(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 $\gamma$, and the reciprocal cell angle, $\gamma^*$. 

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 ($\alpha=\beta=90.,\gamma=120.$). 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 $\alpha^*$, $\beta^*$, and $\gamma^*$. The real-space angle between $a$ and $b$ is $\gamma = 120.$°

(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, FP, FPH1 and FPH2. Each reflection has a measured sigma value. You determined the heavy atom positions (see problem 2) and calculated the FH1 and FH2 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.

\[
\begin{align*}
F_P &= 50 \quad \sigma_P = 2.5 \\
F_{PH1} &= 57 \quad \sigma_{PH1} = 8.0 \\
F_{PH2} &= 46 \quad \sigma_{PH2} = 9.0 \\
|F_{H1}| &= 21.1 \quad \alpha_{H1} = 174.8^\circ \\
|F_{H2}| &= 13.8 \quad \alpha_{H2} = -24.6^\circ
\end{align*}
\]

(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 \( \alpha_{\max} \) 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 \( \alpha_{\text{best}} \) based on your drawing.
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.

<table>
<thead>
<tr>
<th>$F_{\lambda_1}$</th>
<th>4.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F^{+\lambda_2}$</td>
<td>5.3</td>
</tr>
<tr>
<td>$F^{-\lambda_2}$</td>
<td>4.4</td>
</tr>
<tr>
<td>$F_{\text{Se}}$</td>
<td>1.8 (real part)</td>
</tr>
<tr>
<td>$\alpha_{\text{Se}}$</td>
<td>45° (real part)</td>
</tr>
</tbody>
</table>

(a) Draw the Harker diagram. Plot circles for $F_{\lambda_1}$, $F^{+\lambda_2}$ and $F^{-\lambda_2}$, and vectors for $F^{+\text{Se(real)}}$, $F^{+\text{Se(imag)}}$, $F^{-\text{Se(real)}}$ and $F^{-\text{Se(imag)}}$. (Star denote complex conjugate.) Use 1 cm = 1 amplitude unit.

(b) What is the phase of $F_{\lambda_1}$ ?