

## Take Home Exam Instructions.

The spreadsheet is located at <http://ruby.colorado.edu/~smyth/G3010/Exam209.xls>

This take-home exam is intended to be done on Excel. There are two problems on separate worksheets.

### Problem 1. Mineral Stoichiometry and Density

The first work sheet contains chemical compositions in cations per formula unit for seven enstatites and polymorphs of enstatite.

For each sample there are also the unit cell parameters,  $a$ ,  $b$ ,  $c$  (in Å) angles,  $\alpha$ ,  $\beta$ , and  $\gamma$  (in degrees). (Remember that Excel assumes angles are in radians!!) (You can convert a value in degrees in cell c10 to radians with the 'RADIANS' function [=RADIANS(c10)] and back with the 'DEGREES' function)

- A. Row 31 Calculate the formula weight from the numbers of oxygens and cations. (i.e. six (or 12) times the atomic weight of oxygen (15.9994), plus the number of Si cations times the atomic weight of Si (28.086) and so on through all of the cations.) Alternatively, you can also calculate this from the oxides.
- B. Rows 18-26: recalculate the compositions to weight percent oxides normalized to 100 percent.
- C. Row 42: Calculate the unit cell volume from the unit cell parameters ( $V = a*b*c*\sin \beta$ ) or ( $V = a*b*c*\sin 120^\circ$ ) for the trigonal one.
- D. Row 45: Calculate the density in  $\text{g/cm}^3$ . Remember that densities are going to be somewhere between 2.5 and 6.0.
- E. You're done when you have done this for all of the analyses. (Remember how to control the iteration of column and row numbers using the \$ sign.)
- F. The least dense phase will be the one stable to highest temperature at low pressure, and the densest phase will be the one stable to highest pressures. Which are they? (write your answer in a cell below the calculations.)

Problem II. X-ray diffraction calculation of  $d$  and  $2\theta$ .

Given are the unit cell parameters  $a$ ,  $b$ , and  $c$  for the enstatite polymorphs with orthogonal structures.

A. Row 10: Calculate the unit cell volume of each.

B. In the space indicated, calculate  $d$  and  $2\theta$  in degrees for  $\text{CuK}\alpha$  ( $\lambda = 1.5405\text{\AA}$ ) for the following reflections:

(200), (020), (002), (040), (042), (220), (113), (222), (331), and (224).

Again, remember that Excel assumes angles are in radians.

The  $h$ ,  $k$ , and  $l$  values are provided in columns B, C, and D for your convenience.

You do not have to use these, but can embed the values directly in the formulas if you choose. A reflection may not be accessible with this radiation if its  $d$ -spacing is too small.

Listed below are the molecular weights of the oxides and atomic weights of the elements that you will need.

<u>Oxide</u>	<u>MolWtOxide</u>	<u>Element</u>	<u>AtomicWeight</u>
$\text{SiO}_2$	60.086	Si	28.087
$\text{TiO}_2$	79.8988	Ti	47.90
$\text{Al}_2\text{O}_3$	101.963	Al	26.9824
$\text{Cr}_2\text{O}_3$	151.9974	Cr	51.9996
$\text{Fe}_2\text{O}_3$	159.6922	Fe	55.847
FeO	71.8464	Fe	55.847
MgO	40.3114	Mg	24.312
MnO	70.9374	Mn	54.938
CaO	55.96	Ca	39.961
$\text{Na}_2\text{O}$	61.980	Na	22.9809
$\text{K}_2\text{O}$	94.2032	K	39.102
$\text{H}_2\text{O}$	18.0153	H	1.008
		O	15.9994