**X-ray Crystallography 12650 - CHM 69600-006**

***Homework Assignment 3:***

***Space Groups and Symmetry***

*Questions are 5, 10 or 15 points, as indicated. Due date: One week after assignment.*

1) To which point groups do the following space groups belong? *P*$\overline{1}$, *P*21/c, *P*212121, *P*mmm, *C*mca, *I*$\overline{4}$, *P*3121, *R*$\overline{3}$m, *P*63/mmc, *P*a$\overline{3}$. Give both the Herman-Maugin as well as the Schoenfliess symbols for the point groups.

10 pts

2) List some of the important differences between space groups P21/m, P21 and Pm; and between space groups Pm$\overline{3}$ and P$\overline{3}$m1

5pts

3) A space group has a three-fold axis, another a four-fold screw axis as one of its symmetry elements. What Crystal Systems can each belong to?

5 pts

4) Which of the following space groups contain translational symmetry of one kind or another within their unit cells?

*P*$\overline{1}$, *P*2, *P*21/c, *P*212121, *C*mca, *I*$\overline{4}$, *P*$\overline{3}$, *R*$\overline{3}$m, *P*63/mmc, *P*a$\overline{3}$

For each, name the type of symmetry elements that contains the translational component (leave out symmetry elements not given in the shortened Hermann-Maugin symbol used above).

5 pts

5) Can systematic absences distinguish between the following space groups:

*P*$\overline{1}$ and *P*1; *P*2 and *C*2; *P*2 and *P*m; *P*2 and *P*c; *P*2/c and *P*c; *I*$\overline{4}$ and *I*4/m; *I*41 and *I*a; *R*3/m and *P*3

Explain your answers.

10 pts

6) Imagine an organometallic compound with three fold molecular symmetry. Would you be worried if unit cell determination on the diffractometer proposed a C-centered monoclinic space group?

10 pts

7) What information can be extracted from the positions of a sufficiently large number of diffraction spots? No information is available about the intensity other than if a reflection is observed or not. Explain your thoughts.

5 pts