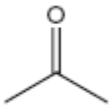
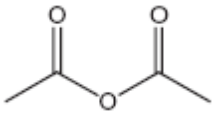
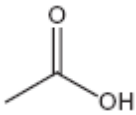
Miscellaneous Stuff

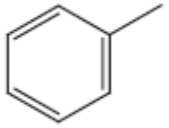
- Common abbreviations:
  - **Me** – methyl group, -CH_3
  - Et – ethyl group, -CH_2CH_3
  - ***n*Pr** – normal propyl group – $CH_2CH_2CH_3$
  - ***i*Pr** – isopropyl group – CH_3-$CHCH_3$
  - ***n*Bu** – normal butyl group – $(CH_2)_3CH_3$
  - ***t*Bu** – tertiary butyl group –$C(CH_3)_3$
  - **Ac** – acetyl group –$COCH_3$
  - **Ph** – pehyl group –C_6H_5 (<u>specifically</u> – no more than one subsistent)
  - **R** – any alkyl group.
  - **Ar** – any aryl group.
- Common names:

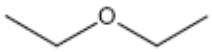

Acetone (propanone)


Acetic anhydride



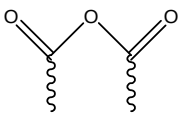
Acetic acid (ethanoic aicid)

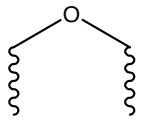

Toluene (methylbenzene)


Ether (diethyl ether)

$CHCl_3$ Chloroform (trichloromethane)

Note*:*


Anhydride functional group


Ether functional group

In both cases, the resulting compounds are named by putting the name of the two substituents one after each other, followed by "anhydride" or "ether".

- When writing formulae, write CHNO and then other stuff.
- **Mass spectrometry** effectively weighs molecules very accurately (up to one part per ten million) by vaporising and ionising them and being focused on a detector by magnetic and electric fields.
  - There are several ways to ionise the sample. The crudest is to bombard the vapour with **high energy electrons** thereby knocking some off. A more gentle technique is **electrospray**, where the sample is introduced into the chamber as

charged aerosol droplets and evaporates in the vacuum. The detected ion is then not M^+, but the molecule with an ion stuck on.

- For elements that occur naturally as several different isotopes, one peak will appear per isotope.
- The fragmentation pattern for each compound is complex and can act as a "fingerprint". Mass spec is therefore very good for identifying compounds whose spectra have already been recorded, especially since only a very small sample is needed (a few million molecules).
- Advantages of MS are that (a) it gives us the molecular formula (b) it uses only a very small amount of material (c) it's excellent for analysing mixtures. However, mass spectra are often hard to interpret.

- If a molecule has formula $C_xH_yN_zO_aHal_b$, then, as long as there are no nitro groups in the molecule, z must have the same parity (even or odd) as $y + b$. Double bond equivalents are also helpful:
  - The *saturated* compound would have $2x + 2 + z$ hydrogen and halogen atoms.
  - Subtracting $y + b$ from that and dividing by 2 gives the number of double bond equivalents in the molecules.
  - Each double bond (including C=O) counts as *one* DBE, and each ring also counts as one DBE (thus, a benzene ring counts as *four* DBEs).
  - Each nitro group counts as *one* DBE only.
- **X-Ray Crystalography** works by diffracting X-rays through a crystal, to produce a diffraction pattern. Notes:
  - The wavelength of X-rays (around 1 Å = 100 pm) is comparable to the spacing between atoms in most compounds.
  - The crystal structure obtained reveals bond lengths and angles as well as how all the molecules pack together.
  - X-Rays are diffracted by interaction with electrons, not nucleons. Therefore, the technique produces **electron density maps**. Sometimes, hydrogen atoms do not show up due to the little electron density associated with them.
  - X-Ray crystallography is certainly the ultimate method of structural identification, but it has a few disadvantages: (a) it needs samples in crystal state – samples that are liquid or do not crystallise well can't be examined (b) the hydrogen atoms are sometimes hard to locate (c) X-Ray crystallography is a science in its own right, and structure determination can take a long time.