CH3F8-15 Advanced Coordination and Bio-Inorganic Chemistry

24/25

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Claudia Blindauer
Credit value
15
Module duration
19 weeks
Assessment
100% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

This module will examine the ways in which biological systems use the specific chemical properties offered by the full range of elements in the periodic table to perform a wide variety of functions, and how synthetic coordination compounds, including those with f-block elements, can be used in a bio-medical context. The module will introduce the chemical principles that govern the use of essential metal ions in biological systems, and selected examples will be discussed, to illustrate these principles. The impact of bio-inorganic chemistry on human health will be discussed in both the context of the consequences of aberrations in metal ion housekeeping and the use of metallo-based drugs.

Module web page

Module aims

1. To provide an introduction to bio-inorganic chemistry
2. To demonstrate how underlying coordination chemistry concepts and principles can be applied to bio-inorganic problems
3. To introduce and use biophysical techniques pertinent to bio-inorganic chemistry

4. To introduce f-block coordination chemistry and spectroscopy, as well as applications (e.g. MRI and other imaging approaches including radio-diagnostics).

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

INTRODUCTION
The importance of metal ions in biology and their relative abundances in the body. Natural selection of the elements, chemical limitation imposed by biological systems.
Relevant coordination chemistry principles (hard and soft acids and bases, stability constants, ligand exchange rates).
Biological Ligands: Proteins, Nucleic Acids and Nucleotides, Porphyrins, related ligands, antibiotics.

PHYSICAL TECHNIQUES TO STUDY METAL ION-BIOMOLECULE INTERACTIONS
Applictions of optical spectroscopies, NMR, EPR, X-ray absorption, Mössbauer spectroscopy

ION TRANSPORT AND SIGNALLING
Importance of balanced distribution of elements, composition of cell membranes. Mechanisms of ion transport: Ionophores, Channels, Pumps.

REGULATION OF METAL UPTAKE AND STORAGE
Why regulation of metal ion concentration is crucial in a biological system. Examples for metalloregulation; the iron cycle, siderophores, transferrin, ferritin.

CONTROL OF PROTEIN STRUCTURE AND DYNAMICS BY METAL IONS
Calmodulin: tuning of protein structure and dynamics by metal binding. Cooperativity. Zinc fingers: structural role of zinc, composition of binding sites, roles of zinc fingers, sequence-specific DNA-recognition and artificial zinc fingers.

METALLOPROTEINS AND METALLOENZYMES: HYDROLYTIC ENZYMES
Zinc. Properties and relevance to biology. Example carbonic anhydrase. The importance of coordination number, electrostatics, and the enzymatic cavity. Model complexes.

METALLOPROTEINS AND METALLOENZYMES: OXYGEN CARRIERS
Dioxygen binding. Iron and copper. Haemoglobin and myoglobin: Structure, Physiological role, Oxygenation Equilibria, Oxygen Coordination, MO Interpretation, Model Systems. Haemerythrin and Haemocyanin.

METALLOPROTEINS AND METALLOENZYMES: REDOX CHEMISTRY
Biological electron transfer: Redox active metal centres. Iron and copper. Importance and overview of range of standard potentials. Redox potentials and how to tune them. Iron-Sulfur Proteins: Rubredoxins, 2Fe Ferredoxins, Polynuclear Clusters. Heme proteins; Cytochromes, Cytochrome P-450. Non-heme Fe-binding enzymes: Methane monooxygenase and other oxygenases.

F-BLOCK (COORDINATION) CHEMISTY AND ELEMENTS IN MEDICINE
Revision: Definition of the f elements; position in the periodic table Properties of the atoms and

ions: ionisation energies, electrode potentials, metallic and ionic radii, preferred oxidation states and speciation (=> coordination chemistry), Electronic spectra and luminescence of lanthanide and actinide complexes, Magnetism Applications including lanthanides for bio-imaging/bio-sensing, and radioactivity of actinides.

INTRODUCTION TO MEDICINAL INORGANIC CHEMISTRY
Examples of metal-based drugs, radiopharmaceuticals, and diagnostic metal complexes (inc. lanthanide-based imaging agents).

Learning outcomes

By the end of the module, students should be able to:

- Understand and rationalise roles that essential metal ions play in biological systems: Control of protein structure and dynamics, enzymatic catalysis, signalling.
- Understand the rationales for the selection of metal ions to perform biological functions.
- Identify metal-binding portions of biomolecules, recognise and describe the differences between metal sites in small molecule complexes and proteins.
- Understand the principles of metal ion homeostasis: metalloregulation of gene expression and translation, metal ion transport through membranes and cytosols.
- Understand and rationalise the effects that the binding of metal ions to proteins and nucleic acids has on the structure and dynamics of biomolecular structures.
- Understand and rationalise the mode of actions of metal ions in hydrolytic and redox metalloenzymes.
- Understand and rationalise the impact of metal binding residues and protein environment (coordination numbers and geometry, hydrophobic and electrostatic effects) on reactivity of metal ions.
- Understand and rationalise the mode of action and design features of selected metallodrugs.
- Understand and rationalise diagnostic metal complexes for biological imaging
- Understand and rationalise the coordination chemistry of f-block metal ions

Indicative reading list

Shriver/Atkins, 7th edition, Chapters 23 (f-block), 26 (Biological Inorganic Chemistry) and 27 (Metals in
Medicine)

Lippard, S J, Berg J: ‘Principles of bioinorganic chemistry’, QD 2400.L4
Biological Inorganic Chemistry: Structure and Reactivity
by I. Bertini, H.B. Gray, E.I. Stiefel, J.S. Valentine (Editors), University Science Books, U.S. (2006).

J J R Frausto da Silva and R J P Williams, The Biological Chemistry of the Elements, Clarendon Press, Oxford, 1991. QD 2400.S4

W Kaim and B Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, Wiley, 1994. QD 2400.K2

Metals in Medicine

by James C Dabrowiak, Wiley & Sons Ltd., 2009

Any further reading matter is available on the Moodle site.

View reading list on Talis Aspire

Interdisciplinary

Bio-Inorganic Chemistry is a topic at the interface between Biological, Inorganic and Analytical Chemistry, and also requires a degree of familarisation with biological and medicinal concepts.

Subject specific skills

Proficiency in interpreting biophysical data in the context of bio-inorganic and medicinal inorganic chemistry.
Proficiency in interpreting f-block element spectroscopic data.
Apply year 1 and 2 coordination chemistry principles to complex biomolecular systems.

Transferable skills

Problem solving,
Critical thinking ,
Numeracy

Study

Study time

Type	Required
Lectures	24 sessions of 1 hour (16%)
Seminars	9 sessions of 1 hour (6%)
Practical classes	(0%)
Private study	117 hours (78%)
Total	150 hours

Private study description

Self study (including exercises provided), directed reading, and revision

Costs

No further costs have been identified for this module.

Assessment

You must pass all assessment components to pass the module.

Students can register for this module without taking any assessment.

Assessment group B5

	Weighting	Study time
In-person Examination	100%	

Feedback on assessment

Cohort level examination feedback provided via Moodle.

Past exam papers for CH3F8

Availability

Pre-requisites

To take this module, you must have passed:

- All of
  - CH267-15 Transition Metal Chemistry: Structure, Reactivity & Organometallic Chemistry

Courses

This module is Optional for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 4 of F101 Chemistry (with Intercalated Year)
  - Year 4 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 3 of F100 Chemistry
  - Year 3 of F100 Chemistry
  - Year 3 of F121 Chemistry with Medicinal Chemistry
- Year 3 of UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
- Year 4 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 3 of F109 MChem Chemistry (with International Placement)
  - Year 3 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants

    - Year 3 of F100 Chemistry
    - Year 3 of F105 Chemistry
    - Year 3 of F109 MChem Chemistry (with International Placement)
    - Year 3 of F125 MChem Chemistry with Medicinal Chemistry
- Year 4 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)