

Assignment 3

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Question 1

1. What is the primitive cell vectors and the transformation matrix (conventional to primitive cell) for Na and Si structures?

For Na which has BCC lattice, transformation matrix is:

$$\begin{bmatrix} 0.5 & 0.5 & -0.5 \\ -0.5 & 0.5 & 0.5 \\ 0.5 & -0.5 & 0.5 \end{bmatrix}$$

Primitive cell vectors are:

$$\begin{bmatrix} 2.145 & 2.145 & -2.145 \\ -2.145 & 2.145 & 2.145 \\ 2.145 & -2.145 & 2.145 \end{bmatrix}$$

For Si, which has FCC lattice, transformation matrix is:

$$\begin{bmatrix} 0.5 & 0 & 0.5 \\ 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0.5 \end{bmatrix}$$

Primitive cell vectors are:

$$\begin{bmatrix} 2.715 & 0 & 2.715 \\ 2.715 & 2.715 & 0 \\ 0 & 2.715 & 2.715 \end{bmatrix}$$

Question 2

1. Which Bravais lattices (P, C/A/B, I, F) does NaCl and CsCl belongs to?

NaCl has an FCC lattice, which is represented as "F".

CsCl has a BCC lattice, which is represented as "I".

2. What are the primitive cell vectors for NaCl and CsCl?

$$\begin{array}{c} \text{NaCl :} \\ \begin{bmatrix} 1.405 & 0 & 1.405 \\ 1.405 & 1.405 & 0 \\ 0 & 1.405 & 1.405 \end{bmatrix} \end{array}$$

$$\begin{array}{c} \text{CsCl:} \\ \begin{bmatrix} 1.785 & 1.785 & -1.785 \\ -1.785 & 1.785 & 1.785 \\ 1.785 & -1.785 & 1.785 \end{bmatrix} \end{array}$$

3. What constitutes the motif for NaCl and CsCl?

In NaCl, motif consists of two types of ions: Na^+ and Cl^- , where each Na^+ is surrounded by 6 chloride ions and each Cl^- ion is surrounded by 6 Na^+ ions. The ratio of sodium ions to chloride ions is 1:1, which reflects the chemical composition of the compound.

In CsCl, motif consists of two types of ions: Cs^+ and Cl^- , where each Cs^+ is surrounded by 8 chloride ions and each Cl^- ion is surrounded by 8 Cs^+ ions. The ratio of caesium ions to chloride ions is 1:1, which reflects the chemical composition of the compound.

4. Visualize NaCl and CsCl in VESTA and find out the bond lengths (Na-Cl, Cs-Cl) and coordination number (first nearest neighbors) to each atom in the respective structure.

Bond length of Na-Cl is 2.81 Å and the coordination number is 6:6.

Bond length of Cs-Cl is 3.57 Å and the coordination number is 8:8.