November Lectures 2015
Workshop B7

Using light to solve chemical puzzles

Year 11 research assessment task which presents independent findings as a scientific digital poster

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Study design

Unit 1 – Area of Study 3: Research Investigation

In this area of study students apply and extend their knowledge and skills developed in Area of Study 1 and/or Area of Study 2 to investigate a selected question related to materials.

10 Options offered:

- Option 1: The origin of the elements
- Option 2: The development of the periodic table
- Option 3: The lanthanoids and actinoids
- Option 4: Using light to solve chemical puzzles
- Option 5: Glass
- Option 6: Crude oil
- Option 7: Surfactants
- Option 8: Polymers and composite materials
- Option 9: Nanomaterials
- Option 10: The life cycle of a selected material or chemical

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Option 4: Using light to solve chemical puzzles

Questions that may be explored in this investigation include:

- What is a crystal, and why do crystals have regular faces?
- What makes synchrotron light useful?
- What can a synchrotron tell us about the differences between salt and sugar crystals?
- How does the composition of a crystal relate to the bonding within and the ratios of the elements present?
- Given that crystals are not alive or functioning, how is it that crystal structures are used to understand biological functions?
- What significant discoveries contributed to the development of X-ray crystallography as an analytical technique?
- How does cryoprotection preserve protein samples for analysis in a synchrotron?
- How has the use of a synchrotron enabled Nobel Prize winning research to occur?
- Why use synchrotron light to determine crystal structure when other sources of X-rays can be used?
- How does the IR beamline in the Australian Synchrotron enable the study of organic molecules and covalent bonding patterns?

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Students undertake a research investigation relevant to one of the following ten options.

A question from the list under each option may be selected or students may develop their own research question relevant to Area of Study 1 and/or Area of Study 2 in conjunction with their teacher.

For the selected question, students outline, analyse and evaluate relevant evidence to support their conclusions.

For Area of Study 3, between 4 and 6 hours of class time should be devoted to undertaking the investigation and communicating findings.

Three suggested themes for the assignment

A. Obtaining chemical information from synchrotron radiation

B. The use of synchrotron X-rays to determine molecular structure via diffraction methods

C. Using the results of X-ray diffraction experiments to understand important biological systems

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Background research on light (the electromagnetic spectrum)

1. Resources relating to the electromagnetic spectrum – background reading for all three themes.

https://en.wikipedia.org/wiki/Electromagnetic_spectrum

http://missionscience.nasa.gov/ems/01_intro.html

http://www.physicsclassroom.com/class/light/Lesson-2/The-Electromagnetic-and-Visible-Spectra

https://www.youtube.com/watch?v=hXe7EVv1y0Q
- a 30 minute video providing an introduction to the EMS

http://earthguide.ucsd.edu/eoc/special_topics/teach/sp_climate_change/p_emspectrum_interactive.html
- interactive web site

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Important concepts to grasp concerning electromagnetic radiation

- light behaves like a wave
- the wavelength of light determines the type of radiation
- the shorter wavelength the higher the energy of the wave
- visible light is only a small part of the EMS

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Australian Synchrotron

The Australian Synchrotron is located on Blackburn Road, Clayton

It provides light ranging from microwaves to very high energy X-rays.

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In a synchrotron electrons are accelerated to a speed very close to the speed of light around a giant loop.

This process results in the emission of very bright light – more than a million times brighter than the sun.

Light is directed into *beamlines* and the light is tuned to specific wavelengths.

We are able to probe the nature of matter by studying how the radiation interacts with samples being investigated.

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Australian Synchrotron

The brighter the light, the more information we obtain.

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Information about synchrotrons provides direct introductory information for the following two themes:

A. Obtaining chemical information from synchrotron radiation

B. The use of synchrotron X-rays to determine molecular structure via diffraction methods

It provides background information for the third topic:

C. Using the results of X-ray diffraction experiments to understand important biological systems

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Resources for Synchrotron
– important information for topics A and B and background for C

The following resources provide a general overview of synchrotron radiation:

http://www.synchrotron.org.au/synchrotron-science/what-is-a-synchrotron

http://www.synchrotron.org.au/synchrotron-science/what-is-synchrotron-light

http://www.synchrotron.org.au/synchrotron-science/how-is-synchrotron-light-created

http://www.synchrotron.org.au/images/newsEventsPublications/Publications/as_introduction%20brochure_final.pdf

http://www.lightsources.org/what-light-source

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Theme A
Obtaining chemical information from synchrotron radiation

Consider the technique of

Infra-red spectroscopy
http://www.rsc.org/learn-chemistry/collections/spectroscopy/introduction#IRSpectroscopy

https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay/infrared-spectroscopy-theory/v/introduction-to-infrared-spectroscopy
-useful video

IR spectroscopy provides qualitative information concerning functional groups

It can provides quantitative information about the strength of bonds.

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Theme A
Obtaining chemical information from synchrotron radiation

Consider the technique of

X-ray Photoelectron Spectroscopy
http://xpssimplified.com/whatisxps.php

XPS provides information regarding elemental composition on a surface.

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X-ray diffraction – maybe used for theme A but important for themes B and C

If radiation with a wavelength comparable to atomic separations is used, then it is possible to generate a diffraction pattern from the crystal.

Through analysis of the diffraction pattern we can determine molecular structure.

A crystal diffracts X-rays because of the the regular, periodic repetition of atomic and molecular components in the crystal.

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Bragg's Law
(theme B with background for theme C)

When X-rays strike a crystal, reflection from lattice planes can occur.

The reflected waves interfere with each other in a destructive or constructive manner.

$$n\lambda = 2d\sin\theta$$

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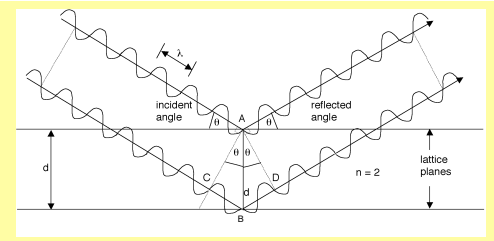
The conditions required for reflection are represented by Bragg's Law:

$n\lambda = 2d\sin\theta$

where n = an integer (the order of the reflection)
λ = the wavelength of the radiation
d = the interplanar separation
θ = the angle of incidence of the reflection



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Resources for X-ray diffraction – information for all three themes but in particular B and some background for C

http://web.pdx.edu/~pmoeck/phy381/Topic5a-XRD.pdf
- some highly technical information but some good material on the basics

http://www-outreach.phy.cam.ac.uk/camphy/xraydiffractionxraydiffraction_exp.htm
- interactive demonstration of Bragg's Law

http://chemwiki.ucdavis.edu/Analytical_Chemistry/Instrumental_Analysis/Diffraction/X-ray_Crystallography
- highly technical in parts but a nice overview with good pictures

https://www.youtube.com/watch?v=fZ0m8wustVk - a nice video

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For theme C – students will need some background on proteins

Students need to appreciate that proteins are large, complex biomolecules whose structure is linked to its function.
- textbooks
- general web references

If we can understand the structure then when we can understand how it performs the various roles it has.

The structure-function relationship needs to be established.

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Protein crystal structures – important information for topic C

https://www.jic.ac.uk/staff/david-lawson/xtallog/summary.htm
- the introductory material is good

https://www.youtube.com/watch?v=fZ0m8wustVk
- a nice video

http://www.rcsb.org/pdb/home/home.do#Category-welcome
- the protein crystallographic database – a useful and very powerful research tool

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For theme C, propose that students select an important protein and then investigate how its structure relates to its function.

Suggested proteins:

Haemoglobin – oxygen transport

Carbonic anhydrase – catalyses the reaction of CO_2 with water so that CO_2 can be removed from our system

Ferritin - Iron storage protein

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Haemoglobin

The haem group

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Haemoglobin

https://en.wikipedia.org/wiki/Hemoglobin

http://www.chemistry.wustl.edu/~edudev/LabTutorials/Hemoglobin/MetalComplexinBlood.html

http://www.rcsb.org/pdb/101/motm.do?momID=41

https://www.youtube.com/watch?v=qs3xONv548I

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Carbonic anhydrase – a zinc enzyme

Consider the reaction of CO_2 and water

$$CO_2 + OH_2 \rightleftharpoons HCO_3^- + H^+$$

In tissue the forward reaction is favoured.
In lungs the backward reaction is favoured.

The transport of "CO_2" is more efficient as the bicarbonate ion.

Problem: the reaction is too slow under physiological conditions

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Carbonic anhydrase

Nature has evolved the catalyst carbonic anhydrase to increase these rates by factor of 10^8 !

Molar mass: 30,000

1 Zn atom

X-ray diffraction has revealed the molecular structure at the active site.

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Carbonic anhydrase

The reaction between H_2O and CO_2 is faster if the the reactants are bound to a Zn(II) centre.

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Carbonic anhydrase

http://www.rcsb.org/pdb/101/motm.do?momID=49

https://en.wikipedia.org/wiki/Carbonic_anhydrase

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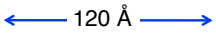
Ferritin: A protein coat with a "rust" core



ribbon models

ball & stick model

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Ferritin

Single protein chain as subunit

24 subunits associate via ionic bonds, H-bonds, etc
→ "hollow sphere" ~ 120 Å external diameter

subunit

Ferritin – Protein outer coat or shell

Subunits –
roughly cylindrical

163 amino acids

predominantly
α-helices

24 subunits – cubic symmetry

Ferritin core

Ferritin core 70-75 Å -
entire structure 120 Å

(C-C single bond ~1.54 Å;
Fe(III)-O bond ~1.96 Å)

predominantly FeO(OH)
with phosphate

Ferritin core

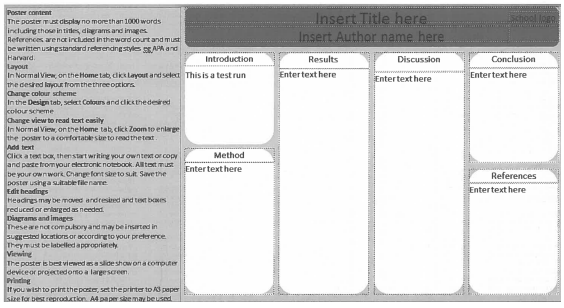
Core MW ~ 418,000

~ 4500 Fe atoms !!

Ferritin

http://www.chemistry.wustl.edu/~edudev/LabTutorials/Ferritin/Ferritin.html
http://www.rcsb.org/pdb/101/motm.do?momID=35

Poster Presentation



Poster Structure – emphasis on pictures rather than words

Introduction
Background information regarding the topic
Finish with a research question

Results and Discussion
- For posters, readers do not want to wade through long sections of text
- Use clear pictures that tell a story
- Figure captions should explain the picture
- Use sub-headings to break it into manageable "bites"
- It is often useful to pose sub-questions and use these as headings
  e.g. *What is a synchrotron?*

Conclusion
This should be brief and describe the main findings of the research

References

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Proposed questions

Theme A - Obtaining chemical information from synchrotron radiation

What is synchrotron radiation and how can we use it to investigate molecules through infra-red spectroscopy?

What is a synchrotron and how can we use it to investigate the composition of matter using X-ray photoelectron spectroscopy?

What is synchrotron radiation and how can we use it to investigate the composition and structure of materials?

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Proposed questions

Theme B - The use of synchrotron X-rays to determine molecular structure via diffraction methods

How can synchrotron radiation allow us to determine the molecular structure within crystals?

What is X-ray diffraction and how is it used in a synchrotron to determine the structure of molecules?

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Proposed questions

Theme C - Using the results of X-ray diffraction experiments to understand important biological systems

How can synchrotron radiation help us to understand the transport of oxygen in blood?

How can synchrotron radiation help us to understand how the body is able to transport CO_2 from tissue to the lungs?

How does the body store iron and how has synchrotron radiation helped us to understand this process?

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Poster presentation assessment rubric

Group name _____ Group topic _____

Name of examiner _____

Criteria	0	1	2	3	4
Organisation	Cluttered organisation with no clear sections or headings. Audience cannot understand the presentation.	Headings and sections present but no transition between sections or logical flow. Audience has difficulty following the presentation.	Headings and sections present, sections flow logically but little relationship between visuals and text. Audience must ask questions to make sense of the presentation.	Headings and sections present, text to visuals relationship is good. Sequence is logical but audience must re-read for clarity.	Clear headings and well-defined sections. Easy to navigate flow to assist the reader understand message. Presentation is logical, creative and interesting; audience follows easily.
Content	Key concepts and issues not addressed	Adequate identification of key concepts and issues and sufficient response to the task.	Good identification of key concepts and issues and credible response to the task.	Convincing response to the key concepts and issues and very good response to the task.	Excellent identification of key concepts and issues and response to task demonstrates originality and insight.

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Poster presentation assessment rubric

Criteria	0	1	2	3	4
Critical thinking	Absence of demonstrable critical thinking and analysis and synthesis of concepts.	Attempt to demonstrate critical thinking and analysis and synthesis of concepts.	Demonstrates emerging critical thinking skills with analysis and synthesis of concepts.	Highly developed critical thinking skills are displayed with demonstrated analysis and synthesis of concepts.	Excellent critical thinking skills are displayed with highly developed analysis and synthesis of concepts.
Visual appeal	Unclear presentation of results and no use of colour, layout or visuals (images, tables, charts, diagrams, etc.).	Unclear presentation of results and no balance between visuals and text. The poster is text heavy.	Clear presentation of results but very little use of colour or visuals to engage the audience.	Good presentation of results and discussion and sufficient use of colour and visuals to engage the audience but not stimulate.	Layout is engaging and intuitive, and supports the message of the presentation. Interesting, relevant visuals and use of colour and space.

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Poster presentation assessment rubric

Criteria	0	1	2	3	4
Communication	Sentence construction, grammar and expression are incoherent. Absence of appropriate use of discipline specific language. Interaction with audience does not clarify information.	Sentence construction, grammar and expression are fluent in patches. Attempts to use appropriate and discipline specific language. Interaction with audience is prompted and scant.	Sentence construction, grammar and expression are predominantly coherent. Emerging use of appropriate and discipline specific language to demonstrate understanding to audience. Engages audience in discussion of topic, adding further detail.	Sentence construction, grammar and expression are coherent. Frequent use of appropriate and discipline specific language to demonstrate understanding to audience. Audience is drawn into discussion and concepts are discussed in great detail.	Sentence construction, grammar and expression are very coherent. Comprehensive use of appropriate and discipline specific language to demonstrate understanding to audience. Excellent rapport with audience, engaging them in the topic and exploring further ideas.

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Thank you and good luck

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Additional slides re carbonic anhydrase

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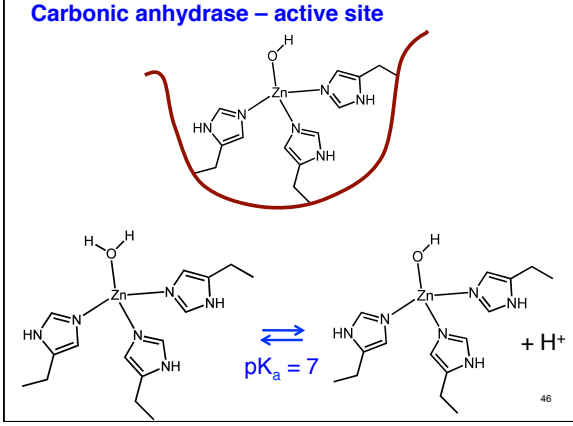
Carbonic anhydrase – active site



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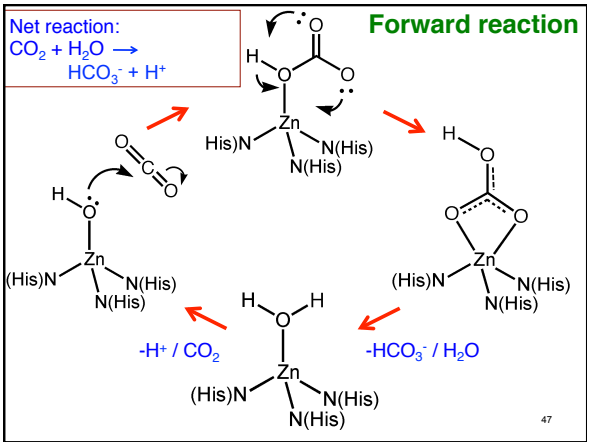
Net reaction:
$CO_2 + H_2O \longrightarrow HCO_3^- + H^+$

Forward reaction



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