Chemistry 208—Spring 2009 **Problem Set 3**
Professor K. N. Raymond **Due 02/18/09**

1) Complete the following table

Initial Position	*Final Position*	*Symmetry operation (and direction if applicable)*
x,y,z	*-x ,-y, -z*	
x,y,z		4-fold // to *a*
x,y,z	x + ½, -y, -z	
x,y,z	*-x, y, -z*	
x,y,z	*-x, y + ½ ,z*	
x,y,z		*n* glide perpendicular to *b*
x,y,z	*-x, y + ¼, z + ¼*	

2) Construct a space-group diagram for $P2_1/c$.
a) What conventions exist for the choice of axes (a,b,c) in this space group? What is the name for this convention?
b) An alternative cell choice allows this space group to 'become' $P2_1/a$. What is the relationship of this cell to the cell which gives the original $P2_1/c$?
c) What is the difference between the c and a symmetry operations (i.e., what do they have in common, and what is different between them?)

3) Write the systematic absences which would be predicted for each of the space groups or crystallographic symmetry elements below:

a) two-fold axis of rotation (2) [monoclinic cell, Laue symmetry 2/m]
b) two-fold screw axis (2_1) [monoclinic cell, Laue symmetry 2/m]
c) center of inversion [monoclinic cell, Laue symmetry 2/m]
d) mirror plane (*m*) [monoclinic cell, Laue symmetry 2/m]
e) glide plane perpendicular to **b**, translation in **c** (*c*)
[monoclinic cell, Laue symmetry 2/m]
f) Pbca
g) $Fd\bar{3}c$

4) Correlate the above diffraction gratings with their diffraction patterns, below. Explain your reasoning.