Unit title: Inorganic Chemistry of Crystal Structures and Transition Metal Complexes

Unit code: **M/601/0360**

Level: **5**

Credit value: **15**

Aim

This unit enables learners to gain an understanding of the first row d block elements. The three main areas covered are the solid state, the first row d block metals and their complexes and catalysis.

Unit abstract

This unit is an in-depth study of some current aspects of inorganic chemistry. The solid state, the first row d block elements and transition metal complexes are examined in detail. These topics are then expanded to cover homogeneous and heterogeneous catalysis.

The unit offers opportunities for learners to research specialised areas and is appropriate for employees working in a research environment or for learners wishing to work in this area or to continue study at a higher level.

Learning outcomes

On successful completion of this unit a learner will:

1 Understand the structure of crystalline materials

2 Understand first row d block metal chemistry

3 Understand models of bonding in transition metal coordination complexes

4 Be able to report on homogeneous and heterogeneous catalysis.

Unit content

1 **Understand the structure of crystalline materials**

Metallic crystal structures: bcc - body centred cubic; ccp - cubic close-packed (face-centred cubic) and hcp - hexagonal close packed structures; examples of metals adopting bcc, ccp and hcp; coordination number of bcc, ccp and hcp structures; unit cells; packing efficiency

Ionic crystal structures: use of x-ray crystallography for determining structure; MX and MX_2 structures including coordination number; ionic radii; limiting radius ratios for NaCl and CsCl structures; structural predictions from radius ratio rule; Born-Haber cycles and lattice enthalpies; factors affecting lattice enthalpies for halides of groups 1 and 2

Theoretical model for ionic crystal lattice: forces of attraction and repulsion between point charges, use of Madelung constant; Born exponent; Born-Lande equation; calculation of lattice enthalpy; comparison of Born-Lande theoretical value of lattice energy with experimental values from Born-Haber cycle

2 **Understand first row d block metal chemistry**

Electron arrangements: distinction between the terms transition metal and d block metal as given by IUPAC definitions; the electronic arrangement of the first row d block metals Sc-Zn, including the deviation of Cr and Cu; order of filling (4s before 3d) and order of loss on cation formation (4s lost before 3d)

Chemistry of first row d-block elements: trends in oxidation states; oxides and halides; redox reactions of first row d block metals; use of standard reduction potentials; $[Cr_2O_7]^{2-}$ and $[MnO_4]^-$ as examples of powerful oxidising agents; hydrolysis e.g. $[Sc(H_2O)_6]^{3+}$ gives acidic solutions in water

Coordination chemistry: ligands; denticity to include examples of monodentate, bidentate, tridentate and ethylene diamine tetra-acetic acid (EDTA) as a hexadentate ligand; formation of complexes; coordination numbers and coordination geometry limited to examples of tetrahedral, square planar, octahedral; naming coordination compounds; isomerism to include structural isomerism, ionisation, hydrate, coordination, linkage and stereoisomerism; geometric and chiral complexes

Stability of complexes: ligand exchange; coordination equilibria; stability constants; stepwise formation constants; trends in formation constants; chelate effect

Experimental work: suitable experiments illustrating relevant content e.g. colours of complexes, colorimeter or UV experiments, ligand exchange and stability constants

3 Understand models of bonding in transition metal coordination complexes

Crystal field model: shapes and orientations of d orbitals; crystal field splitting effects in octahedral and tetrahedral complexes; crystal field splitting parameter; spectrochemical series; effect of metal ion on crystal field splitting parameter; absorption spectra; stabilisation energy; high and low spin configurations; magnetic properties (diamagnetic and paramagnetic); Gouy balance

Ligand field model: comparison of crystal field and ligand field theory; combination of metal and ligand orbitals to give molecular orbitals; energy level diagrams for simple systems (σ bonds only)

4 Be able to report on homogeneous and heterogeneous catalysis

Catalysts: homogeneous and heterogeneous; catalytic efficiency; catalytic cycles; energetic; selectivity; lifetime; poisoning

Homogeneous catalysis: industrial e.g. alkene hydrogenation, hydroformylation (Oxo-process), methanol carbonylation (ethanoic acid synthesis); recent advances to include polymer supported catalysts; biphasic catalysis

Heterogeneous catalysis: surface properties of heterogeneous; physisorption and chemisorption; desorption; catalytic converters; hydrogenation of alkenes; ammonia synthesis; oxidation of sulfur (IV) oxide; structure and applications of zeolites

Learning outcomes and assessment criteria

Learning outcomes On successful completion of this unit a learner will:	**Assessment criteria for pass** The learner can:
LO1 Understand the structure of crystalline materials	1.1 explain the structures of metals 1.2 explain the structure of ionic crystal structures 1.3 analyse data using specified methods for determining lattice enthalpy
LO2 Understand first row d block metal chemistry	2.1 discuss electron arrangements and explain the chemistry of first row d block metals 2.2 explain specified coordination chemistry of first row d block metals 2.3 discuss the stability of complexes in terms of stability constants 2.4 explain experimental observations in terms of the relevant theory
LO3 Understand models of bonding in transition metal coordination complexes	3.1 discuss the application of crystal field theory to account for behaviour of tetrahedral and octahedral complexes of first row d metal elements 3.2 discuss the application of ligand field theory to account for behaviour of octahedral complexes of first row d metal elements 3.3 compare the ligand field and crystal field approach to bonding in complexes
LO4 Be able to report on homogeneous and heterogeneous catalysis.	4.1 report on how catalysts function 4.2 review industrial homogeneous catalysis 4.3 research the use of industrial heterogeneous catalysts including characteristics of their mode of action

Guidance

Links

This unit has particular links with the following units within this qualification:

- *Unit reference number R/601/0349: Inorganic Chemistry*
- *Unit reference number Y/601/0353: Physical Chemistry*
- *Unit reference number M/601/0410: Analytical Chemistry*
- *Unit reference number F/601/0413: Industrial Chemistry.*

Essential requirements

Delivery

There are a number of opportunities to integrate the use of computer software or interactive internet sites. This is particularly valuable when dealing with complex three dimensional structures. Specific examples include hcp, ccp and bcc packing arrangements, visual examples of complex ionic structures, transition metal complexes and d orbital diagrams. There are now many online video demonstrations of coordination chemistry and these may be useful when resources are limited.

Assessment

Learning outcome 1 may be assessed via a structured assignment, although centres may wish to involve some practical tasks, for example using molecular model kits for packing structures. It is advisable to assess learning outcomes 2 and 3 together since they are closely related topics. However, there is flexibility in the assessment of the other learning outcomes. Learning outcome 4 could be assessed in isolation as a learner-centred literature research project.

Resources

Equipment for practical work should be within normal laboratory resources.

The Royal Society of Chemistry website (www.rsc.org) has a large range of resources including the CD ROM *The Molecular World* series: Molecular Modelling and Bonding.

Employer engagement and vocational contexts

The unit content, especially learning outcome 4, may have local relevance. Use of site visits or guest speakers would enhance delivery.