Quiz 1
ChE386k

I certify that I have not received any help with this examination. I did not consult with anyone and it represents my own individual effort. I am fully aware of the consequences of dishonesty when taking examinations. The use of all books and notes is encouraged.

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Signature

1. Show by matrix development that a point group denoted by $\bar{6}$ is actually the same as the point group $\frac{3}{\mathrm{m}}$. You can use the $\bar{6}$, 3 and m matrices for from the Burns and Glazer handout as starting points. Assume they are either parallel or perpendicular to the c-axis.

2. Evaluate the metric tensor for the mineral augite which is monoclinic with a = 9.73Å, b = 8.91Å, c = 5.29Å, β = 105.83°. Determine the angle between [101] and [121] and also the interplanar angle (101):(121).

3. Th_2Fe_{17} has been reported to be monoclinic with a = 9.68 Å, b = 8.56 Å, c = 6.46 Å, β = 99.3 °, space group C2/m. The Th atoms are loca ted in position 4i: ±(x , 0 , z) + (0, 0, 0 ; ½, ½, 0), with x = 0.167, z = 0.333. (This you might remember was our class example). Find the dimensions and volume of a new unit cell in using the following alternate transformation matrix

$$T = \begin{bmatrix} 0 & 1 & 0 \\ 1/2 & -1/2 & 1 \\ 1 & 0 & -1 \end{bmatrix}$$

   Also find the locations of all the Th atoms in the new cell.

4. In the tetragonal system there are two accepted Bravais lattices, P and I. Show why the others (A, B, C, F) either cannot exist or how they can be converted to another centering.

5. Examine the three interactive figures listed in the following URL's:

   a. http://capsicum.me.utexas.edu/ChE386K/html/5a.html
   b. http://capsicum.me.utexas.edu/ChE386K/html/5b.html
   c. http://capsicum.me.utexas.edu/ChE386K/html/5c.html

   For each figure assign a point group giving both the Schoenflies and International notations.

6. A crystal with $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90°$ has atoms of the same kind in the following positions.

0.29 0.04 0.22	−0.29 −0.04 −0.22
0.79 0.46 0.28	0.21 0.54 0.72
−0.29 0.54 −0.22	0.29 0.46 0.22
0.21 −0.04 0.72	0.79 0.04 0.28

   Identify the space group. A copy of the International Tables Vol. A is located in ETC 9.120 and will be helpful in determining the proper group.

7. The structure of Cuprite, Cu_2O, was among the first to be determined. From the unit cell parameter (a = 4.26 Å), crystal system (cubic), and the density (ρ = 6.1 g cm^{-3}) determine the space group or groups in which Cuprite could possibly crystallize and the crystal structure (atomic positions) of Cuprite. Hint: Once you find Z, use the International Tables to locate cubic groups that have the correct Wycoff positions.

8. Find the type and position of the conventional symmetry element that is involved in the following transformations:
   a. x, y, z → ½-x, ½-y, ½+z.
   b. ¼+x, ¼+y, ¼-z → ½+x, y, ½+z.

9. Identify the plane group of each of the attached Escher images.

   http://capsicum.me.utexas.edu/ChE386K/Images/Escher/escher3pmm.jpg

   http://capsicum.me.utexas.edu/ChE386K/Images/Escher/10.jpg