Unit title: Organic Chemistry of Aromatic and Carbonyl Compounds

Unit code: **A/601/0362**
Level: **5**
Credit value: **15**

Aim

This unit covers understanding of aromaticity and optical activity. The chemistry of aromatic and carbonyl compounds are examined with respect to reaction mechanisms and use in synthesis.

Unit abstract

This unit develops and enhances the knowledge of organic chemistry that underpins both the industrial chemistry and the biological applications of organic molecules. The unit covers the concept of aromaticity and examines the chemistry of aromatic and carbonyl compounds from the viewpoint of their reactions, mechanisms and use in synthesis. Stereochemistry and functional group chemistry are also studied to unify the underlying chemistry.

The concept of aromaticity together with mechanisms for electrophilic substitution in both aromatic and substituted aromatic compounds are examined. Knowledge of these mechanisms is used to rationalise an understanding of the use of aromatic compounds in the synthesis of di-and tri-substituted benzene derivatives. The organic chemistry of carbonyl compounds is treated in a similar manner with knowledge of mechanistic pathways being used to support their varied synthetic uses.

The unit concludes by focusing on aspects of optical isomerism including stereochemical representation and nomenclature. The relevance of stereochemistry in chemical reactions and biological systems is considered in terms of asymmetric synthesis and examples of biologically active compounds.

Learning outcomes

On successful completion of this unit a learner will:

1. Understand the structure of aromatic compounds
2. Understand the synthetic use of substitution reactions of aromatic compounds
3. Understand the synthetic use of carbonyl compounds
4. Understand structures and reactions of optically active molecules.

Unit content

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1 Understand the structure of aromatic compounds

The electronic structure of benzene: physical structure; methods of representation; bonding, sp^2 hybridisation, bond lengths, resonance, stabilisation in terms of resonance energy or delocalisation energy; molecular orbital model

Experimental evidence: hydrogenation enthalpy; bond lengths; resistance to typical electrophilic addition reactions

Categorise aromatic hydrocarbon systems: identification of aromatic and anti-aromatic hydrocarbon systems using Hückel's rule to the following systems (planar, fully conjugated, monocyclic systems with $4n + 2$ π electrons)

Aromatic heterocycles: application of Hückel's rule to simple heterocyclic systems e.g. pyridine, pyrrole, furan

Experimental data: use of chemical and spectroscopic evidence to elucidate structures e.g. characteristic ^1H NMR signals of aromatic hydrogens, characteristic infrared bands

2 Understand the synthetic use of substitution reactions of aromatic compounds

Mechanisms of electrophilic substitution: nitration; sulfonation; Friedel-Crafts alkylation; Friedel-Crafts acylation and halogenations using halogen carrier

Reactivity of substituted benzenes: in electrophilic substitutions*;* effect of existing substituent on rate and position of further electrophilic substitution; nucleophilic substitution; effect of leaving groups; use in synthesis

Synthetic pathways: applications to synthesis of di-substituted and tri-substituted benzene compounds

Commercial applications: examples of substituted benzenes e.g. ibuprofen, salbutamol, aspirin, paracetamol, phenols

3 Understand the synthetic use of carbonyl compounds

Acidity of carbonyl compounds: acidity of α-hydrogens and formation of enolate ions; enolisation of carbonyl compounds including aldehydes, ketones and esters; use of equilibrium constants as a measure of stability of carbonyl compound relative to corresponding enol; examples of stable enols e.g. those that form intramolecular hydrogen bonds; acid catalysed α-halogenations of aldehydes and ketones; halogenations of aldehydes and ketones in base e.g. haloform reaction, iodoform test

Aldol addition and aldol condensation: base catalysed aldol addition reactions; dehydration of aldol addition products leading to formation of α,β-unsaturated carbonyl compounds; crossed aldol reactions e.g. Claisen-Schmidt condensation

Condensation reactions involving ester enolate ions: Claisen condensation and crossed Claisen condensations; synthesis using Claisen condensations e.g. β-keto esters, β-diketones

Alkylation of ester enolate ions: malonic ester synthesis; acetoacetic ester synthesis

Conjugate addition reactions: conjugate addition to α,β unsaturated carbonyl compounds e.g. α,β-unsaturated esters, α,β-unsaturated ketones, enolate ions, Michael addition, Robinson annulations; conjugate addition reactions versus carbonyl addition as an example of kinetic versus thermodynamic control

4 Understand structures and reactions of optically active molecules

Chiral molecules: molecules containing chiral carbon atoms; R/S notation and nomenclature

Optical rotation: simple calculations involving optical rotation and specific optical rotation; racemic mixtures

Resolution of enantiomers: chemical and chromatographic resolution and separation of enantiomers

Diastereoisomers: limited to examples with two chiral centres; physical properties

Stereochemical representations: use of molecular models to demonstrate the stereochemical nature of molecules; Fischer and Newman projections; use of (R) and (S) sequence rules

Reactions involving optical activity: examples of reactions that involve optical isomers; formation of racemic mixtures; asymmetric synthesis

Biological systems: examples of optical isomerism in biological systems e.g. drug synthesis in the pharmaceutical industry, taste (flavours), sugars, amino acids, pesticides/fertilisers, natural products

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 aromatic compounds	1.1 explain the structure of benzene in terms of a delocalised π system and molecular orbitals 1.2 review experimental evidence to support current model of benzene structure 1.3 categorise hydrocarbon and heterocyclic structures as aromatic or anti-aromatic using Hückel's rules 1.4 analyse experimental data to elucidate structures of aromatic compounds
LO2 Understand the synthetic use of substitution reactions of aromatic compounds	2.1 explain, using mechanisms, specified electrophilic substitution reactions 2.2 explain the effect of substituent on electrophilic and nucleophilic reactivity of substituted benzenes 2.3 discuss different synthetic pathways for the synthesis of substituted benzene compounds 2.4 explain the importance of aromatic compounds in a commercial context
LO3 Understand the synthetic use of carbonyl compounds	3.1 review acidity of carbonyl compounds in enolisation and explain the role of aldol reactions in synthesis 3.2 discuss the synthetic role of ester enolate condensation reactions 3.3 explain alkylation of ester enolates in a synthetic context 3.4 discuss synthetic pathways using conjugate addition reactions
LO4 Understand structures and reactions of optically active molecules	4.1 explain (+) (-) and R/S notation and calculate optical rotations using given data 4.2 explain the resolution of enantiomers 4.3 discuss the properties of diastereoisomers 4.4 use Fischer stereochemical representations for R/S enantiomers 4.5 discuss reactions involving optical activity and the importance of optical activity in biological systems

Guidance

Links

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

- *Unit reference number R/601/0352: Organic Chemistry*
- *Unit reference number H/601/0355: Chemical Laboratory Techniques*
- *Unit reference number M/601/0410: Analytical Chemistry*
- *Unit reference number R/601/0416: Medicinal Chemistry*
- *Unit reference number F/601/0413: Industrial Chemistry*
- *Unit reference number F/601/0217: Biochemistry of Macromolecules and Metabolic Pathways*
- *Unit reference number L/601/0415: Polymer Chemistry*

Essential requirements

Delivery

Where possible, tutors must select illustrative material to emphasise the relevance of the learning outcomes to everyday life or industrial application.

It may be appropriate to develop and organise the unit in a relatively classical manner around a theme that illustrates concepts of organic chemistry. Possible themes and features include emphasis on industrial, biological, medical, environmental, cosmetics and nutritional applications of organic chemistry.

Assessment

The learning outcomes can be treated individually if desired, although there are opportunities to integrate learning outcome 4 with some of the reactions in learning outcome 3. Similarly, learning outcomes 1 and 2 may be assessed together since they are both aromatic themes.

Resources

Learners will need access to library and information technology resources, tutorial and technical support, molecular models and laboratory facilities to demonstrate experiments.

Employer engagement and vocational contexts

Where possible, the content should be delivered within a vocational context. The emphasis should be on synthetic routes and there are numerous industrial examples. Site visits or visiting speakers may also enhance content.