

Student	
Course	Module 4 -- Characterization I: Physical-Chemical Techniques X-Ray Diffraction
Lecturer	L. R. Falvello
Date of assessment	

Answer questions 1 and 2 and either 3, 4, or 5.

1. The reciprocal lattice is a construct used to:

- (a) Interpret the intensities of diffraction maxima.
- (b) Calculate a Fourier transformation to obtain phases of diffracted beams.
- (c) Interpret the geometry of diffraction from crystalline solids.
- (d) Determine the number of molecules in the unit cell.

2. (a) What is the energy of x-rays with wavelength $\lambda = 0.711 \text{ \AA}$?

(b) What is the energy of a neutron beam with the same wavelength, $\lambda = 0.711 \text{ \AA}$?

Show your work for both parts (a) and (b).

3. (a) What is the principal difference between a point group and a space group?

(b) What is the relationship between the crystallographic asymmetric unit and the space group?

(c) For a given crystal, is it necessary for the number of molecules in a unit cell to be equal to the number of operations in the space group? Explain.

4. In the structure factor equation for x-ray or neutron diffraction:

- (a) Which terms or symbols represent variable atomic parameters?
- (b) Which term depends on the type of element of a given atom?
- (c) What characteristic of an atom is described by the parameters U_{ij} ?

5. (a) What is the most fundamental difference between neutron diffraction and x-ray diffraction?

(b) Why do C---H and O---H bond distances, when analyzed by neutron diffraction, have different values from those obtained for the same substance using x-ray diffraction?