PSD -- Fall 2020 -- Xray Homework 2

due thursday Nov 12, 2018

http://www.bioinfo.rpi.edu/bystrc/courses/bcbp4870/homework.html

(1) Reciprocal Lattice

Using crystal lattice paper.

Draw the reciprocal lattice over the real space lattice. (Use any point as the origin of reciprocal space). Cell vector **a** is the long axis and **b** is the short axis.
Draw **a* and b*** with correct relative lengths. Label the real cell angle γ, and the reciprocal cell angle, **γ***.

Suggested scaling: 1mm = 1Å for real space.
1mm = 0.005Å^{-1} for reciprocal space.

(2) Solving a Patterson

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* $P3_1$ or $P3_2$ (*You cannot distinguish between enantiomeric space groups such as $P3_1$ and $P3_2$ based on the Patterson map alone.*)

(a) **Write the three symmetry operators for space group $P3_1$** in matrix + vector form. Use the International Tables of Crystallography.

(b) A heavy-atom-to-heavy-atom peak was found at the Patterson space position **(0.355, 0.241, 0.333)** in the Patterson map. Using this peak, **solve for the real-space location** of the 3 heavy atoms, using matrix algebra. Find two solutions, one for $P3_1$ and one for $P3_2$.

(c) Using atom positions**, write the Patterson space locations of all 6 Patterson peaks,** using space group $P3_1$ (all z values must be -1/3 or +1/3).

(d) **Calculate the amplitude and phase** of the heavy atom structure factor **F_h(11 15 0)** by applying the Fourier transform to the three heavy atoms. Calculate using both $P3_1$ and $P3_2$ symmetry.

(e) **Calculate the lengths of the reciprocal lattice vectors a*, b* and c* in Å^{-1} and reciprocal cell angles angles α*, β*, and γ***. The real-space angle between **a** and **b** is **γ** =120.°

(f) Determine the length of the scattering vector **|S|** for the **F(11 15 0)** reflection by summing **a*** and **b*** vectors. Based on this measurement, calculate the resolution (*d*) of the reflection **F(11 15 0)**. Suggested scaling: 1mm = 0.005Å^{-1} for reciprocal space. Hint $d = 1/|S|$.

(3) MIR : Harker diagram

You have made two isomorphous heavy atom derivatives. PH1= protein + PtCl4, and PH2 = protein + Pb-acetate. You collected three datasets, F_P, F_{PH1} and F_{PH2} . Each reflection has a measured sigma value. You determined the heavy atom positions (see problem 2) and calculated the F_{H1} and F_{H2} heavy atom vectors. Solve for the phase of one reflection (Miller indeces unspecified, because you don't need them), using the amplitudes and heavy atom vectors below. Then use the sigma value to estimate the phase distribution. From that give a rough estimate of the Figure of Merit.

$F_P = 50 \quad \sigma_P = 2.5$
$F_{PH1} = 57 \quad \sigma_{PH1} = 8.0$
$F_{PH2} = 46 \quad \sigma_{PH2} = 9.0$
$|F_{H1}| = 21.1 \quad \alpha_{H1} = 174.8°$
$|F_{H2}| = 13.8 \quad \alpha_{H2} = -24.6°$

(a) Draw the Harker diagram showing amplitudes ± sigmas.

(b) On the Harker diagram, shade in the zone of solution. Mark the *estimated* centroid of that space. (label it C)

(c) Draw and label the probable phase α_{max} of F_P

(d) Graph (in radial coordinates) the phase probability distribution. Draw it around the F_P circle.

(e) Estimate the Figure of Merit, m, and the best phase α_{best} based on your drawing.

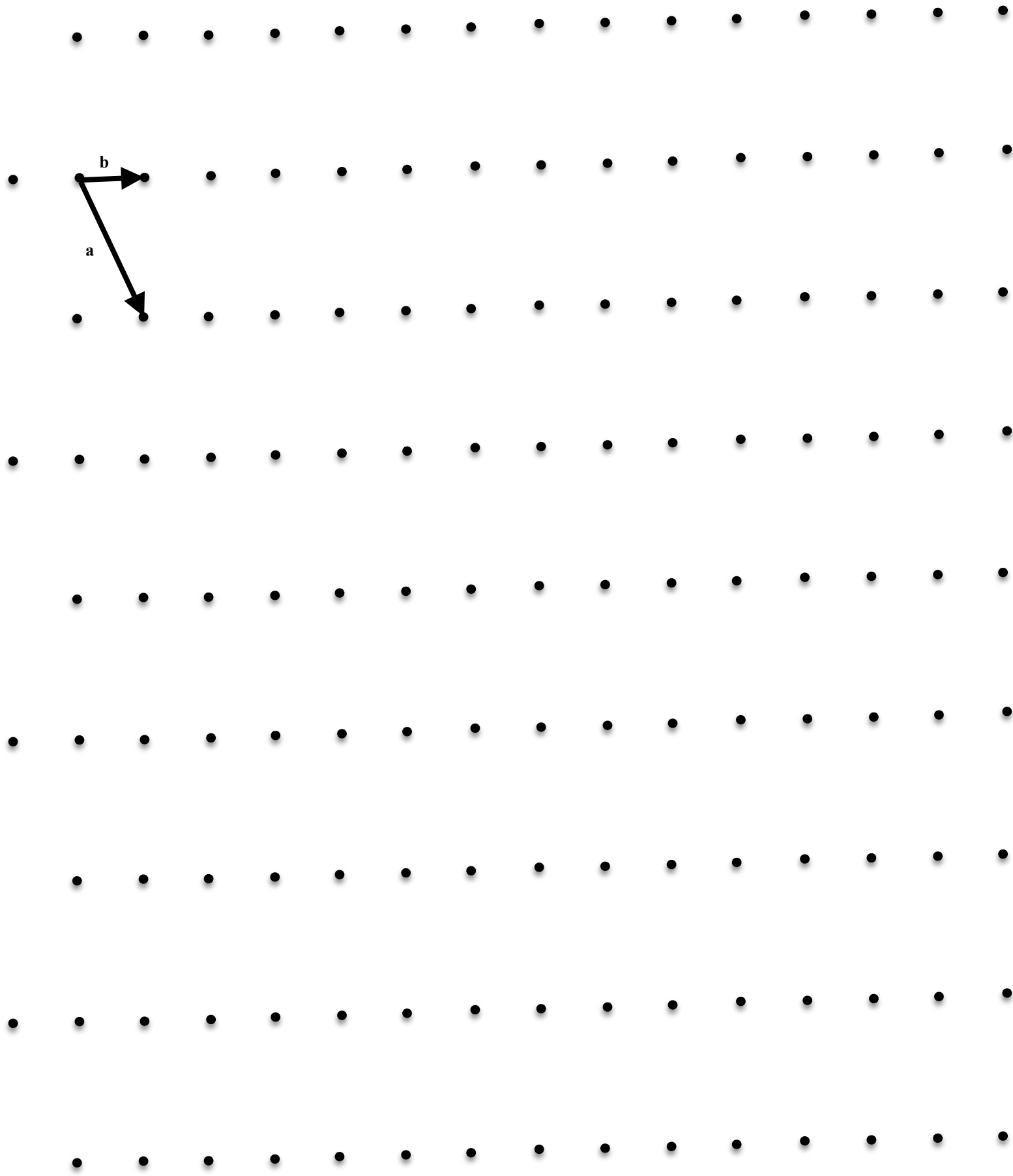
(4) MAD : Harker diagram

You have collected data on a crystal containing selenomethionine, at two different wavelengths. $F_{\lambda 1}$ is the dataset at the non-anomalous wavelength, while $F^{+}_{\lambda 2}$ and $F^{-}_{\lambda 2}$ are the dataset for the + and - Friedel mates at the anomalous wavelength. Using Patterson maps, you have determined the heavy atom positions and calculated the amplitude and phase of the selenium atoms (real part). By looking up selenium in the International Tables of Crystallography, you have determined that the amplitude of the imaginary part is 25% of the amplitude of the real part, and the phase of the imaginary part is +90° from the phase of the real part.

$| F_{\lambda 1} | = 4.5$
$| F^{+}_{\lambda 2} | = 5.3$
$| F^{-}_{\lambda 2} | = 4.4$
$| F_{Se} | = 1.8$ (real part)
$\alpha_{Se} = 45°$ (real part)

(a) Draw the Harker diagram. Plot circles for $F_{\lambda 1}$, $F^{+}_{\lambda 2}$ and $F^{-}_{\lambda 2}$, and vectors for $F^{+}_{Se(real)}$, $F^{+}_{Se(imag)}$, $F^{-}_{Se(real)}$* and $F^{-}_{Se(imag)}$*. (Star denote complex conjugate..) Use 1 cm = 1 amplitude unit.

(b) What is the phase of $F_{\lambda 1}$?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