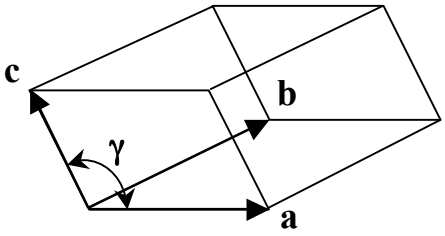
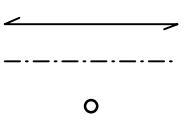
January the 5th 2012

Consider a monoclinic crystal with cell parameters a,b,c and β such that a=8.00Å, b = 6.67Å, c=10.00Å and β=115.84°.



The space group is P21/n which means: Primitive cell, 2-fold screw axis along **b** axis and glide plane perpendicular to **b** axis with fractional translation along ½ (**a**+**c**).

1. The intersection of the 2-fold screw axis with the (**a**, **c**) plane is given by the three coordinates (x_2, 0, z_2). Give the coordinates (x', y', z') of the transform of a general position (x, y, z) by this 2-fold screw axis.
2. The intersection of the glide plane with the **b** axis is given by the three coordinates (0, y_n, 0). Give the coordinates (x'', y'', z'') of the transform of a general position (x, y, z) by this glide plane.
3. Assuming that the only additional symmetry elements are the identity and inversion, show from the composition of the 2-fold screw axis and glide plane operations that the values x_2, y_n and z_2 are fixed (give these values).
4. Draw the symmetry elements in the plane (x,y,1/4), using the following notation:



2-fold axis

glide plane

inversion center

5. Give the reciprocal unit cell vectors $(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)$ and draw the Brillouin Zone in the $(\mathbf{a}^*, \mathbf{c}^*)$ plane.
6. Consider the case of such a crystal with space group P21/n made of diatomic molecules A-A where one atom A has coordinates (x_o, y_o, z_o) = (u,0,0) with |u| < 0.2. Draw all atomic positions in the unit cell in projection onto the (**a**,**b**) plane. Use "+" (or "-" if necessary) sign to indicate position above (below) basal (**a**,**b**) plane.
7. Compute the unit cell structure factor F(h,k,l) where h,k,l are integer components of the scattering **Q** vectors in the reciprocal base, as function of coordinates (x_o, y_o, z_o) ignoring first the particular values. What are the systematic extinctions induced in the diffraction pattern by the presence of these symmetry elements?
8. What are the additional systematic extinctions due to the particular atomic positions (x_o, y_o, z_o) = (u,0,0) ? How can you interpret it?
9. Imagine this crystal undergoes a phase transition where the symmetry goes from $P2_1/n$ space group to a new space group Pn (2_1 screw axis and inversion center are lost). The new positions of the two A atoms of one molecule are then respectively (u,ε,0) and (u,-ε,0) and where ε is small compared to u. Draw all atomic positions in the unit cell in projection onto the (**a**,**b**) plane with the same scale as that of question 7.
10. Compute the structure factor of this new phase.
11. Show that the Bragg intensity for h+k+l odd goes approximately like ε^2.

Math hints: $\sin(x) \underset{x\to 0}{\approx} x$ $\theta = \dfrac{e^{i\theta} + e^{-i\theta}}{}$ $\sin(\theta) = \dfrac{e^{i\theta} - e^{-i\theta}}{2i}$