Al-Mustaqbal University College

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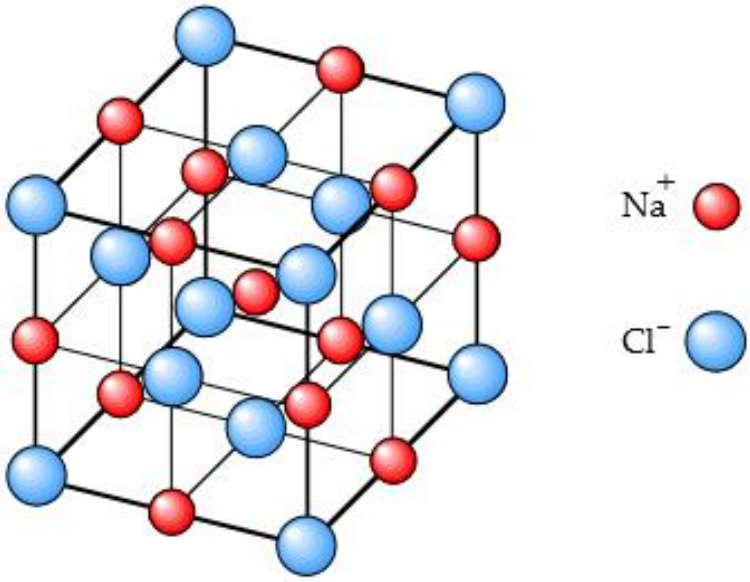
Dr. Aiyah Sabah Noori

THE MOST IMPORTANT CRYSTAL STRUCTURES

- Sodium Chloride Structure Na+Cl
- Cesium Chloride Structure Cs+Cl
- Hexagonal Closed-Packed Structure
- Diamond Structure
- Zinc Blende

Sodium Chloride Structure (Na^+Cl^-)

The Bravais lattice is FCC and the basis comprises one Na atom and one Cl atom separated by half the body diagonal of the unit cell cube.



Examples of this structure include KCl, PbS, MgO, MnO, KBr.

■Sodium chloride also crystallizes in a cubic lattice, but with a different unit cell.

■ Sodium chloride structure consists of equal numbers of sodium and chlorine ions placed at alternate points of a simple cubic lattice.

■ Each ion has six of the other kind of ions as its nearest neighbors.

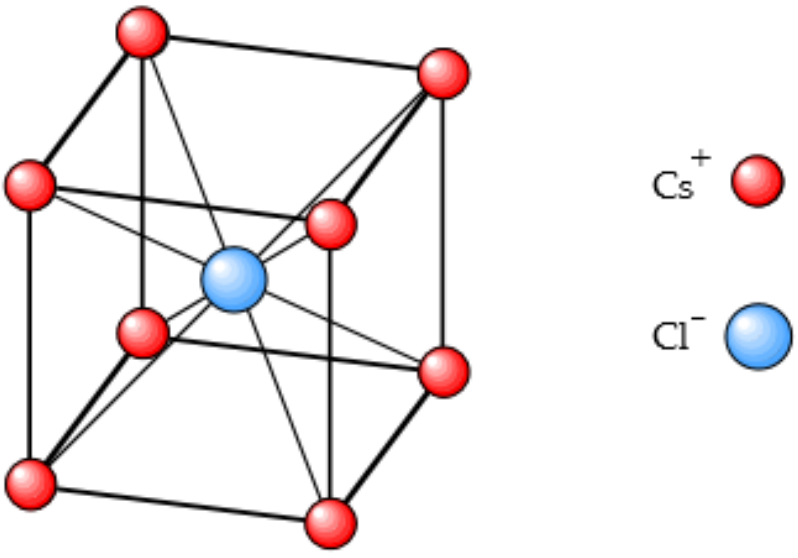
■ This structure can be considered as a face centered-cubic Bravais lattice with a basis consisting of a sodium ion at 0 and a chlorine ion at the center of the conventional cell.

$$a / 2 (\vec{x} + \vec{y} + \vec{z})$$

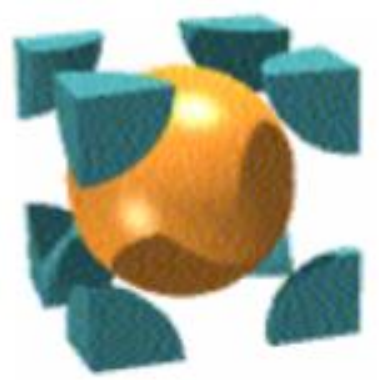
■ The lattice constants are in the order of 4-7 angstroms

Cesium Chloride Structure Cs+Cl-

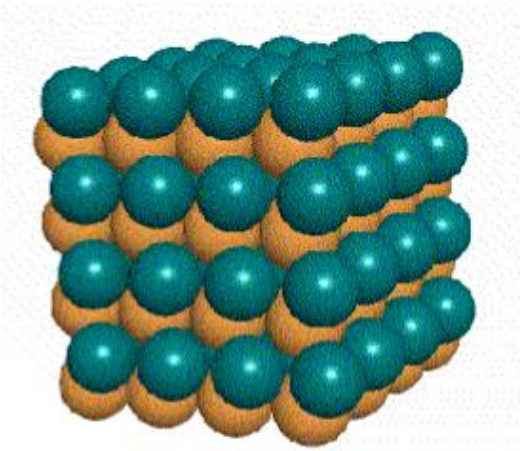
The structure of CsCl is similar to that of NaCl in that it has a basis of two different species of atom, separated by half of the body diagonal of the unit cell cube. The lattice, by comparison, is a simple cubic and so the resultant structure is more easily visualised.



■Cesium chloride crystallizes in a cubic lattice. The unit cell may be depicted as shown. (Cs+ is teal, Cl-is gold)



■Cesium chloride consists of equal numbers of cesium and chlorine ions, placed at the points of a body-centered cubic lattice so that each ion has eight of the other kind as its nearest neighbors.



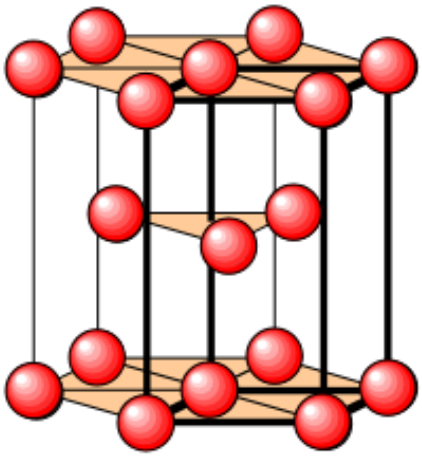
The translational symmetry of this structure is that of the simple cubic Bravais lattice, and is described as a simple cubic lattice with a basis consisting of a cesium ion at the origin 0 and a chlorine ion at the cube center

$$a/2(\vec{x}+\vec{y}+\vec{z})$$

CsBr,CsI crystallize in this structure.The lattice constants are in the order of 4 angstroms.

Hexagonal Close-Packed (HCP)

The HCP structure is based on the simple hexagonal lattice and has a two-atom basis. The second atom of the basis is positioned half way up the cell and so forms another hexagonal layer of close-packed atoms half-way between the top and bottom layers of the unit cell.



There is no way of choosing a primitive unit cell such that the basis contains only one atom.

The primitive cell usually drawn for the HCP crystal structure is shown in bold.

It is conventional to refer to the lattice constant (interatomic separation) in the plane of hexagons as a and that in the perpendicular, or axial, direction as c (where the latter is the height of the unit cell, and not the separation of adjacent layers of hexagonal planes).