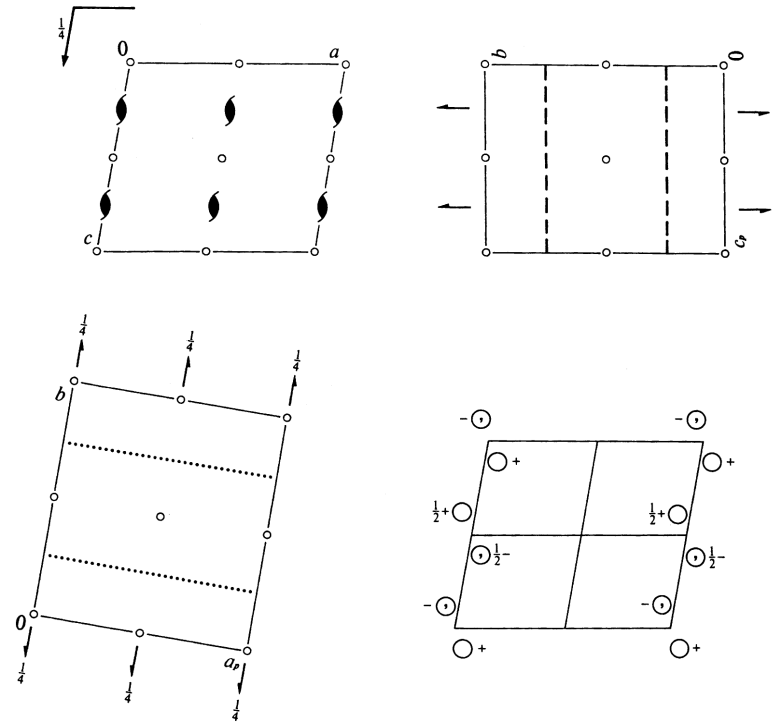
Chemistry 208—Spring 2008 **Problem Set 3**
Professor K. N. Raymond **Answer Key**

1)

Initial Position	*Final Position*	*Symmetry operation (and direction if applicable)*
x,y,z	*-x ,-y, -z*	***inversion***
x,y,z	***x, -z, y***	4-fold // to *a*
x,y,z	x + ½, -y, -z	2_1 // to *a*
x,y,z	*-x, y, -z*	***2-fold // to b***
x,y,z	*-x, y + ½ ,z*	***b-glide perpendicular to a***
x,y,z	*x + ½, -y, z + ½*	*n* glide perpendicular to *b*
x,y,z	*-x, y + ¼, z + ¼*	***d glide perpendicular to a***

2) $P2_1/c$



a) Like all monoclinic systems, the space group $P2_1/c$ uses the *second setting*. In monoclinic cells, the 'unique' axis which is perpendicular to the other two, is chosen as the **b** axis rather than the **c** axis. As a result, the unrestricted (non-90°) angle is the angle β.

b) (Refer to the Crystallographic Tables for figures). Let **a** and **c** represent the vectors for cell choice 1 (2_1/c) and **a'** and **c'** represent the indexing vectors for cell choice 2. **a'= c** and **c'=** $\bar{a} + \bar{c}$**.**

c) Both symmetry operations involve reflection across the mirror plane perpendicular to the unique **b** axis. The *c* glide involves translation in the *c* direction, while the *a* glide involves translation in the *a* direction. [Note that, because of the cell choice definitions in b), these operations are precisely equivalent, as you would expect.]

3)

a) 0 *k* 0, *k* = 2 n

b) no systematic absences

c) no systematic absences

d) no systematic absences

e) *0 k l*, *l* = 2n.

f) (Orthorhombic)

0 *k l*, *k* = 2 n; b glide perpendicular to a

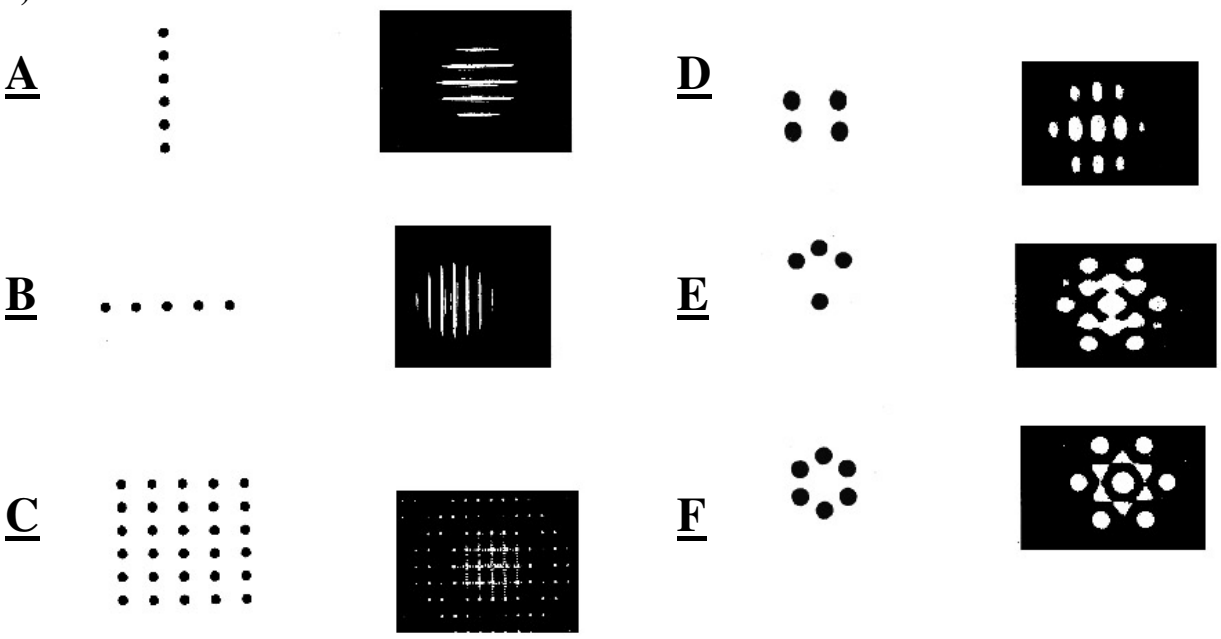
h 0 *l*, *l* = 2 n; c glide perpendicular to b

h k 0, *h* = 2 n; a glide perpendicular to c

These systematic absences are unique to *Pbca*.

g) $Fd\bar{3}c$: *h k l*, all even or odd, 0 *h l*, etc., *k* + *l* = 4n, *h h l*, etc. *l* = 2n. (Almost certainly easiest to obtain these directly from the crystallographic tables. While you should be able to produce the above without, this is almost certainly beyond the limits of most mortals.)

4)



(a) Vertical points create horizontal lines
(b) Horizontal points create vertical lines
(c) An array of points creates a diffraction pattern with corresponding symmetry
(d) Four large points, generates diffraction pattern with same symmetry, but poor resolution due to the small number of points in the lattice
(e) Not a well defined lattice so the diffraction pattern is poorly formed. The diffraction pattern has only *m* symmetry like the lattice.
(f) 6-fold symmetry shown in the diffraction pattern