University of Windsor
Chemistry and Biochemistry
Chemistry 59-553, Winter Term 2017

Assignment 2

Due: Tuesday, March 14

Question #1

1. A study of crystalline sample of molybdenum hexacarbonyl, $Mo(CO)_6$, showed to be molecular and to crystallize in the space group *Pnma* (No. 62). Discuss the possible locations and the symmetries of the molecules if there were: (i) 8 formula units per cell (ii) 4 formula units per cell (iii) 2 formula units per cell.

2. Me_3NHCl crystallizes in a monoclinic centrosymmetric space group, with a = 6.09, b = 7.03, c = 7.03 Å, β = 95.73 and Z = 2. The only limiting condition is *0k0* k = 2n. What is the space group? Comment on the probable positions of (a) Cl (b) C (c) N (d) H atoms.

3. Calcium (Ca) crystallizes in a cubic space group with a = 5.56 Å and we observe a reflection corresponding to a d-spacing of 1.85 Å. What families of planes (*hkl*) could contribute to this reflection?

4. The default setting for the analysis software on the powder X-ray diffractometer lists peaks by their d-spacing instead of by their diffraction angle. Explain why d-spacing is a more useful default using a plane from Ca as an example.

5. For a primitive cubic lattice composed of only one type of atom:
   (a) What are the positions of each of the atoms in the unit cell (using the standard setting with positions in fractional coordinates)?
   (b) What fraction of each atom is contained within the unit cell?
   (c) Using the information from (a) and (b), calculate the value of a general structure factor, *F(hkl)*, for this structure in terms of the atomic scattering factor f_{atom}. Remember that: $\exp(\theta i) = \cos(\theta) + i\sin(\theta)$.
   (d) Comment on the importance/utility of your result in part (c).
   (e) Calculate the general structure factor for a face-centered cubic lattice.

6. Tantalum (Ta) crystallizes in a cubic space group with a = 3.3013 Å. Reflections for the following families of planes are observed:
(*110*), (*200*), (*211*), (*220*), (*310*), (*222*), (*321*), (*400*), (*411*), (*420*), (*332*), (*431*)

   (a) What type of cubic lattice do these data imply?
   (b) Which reflection (*110*) or (*200*) should be more intense? (note: just draw one representative plane for each (*hkl*) to help you make your decision)
   (c) Determine the structure factors for the (*110*) and (*200*) planes. Note that the atomic scattering

factors in units of electrons are: $f_{Ta}(110) = 57$; $f_{Ta}(200) = 50$.
(d) Determine the structure factor for the (*111*) plane if $f_{Ta}(111) = 54$. Draw an Argand diagram to illustrate your result.

7. Determine the final magnitude |F| and phase α obtained by the addition of the following atomic scattering factors (or waves) and draw an approximate Argand diagram to illustrate the process:

f_j	$\phi_j(^o)$
33	45
9	120
7	140
7	-10
7	180
6	-90
1	-110
1	-100
1	-105

Comment briefly on the phase you have calculated.