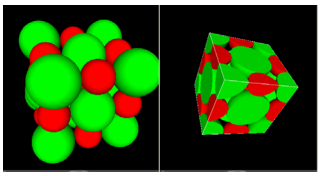
3D Images of Crystal Structures

Student Handout

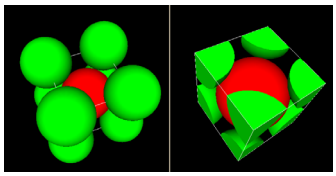
Purpose: To visualise structures of ionic crystals using three-dimensional images.

Introduction

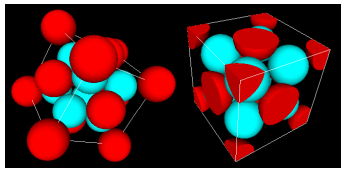
Computer program can be used effectively to help us visualise the structures of crystals. In this activity you will employ VRML (Virtual Reality Modeling Language) to display three-dimensional images of the structures of some ionic crystals namely, sodium chloride, caesium chloride and calcium fluoride (fluorite). VRML images can be manipulated as if one is examining a real model, i.e. one can view the entire structure at all angles.



sodium chloride



caesium chloride



calcium fluoride

Tasks

1. Start a web browser equipped with VRML e.g. Cortona VRML Client available at http://www.parallelgraphics.com/products/cortona/download/iexplore.

2. Examine the VRML images of the 3 ionic crystals by entering the following URLs:
   - http://www.chm.davidson.edu/ChemistryApplets/Crystals/IonicSolids/NaCl.html
   - http://www.chm.davidson.edu/ChemistryApplets/Crystals/IonicSolids/CsCl.html
   - http://www.chm.davidson.edu/ChemistryApplets/Crystals/IonicSolids/Fluorite.html

3. Complete the following table.

	Coordination No.		**Lattice structure for larger ions**	**No. of cations in a unit cell**	**No. of anions in a unit cell**
	cation	**anion**			
NaCl(s)					
CsCl(s)					
CaF_2(s)					

Discussion Questions

1. What is the relationship between the relative size of cation and anion and the coordination numbers of ions?

2. What is the relationship between the empirical formula and the number of ions in a unit cell for an ionic solid?