INVESTIGATION 2
Notes for the Instructor

PURPOSE

To have students become familiar with the structure of magnetite and based upon this structure to determine the empirical formula for the compound. It is also possible to discuss why this substance is magnetic from these structural considerations, but this involves a discussion of octahedral and tetrahedral holes. Noting that the iron ions are occupying different types of holes in the oxide ion structure that are not chemically equivalent is worthwhile.

METHOD

The students are provided with a model of the conventional cubic unit cell and asked to construct a model of the tetragonal unit cell that is considerably easier to build. Both models can be constructed using the ICE Solid State Model Kit, but it should be noted that the cubic cell requires three (3) kits and the tetragonal model two (2) kits in order to obtain the necessary number of larger oxide spheres. Construction directions are included in the Appendix for this module. Appendix A in the Memory Metal Module of this manual contains a detailed discussion of unit cells. Be sure to emphasize that some atoms in a structure are shared by more than one unit cell and the fraction belonging to a given cell must be determined.

ANSWERS TO THE 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)	**8**	**12**	**30**	**13**
TETRAGONAL UNIT CELL (B)	**8**	**12**	**6**	**9**

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)	**0**	**0**	**0**	**8**
TETRAGONAL UNIT CELL (B)	**0**	**0**	**4**	**2**

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)	**0**	**12**	**12**	**7**
TETRAGONAL UNIT CELL (B)	**0**	**4**	**8**	**3**

4. Convince yourself that each of the corner atoms is shared with seven <u>other</u> unit cells; that the edge atoms are shared with three <u>other</u> 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 =	**1**	**1**
__EDGES X 1/4 =	**3**	**3**
__FACES X 1/2 =	**15**	**3**
__INSIDE X 1 =	**13**	**9**
__ TOTAL IN CELL =	**32**	**16**

PINK	CUBIC UNIT CELL (A)	TETRAGONAL UNIT CELL (B)
__CORNERS X 1/8 =	0	0
__EDGES X 1/4 =	0	0
__FACES X 1/2 =	0	2
__INSIDE X 1 =	8	2
__ TOTAL IN CELL =	8	4

RED AND BLUE	CUBIC UNIT CELL (A)	TETRAGONAL UNIT CELL (B)
__CORNERS X 1/8 =	0	0
__EDGES X 1/4 =	3	1
__FACES X 1/2 =	6	4
__INSIDE X 1 =	7	3
__ TOTAL IN CELL =	16	8

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 $Fe_{24}O_{32}$. And the simplest ratio is Fe_3O_4.

   b. For the tetragonal cell $Fe_{12}O_{16}$. And the simplest ratio is Fe_3O_4.