

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 \AA^{-1} and reciprocal cell 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 \mathbf{a} as the long dimension and \mathbf{b} as the short dimension. Define the “beam” position (origin) somewhere near the middle of the page. Draw and label \mathbf{a}^* and \mathbf{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. $1\text{mm} = 1\text{\AA}$ for real space. $1\text{mm} = 0.005\text{\AA}^{-1}$ 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 = 1.5418\AA .





