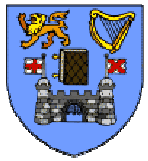
Chemistry for Health Sciences

2007



These notes can be found on:

http://www.tcd.ie/Chemistry/People/gunnlaugsson/resources.php

Organisation

Michaelmas term

- **Organic Chemistry**
  - Me! Prof. Thorfinnur Gunnlaugsson
    - 5 weeks (almost!)
- Physical Chemistry
  - Prof. John Corish
  - Dr. Dónall Macdónaill
    - 4 weeks

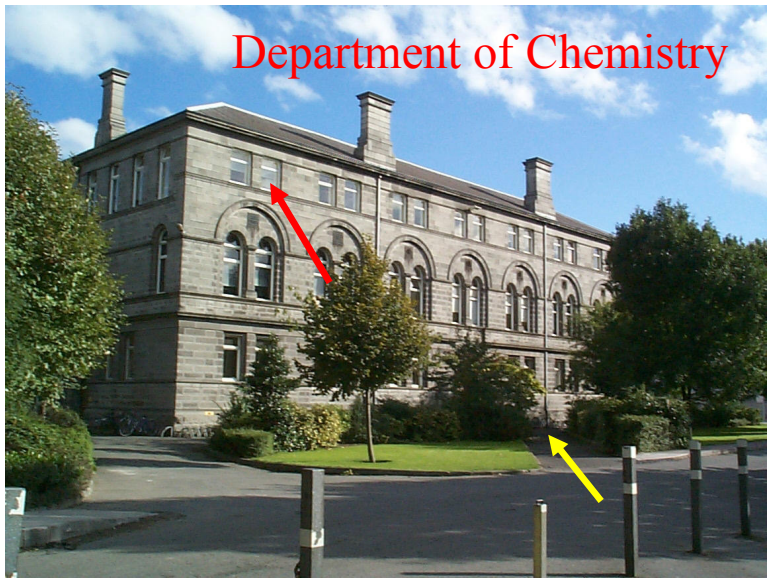
Organisation

Lecturer:

- Professor Thorfinnur Gunnlaugsson.
  - Room: 2.4
  - E-mail: gunnlaut@tcd.ie
  - Phone: 608 3459

Textbooks:

- **Organic Chemistry: A Short Course**
  - **by H. Hart or McMurray**
- Organic Chemistry. 8th Ed
  - by T. W. Solomons
- Organic Chemistry
  - by Clayden, Greeves, Warren and Wothers



Organisation

Overview

- Introduction
  - **Simple functional groups**
  - **Drawing organic structures**
  - **Nomenclature of Organic chemistry**
- Bonding
  - **Intramolecular**
    - **Ionic bonds, covalent bonds (hybridisation)**
  - **Intermolecular**
    - **Hydrogen bonding, Dipole-dipole interactions**

Organisation

Overview

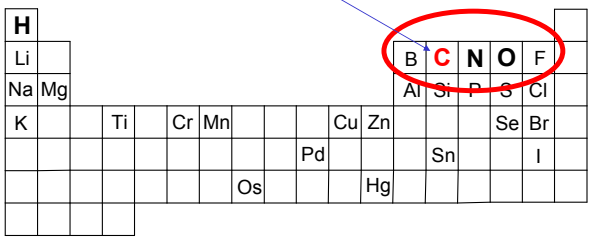
- **Alkanes, Alkenes, Alkynes and Benzene**
- **Halogen Compounds, Alcohols,**
  - Stereochemistry
  - Isomers, chirality
- **Phenols, Ethers, Amines**

Duration

- **4-5 weeks**

Introduction

- Deals with compounds in which **carbon** (C) is the principle element
- Not whole periodic table



Introduction

What is Organic Chemistry?

- **Chemistry:**
  - Small or large assembly of covalently liked atoms where carbon and hydrogen dominate!

  eg. Alcohols, small drugs *etc.*
- **Biology:**
  - The living organisms: *eg.* Cells, plants and animals
- **Biochemistry:**
  - The chemistry of life: *eg.* Enzymes and their role, DNA, Carbohyhdrates, *etc.*

Introduction

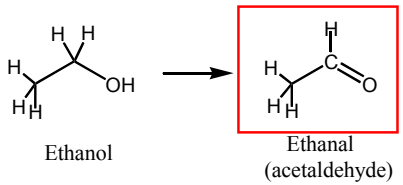
Organic Chemistry

- **May/may not involve natural process**

A → B

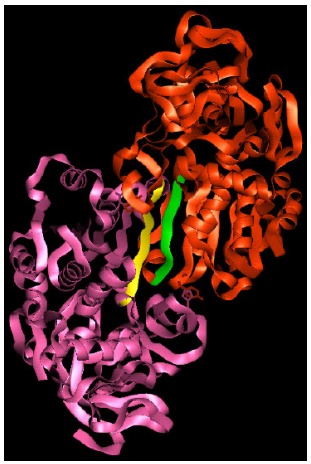
- **Organic chemists use** REAGENTS / CATALYSTS in SYNTHESIS, **employing solvents, heat, pressure, *etc*.**
- Nature uses ENZYME, cofactors, *etc*.

Introduction



Ethanol

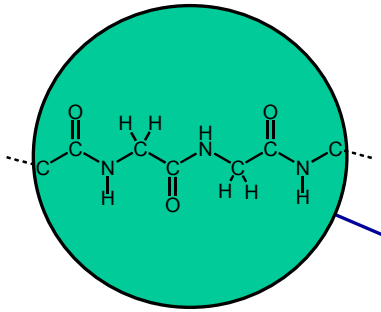
Ethanal (acetaldehyde)

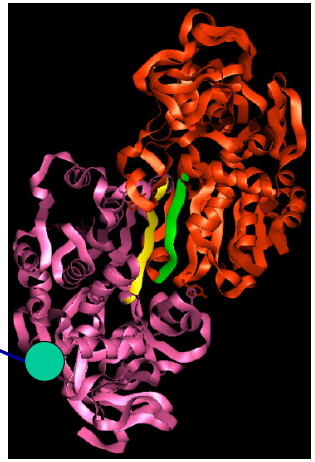


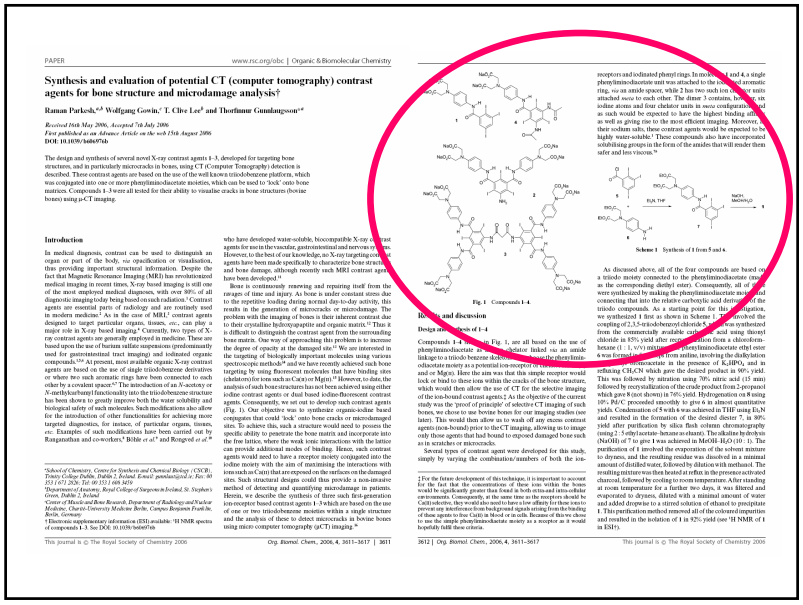
- Nature uses ADH
- Organic chemist uses:
  - Oxidising agent
  - H_2O_2, HNO_3, *etc.*

Introduction

- Even enzymes are organic!







PAPER www.rsc.org/obc | Organic & Biomolecular Chemistry

Synthesis and evaluation of potential CT (computer tomography) contrast agents for bone structure and microdamage analysis†

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The design and synthesis of several novel X-ray contrast agents 1–3, developed for targeting bone structures, and in particularly microcracks in bones, using CT (Computer Tomography) detection is described. These contrast agents are based on the use of the well known triiodobenzene platform, which was conjugated into one or more phenyliminodiacetate moieties, which can be used to 'lock' onto bone matrices. Compounds 1–3 were all tested for their ability to visualise cracks in bone structures (bovine bones) using μ-CT imaging.

Introduction

In medical diagnosis, contrast can be used to distinguish an organ or part of the body, *via* opacification or visualisation, thus providing important structural information. Despite the fact that Magnetic Resonance Imaging (MRI) has revolutionized medical imaging in recent times, X-ray based imaging is still one of the most employed medical diagnoses, with over 80% of all diagnostic imaging today being based on such radiation.[1] Contrast agents are essential parts of radiology and are routinely used in modern medicine.[2] As in the case of MRI,[3] contrast agents designed to target particular organs, tissues, *etc.*, can play a major role in X-ray based imaging.[4] Currently, two types of X-ray contrast agents are generally employed in medicine. These are based upon the use of barium sulfate suspensions (predominantly used for gastrointestinal tract imaging) and iodinated organic compounds.[5,6] At present, most available organic X-ray contrast agents are based on the use of single triiodobenzene derivatives or where two such aromatic rings have been connected to each other by a covalent spacer.[6,7] The introduction of an *N*-acetoxy or *N*-methylcarbamoyl functionality into the triiodobenzene structure has been shown to greatly improve both the water solubility and biological safety of such molecules. Such modifications also allow for the introduction of other functionalities for achieving more targeted diagnostics, for instance, of particular organs, tissues, *etc.* Examples of such modifications have been carried out by Ranganathan and co-workers,[8] Böhle *et al.*[9] and Rongved *et al.*[10]

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† Electronic supplementary information (ESI) available: 1H NMR spectra of compounds 1–3. See DOI: 10.1039/b606970b

Fig. 1 Compounds 1–4.

who have developed water-soluble, biocompatible X-ray contrast agents for use in the vascular, gastrointestinal and nervous systems.[11] However, to the best of our knowledge, no X-ray targeting contrast agents have been made specifically to characterize bone structure and bone damage, although recently each MRI contrast agents have been developed.[12]

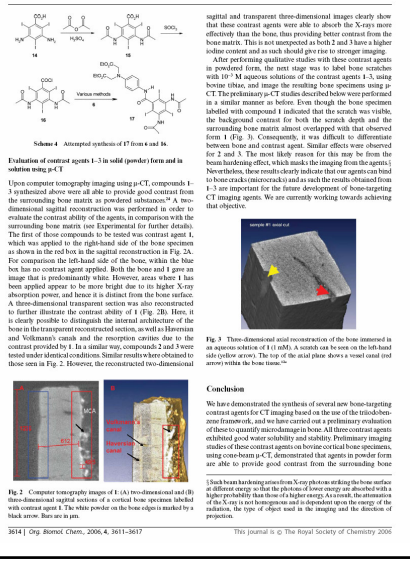
Bone is continuously renewing and repairing itself from the ravages of time and injury. As bone is under constant stress due to the repetitive loading during normal day-to-day activity, this results in the generation of microcracks or microdamage. The problem with the imaging of bones is their inherent contrast due to their crystalline hydroxyapatite and organic matrix.[13] Thus it is difficult to distinguish the contrast agent from the surrounding bone matrix. One way of approaching this problem is to increase the degree of opacity at the damaged site.[13] We are interested in the targeting of biologically important molecules using various spectroscopic methods[14] and we have recently achieved such bone targeting by using fluorescent molecules that have binding sites (chelators) for ions such as Ca(II) or Mg(II).[15] However, to date, the analysis of such bone structures has not been achieved using either iodine contrast agents or dual based iodine/fluorescent contrast agents. Consequently, we set out to develop such contrast agents (Fig. 1). Our objective was to synthesize organic-iodine based conjugates that could 'lock' onto bone cracks or microdamaged sites. To achieve this, such a structure would need to possess the specific ability to penetrate the bone matrix and incorporate into the free lattice, where the weak ionic interactions with the lattice can provide additional modes of binding. Hence, such contrast agents would need to have a receptor moiety conjugated into the iodine moiety with the aim of maximising the interaction with ions such as Ca(II) that are exposed on the surfaces on the damaged sites. Such structural designs could thus provide a non-invasive method of detecting and quantifying microdamage in patients. Herein, we describe the synthesis of three such first-generation ion-receptor based contrast agents 1–3 which are based on the use of one or two triiodobenzene moieties within a single structure and the analysis of these to detect microcracks in bovine bones using micro computer tomography (μCT) imaging.[16]

receptors and iodinated phenyl rings. In molecules 1 and 4, a single phenyliminodiacetate unit was attached to the iodinated aromatic ring, *via* an amide spacer, while 2 has two such ion receptor units attached *meta* to each other. The dimer 3 contains, however, six iodine atoms and four chelator units in *meta* configuration, and as such would be expected to have the highest binding affinity as well as giving rise to the most efficient imaging. Moreover, as their sodium salts, these contrast agents would be expected to be highly water-soluble.[1] These compounds also have incorporated solubilising groups in the form of the amides that will render them safer and less viscous.[16]

Scheme 1 Synthesis of 1 from 5 and 6.

As discussed above, all of the four compounds are based on a triiodo moiety connected to the phenyliminodiacetate (not as the corresponding diethyl ester). Consequently, all of these were synthesized by making the phenyliminodiacetate moiety and connecting that into the relative carboxylic acid derivatives of the triiodo compounds. As a starting point for this investigation, we synthesized 1 first as shown in Scheme 1. This involved the coupling of 2,3,5-triiodobenzoyl chloride (6) (which was synthesized from the commercially available carboxylic acid using thionyl chloride in 83% yield after recrystallization from a chloroform–hexane (1 : 1, v/v) mixture) to phenyliminodiacetate ethyl ester 6 was formed in 65% yield from aniline, involving the dialkylation of ethyl bromoacetate in the presence of K_2HPO_4 and in refluxing CH_3CN which gave the desired product in 90% yield. This was followed by nitration using 70% nitric acid (15 min) followed by recrystallization of the crude product from 2-propanol which gave 8 (not shown) in 74% yield. Hydrogenation on 8 using 10% Pd/C proceeded smoothly to give 6 in almost quantitative yields. Condensation of 5 with 6 was achieved in THF using Et_3N and resulted in the formation of the desired diester 7, in 80% yield after purification by silica flash column chromatography (using 2 : 5 ethyl acetate–hexane as eluant). The alkaline hydrolysis ($NaOH$) of 7 to give 1 was achieved in MeOH–H_2O (10 : 1). The purification of 1 involved the evaporation of the solvent mixture to dryness, and the resulting residue was dissolved in a minimal amount of distilled water, followed by dilution with methanol. The resulting mixture was then heated at reflux in the presence activated charcoal, followed by cooling to room temperature. After standing at room temperature for a further two days, it was filtered and evaporated to dryness, diluted with a minimal amount of water and added dropwise to a stirred solution of ethanol to precipitate 1. This purification method removed all of the coloured impurities and resulted in the isolation of 1 in 92% yield (see 1H NMR of 1 in ESI†).

‡ For the future development of this technique, it is important to account for the fact that the concentrations of these ions within the bones would be significantly greater than found in both extra-and intra-cellular environments. Consequently, at the same time as the receptors should be Ca(II) selective, they would also need to have a low affinity for those ions to prevent any interference from background signals arising from the binding of these agents to free Ca(II) in blood or in cells. Because of this we chose to use the simple phenyliminodiacetate moiety as a receptor as it would hopefully fulfil these criteria.



Scheme 4 Attempted synthesis of 17 from 6 and 16.

Evaluation of contrast agents 1–3 in solid (powder) form and in solution using μ-CT

Upon computer tomography imaging using μ-CT, compounds 1–3 synthesized above were all able to provide good contrast from the surrounding bone matrix as powdered substances.[16] A two-dimensional sagittal reconstruction was performed in order to evaluate the contrast ability of the agents, in comparison with the surrounding bone matrix (see Experimental for further details). The first of those compounds to be tested was contrast agent 1, which was applied to the right-hand side of the bone specimen as shown in the red box in the sagittal reconstruction in Fig. 2A. For comparison the left-hand side of the bone, within the blue box has no contrast agent applied. Both the bone and 1 gave an image that is predominantly white. However, areas where 1 has been applied appear to be more bright due to its higher X-ray absorption power, and hence it is distinct from the bone surface. A three-dimensional transparent section was also reconstructed to further illustrate the contrast ability of 1 (Fig. 2B). Here, it is clearly possible to distinguish the internal architecture of the bone in the transparent reconstructed section, as well as Haversian and Volkmann's canals and the resorption cavities due to the contrast provided by 1. In a similar way, compounds 2 and 3 were tested under identical conditions. Similar results were obtained to those seen in Fig. 2. However, the reconstructed two-dimensional sagittal and transparent three-dimensional images clearly show that these contrast agents were able to absorb the X-rays more effectively than the bone, thus providing better contrast from the bone matrix. This is not unexpected as both 2 and 3 have a higher iodine content and as such should give rise to stronger imaging.

After performing qualitative studies with these contrast agents in powdered form, the next stage was to label bone scratches with 10^{-3} M aqueous solutions of the contrast agents 1–3, using bovine tibiae, and image the resulting bone specimens using μ-CT. The preliminary μ-CT studies described below were performed in a similar manner as before. Even though the bone specimen labelled with compound 1 indicated that the scratch was visible, the background contrast for both the scratch depth and the surrounding bone matrix almost overlapped with that observed form 1 (Fig. 3). Consequently, it was difficult to differentiate between bone and contrast agent. Similar effects were observed for 2 and 3. The most likely reason for this may be from the beam hardening effect, which masks the imaging from the agents.‡ Nevertheless, these results clearly indicate that our agents can bind to bone cracks (microcracks) and as such the results obtained from 1–3 are important for the future development of bone-targeting CT imaging agents. We are currently working towards achieving that objective.

Fig. 3 Three-dimensional axial reconstruction of the bone immersed in an aqueous solution of 1 (1 mM). A scratch can be seen on the left-hand side (yellow arrow). The top of the axial plane shows a vessel canal (red arrow) within the bone tissue.[16]

Fig. 2 Computer tomography images of 1: (A) two-dimensional and (B) three-dimensional sagittal sections of a cortical bone specimen labelled with contrast agent 1. The white powder on the bone edges is marked by a black arrow. Bars are in μm.

Conclusion

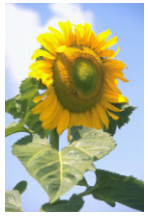
We have demonstrated the synthesis of several new bone-targeting contrast agents for CT imaging based on the use of the triiodobenzene framework, and we have carried out a preliminary evaluation of these to quantify microdamage in bone. All three contrast agents exhibited good water solubility and stability. Preliminary imaging studies of these contrast agents on bovine cortical bone specimens, using cone-beam μ-CT, demonstrated that agents in powder form are able to provide good contrast from the surrounding bone

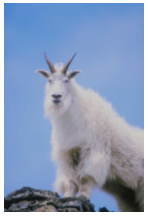
‡ Such beam hardening arises from X-ray photons striking the bone surface at different energy so that the photons of lower energy are absorbed with a higher probability than those of a higher energy. As a result, the attenuation of the X-ray is not homogenous and is dependent upon the energy of the radiation, the type of object used in the imaging and the direction of projection.

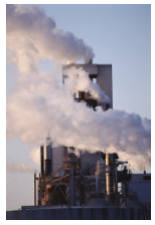
Introduction

Organic substances are everywhere

plants | animals | industry | research labs



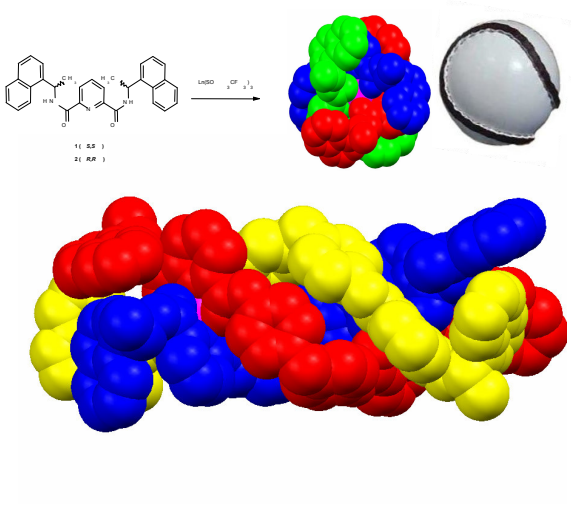


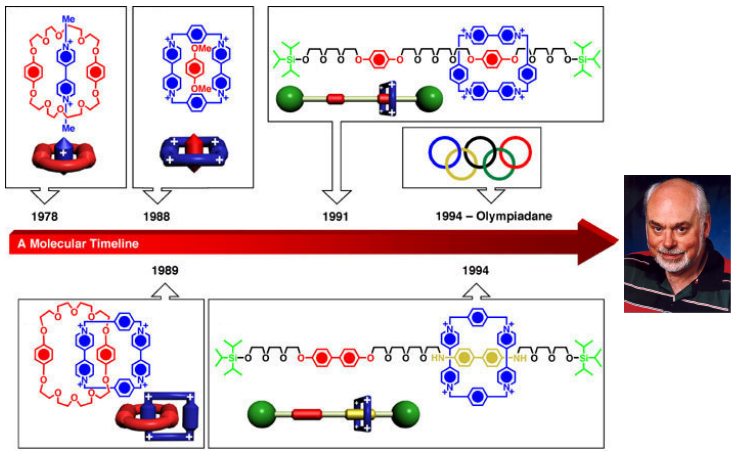


Introduction

Organic Chemistry

- **Many branches**
  - Medicinal and pharmaceutical chemistry
  - **Perfume and Food chemistry**
  - Synthesis
  - Mechanistic
  - **Natural product chemistry**
  - **Polymers**
  - Supramolecular!



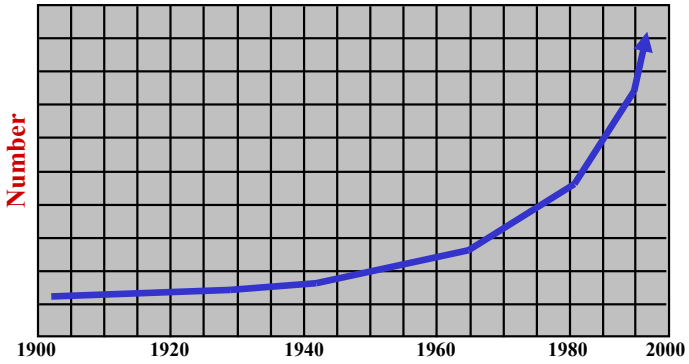


http://stoddart.chem.ucla.edu/ **Professor J Fraser Stoddart**

Introduction

~ 12 million organic substances

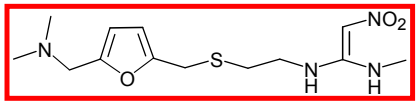
- increases by 10,000 per week!



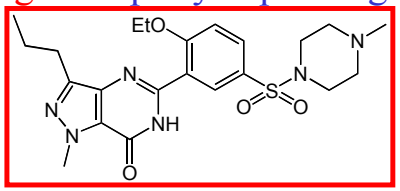
Introduction

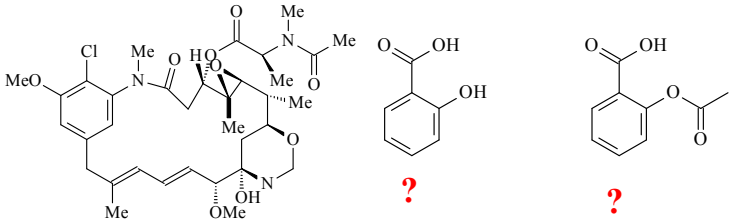
Pharmaceuticals

- *eg*. Ranitidine: sales > £1,000,000,000 per annum for Glaxo-Wellcome



- *eg*. Viagra: Rapidly expanding market!

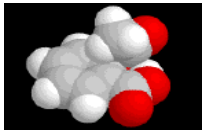




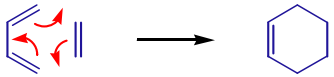
MAYTANSINE
A very potent anti-tumour agent
E. J. Corey *et. al.* 1978-1980

Aims of Course

To understand ….



- Structures and shapes
  - BONDING
- Basic reaction mechanisms
  - HOW SHAPES ARE CREATED



The Basics

Drawing Chemicals

- **Molecular Formula**
- **Condensed Structural Formula**
- **Lewis Forms**
- **Kekule Structure**
- **Skeletal Structure**

Nomenclature

- **Functional Groups**
- **Examples**

Molecular Formula / Drawing Structures

Drawing Chemicals

Molecular Formula

- **Actual number and type of atoms**

eg. Ethanol = C_2H_6O

eg. Dimethyl Ether = C_2H_6O

Condensed Structural Formula

- **Shows which way atoms are** bonded/connected, but doesn't require all bonds to be drawn

eg. Ethanol = CH_3CH_2OH

eg. Dimethyl Ether = CH_3OCH_3

Drawing Chemicals

Valence shell!

- **We know that eight electrons in –an electron octet- in the outermost shell, or valence shell, impart special stability to the noble-gas elements: Neon 2+8, Argon (2+8+8) etc.**
- **These valence electrons are the one that participate in bonding.**
- **Methane is one of these molecules that forms an octet. Carbon has $1s^2\ 2s^2\ 2p^3$ electrons and needs 4 more to form the octate. Hydrogen has $1s^1$, *i.e.* we need four of these:**

CH_4 is methane!

Drawing Chemicals

8 max!!

Structural Formula

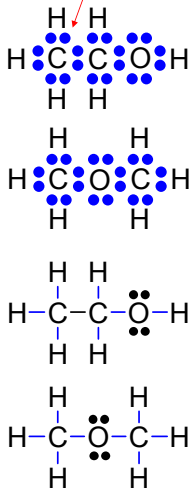
Lewis Structure

- Dots are used to represent all valence electrons

Kekule Structure

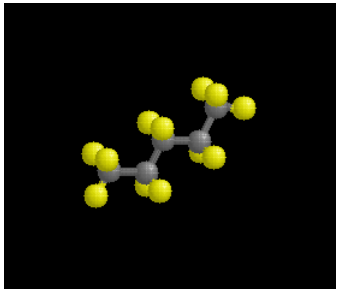
- Dots represent nonbonding valence electrons (not used e^-), or lone-pair electrons! *e.g.* NH_3!!
- Lines represent bonding valence electrons

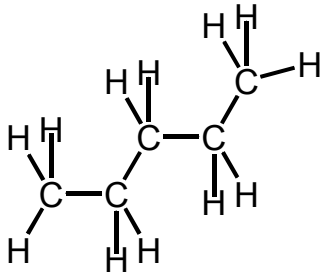
Example: CH_3Cl (Chloromethane)



Drawing Structures

- Structures in Reality!

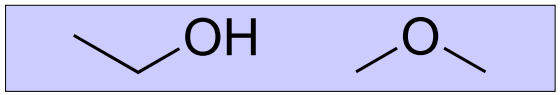




Drawing Chemicals

Skeletal Structure

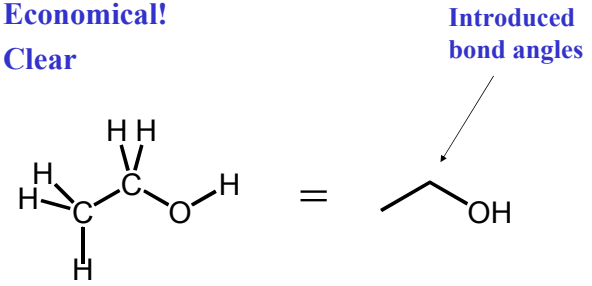
- The carbon backbone is represented by a zig-zag line (reflects reality)
- All hydrogens attached to the carbon backbone are neglected (convenient and fast)
- Carbon atoms are the corners and ends
- Important for drawing larger chemicals and highlighting functional groups



Drawing Chemicals

Guidelines

- Realistic
- Economical!
- Clear



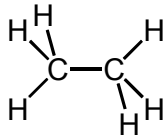
Ethanol, Ethan-2-ol

Functional Groups

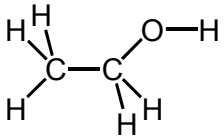
Definition

- An atom or group **of atoms that is part of a larger molecule and that has a characteristic reactivity**

eg. alcohol



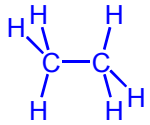
Ethane



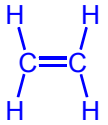
Ethanol

Functional Groups

Hydrocarbons

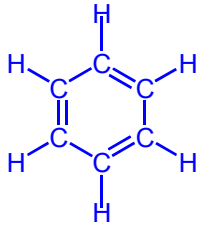


Alkanes



Alkenes

Alkynes



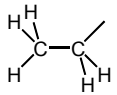
Aromatic Hydrocarbons

Functional Groups

Hydrocarbon Derivatives

- R is chemists shorthand for 'alkyl'

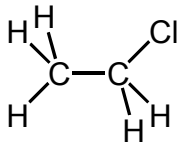
eg. R = ethyl =



R—Cl

Alkyl Halides

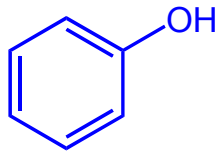
eg.



Functional Groups

Hydrocarbon Derivatives *cont.*

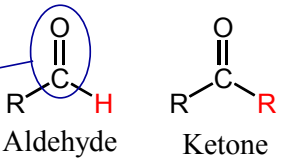
- **Alcohols** R—OH
- **Ethers** R—O —R
- **Amines** R—NH_2
- **Phenols**



Functional Groups

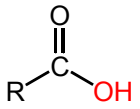
Hydrocarbon Derivatives *cont.*

Carbonyl group

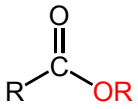


Aldehyde

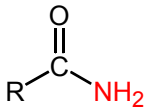
Ketone



Carboxylic acids



Esters

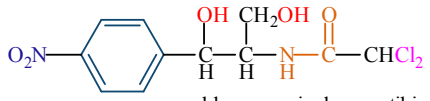


Amides

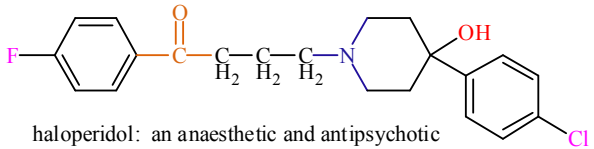
Functional Groups

Importance

- Determine chemical behaviour



chlorampenicol: an antibiotic



haloperidol: an anaesthetic and antipsychotic

Naming Chemicals/Structures

Naming Chemicals

Overview (IUPAC system)

- Names of chemicals have 4 main parts:
  - Parent name: describes the main **carbon** section of the molecule.
  - Suffix: identifies the principle **functional group**
  - Prefix: identifies the **substituents** on the main chain or ring
  - Locants: shows where the substituents are **located**

Naming Chemicals

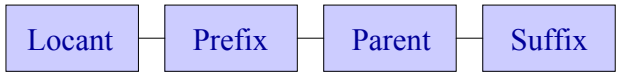
Common Parent and Substituent Names

Number of Carbons	Parent Name	Substituent Name
1	**methane**	**methyl**
2	**ethane**	**ethyl**
3	**propane**	**propyl**
4	**butane**	**butyl**
5	**pentane**	**pentyl**
6	**hexane**	**hexyl**
7	**heptane**	**heptyl**
8	**octane**	**octyl**
9	**nonane**	**nonyl**
10	**decane**	**decyl**

Naming Chemicals

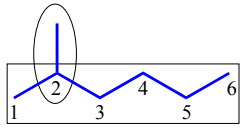
Overview

- Names of chemicals have 4 main parts:



eg. 2-Methylhexane

locant: 2-
prefix: methyl
parent: hex
suffix: ane



Naming Chemicals

Rules

1. Name the Parent
   - Identify the longest carbon chain containing the most important functional group
2. Add the Suffix
   - Identify the most important functional group and add the appropriate suffix

   eg. Alkanes = 'ane'

Naming Chemicals

3. Add the Prefix

➢ Name any substituents

- Substituents are arranged in alphabetical order
- If more than one group is present use 'di', 'tri', 'tetra', 'penta', 'hexa', 'hepta', 'octa', 'nona' or 'deca' before the group

Note: these additional prefixes do not count when alphabetising the substituents

Naming Chemicals

4. Include the Locants

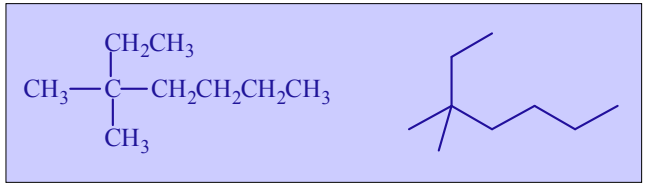
➢ Specify substituent location

- Number the parent chain **from the end closest to the functional group**
- Different substituents can have the same number if they are attached to the same carbon
- Use hyphens to separate no. and letters
- Use commas to separate no. form no.

Naming Chemicals

Alkanes

➢ name the following alkane:

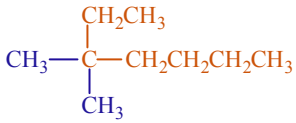


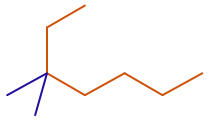
Naming Chemicals

Alkanes

Step 1: Name the Parent Chain

- find the longest continuous chain





- assign appropriate parent name

→ hept

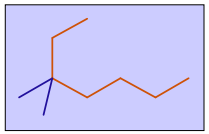
Naming Chemicals

Alkanes

Step 2: Add the Suffix

- The chemical is an alkane

→ heptane



Step 3: Add the Prefix

- Describe any substituents attached to the parent chain

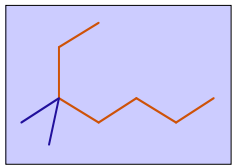
→ Dimethylheptane

Naming Chemicals

Alkanes

Step 4: Include the Locants

- Include the position of attachment
  - use the lowest possible option
- 3,3-Dimethylheptane
  - Not 5,5-Dimethylheptane



Naming Chemicals

Alkanes

1. Name the Parent Chain

- oct

2. Add the Suffix

- octane

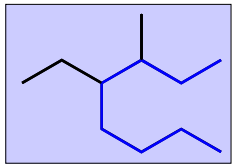
3. Add the Prefix

- Ethylmethyloctane

4. Include the Locant

- 4-Ethyl-3-methyloctane

Example 2:



Naming Cyclic Chemicals

Cycloalkanes

1. Name the Parent

- cyclohex

2. Add the Suffix

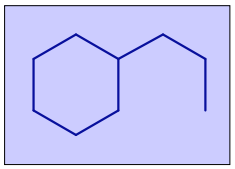
- cyclohexane

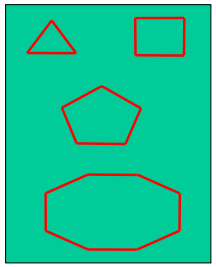
3. Add the Prefix

- propylcyclohexane

4. Include the Locant

- 1-propylcyclohexane





Naming Chemicals

Alkenes and Alkynes

*1. Name the Parent Chain (**must include functional group**)*

- hept

2. Add the Suffix

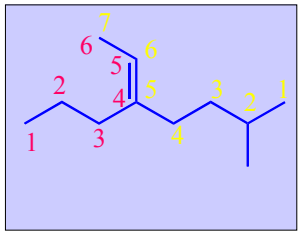
- heptene

3. Add the Prefixes

- methylpropylheptene

4. Include the Locants

- 6-methyl-3-propylhept-2-ene

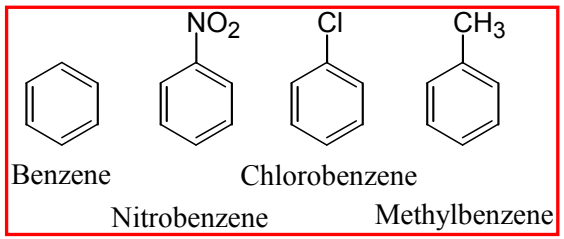


Naming Chemicals

Aromatic Hydrocarbons

- 'Substituent name' followed by 'Benzene'

eg.

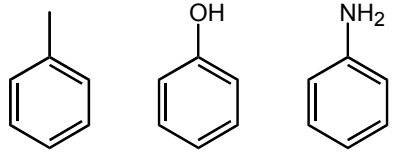


Naming Chemicals

Aromatic Hydrocarbons

- A large number of aromatic hydrocarbons have *non-systematic (common)* names

eg.



Toluene (Methylbenzene)

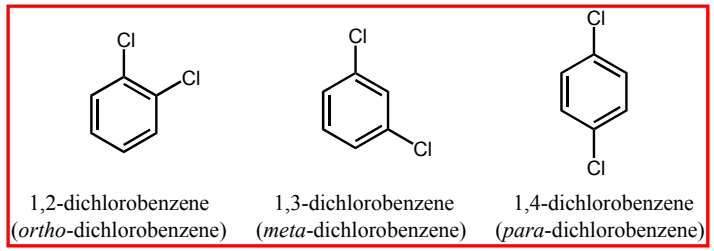
Phenol (Hydroxybenzene)

Aniline (Aminobenzene)

Naming Chemicals

Aromatic Hydrocarbons

- When there is >1 substituent, locants are used to specify their relative position
- *ortho-*, *meta-* and *para-* maybe used in place of numerical locants

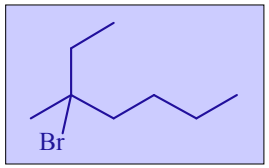


1,2-dichlorobenzene (*ortho*-dichlorobenzene) | 1,3-dichlorobenzene (*meta*-dichlorobenzene) | 1,4-dichlorobenzene (*para*-dichlorobenzene)

Naming Chemicals

Halogen Compounds

- As for alkanes
- The halogen is named as a substituent with an 'o' (*eg*. bromine becomes bromo)



→ 3-Bromo-3-methylheptane

Naming Chemicals

Alcohols

1. Name the Parent Chain

- octane

2. Remove 'e' and add the Suffix 'ol' to alkane name

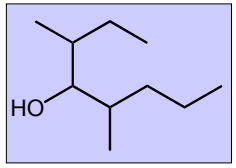
- octanol

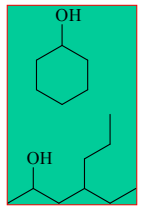
3. Add the Prefix

- Dimethyloctanol

4. Include the Locants

- 3,5-Dimethyloctan-4-ol





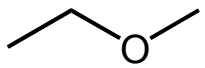
You try these!

Naming Chemicals

Ethers

- substituents are listed alphabetically followed by the word 'ether'

eg.



→ Ethyl methyl ether

Naming Chemicals

Amines

1. Name the Parent Chain as substituent

- propyl

2. Add the Suffix

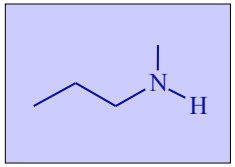
- propylamine

3. Add the Prefix

- Methylpropylamine

4. Include the Locant

- *N*-Methylpropylamine



Naming Chemicals

Aldehydes

1. Name the Parent Chain

- heptane

2. Remove 'e' and add Suffix 'al' to alkane

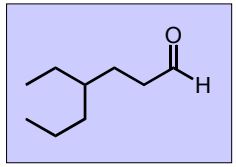
- heptanal

3. Add the Prefix

- Ethylheptanal

4. Include the Locant

- 4-Ethylheptanal



Naming Chemicals

Ketones

1. Name the Parent Chain

- heptane

2. Remove 'e' and add Suffix 'one' to alkane

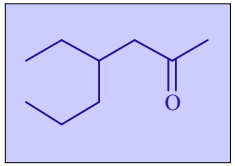
- heptanone

3. Add the Prefix

- Ethylheptanone

4. Include the Locants

- 4-Ethylheptan-2-one



Naming Chemicals

Carboxylic Acids

1. Name the Parent Chain

- heptane

2. Remove 'e' and add Suffix 'oic acid' to alkane

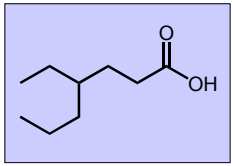
- heptanoic acid

3. Add the Prefix

- Ethylheptanoic acid

4. Include the Locant

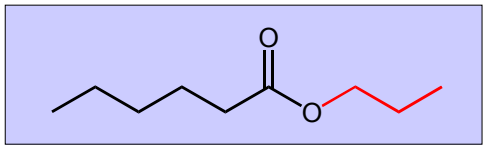
- 4-Ethylheptanoic acid



Naming Chemicals

Esters

1. *Parent:*
   - Hexane
2. *Remove 'e' and add 'ate':*
   - Hexanate
3. *Prefix: the other alkyl segment with a space:*
   - propyl Hexanoate
4. *Locants:* Not required for this example



Naming Chemicals

Acid Chlorides

- replace 'ic acid' with 'yl chloride'

Anhydrides

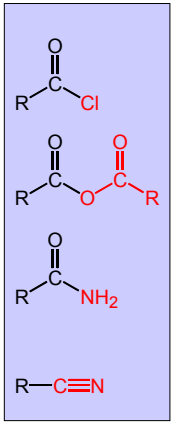
- replace 'acid' with 'anhydride'

Amides

- replace 'ic acid' with 'amide'

Nitriles

- replace 'ic acid' with 'nitrile'



Naming Chemicals

>1 Functional Group

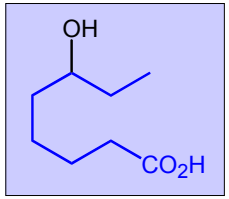
Priority List

1. Carboxylic acids
2. Aldehydes
3. Ketones
4. Alcohols
5. Amines
6. Alkenes
7. Alkynes
8. Alkanes

Naming Chemicals

>1 Functional Group

1. *Identify Priority gp.*
   Carboxylic acid, alcohol
2. *Name parent and suffix as usual*
   octanoic acid
3. *prefix for alcohol substituent*
   hydroxyoctanoic acid
4. *Locants*
   6-hydroxyoctanoic acid



Naming Chemicals

Suffix and Prefix

Group	suffix	prefix
aldehyde	-al	formyl-
ketone	-one	oxo-
alcohol	-ol	hydroxy-
amine	-amine	amino-

Naming Chemicals

Suffix and Prefix

- Alkenes and alkynes
  - Specify location 'within' parent
  - Essentially as before!

But-2-yne

But-2-ynoic acid

Naming Chemicals

Further Example

1. *Priority*
   alcohol aldehyde and alkene
2. *Parent + suffix*
   oct, ene and al = octenal
3. *Substituents*
   hydroxy
4. *Locants*
   5-hydroxyoct-3-enal