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

(A) Using a Bragg plane diagram, explain why a crystal with P2₁ 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 (α=β=90.,γ=120.). The space group is either P3₁ or P3₂ (you cannot distinguish enantiomorphic space groups without additional data)

1) Write the three symmetry operators for P3₁ (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 P3₁ (z within -1/3 ≤ z ≤ 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 P3₁ and one for P3₂.
4) Calculate the amplitude and phase of the reflection F₀(15 12 0) by applying the Fourier transform to the three heavy atoms. Do both solutions P3₁ and P3₂.
5) Write the lengths of the reciprocal lattice vectors a*, b* and c* in Å⁻¹ and reciprocal cell angles angles α*, β*, and γ*.
6) Writing 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.