

CHEM 281 LAB: SOLID STATE STRUCTURE OF IONIC COMPOUNDS

Crystal lattice

The structures of ionic compounds are crystalline (**crystal lattice**) with regular arrangement of spherical ions in one of the above ionic lattice types.

Coordination number (CN): The number of nearest neighboring metal atoms (four, six, eight to twelve) which each atom is surrounded in the crystal lattice.

Crystal Packing

Unit cell:

Wallpaper has regular repeating design that extends from one edge to the other. Crystals have a similar repeating unit called unit cell that extends in 3-D from one edge of the solid to the other. Unit cell has, three edges, a , b , c and there angles, α , β , γ .

Cubic crystal system ($a = b = c$ and there angles, $\alpha = \beta = \gamma = 90^\circ$).

For the cubic crystals, there are four basic unit cells.

Ionic crystals are found among all 7 crystal systems with specific unit cells.

Crystal Systems	Unit cell Constraints	Fourteen Bravis Lattices
1. Cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	P, I, F (3)
2. Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, I (2)
3. Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, C, I, F (4)
4. Trigonal	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	R/P (1)
5. Monoclinic	$a \neq b \neq c, \beta \neq \alpha = \gamma = 90^\circ$	P, C (2)
6. Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	P (1)
7. Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	P (1)

Part of the Atom in the Unit Cell

The part of the atom in the unit cell is counted according to the following locations

corner = 1/8	edge = 1/4	face = 1/2	body = 1
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Number of Atoms in the Cubic Unit Cell

SC = 1 (8 corners)	FCC = 4 (8 corners, 6 faces)
BCC = 2 (8 corners, 1 body)	Other unit cells?

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Number of Atoms in the Cubic Unit Cell

SC = 1 (8 corners)	FCC = 4 (8 corners, 6 faces)
BCC = 2 (8 corners, 1 body)	Other unit cells?

Interstitial Sites and Holes: The remaining unoccupied space in any host ion packing scheme of host unit cell is found as void space. This void space occurs between the spheres and gives rise to so-called holes. These holes could be filled with a smaller ion to give various ionic lattices.

Holes: The easiest way to determine the type of hole is by looking at how the atoms surround the ion in the hole.

Hexagonal (HCP) and cubic close packing (CCP-FCC):

Octahedral hole: Space in an octahedral hole is surrounded by six other metals oriented octahedrally.

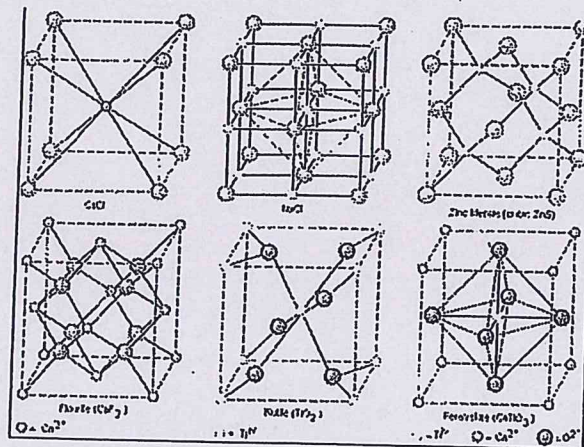
Octahedral hole: Space in an tetrahedral hole is surrounded by four other metals oriented tetrahedrally.

Bravais Lattice: A Bravais Lattice is a three dimensional lattice. A Bravais Lattice tiles space without any gaps or holes. There are 14 ways in which seven crystal systems this can be accomplished. Basic types of Bravais unit cells P (primitive), I (body centered), F (face centered), C (centered on c axis) and R/P (rhombohedral/primitive)

Seven Crystal Systems

Ionic crystal structures:

Crystal structure
Cesium chloride structure:
Rock Salt Structure:
Fluorite Structure:
Sphalrite Structure:
Wurtzite:
Rutile:
Pervoskite structure:



CHEM 281 LAB #5 Activity (Lattices of ionic compounds):

1. Using the model kit build the following lattice types. Give the page number and card number and draw the structures:

a) Cesium chloride structure: (CsCl)

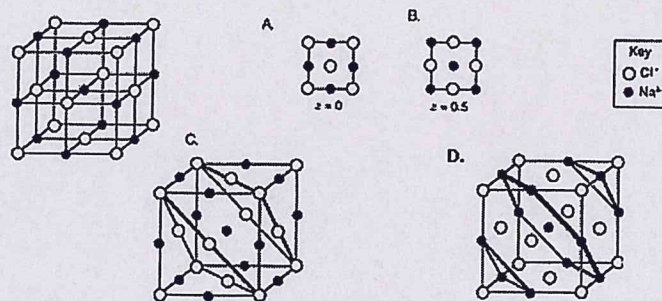
b) Rock Salt Structure: (NaCl)

c) Fluorite Structure: (CaF₂)

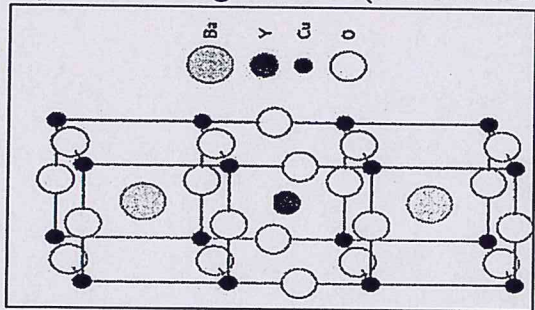
d) Sphalrite Structure: (ZnS)

e) Wurtzite: (ZnS)

5. Identify the Miller indices of the planes in crystalline lattices of rock salt structure:



6. Give the number of ions per unit cell of the perovskite structure of superconducting material (1-2-3:Y-Ba-Cu) given below:



7. Complete the table:

	Crystal structure	a) Unit Cell	b)M(CN)	c) M Hole	X(CN)	c) X Hole	Formula, MX
1	Cesium chloride structure:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Cs}^+ =$		$\text{Cl}^- =$		CsCl
2	Rock Salt Structure:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Na}^+ =$		$\text{Cl}^- =$		NaCl
3	Fluorite Structure:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Ca}^{2+} =$		$\text{F}^- =$		CaF_2
4	Antifluorite	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{K}^+ =$		$\text{O}^{2-} =$		K_2O
5	Sphalrite Structure:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Zn}^{2+} =$		$\text{S}^{2-} =$		ZnS
6	Wurtzite:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Zn}^{2+} =$		$\text{S}^{2-} =$		ZnS
7	Rutile:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Ti}^{4+} =$		$\text{O}^{2-} =$		TiO_2
8	Pervoskite structure:	$a = b = c,$ $\alpha = \beta = \gamma = 90^\circ$	$\text{Ca}^{2+} =$ $\text{Ti}^{4+} =$	$=$ $=$	$\text{O}^{2-} =$		CaTiO_3