

MASTER OF SCIENCE EXAMINATION, 2024

(2nd Year, 1st Semester)

PHYSICS

PAPER : PHY/TH/203

[X-Ray Crystallography (I)]

Time : Two Hours

Full Marks : 40

Answer **any four** questions.

1. (a) From Fourier synthesis of electron density, show that the electron density function and structure factor function are Fourier transforms of each other.
 (b) Determine the structure factor of NaCl and indicate the cases where intensity can be observed. The atomic positions of Na⁺ and Cl⁻ in the unit cell are

$$\begin{array}{l} \text{Na}^+ \quad (000) \quad \left(\frac{1}{2} \frac{1}{2} 0 \right) \quad \left(\frac{1}{2} 0 \frac{1}{2} \right) \quad \left(0 \frac{1}{2} \frac{1}{2} \right) \\ \text{Cl}^- \quad \left(\frac{1}{2} 0 0 \right) \quad \left(0 \frac{1}{2} 0 \right) \quad \left(0 0 \frac{1}{2} \right) \quad \left(\frac{1}{2} \frac{1}{2} \frac{1}{2} \right) \end{array}$$

[6+4]
2. (a) What is “Phase problem” in crystallography? What are the ways to solve a structure by overcoming the phase problem?

(2)

- (b) From the ‘Convolution function’ of Fourier theory, show that the Patterson function has a center of symmetry in origin, whether the crystal is centrosymmetric or not. What are the limitations of the Patterson method for structure solution? [(2+2)+(5+1)]
3. (a) What do you mean by “Structure Refinement”? What is meant by “Difference Fourier map”?
 (b) What are the characteristic features of Burn Error Synthesis method of structure refinement? How are the different density maps nearly free from ‘series termination errors’?
 (c) Discuss whether an R-factor 0.0 can be attained practically or not. [(2+2)+(2+2)+2]
4. Consider the classical scattering of unpolarized X-rays by a single free electron and obtain an expression for the scattered intensity at a given point *P*. Thus obtain an expression for the power of the scattered X-ray beam. How can polarized X-ray beam be obtained? [7+2+1]
5. (a) Obtain an expression for the crystal structure factor and show how the observed-ray intensity vanishes for planes of a bcc crystal satisfying the condition $h + k + l = 2n$, where symbols have their usual meaning.
 (b) What is the fundamental requirement of observing X-ray/electron diffraction from single crystals?
 (c) What is Weiss Zone law? Analyze if the set of planes (-224) and $(1-13)$ belong to the zone axis $[110]$. [(4+2)+1+(1+2)]

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