**622 Chem.**

This graduate level course in crystal structure refinement focuses on practical aspects of crystal structure determination from data collection strategies to data reduction and basic and advanced refinement problems of organic and inorganic molecules:

**Tools and Concepts:**

**Introduction**

**Timescales**

**Diffraction Methods:**

Introduction

Diffraction of electrons, neutrons and X-ray

Diffraction by single crystals; symmetry

* The unit cell
* Symmetry elements within the unit cell
* The seven crystal systems
* Three-dimensional periodic symmetry; space groups
* Close packed structural-Cubic and hexagonal close packing
* Materials that can be descried as close packed
* Metals
* Alloys
* Ionic structure
* Covalent network structure

**Diffraction by single crystals; the theoretical basis**

**Diffraction by single crystals; the experiment**

* Crystal growth
* Experimental set-up
* Indexing and determining unit cell dimensions
* Data collection
* Experimental problems: X-ray absorption and extensions
* Data analysis

**Diffraction by single crystals; interpretation of results**

* How good is structure
* Common problems: incorrect atom assignment
* Common problems: disorder
* Recognizing chemical bonds
* Absolute structure determination
* How big can we go

**Diffraction by single crystals; electron density determination**

**Topological features of the electron density**

* Displaying topological features of the electron density
* Definition of topological atom and its properties
* Critical points
* Bonding description
* The Laplacian of the electron density
* Some examples of electron topology studies

**Phase dependence of molecular structures**

* SHELXLCrystal structure refinement
* Hydrogen atomsAtom type assignment
* Disorder
* Pseudo-Symmetry
* Twining
* Artefacts
* Structure Validation

**Diffraction by powder**

**High-pressure crystallography**

**Extended x-ray absorption fine structure.**

**Nuclear Magnetic Resonance Spectroscopy**

**Electron Paramagnetic Resonance Spectroscopy**

**Mossbauer Spectroscopy**

**Electronic Characterization technique**

**References:**

1. **Structural Methods in Molecular Inorganic Chemistry, Wiley (2013) D.Rankin, N.Mitzel, C.Morrison**
2. **Crystal Structure Analysis: Principles and Practice, Alexander J. Blake, William Clegg, Oxford(2004).**
3. **Crystal Structure Determination, W.Clegg, Oxford (1998).**
4. **Crystal Structure Refinement, A crystallographer’s guide to SHELXL, P.Muller and others, Oxford(1998).**
5. **Basic Solid State Chemistry , A.West, Wiley(1997)**
6. **Solid State Chemistry, E.Lesley Smart and Eliane.Moore, Taylor (2005).**
7. **NMR,NQR,ERP,Mossbauer Spectroscopy in Inorganic Chemistry, R.V.Parish(1990)**

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**Midterm exam=30**

**Showcase=30**

**Final exam=40**