 Year 12 Chemistry

Module 8 – Analysis of Organic Substances

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Duration

5-6 hours

Description of unit

The identification and analysis of chemicals is of immense importance in scientific research, medicine, environmental management, quality control, mining and many other fields.

Students investigate a range of methods used to identify and measure quantities of chemicals. They investigate and process data involving the identification and quantification of ions present in aqueous solutions. This is particularly important because of the impact of adverse water quality on the environment. Students deduce or confirm the structure and identity of organic compounds by interpreting data from qualitative tests of chemical reactivity and determining structural information using proton and carbon-13 nuclear magnetic resonance (NMR) spectroscopy.

Focus questions

* How is information about the reactivity and structure of organic compounds obtained?

Working scientifically skills

* CH11/12-1 Develops and evaluates questions and hypotheses for scientific investigation
* CH11/12-3 Conducts investigations to collect valid and reliable primary and secondary data and information
* CH11/12-4 Selects and processes appropriate qualitative and quantitative data and information using a range of appropriate media
* CH11/12-7 Communicates scientific understanding using suitable language and terminology for a specific audience or purpose

Outcomes

* CH12-15 Describes and evaluates chemical systems used to design and analyse chemical processes

Assessment

* Formative assessment of depth study

| Outcomes and content | Teaching and learning | Evidence of learning |
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| Conduct qualitative investigations to test for the presence in organic molecules of the following functional groups:* Carbon-carbon double bonds
* Hydroxyl groups
* Carboxylic acids (ACSCH130)
 | Using molecular molecule kits, students are to create models of an alkene, an alkanol and an alkanoic acid. They should recall how to name them.Students are to use their models to demonstrate the chemical reactions that occur in each of the three tests outlined below.Students are to perform a first-hand investigation to identify the presence of different functional groups on organic molecules.Samples of hexane, hexene, hexanol and hexanoic acid in separate test tubes are to undergo three tests (a fresh sample is to be used for each).1. C=C bonds – Bromine Water Test
	* Add a few drops of bromine water to each test tube and observe any colour changes.
2. -OH groups – Ester Test
	* Add ethanoic acid along with a few drops of concentrated H2SO4. Allow to sit for 30 minutes and test for a fruity odour.
3. -COOH – Ester Test
	* Add ethanol along with a few drops of concentrated H2SO4. Allow to sit for 30 minutes and test for a fruity odour.

Summarise results in an appropriate table. Include balanced chemical reactions for the confirmatory reaction in each test. | Students should be able to:* Outline the method used to identify each of the functional groups
* Clearly state the criteria for determining the presence of each functional group and support each with a suitable chemical equation
* Infer the presence of various functional groups from experimental data
* Outlinine the set of tests required to identify an unknown substance containing one of the named functional groups
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| Investigate the processes used to analyse the structure of simple organic compounds addressed in the course, including but not limited to:* Proton and Carbon-13 NMR
* Mass spectroscopy (ACSCH19)
* Infrared spectroscopy (ACSCH130)
 | EngageBrainstorm where fast and accurate analysis of chemical composition would be useful.ExploreResearch question* How do IR/MS/NMR spectrums identify or distinguish between:
	+ Chemicals in a homologous series (initially limited to COOH, -OH and C=C/C-C)
	+ Different functional groups
	+ Structural isomers

In small groups or as individuals, students are to investigate one of these questions by first collecting a relevant set of spectral data. Sources may include:* [Search for Species Data by Chemical Name](http://webbook.nist.gov/chemistry/name-ser/) (NIST)
	+ Provides IR and mass spectral data. Students can search for a compound by name or by formula.
* [Spectral Database for Organic Compounds](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi) (AIST Japan)
	+ Provides IR, mass and NMR spectral data; however, the NIST site has a clearer layout. Again, students can search by name or formula.

Groups are to collate spectral graphs of at least three compounds and describe results through presentation of the selected spectra so that they can be easily compared. (Sample sets of spectra have been provided with the additional resources.)ExplainEach group is to describe to the class the type(s) of spectra that are useful for the task they were investigating and describe the key features of the spectra. Tabulate results on board.Next provide students some examples of pairs of chemicals with similar/contrasting properties. Using the Predict-Observe-Explain method:1. Students predict the features/similarities/differences they expect to see in the spectra.
2. Teacher presents the spectra to students, side by side using a projector (or handout if necessary). Use think-pair-share to describe what students observe. Write points on the board.
3. Each student is to develop an explanation for one or more of the points written on the board.

ElaborateAs a class, generate a simple set of rules for:* Which spectra can identify particular functional groups
* Which spectra can determine molecular size/mass
* Which spectra can distinguish between structural isomers

Along with which features of each spectra are used.Ask students to consider why using a variety of techniques would be useful.Show students the infographics on IR, mass and C-13 NMR spectroscopy from the Compound Interest website (these are also provided in the additional resources).EvaluateClass discussion:* How complete is your understanding?
* What questions do you have that remain unexplained?

Follow-up Activity – Individual ResearchStudents are to complete a case study, researching an application of at least one of the techniques studied. The application may be drawn from the following fields: scientific research, medicine, environmental management, quality control or mining. | Students should be able to:* Describe the useful information obtained from a range of analytical processes used for investigating organic substances.
* Correctly deduce the compound name or homologous series when given a spectral graph, an appropriate reference sheet and a list of possible compounds or molecular formula.
* Discuss the importance of analytical techniques to a variety of fields and support their discussion with a case study.
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| (Alternative approach)Investigate the processes used to analyse the structure of simple organic compounds addressed in the course, including but not limited to:* Carbon-13 NMR
* Mass spectroscopy (ACSCH19)
* Infrared spectroscopy (ACSCH130)
 | For each of the three processes:* Define the key terms
* Outline the function of apparatus
* Describe the results obtained from process
* Relate features of the results to the structure/function of analyte
* Discuss the strengths/weaknesses of the technique
* Provide examples of application
* Suggest further confirmatory tests

Demonstrate the usefulness/limitations of each technique by comparing the results observed for at least two similar substances. For example:* Comparison of two compounds with same molecular formula
	+ C6H12O (either Cyclohexanol or 3-Hexanone) – While the mass spectrum hints at some difference, the IR spectrum clearly indicates the presence of O-H and C=O bonds respectively. C13-NMR also clearly distinguishes between the ketone and alcohol.
* Comparison of two compounds with same functional groups
	+ Hexane and Pentane produce almost identical IR spectra. They can, however, be easily distinguished from the molecular ion peaks on their respective mass spectra. The C-13 NMR spectra are very similar in terms of the number of peaks, however, the relative intensity of the peak associated with the centre two carbons in hexane is approximately double that of the corresponding peak in pentane.

Discuss the value of combining techniques.Students are to complete a case study, researching an application of at least one of the techniques studied. The application may be drawn from the following fields: scientific research, medicine, environmental management, quality control or mining. | Students should be able to:* Describe the useful information obtained from a range of analytical processes used for investigating organic substances.
* Correctly deduce the compound name or homologous series when given a spectral graph, an appropriate reference sheet and a list of possible compounds or molecular formula.
* Discuss the importance of analytical techniques to a variety of fields and support their discussion with a case study.
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| Additional resources | Sample Spectral Data* [C-13 Chemical Shifts](http://www.chem.wisc.edu/areas/reich/nmr/c13-data/cdata.htm) (University of Wisconsin)
* [Search for Species Data by Chemical Name](http://webbook.nist.gov/chemistry/name-ser/) (NIST)
* [Spectroscopy Learning Goals](http://www.science.oregonstate.edu/~gablek/CH335/Chapter10/Spectroscopy_LG.htm) (Oregon State University)
* [Spectral Database for Organic Compounds](http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi) (AIST Japan)

All of the above sites can be used to source spectral data for use by students.Further Reading* [The power of ion mobility – mass spectrometry for structural characterisation and the study of conformational dynamics](https://www.nature.com/articles/nchem.1889?foxtrotcallback=true)
	+ Table of advantages and disadvantages of analytical techniques from a Nature Chemistry article. To be used to support further understanding of the need for effective selection of analytical technique(s).
* [C-13 NMR](http://www.chemguide.co.uk/analysis/nmr/backgroundc13.html)
* [Simplified MRI](https://phet.colorado.edu/en/simulation/legacy/mri) (PhET)
	+ A simulated model of NMR demonstrating the relationship between applied magnetic field and resonant frequency.
* [Applications of NMR](http://sydney.edu.au/science/chemistry/facilities/nmr/nmr-applications.shtml) (University of Sydney)
	+ Outlines the applications of NMR Spectroscopy along with some advantages of this method and particular applications.
 |  N/A |
| Potential areas for depth study | * Research the historic significance and/or current research utilising x-ray crystallography.
* Construct a model to demonstrate the principle of operation of one of the analytical techniques studied.
* Complete a comprehensive study on the operation and potential applications of 1H and 13C NMR.
* Investigate and present the mathematics of the Fourier Transform as it applies to spectroscopy.
* Research and present how NMR is used in MRI for diagnostic purposes along with its relative advantages over other diagnostic techniques.
* QA processes in polymer production
 | N/A |

Reflection and evaluation