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Course Subject: Bio-Inorganic Chemistry

Prerequisite: CHEM 3II3.

Tutorials: BSB-119 / Monday at 1.30-2.20

Course Textbook:

There is no prescribed textbook for the course – lecture notes and overheads/handouts will provide the required material (all overheads, or their content in the form of a handout, will be posted on Avenue to Learn). However, the textbooks below are useful references.

Useful References:

- Your textbook for CHEM 3II3 (presumably Shriver & Atkins or Housecroft)

Contents:

1. Brief review of important concepts from CHEM 3II3.  
3. Bio-mimetic chemistry (integrated with the section above)  
4. Metal-containing imaging agents, drugs and radiopharmaceuticals  
5. Methods for characterization of metal-containing molecules (in biological and synthetic systems) will be discussed where appropriate throughout the course.

Evaluation:

- Assignment 1 = 15 % (probably due date in first week of February)  
- Midterm = 20 % (likely to be late February / early March; not during class)  
- Assignment 2 = 15 % (probably due around the end of March)  
- Final exam = 50 % (TBA)
More Detailed List of Topics for 4IB3 (may be subject to change):

- Inorganic elements in biology, and biological ligands
- Biological functions of metals – an overview
  - ** X-ray crystallography
  - ** Raman spectroscopy
- Myoglobin and Hemoglobin (a case study)
- Aerobic respiration (actually a case study of cytochrome c oxidase, with discussion of the whole of aerobic respiration to put the role of this enzyme in perspective)
- FeS Redox Centres
  - ** CV (cyclic voltammetry)
  - ** Mixed Valence Complexes (Robin-Day classification)
  - ** EPR spectroscopy
  - ** Mössbauer spectroscopy
  - ** N₂, CO, H⁺ and H₂ as ligands
- Aconitase
- Industrial NH₃ production
- Biomimetic and Bio-inspired Inorganic Chemistry – Models for myoglobin, cytochrome-c-oxidase, aconitase, nitrogenase (and N₂ fixation in general), and hydrogenases.
- Nitrogenase
- Hydrogenases
- Small molecule toxicity (CO, CN⁻, N₃⁻)
- Heavy metal toxicity [As, Hg, Pu (also briefly Be, Cd, Pb, Tl)]
  - ** Linear geometry
  - ** Relativistic Effects
  - ** Lanthanides versus Actinides
- Chelation therapy (discussed in the context of heavy metal toxicity)
- Contrast agents for MRI
  - ** Different types of radioactive decay
  - Generation of radionuclides
  - Radionuclides for imaging (SPECT and PET)
  - Radionuclides for therapy
  - 1st generation or “metal-essential” radiopharmaceuticals
  - 2nd generation or “metal-tagged” radiopharmaceuticals
- Radionuclides for Palliative Treatment
- Boron Neutron Capture Therapy (BNCT)
- Medicinal inorganic chemistry in general
- Drugs in which the metal has a functional role [Pt (briefly also Ru, Ga)]
- Drugs in which the metal has structural or other role.
- Gold anti-arthritis and anti-cancer drugs
- Vanadium insulin mimics

*Topics preceded by asterisks are focused on background understanding or spectroscopic techniques.*
Relevant background in the area of transition metal chemistry

Topics that should have been covered in CHEM 3I3:

- Construction of MO diagrams for simple molecules (O₂, N₂, CO, H₂C=CH₂, butadiene, C₅H₅⁻, benzene).
- Variation of accessible oxidation states and atomic radii across the transition metals.
- Ligand bonding modes – monodentate, chelating (bidentate, tridentate etc.), bridging.
- A general introduction to coordination complexes, likely geometries for different coordination numbers, possible isomers, and isomerisation mechanisms.
- Crystal field theory – assumptions and limitations of CFT, application of CFT to various geometries, Jahn-Teller distortion, crystal field stabilization energy.
- Ligand field theory / MO diagrams for transition metal complexes.
- \( \sigma \)-Donor ligands, \( \pi \)-donor ligands, \( \pi \)-acceptor ligands, and the spectrochemical series of ligands. Also, the spectrochemical series of metals.
- Thermodynamic aspects of coordination chemistry including: formation constants, chelate effect, macrocycle effect, and the Irving-Williams series.
- Introduction to organometallic chemistry, electron counting, and the 18-electron rule.

Topics that may not have been covered in CHEM 3I3:

- Hard and soft ligands and metals.
- Kinetics and mechanisms of transition ligand substitution reactions: associative, interchange and dissociative mechanisms, activation parameters, and Taube’s rules.