

212027 – STRUCTURAL CRYSTALLOGRAPHY

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Symmetry on the solid state. Diffraction of X-rays. Determination of crystalline structure. Resolution, refinement and design programs of crystalline structures.

SYLLABUS:

1. Solid state symmetry: elements of symmetry, unit cell, Miller indices, point group and spatial group.
2. X-ray diffraction: Bragg law, X-ray scattering, structure factor, spatial group determination, phase problem, structure factor applications.
3. Determination of crystal structures: Patterson methods and direct methods.
4. Programs of resolution, refinement and design of crystal structures: programs Wingx, Shelx97, Ortep and Mercury.

BIBLIOGRAPHY:

1. LADD, Mark F. C.; PALMER, Rex A. Structure determination by X-ray crystallography. 4.ed. New York: Kluwer Academic/Plenum Publishers, 2003.
2. WOOFSOON, Michael M. An Introduction to X-ray Crystallography. 2.ed. Cambridge University Press, 1997.