

## Assignment 2

Due: Wednesday, November 14

### Question #1

1. A study of crystalline sample of ammonium dihydrogen phosphate  $\text{NH}_4\text{H}_2\text{PO}_4$ , showed to be ionic and to crystallize in the space group  $Pbam$  (No. 55). Discuss the possible locations and the symmetries of the ions if there were: (i) 8 formula units per cell (ii) 4 formula units per cell (iii) 2 formula units per cell.

2.  $\text{Me}_3\text{NHCl}$  crystallizes in a monoclinic centrosymmetric space group, with  $a = 6.09$ ,  $b = 7.03$ ,  $c = 7.03$  Å,  $\beta = 95.73$  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:

- What are the positions of each of the atoms in the unit cell (using the standard setting with positions in fractional coordinates)?
- What fraction of each atom is contained within the unit cell?
- 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:  $\exp(i\theta) = \cos(\theta) + i\sin(\theta)$ .
- Comment on the importance/utility of your result in part (c).

6. Tungsten (W) crystallizes in a cubic space group with  $a = 3.1648$  Å. Reflections for the following families of planes are observed:

$(110)$ ,  $(200)$ ,  $(211)$ ,  $(220)$ ,  $(310)$ ,  $(222)$ ,  $(321)$ ,  $(400)$ ,  $(411)$ ,  $(420)$ ,  $(332)$ ,  $(431)$

- What type of cubic lattice do these data imply?
- Which reflection  $(110)$  or  $(200)$  should be more intense? (note: just draw one representative plane for each  $(hkl)$  to help you make your decision)
- Determine the structure factors for the  $(110)$  and  $(200)$  planes. Note that the atomic scattering factors in units of electrons are:  $f_W(110) = 58$ ;  $f_W(200) = 51$ .
- Determine the structure factor for the  $(111)$  plane if  $f_W(111) = 55$ . Draw an Argand diagram to

illustrate your result.

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

$f_j$	$\phi_j(^{\circ})$
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.