CH3F0-15 Advanced Inorganic Chemistry and Laboratory

21/22

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Adrian Chaplin
Credit value
15
Module duration
6 weeks
Assessment
33% coursework, 67% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A

[Module web page]

Module aims

The module aims to give an advanced background to the issues which impact on industrial catalytic reactions. Organometallic chemistry uses principles from organic and inorganic (particularly coordination) chemistry, and also physical chemistry (particularly kinetics). Inorganic materials chemistry uses principles from inorganic chemistry (structures of solids) and physical chemistry (electronic properties of solids). The module draws together aspects of this work developed in Year 2 and extends it to the types of reactions and catalysis used widely in chemical industries (petrochemicals, polymers, fine chemicals and pharmaceuticals).

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

What is catalysis? Homogeneous vs Heterogeneous. Key concepts

Recap: Electron Counting and Coordination Numbers in Organometallics; Covalent Bond Classification

Reactivity of organometallics: Oxidative addition and Reductive Elimination

Reactivity of organometallics: Insertion and Elimination

Homogeneous Catalysis

- Hydrogenation
  Activation of dihydrogen using transition metals
  Mechanisms of alkene hydrogenation
  Mechanisms of ketone hydrogenation (including transfer hydrogenation)
  Asymmetric hydrogenation
  Homogeneous vs. Heterogeneous catalysis (arene hydrogenation)
- Hydroformylation of alkenes (Co, Rh)
- Hydrocyanation (Ni)
- Carbonylation of methanol (Rh, Ir)
- Carbonylation of alkynes (Ni)
- Wacker Process (Pd)
- Heck olefination (Pd)
- Olefin metathesis (Co, Mo, pre Grubbs)
- Ziegler catalysis (Ti, Zr)

Heterogeneous Catalysis

- Zeolites: silicates and alumino-silicates
  Structure description
  Synthesis: solvothermal crystallisation
  the use of templates
  design of new materials
- Zeotypes: AlPOs
- Mixed tetrahedral-octahedral frameworks (transition-metal-containing)
- Mesoporous silicas
- Metal-Organic Frameworks: structures and synthesis
- Ion-exchange properties of nanoporous materials
- Separation (molecular sieving) by porous materials
- Shape-selective catalysis:
  Petroleum cracking
  Solid-acid catalysis
  Transition-metal containing microporous catalysts for oxidation
  Mesoporous solids to tether molecular catalysts
  MOFs – limitations on their use
- Other industrially relevant solid-state catalysts: for example, three-way catalytic convertors, Haber-Bosch, water-gas shift (WGS) reaction, steam reforming, sulphuric acid production

Summary

Homo vs Hetero Fischer-Tropsch (Fe, Co, analogy with homogeneous processes)

Learning outcomes

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

- Apply and understand the limitations of the 18 electron counting rule in rationalising the stability of organometallic complexes by consideration of other properties of the constituent metal and ligands (sterics, coordination number).
- Calculate and interpret the changes in oxidation state, coordination number and valence electron count during elementary reactions and use these to predict outcomes
- For each of the organometallic reaction classes in Syllabus): Understand the mechanistic basis (using e.g. frontier MO descriptions); Recognise the situations (structure, electron count, coordination number, steric/strain) in which the reaction may occur or is promoted/suppressed; Interpret trends in given mechanistic data (i.e. reaction outcomes: rate, structure/reactivity, stability, product distribution, stereochemistry) in terms of the above; Predict the effects of designed changes of complex properties (coordination number, ligand size, charge, electron density, electron count) on reaction outcomes; Suggest & justify modifications to systems in order to effect changes in reaction outcome; Design and interpret chemical and isotopic labelling, and other mechanistic probe experiments.
- For a range of catalytic processes mediated by organometallics (see Syllabus): Identify the fundamental reactions involved and apply; Apply the principles developed above in interpreting, predicting and designing catalytic the outcomes of catalytic reactions; Identify rate-determining and selectivity-determining steps using kinetic and reaction outcome data; Recognise off-cycle processes (such as co-catalytic cycles, decompositions, equilibria)
- Describe the structures of microporous zeolites in terms of primary and secondary building units using the examples of sodalite, zeolite A and zeolite X/Y.
- Describe the structures of microporous phosphates and mixed polyhedral frameworks in relation to zeolites.
- Understand the role of templating in the synthesis of mesoporous solids.
- Describe the structures of metal organic frameworks
- Predict conditions details for porous solids in terms of choice of reagents on the product of reaction
- Rationalise unseen experimental data concerning the uses of porous solids in catalysis, including the following features of their reactivity: Shape-selective adsorption (molecular sieving); Solid-acid catalysis; Transition metal redox catalysis; Ion-exchange
- Rationalise unseen experimental data concerning the uses of transition-metal oxides in heterogeneous catalysis, with reference to their redox activity.
- Design synthetic experiments on the basis of input from laboratory scripts, literature sources, previous experiments and advice from demonstrators.
- Understand and assess the spectroscopic etc. properties of new or unknown inorganic coordination compounds in relation to their identity, purity and physico-chemical properties as appropriate.
- Present the results of their studies, including aspects of research work in a laboratory report for the experimental work.

Indicative reading list

Shriver and Atkins' Inorganic Chemistry, 7th edition, Oxford University Press, 2018, Chapters 24 & 25 (in part for heterogeneous)
Organometallic Chemistry by Spessard and Miessler (Prentice Hall) – several copies in library.
Applied Organometallic Chemistry and Catalysis (Oxford Chemistry Primers) Robin Whyman
Homogeneous Catalysis: Understanding the Art. Piet van Leuven. Superb, expensive, used in development of module materials. Good for kinetics.
Metal-Catalysis in Industrial Organic Processes (RSC) Gian Paolo Chiusoli (Editor), Peter M. Maitlis (Editor) – expensive, used in development of module materials.
The Organometallic Chemistry of the Transition Metals (Wiley) Robert H. Crabtree – expensive, used in the development of the module materials
The f Elements (Oxford Chemistry Primers), Nikolas Kaltsoyannis and Peter Scott – inexpensive but not necessary to purchase. Useful for basic f element chemistry principles.
Principles and Applications of Organotransition Metal Chemistry, James P. Collman, Louis S. Hegedus, Jack R. Norton, and Richard C. Finke (University Science Books,U.S.; 2nd Revised edition) – expensive, was used in development of course materials.
Organotransition Metal Chemistry: From Bonding to Catalysis, John F. Hartwig (Univeristy Science Books) – expensive, was used in the development of course materials.
Smart and Moore Solid-State Chemistry (in part for heterogeneous)

Subject specific skills

Numeracy
Problem solving
Critical thinking

Transferable skills

Numeracy
Problem solving
Critical thinking

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (13%)
Practical classes	5 sessions of 6 hours (20%)
Other activity	3 hours (2%)
Private study	97 hours (65%)
Total	150 hours

Private study description

N/A

Other activity description

Workshop / dropin sessions

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Students can register for this module without taking any assessment.

Assessment group D2

	Weighting	Study time	Eligible for self-certification
Assessment component			
Laboratory Report	33%		Yes (extension)
Reassessment component is the same			
Assessment component			
Online Examination ~Platforms - AEP	67%		No

- Online examination: No Answerbook required

Reassessment component is the same

Feedback on assessment

Cohort level examination feedback provided via Moodle. Written feedback on laboratory report from assessor.

[Past exam papers for CH3F0]

Availability

Pre-requisites

To take this module, you must have passed:

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

Post-requisite modules

If you pass this module, you can take:

- CH403-15 Synthetic Chemistry II (Metallo-organic)
- CH401-60 Research Project & Methodology

Courses

This module is Core for:

- Year 4 of UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
- Year 3 of UCHA-3 Undergraduate Chemistry 3 Year Variants
- Year 4 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 3 of F105 Chemistry
  - Year 3 of F125 MChem Chemistry with Medicinal Chemistry
- Year 4 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)

This module is Core optional for:

- Year 4 of UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
- Year 3 of UCHA-3 Undergraduate Chemistry 3 Year Variants
- Year 3 of UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
- Year 3 of UCHA-4M Undergraduate Master of Chemistry Variants