

CH370: X-ray – Sample Problems

1. Image Formation: You have invented and patented an X-ray laser that emits 8.0 nm light. However, you have trouble selling it to protein crystallographers. Why?

2. X-ray formation: Contrast the generation of X-rays in a sealed tube X-ray generator, a rotating anode X-ray generator, and a synchrotron? Name two major advantages of data collection at a light source like the synchrotron at APS?

3. Crystal formation:

a) Name six variables that influence crystal growth.

- | | |
|----|----|
| 1. | 2. |
| 3. | 4. |
| 5. | 6. |

b) Name three common “methods” for crystallizing proteins or nucleic acids.

- 1.
- 2.
- 3.

4. Electron Density: Given the following equation for calculation of the electron density at a point with fractional coordinates (x,y,z) in the unit cell:

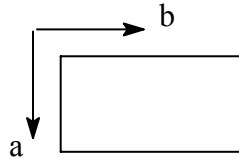
$$\rho(x,y,z) = (1/V)\sum\sum\sum |F_{hkl}| e^{i\alpha_{hkl}} e^{-2\pi i(hx + ky + lz)}$$

Define the meaning of all terms used in the above equation.

5. Crystal Diffraction

a) What information is available from the “spot” spacing? From the relative intensities?

b) Illustrate what “Bragg” planes are involved in the 230 “reflection.”



c) Given that the reciprocal lattice shows three, orthogonal reciprocal lattice vectors, and based on the following data using copper K_{α} radiation ($\lambda = 1.5418\text{\AA}$), calculate the lattice constants and volume of the unit cell.

<i>hkl</i>	2θ
800	5.44°
030	6.48°
006	5.62°

$$a = \underline{\hspace{2cm}}; \quad b = \underline{\hspace{2cm}}; \quad c = \underline{\hspace{2cm}}; \quad V = \underline{\hspace{2cm}}$$

d) Estimate the maximum number of independent reflections that could be measured for this system for a 3.0\AA data set? For a 1.8\AA data set? (Hint: think in reciprocal space)

6. Phase problem

a) Define MIR, MR, MAD

b) List the major advantages and disadvantages of each method.