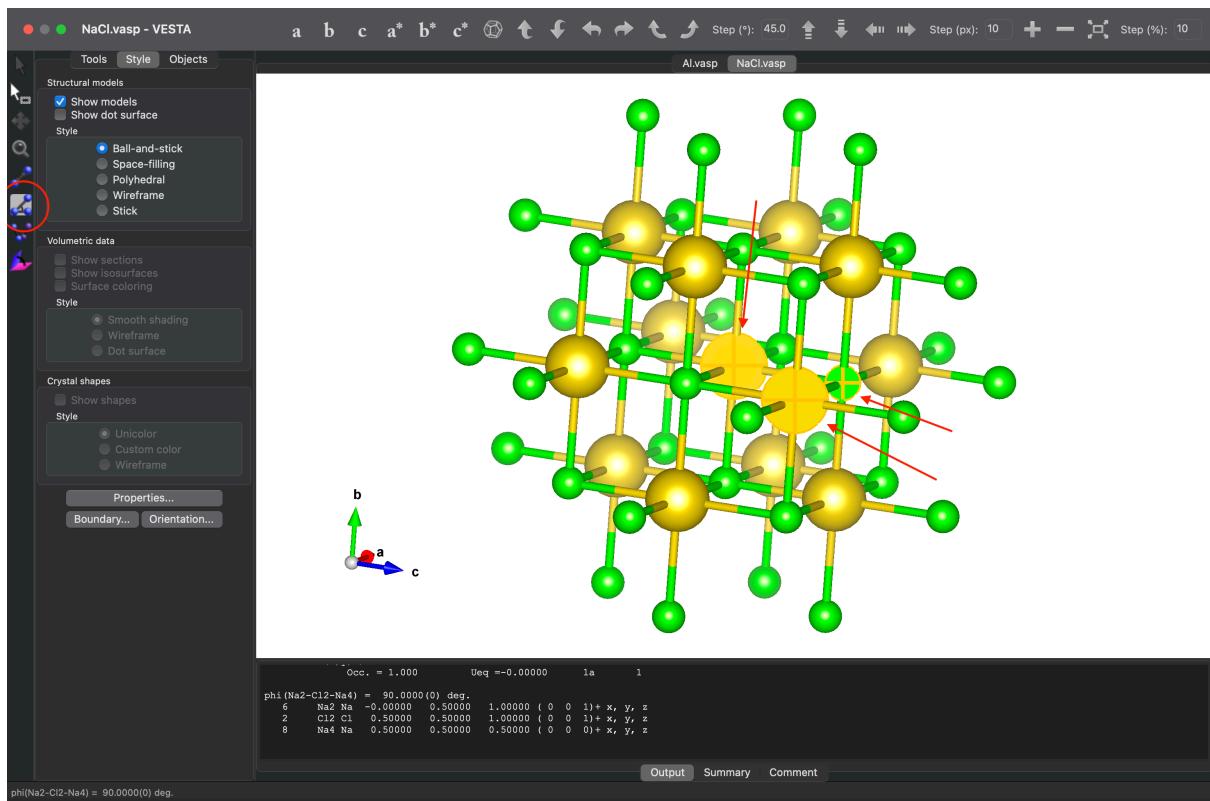
For Al:



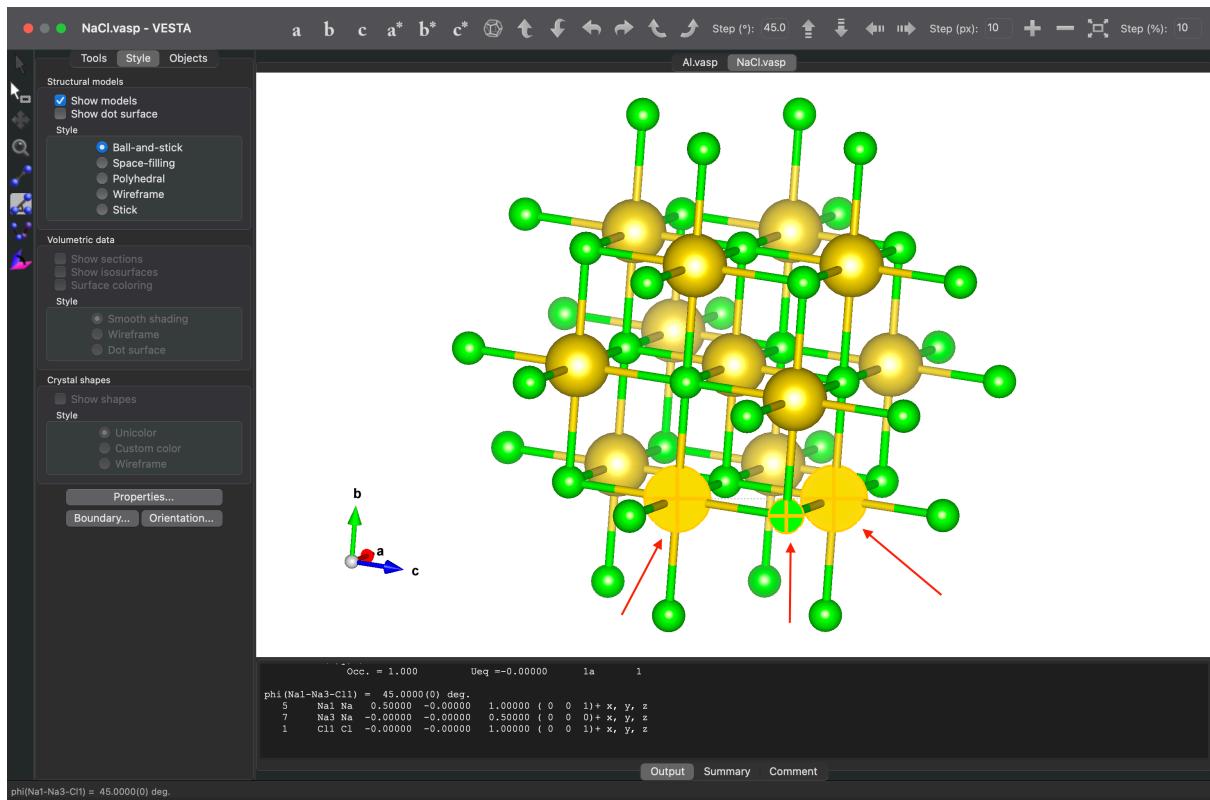
From this, we conclude:

**Al-Al-Al angle is 60°.**

For Na:



From this, we conclude:  
**Na-Cl-Na angle is 90°.**

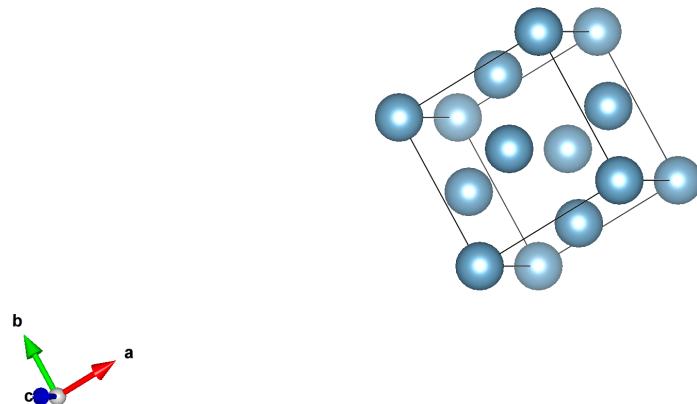
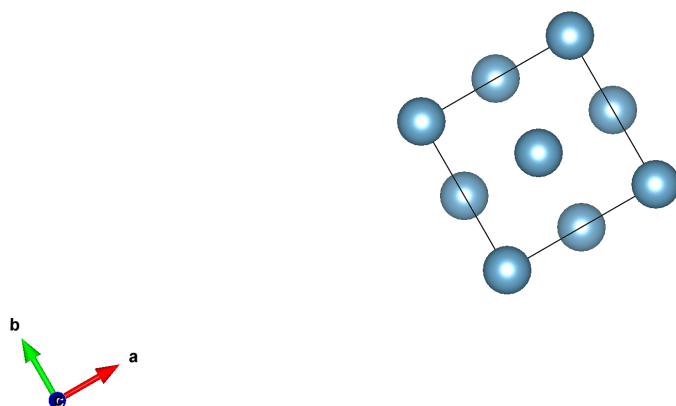


From this, we conclude:

**Na-Na-Cl angle is 45°.**

## Answer 4

To rotate the structure about c-axis by  $30^\circ$  and b- axis by  $20^\circ$ , we follow some steps-



Step-1: Position structure with respect to c-axis.

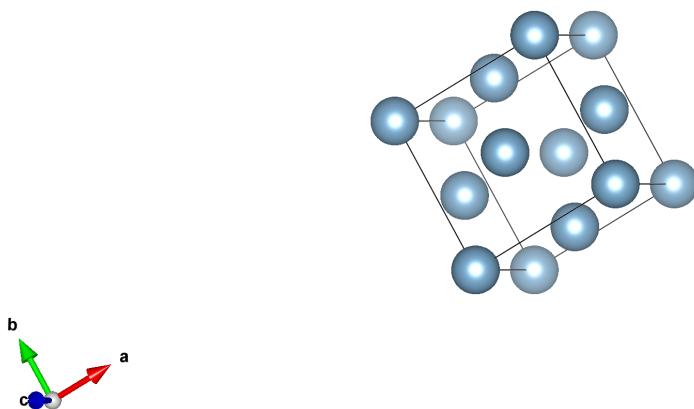
Step-2: Set the angle to  $30^\circ$ .

Step-3: Turn using the marked arrow to rotate about c-axis.

Step-4: Change the angle to  $20^\circ$ .

Step-5: Turn using marked arrow to rotate about b-axis.

We obtain the following picture:



### **Answer 5**

Aluminium (Al) has a face-centred cubic (FCC) structure, where each atom has 12 nearest neighbours.

Focus on the atom at  $(0.5, 0.0, 0.5)$ .

Adjust the coordinates by adding or subtracting in the x, y, and z directions.

The coordinates of the nearest neighbours are:

$(0.5, 0.5, 0.0)$

$(0.5, 0.5, 1.0)$

$(0.0, 0.0, 0.5)$

$(1.0, 0.0, 0.5)$

$(0.5, 0.0, 0.0)$

$(0.5, 0.0, 1.0)$

$(0.0, 0.5, 0.5)$

$(1.0, 0.5, 0.5)$

$(0.5, -0.5, 0.5)$

$(0.5, 0.5, 0.5)$

(0.0, 0.0, 0.0)

(1.0, 0.0, 1.0)