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

Assignment 1

Due: Feb. 16, 2017

Question #1

1. Consider an atom at fractional coordinates *x,y,z*. When operated on by the following symmetry elements, what are the fractional coordinates of the symmetry related atoms?

(a) 2 along b (b) -4 along c (c) m perpendicular to b
(d) -1 centered at (000) (e) 4_3 along c (f) b glide plane perpendicular to a
(g) 2_1 along a (h) n glide perpendicular to b.

2. The compound $[Cp^*_3Pb_2][B(C_6F_5)_4]$ (MW = 1499.09) crystallizes in the space group *C2/c* with a = 22.545(5) Å, b = 14.773(5) Å, c = 17.087(5) Å, β = 114.911(5), Z = 4. Calculate the density of this salt and indicate if there are any other conclusions you can draw about the structure.

3. The ionic compound $[(C_{11}H_{20}N_2)_2P][Cl]\cdot n(C_7H_8)$ crystallizes in the space group *P-1* with a = 10.134(3), b = 12.243(3), c = 13.037(3) Å, α = 103.358(4), β = 99.906(5), γ = 100.772(4). Given that the measured density is 1.145 g cm^{-3} what conclusions can you draw about the structure.

4. (a) Using diagrams explain why a *B* centered cell is not a distinct monoclinic cell.
(b) Using diagrams explain why an *I* centered monoclinic cell is equivalent to a C centered monoclinic cell.

5. Use diagrams to show and explain the relationship between $P2_1/n$ and $P2_1/c$.

6. For a primitive unit cell from each of the 7 crystal systems:
(a) identify the point group of the unit cell (treat it as an isolated box)
(b) use drawing(s) to show the location of the symmetry elements of the cell (again for a box)

7. What systematic absences are expected if the following symmetry elements are present?
(a) *I* centered lattice
(b) c glide perpendicular to a
(c) mirror perpendicular to b
(d) 2_1 along c

8. Explain in detail, the information implied by the space group symbol *Fd-3m*.

9. Identify the possible space groups implied by the following information. Also indicate if the space group is uniquely determined (see section 3.1 of the *International Tables for Crystallography Volume A*).

(a) primitive monoclinic lattice, for *h0l, h00 ,00l* present only for l = 2n.
(b) primitive orthorhombic lattice, for *00l,* present only for l = 2n.
(c) C centered orthorhombic lattice, no other absences observed.
(d) F centered orthorhombic lattice, no other absences observed.
(e) centrosymmetric C centered monoclinic lattice, no other absences observed.

10. At low temperatures, methane crystallizes in a cubic cell with a = 5.89 Å. Assuming that the density of the solid methane is similar to that of liquid methane (d = 0.466 g cm^{-3}), determine whether methane adopts a primitive, body-centered or face-centered structure.

11. What are the Miller indices for planes with the following unit cell intercepts:
(a) ∞ a, 1/3 b, c
(b) a, b, c
(c) -1/4 a, 1/2 b, 3 c
(d) 1/6 a, 1/3 b, 3/4 c
(e) 2/3 a, ∞ b, 1/6 c

12. Draw orthorhombic unit cells with dimensions of a = 4 Å, b = 7 Å and c = 9 Å. Draw the following planes (make sure to label them): (100), (010), (001), (-210), (011), (111), (042), (222), (301), (024)

13. Determine the d-spacing for each family of planes in question 12.

14. Using MoKα X-rays, what would be diffraction angle for each family of planes in question 12.