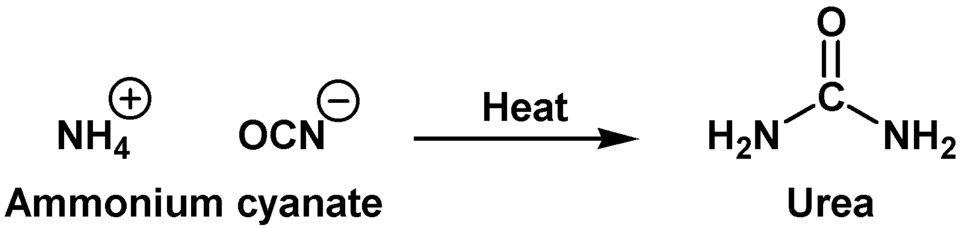
Chemistry: What is it good for?

- To understand the properties of all matter
- To understand the interactions of materials
- To understand biological processes
- To develop new drugs (antibiotics, anti-cancer agents...)
- To develop new materials (plastics, ceramics...)

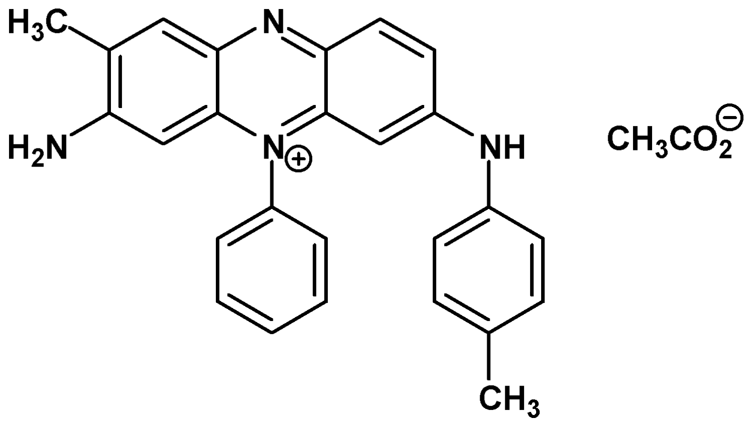
The first synthetic chemists

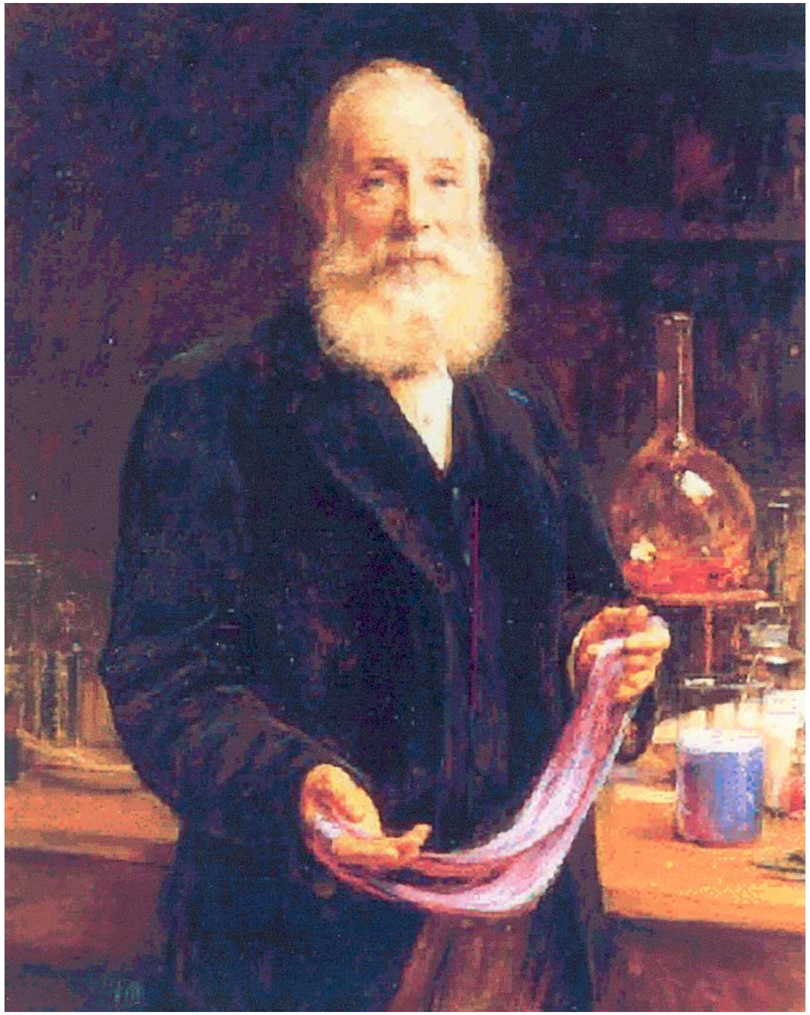
(making new molecules)

- 1828; Wohler prepares urea



- 1857; Perkin makes 'mauveine' from coal tar





Chemical Bonds and Structure

- In addressing the properties of different compounds it is useful to group them into two classes:

Ionic compounds;

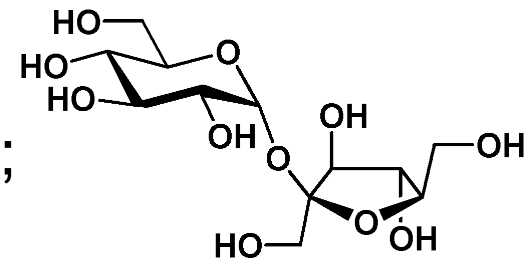
typically inorganic compounds (salts etc.)

Covalent compounds;

typically organic componds

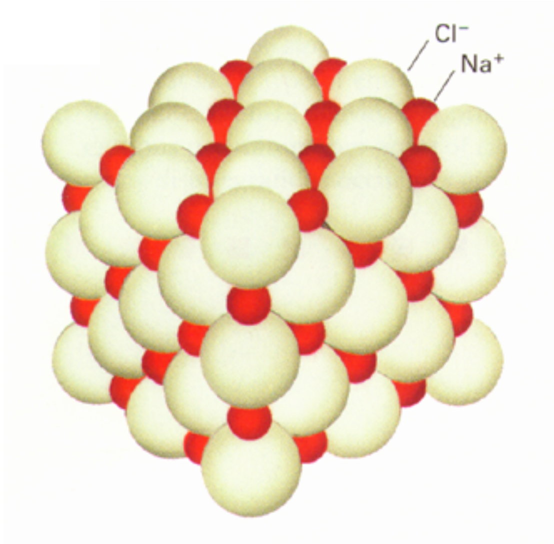
Table salt; $Na^{+}Cl^{-}$

Table sugar;



Ionic Compounds

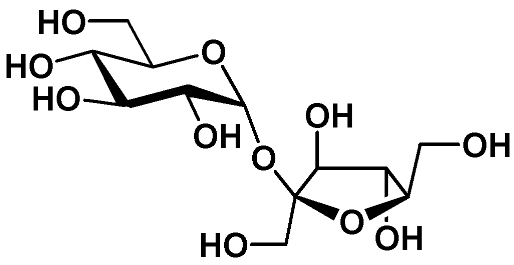
- Complete transfer of one or more electrons occurs, creating ions.

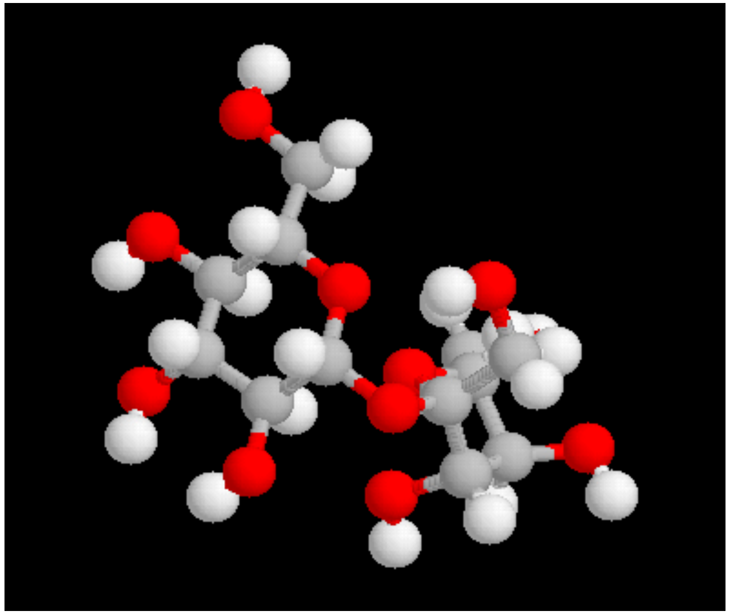


- Ions are held together (in a lattice) by strong electrostactic forces

Covalent Compounds

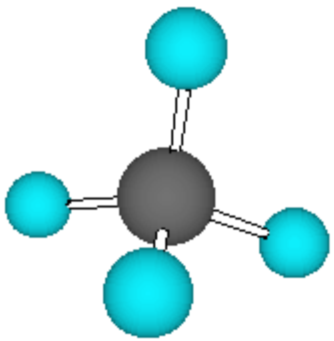
- Bonding electrons are ‘shared’ between atoms
- Overlap of electronic orbitals gives rise to bonding orbitals, or covalent bonds

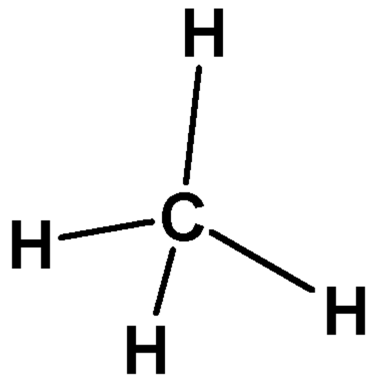


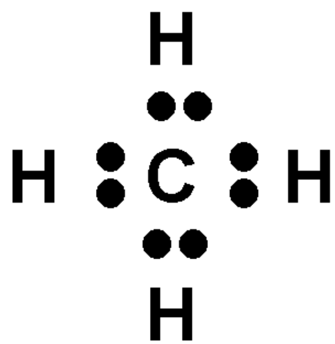


What are covalent bonds?

- Two electrons shared between two atoms







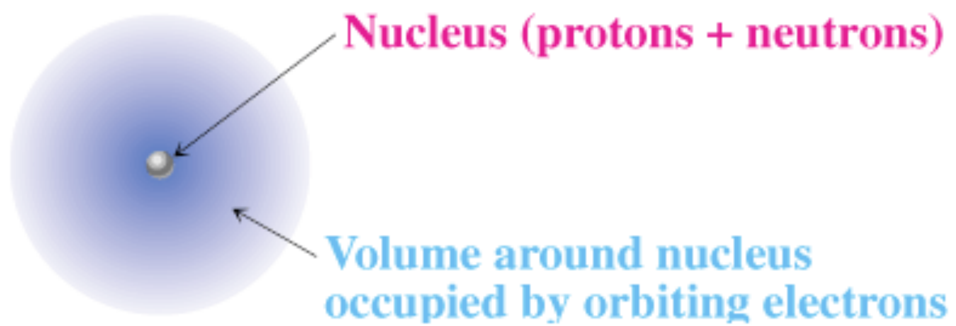
Electronic Configuration

- Describes the orbitals occupied by electrons for a given element

Element	Atomic Number	Electron Configuration
H	1	1s1
He	2	1s2
Li	3	1s2 2s1
Be	4	1s2 2s2
B	5	1s2 2s2 2p1
C	6	1s2 2s2 2p2
N	7	1s2 2s2 2p3
O	8	1s2 2s2 2p4
F	9	1s2 2s2 2p5
Ne	10	1s2 2s2 2p6

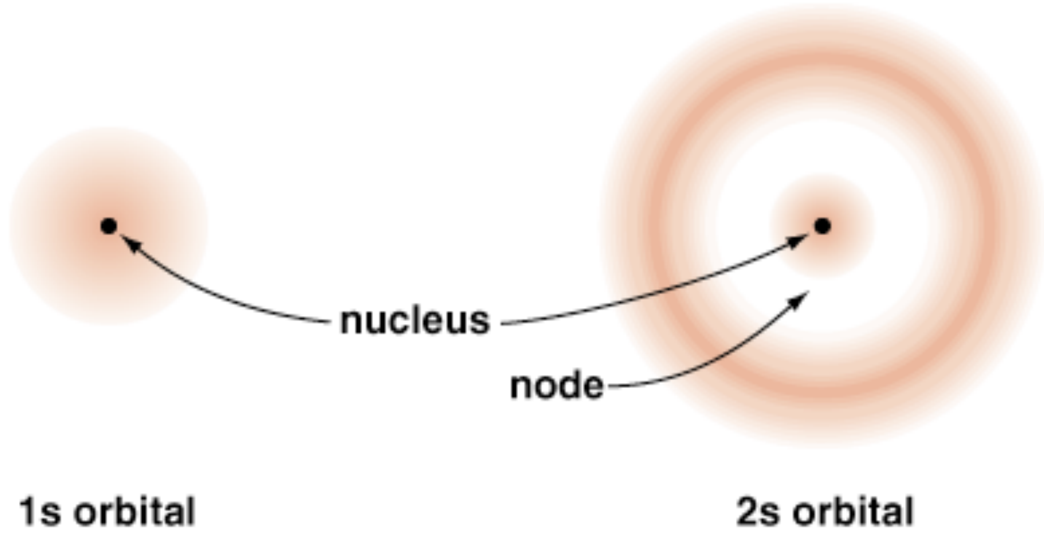
Orbital Theory

- The space around a nucleus in which an electron is most likely to be residing is termed an *orbital*



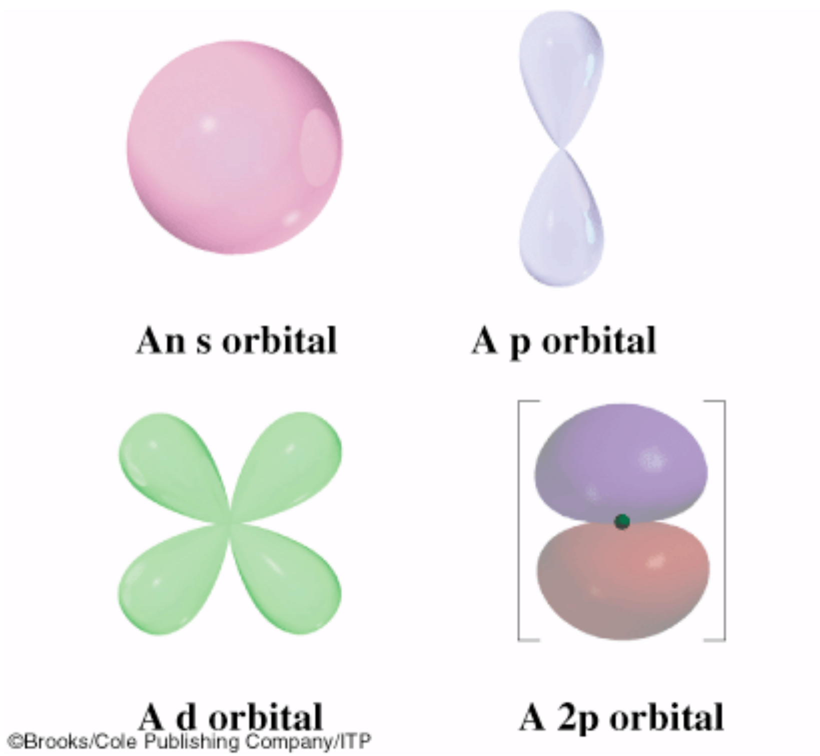
What does an orbital look like?

- The further from the nucleus, the higher the energy of the orbital



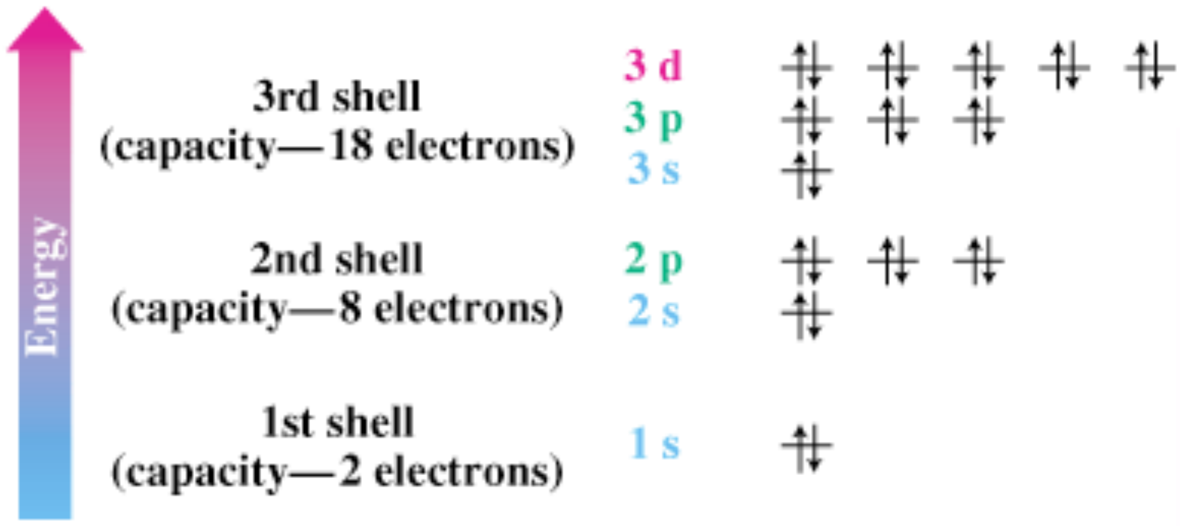
What does an orbital look like?

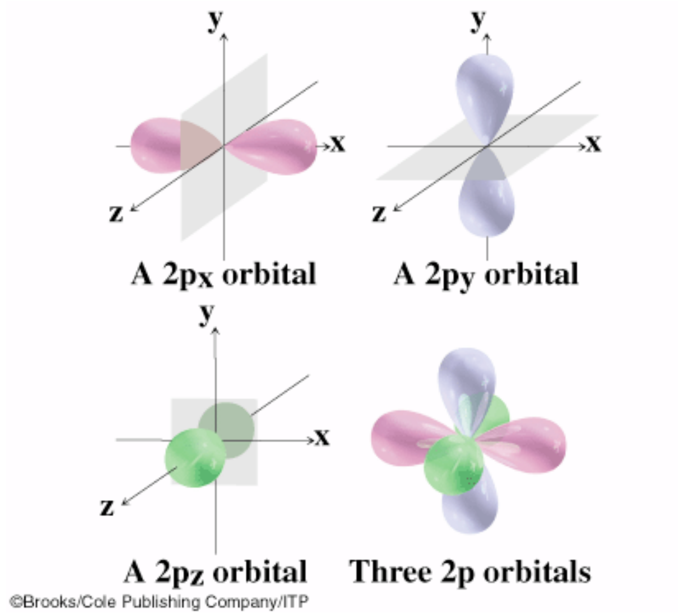
- The shape of an orbital varies with type



Electronic Configuration

- Energy levels of orbitals...





— an orbital

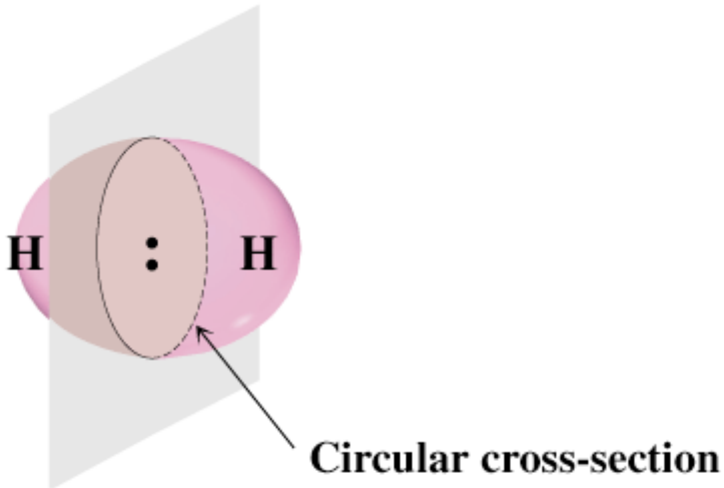
↑ an electron

Formation of covalent bonds

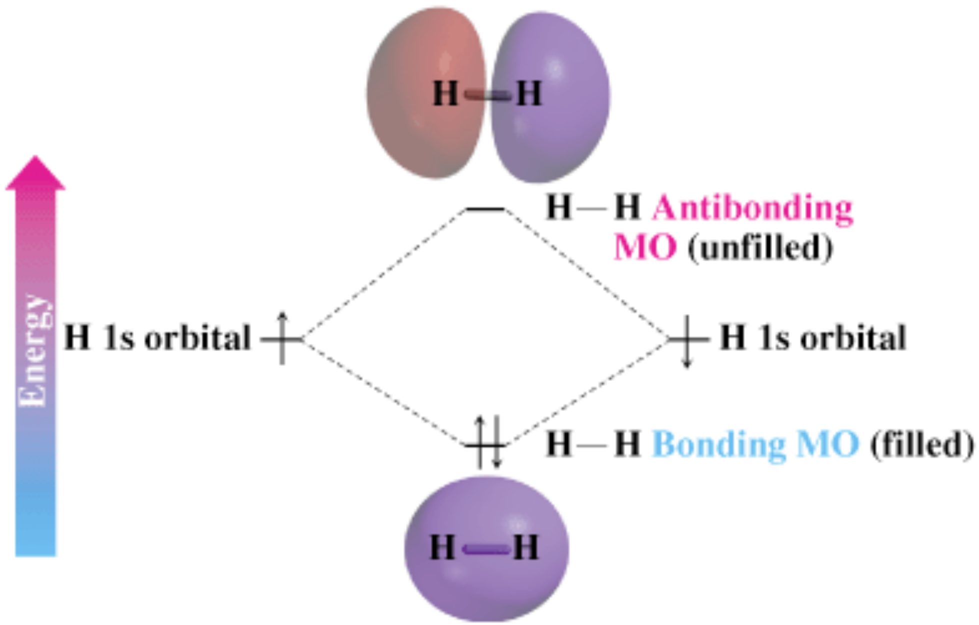
- A covalent bond is formed by the sharing between atoms of unpaired electrons
- Unpaired electrons are always in the outer (valence) shell highest energy occupied orbitals
- Two theories used to describe covalent bond formation;
  - Valence bond theory
  - Molecular orbital theory

Valence bond theory

- overlap of two singly-occupied orbitals gives a bonding orbital
- bonds formed by head-on overlap of orbitals are σ-bonds



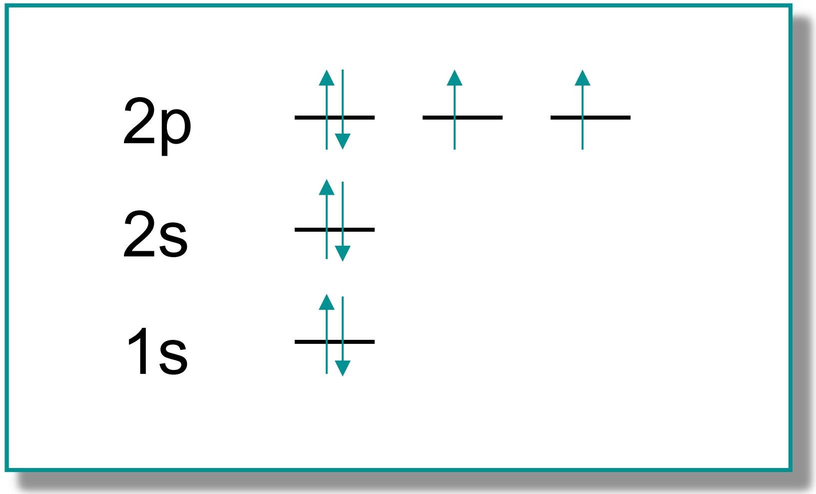
Molecular orbital theory



- combination of
  2 atomic orbitals gives
  2 molecular orbitals
- ‘additive’ combination gives bonding molecular orbital
  (filled, low energy)
- ‘subtractive’ combination gives anti-bonding molecular orbital
  (not filled, high energy)

Formation of covalent bonds

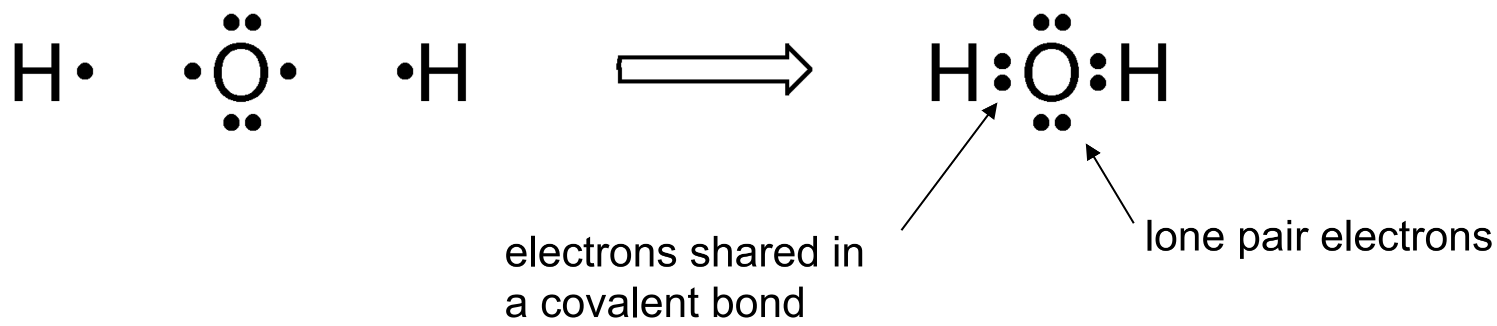
- A covalent bond is formed by the sharing between atoms of unpaired outer shell electrons



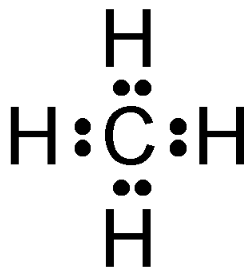
Oxygen: $1s^2\ 2s^2\ 2p^4$

Lewis structures

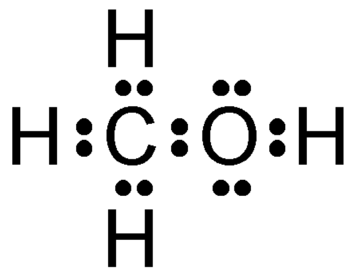
- A simple way of representing covalent bonds is by Lewis structures;
  - valence electrons are represented by dots
  - a stable molecule exists when an inert gas configuration is achieved for all atoms (stable octet rule)



Lewis structures



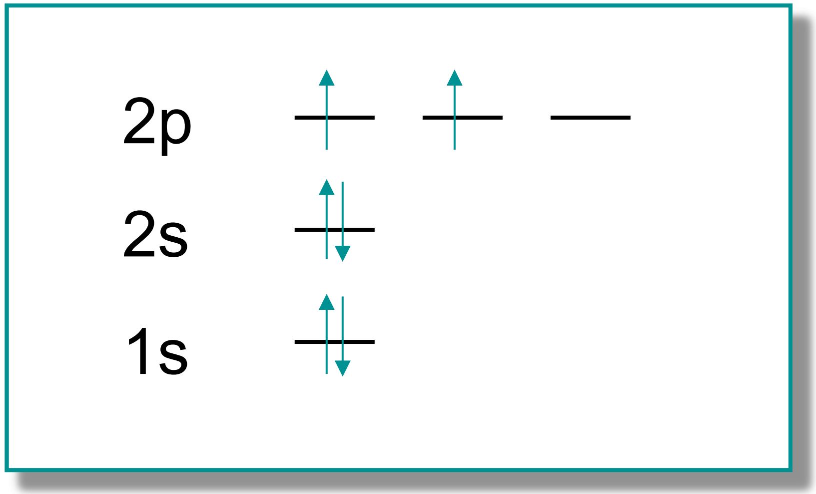
methane



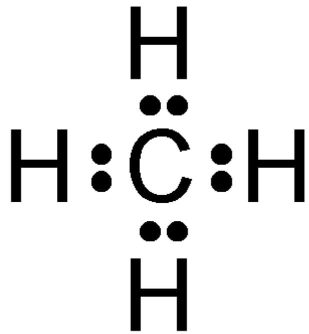
methanol

Orbital theory and carbon?

- The ground state configuration of carbon contains only two unpaired electrons…
- yet carbon forms four covalent bonds to achieve a 'stable octet' …



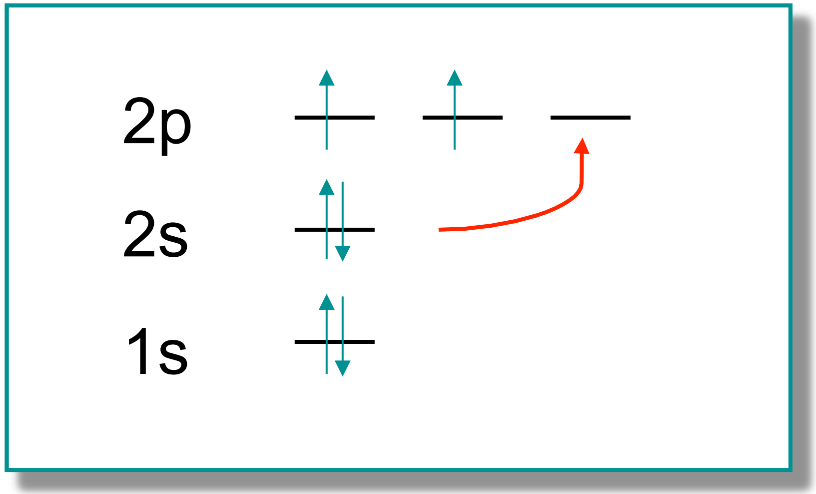
Carbon: $1s^2\ 2s^2\ 2p^2$



methane, CH_4

Excited state configuration

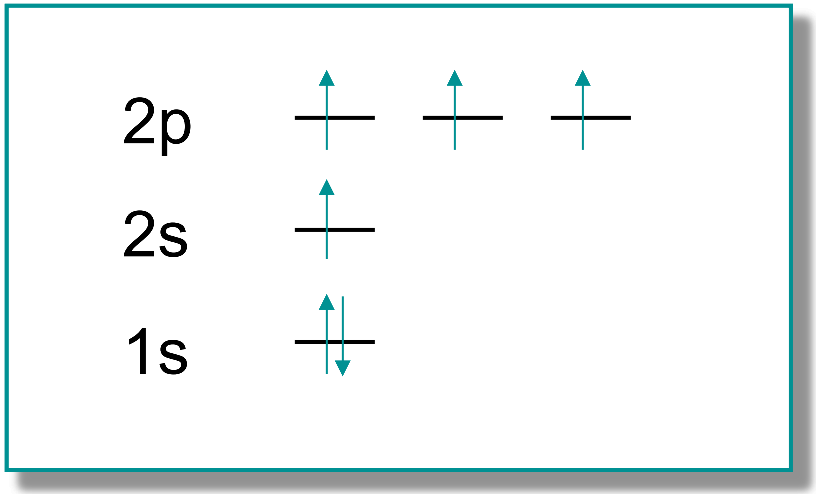
ground state



Carbon: $1s^2\ 2s^2\ 2p^2$

two unpaired valence electrons

excited state



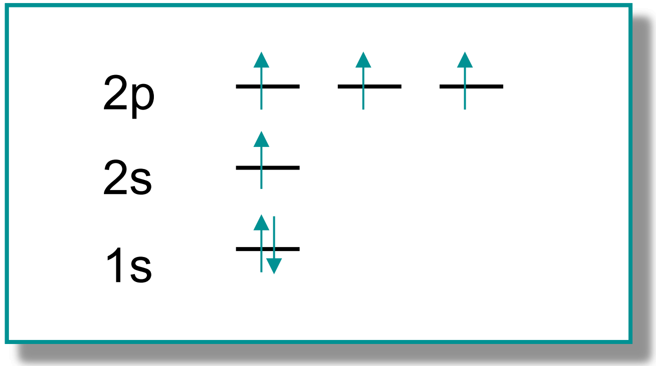
Carbon: $1s^2\ 2s^1\ 2p^3$

four unpaired valence electrons

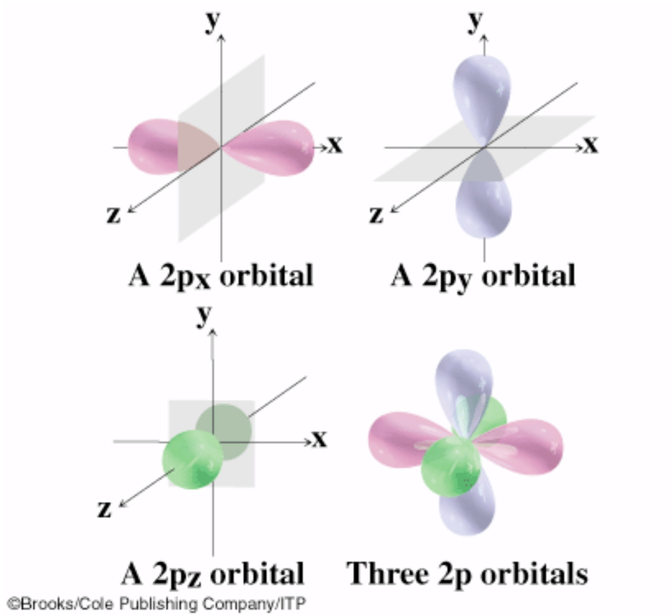
Bonding in carbon

- But…

  bonding in this state would give 3 equivalent bonds (from the 2p orbitals) and 1 different bond (from the 2s orbital).

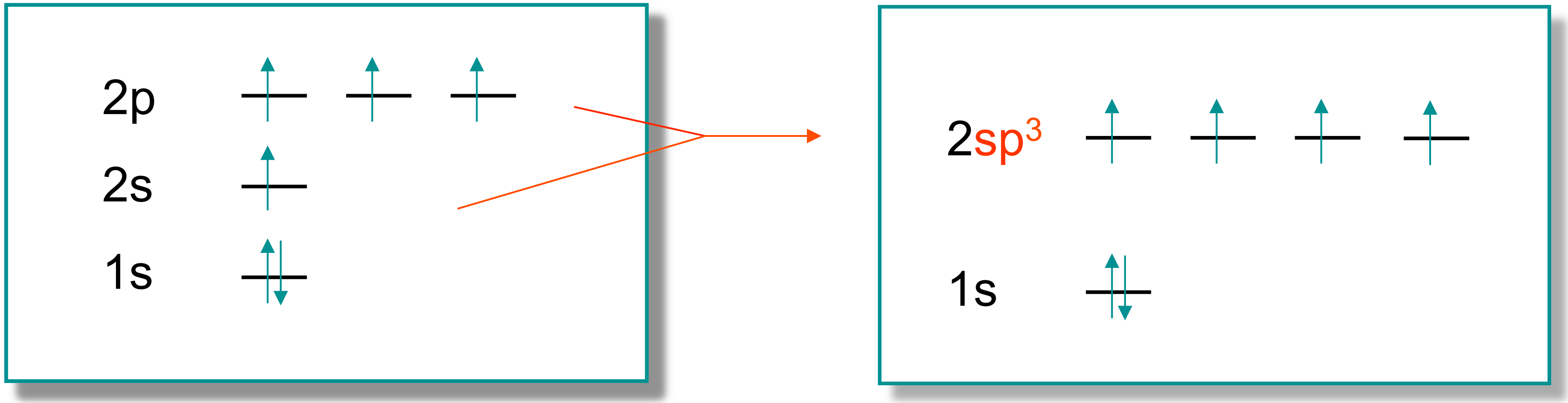


How do we account for experiments that confirm that all four bonds in methane are of the same length and strength?



Hybridisation

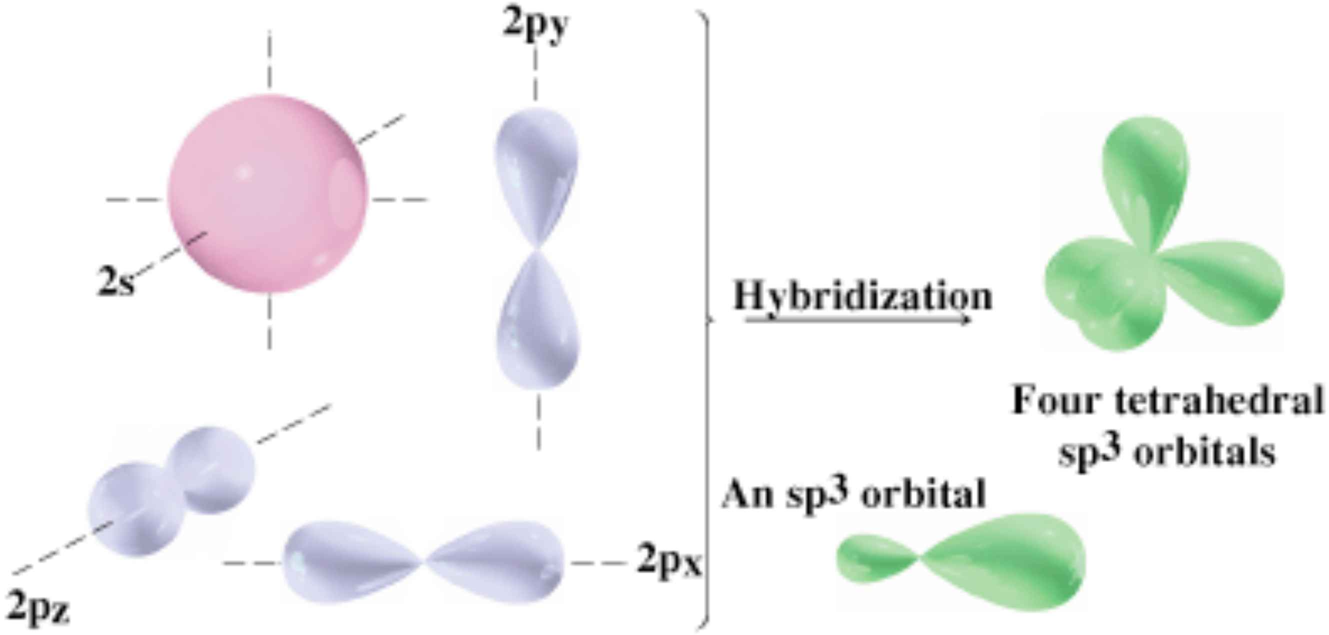
- The 2s, $2p_x$, $2p_{y,}$ & $2p_z$ orbitals are 'hybridised' to generate four equivalent sp^3 orbitals



Carbon: $1s^2\ 2s^1\ 2p^3$
'excited state'

Carbon: $1s^2\ [2sp^3]^4$
possible 'bonding state'

Hybridisation

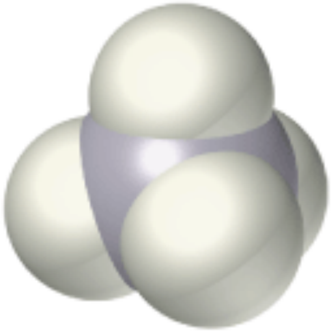


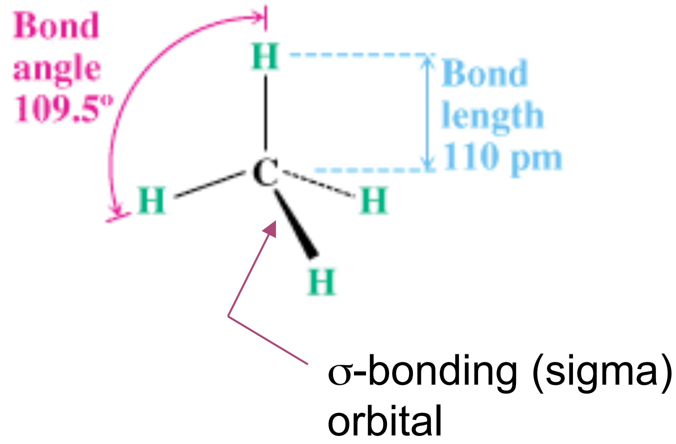
The four sp^3 orbitals have a tetrahedral arrangement around the nucleus

This can be determined mathematically (Schroedinger equation), and/or can be thought of as the arrangement that places the four orbitals as far apart as possible (VSEPR theory).

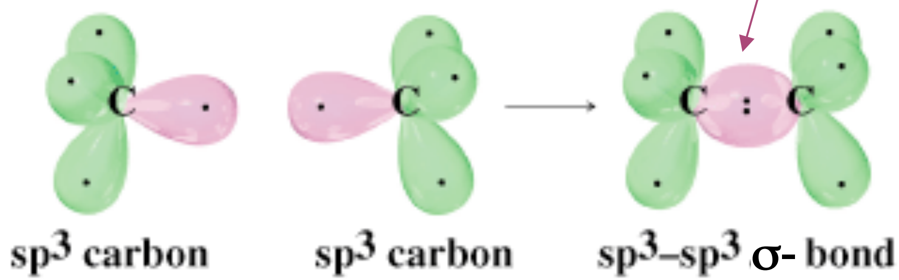
Tetrahedral geometry

- Methane, CH_4



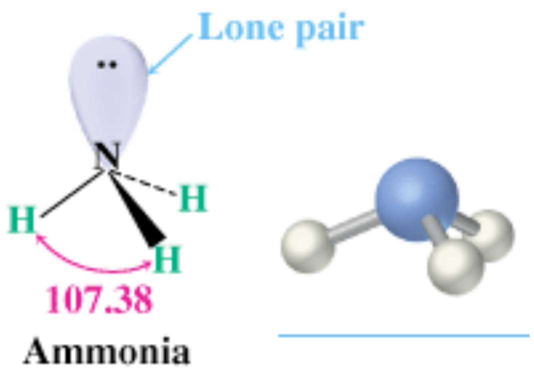


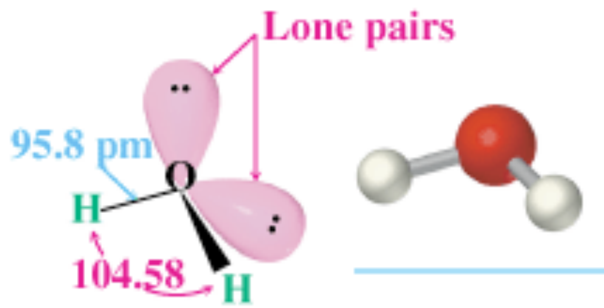
- Ethane, C_2H_6



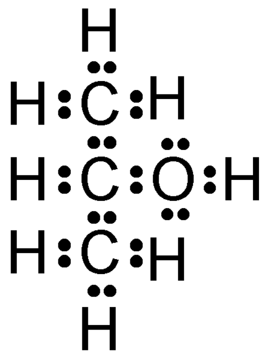
Tetrahedral geometry

- Oxygen and nitrogen can also be sp^3-hybridised;

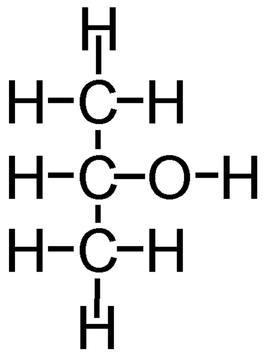




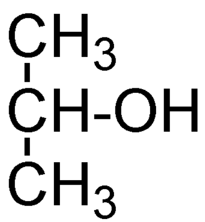
Representation of molecules



- Lewis structure;
  - confusing even with small molecules

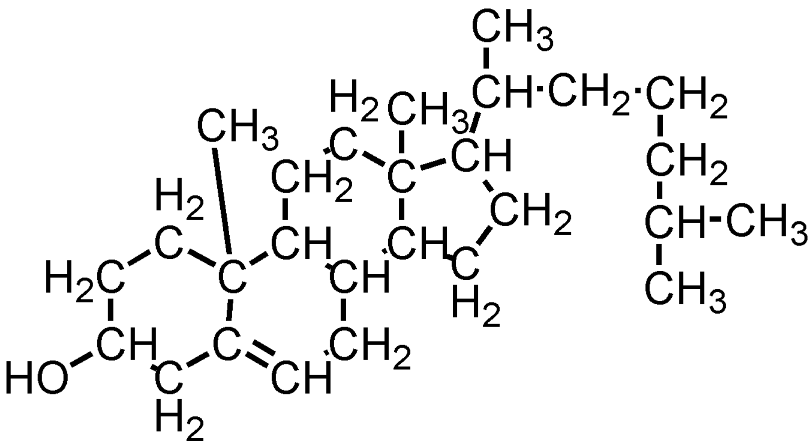


- Kekule structure (Structural formula);
  - covalent bonds represented as lines
  - cumbersome for larger molecules

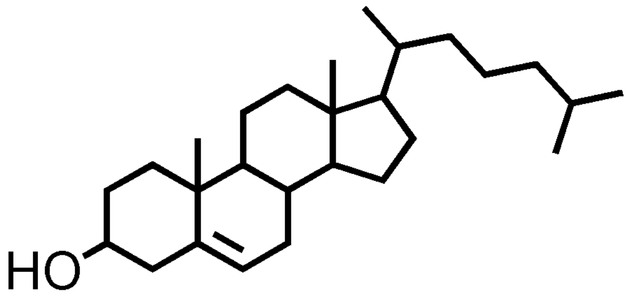


- Condensed structural formula;
  - group H’s together

Representation of molecules



- So what is this molecule?



cholesterol

- Line structure;
  - C-C bonds drawn as lines
  - C-H bonds omitted
  - non-C,H atoms drawn
  - only H's not bonded to C shown

Alkanes

Names of Straight-Chain Alkanes

Number of Carbons(n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{16}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$
11	Undecane	C_{11}H24
12	Dodecane	$C_{12}H_{25}$
13	Tridecane	$C_{13}H_{28}$
20	Icosane	$C_{20}H_{42}$
21	Henicosane	$C_{21}H_{44}$
30	Triacontane	$C_{30}H_{62}$

The number of carbons in the longest chain containing the functional group

$\Downarrow$

Parent — **Ending**

$\Uparrow$

The functional group present

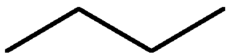
e.g. **octane**

eight carbons

an alkane

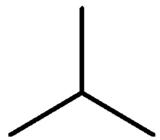
Structural isomers

- Alkanes with four or more carbons can exist as structural isomers
- Structural isomers have the same molecular formula, but have different bond connectivity



$CH_3CH_2CH_2CH_3$

b.p. 0 °C



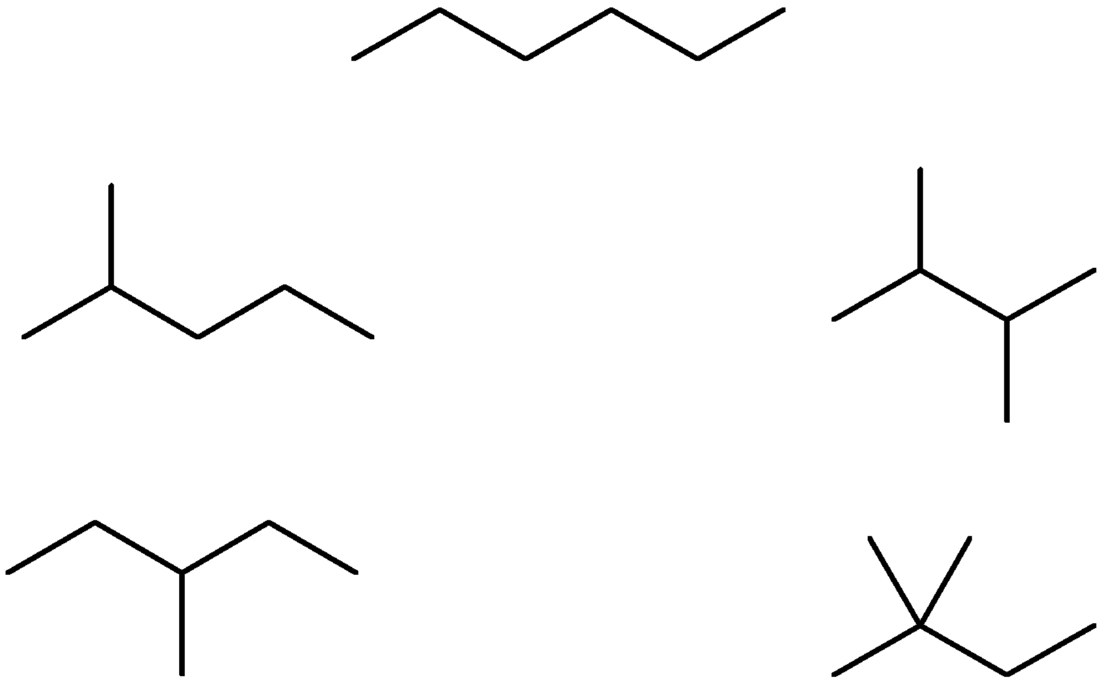
CH_3

CH_3CHCH_3

b.p. –12 °C

- Structural isomers may have different physical and chemical properties

C_6H_{14}



Structural isomers...

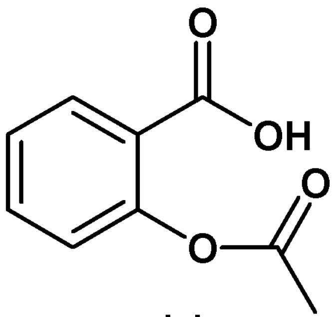
Number of Alkane Isomers

Formula	Number of isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35

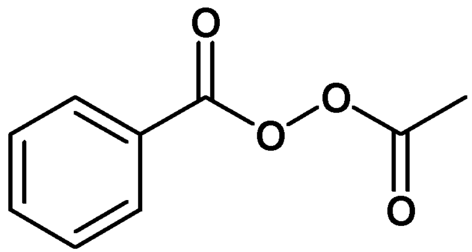
Formula	Number of isomers
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{48}$	366,319
$C_{30}H_{62}$	4,111,846,763

Structural isomers

- $C_9H_8O_4$



aspirin
(analgesic)



acetozone
(disinfectant)

- aspirin and acetozone are structural isomers with different chemical properties
- it is not possible to derive molecular structures from their ‘trivial’ names
- systematic names are required

Nomenclature - the rules

Locates the substituent(s) in the molecule

The number of carbons in the longest chain containing the functional group

Number(s) — **Substituent(s)** — **Parent** — **Ending**

The parts of the molecule that are not the stem

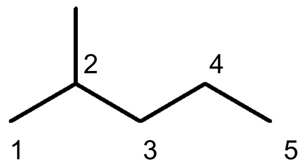
The functional group present

- Identify the longest carbon chain (parent chain)
- Identify the substituent(s)
- Number the longest chain to give the lowest possible numbering for the substituent(s)
- Allocate a number to every substituent
- List substituents in alphabetical order
- Identical substituents are indicated by prefixes: di (2), tri (3), tetra (4) ...then write it all out as one word

Isomers of hexane

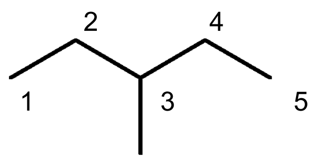
· To name **substituents** just replace the ending -ane with -yl

Alkane		Alkyl substituent	
propane	$CH_3CH_2CH_3$	propyl	$CH_3CH_2CH_2$-
pentane	$CH_3CH_2CH_2CH_2CH_3$	pentyl	$CH_3CH_2CH_2CH_2CH_2$-

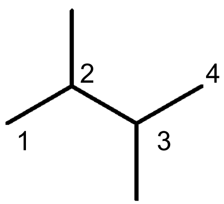


$$\begin{array}{l} \quad\;\; CH_3 \\ \quad\;\; | \\ CH_3CHCH_2CH_2CH_3 \end{array}$$

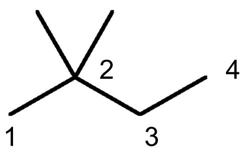
2-methylpentane



3-methylpentane



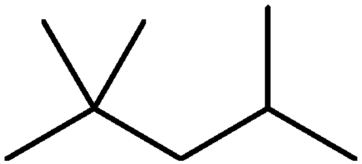
2,3-dimethylbutane



2,2-dimethylbutane

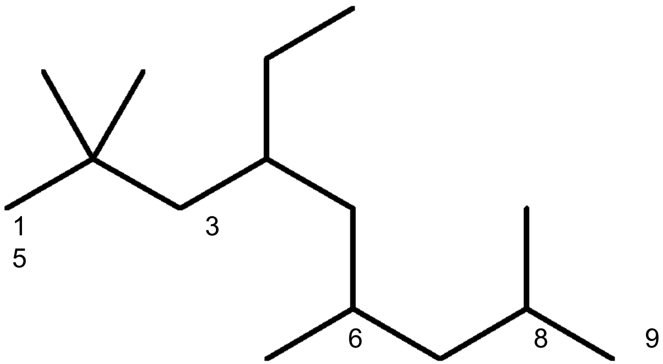
Number(s) — **Substituent(s)** — **Parent** — **Ending**

- isooctane...



2,2,4-trimethylpentane

- a more complicated example...



4-ethyl-2,2,6,8-tetramethylnonane

not

6-ethyl-2,4,8,8-tetramethylnonane

2,2,6,8-tetramethyl-4-ethylnonane

Functional groups

Number(s) — **Substituent(s)** — **Parent** — **Ending**

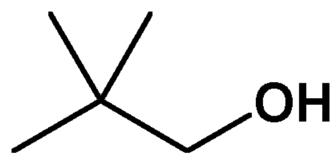
The functional group present

- Organic molecules may incorporate *functional groups*…

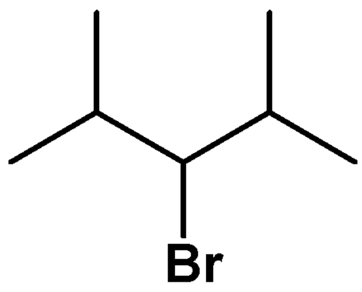
– alcohol	-OH	CH_3CH_2OH	(ethanol)
– halide	-F,Cl,Br,I	CH_3I	(iodomethane)
– carboxylic acid	$-CO_2H$	CH_3CO_2H	(ethanoic acid)
– amine	$-NH_2$	$CH_3CH_2NH_2$	(ethylamine)

… and many others

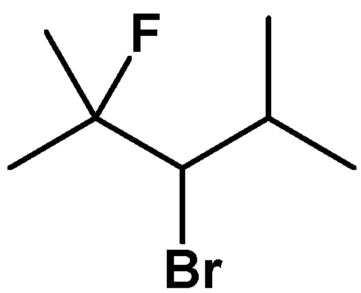
Nomenclature



2,2-dimethyl-1-propanol



3-bromo-2,4-dimethylpentane



3-bromo-2-fluoro-2,4-dimethylpentane