INVESTIGATION 2

PURPOSE

To construct a unit cell of the extended three-dimensional crystalline structure of magnetite (Fe_3O_4) and to verify this empirical formula based on this structure.

INTRODUCTION

The crystalline structure of magnetite consists of a repeating arrangement of oxide ions in what is referred to as cubic close-packed (recall the pattern of spikes that you observed in Investigation 1). Fe(II) and Fe(III) ions are distributed into some of the spaces (holes) that are created between the oxide ions. These holes do not provide the same chemical environment for all the iron ions and it is this difference in environment that results in the magnetic properties of the compound.

PROCEDURE

Following the directions as provided by your instructor, use the Solid State Model Kit to construct the layer sequences for:

Team A: the conventional cubic unit cell.

Team B: the tetragonal unit cell.

Alternatively your instructor may provide you with a completed model of one or both of these unit cells.

FOLLOW-UP QUESTIONS

1. For each of the structures complete the table below, indicating HOW MANY COLORLESS SPHERES LIE WITH THEIR CENTERS AT THE _____OF THE UNIT CELL.

STRUCTURE	CORNERS	EDGES	FACES	INSIDE
CUBIC UNIT CELL (A)				
TETRAGONAL UNIT CELL (B)				

2. For each of the structures complete the table below, indicating HOW MANY PINK SPHERES LIE WITH THEIR CENTERS AT THE _____ OF THE UNIT CELL.

STRUCTURE	CORNERS	EDGES	FACES	INSIDE
CUBIC UNIT CELL (A)				
TETRAGONAL UNIT CELL (B)				

3. For each of the structures complete the table below, indicating HOW MANY BLUE AND RED SPHERES LIE WITH THEIR CENTERS AT THE _____ OF THE UNIT CELL.

STRUCTURE	CORNERS	EDGES	FACES	INSIDE
CUBIC UNIT CELL (A)				
TETRAGONAL UNIT CELL (B)				

Note that the colorless spheres are oxides, small pink spheres are ferric ions in tetrahedral holes, and blue and red are ferrous and ferric ions in octahedral holes.

4. Convince yourself that each of the corner atoms is shared with seven other unit cells; that the edge atoms are shared with three other unit cells; and that the face atoms are shared with one other unit cell. Remember that these structures extend in all three dimensions indefinitely. It may be helpful to stack books or CD cases together to help to visualize the relationships stated above. Given that the stated information is correct, then only part of the spheres occupying each site belong to the unit cell under consideration, i.e., only 1/8 of the corner spheres, 1/4 of the edge spheres, and 1/2 of the face spheres belong to a given unit cell. Those spheres lying totally inside the cell of course belong only to that cell. Using the information above, complete the tables below.

COLORLESS	CUBIC UNIT CELL (A)	TETRAGONAL UNIT CELL (B)
__CORNERS X 1/8 =		
__EDGES X 1/4 =		
__FACES X 1/2 =		
__INSIDE X 1 =		
__ TOTAL IN CELL =		

PINK	CUBIC UNIT CELL (A)	TETRAGONAL UNIT CELL (B)
__CORNERS X 1/8 =		
__EDGES X 1/4 =		
__FACES X 1/2 =		
__INSIDE X 1 =		
__ TOTAL IN CELL =		

RED AND BLUE	CUBIC UNIT CELL (A)	TETRAGONAL UNIT CELL (B)
__CORNERS X 1/8 =		
__EDGES X 1/4 =		
__FACES X 1/2 =		
__INSIDE X 1 =		
__ TOTAL IN CELL =		

5. The ratio between the sum of the Fe (II) and Fe (III) relative to the O^{-2} from the tables above is then:

    a. For the cubic unit cell Fe__O__. And the simplest ratio is Fe__O__.

    b. For the tetragonal cell Fe__O__. And the simplest ratio is Fe__O__.