Protein Structure Determination, BCBP 4870, Fall 2011
Homework 5 – *due Nov 14, 2010*

(A) Using a Bragg plane diagram, explain why a crystal with $P2_1$ symmetry (2-fold screw along the c axis), has only even-numbered reflections in the **c*** direction. i.e. (001), (003), (005) etc are missing, (002), (004),(006), etc are present. (Hint: Rhodes section 5.4.3 , but put it in the form of a drawing.)

(B) A Patterson map was calculated for a crystal with cell dimensions (a=b=60.,c=100.) and cell angles ($\alpha=\beta=90.,\gamma=120.$). The space group is *either* $P3_1$ or $P3_2$ (*you cannot distinguish enantiomeric space groups without additional data*)

(1) **Write the three symmetry operators for $P3_1$** (matrix + vector). Use online sources, such as the International tables of crystallography.

(2) A heavy-atom-to-heavy-atom peak was found at fractional coords **(0.355, 0.241, 0.333)** in the Patterson map. Using symmetry operators**, write the Patterson space locations of 5 other peaks** using space group $P3_1$ (z within $-1/3 \leq z \leq 1/3$).

(3) Using this peak, **solve for the real-space location** of the 3 heavy atoms in real space, using matrix algebra. Find two solutions, one for $P3_1$ and one for $P3_2$.

(5) **Calculate the amplitude and phase** of the reflection **F_h(15 12 0)** by applying the Fourier transform to the three heavy atoms. Do both solutions $P3_1$ and $P3_2$.

(6) **Write the lengths of the reciprocal lattice vectors a*, b* and c* in $Å^{-1}$ and reciprocal cell angles angles α*, β*, and γ***.

(7) Using a*, b* and γ* **find the length of the scattering vector (S), and the resolution (d)** of the **F(15 12 0)** reflection. Show your work.

(C) Using the crystal lattice paper on p.3

(1) **Draw the reciprocal lattice directly on top of the real space lattice,** using lines. Define **a** as the long dimension and **b** as the short dimension. Define the "beam" position (origin) somewhere near the middle of the page. Draw and label **a* and b*** with correct lengths and directions. Measure the real cell angle γ, and the reciprocal cell angle, γ*.

Choose and make a note of the scale for real space and the scale for reciprocal space.
For example. 1mm = 1Å for real space. 1mm = $0.005Å^{-1}$ for reciprocal space.

(2) **Draw the direction of the X-ray beam**, **the reflection**, **and the Bragg planes** (draw at least 2 planes) for the **F(3 2 0)** reflection**.** X-ray wavelength = 1.5418Å.