MOLECULAR STRUCTURE - SUMMARY TABLE

METHOD	SAMPLE STATE	Principle	Information Obtained	Limitation
X-ray Diffraction	Solid crystal or powder	X rays are diffracted by the electrons around atoms. Interference patterns relate to the position and electron density of atoms	Accurate positions of atoms in crystal as well as accurate bond lengths, bond angles, and intermolecular distances	Hydrogen cannot be placed. Slow, tedious calculations (now computerized)
Electron Diffraction	Vapour (or solid surface)	Fast moving electrons behave as waves of definite wavelengths, and interference patterns can form	Accurate bond lengths and angles	Small molecules only (up to 5 atoms) in gas phase. Complex calculations
Infrared Absorption Spectra (I.R)	Solid, liquid, gas, or solution	The energy absorbed to cause different bonds to increase their vibration has definite wavelengths, which may be recognized	Detection of presence of certain bonds and groups C-O, C=O, C=C, -OH, etc. As a fingerprint to identify unknown by comparison with known spectra. To check purity of sample	Too complex to identify entire structure. The bonds must have fluctuating dipole. Although bond lengths can be calculated this can be difficult
Raman Spectra	Gas or transparent liquid	Radiation scattered due to absorption and re-emissions by bonding electrons. If extra energy is taken in or emitted by bonds this shows as a change in wavelength	Bonds present – applies to symmetrical frequencies (no vibrating dipole) so complements I.R.	Very faint, difficult to detect
Ultraviolet and Visible Absorption Spectra	Vapour	Electrons, especially in double bonds, may absorb energy of certain wavelengths. Amount and wavelength absorbed depends on how closely electrons are linked to particular atoms	Identifying bonds present, especially double bonds, conjugated bonds and aromatic systems	Vapour only. Not much use for single bonds
Nuclear Magnetic Resonance (NMR)	Solid, liquid, or solution in low proton solvent	Atoms containing an odd number of protons and even number of neutrons in the presence of a strong magnetic field absorb radio frequency energy. Wavelengths absorbed depend on other atoms or groups to which they are bonded	Particular important for ${}^{1}_{0}\mathrm{H}$. Can show number of hydrogen atoms attached to the other atoms or groups of atoms	Few natural isotopes meet requirements. For other elements artificially produced isotopes must be used. Apparatus cannot be altered for different elements
Electron Spin Resonance (ESR)	Same as NMR	Same as NMR but requires an unpaired electron. Microwave frequency is involved	Investigation of nuclear spin and radicles (particularly reaction intermediates)	Difficult to carry out. Difficult to interpret results
Mass Spectrometry	Vapour	The molecule is changed in the M.S. Some molecules will fragment into further changed particles. The mass of all changed particles present can be detected	Spectrum of masses of particles present gives indication of arrangement in original molecule	Sample must be thermally stable and readily vaporized
Double Focusing Mass Spectrometry	Vapour	Highly accurate mass spectrometers can determine molecular mass to 3 or 4 decimal places	Molecular formulae maybe directly determined from tables since atomic masses differ from integer to varying extents	