SL worksheet IR and Carbon NMR

**Some important concepts from NMR spectroscopy**

1H nucleus is shielded or screened by the electrons that surround it. Each nucleus feels an influence of the main magnetic field to a different extent depending on the efficiency in which it is screened. Each 1H nucleus with a different chemical environment has different shielding HENCE a different chemical shift in an 1H NMR.

The number of different signals in an 1H NMR = the number of chemically distinct environments for the 1H in the molecule. UNLESS two 1H environments are identical by **symmetry** their chemical shifts are different.

1H nucleus is sensitive to presence of neighboring electronegative and electropositive groups that can influence the region the sift appears.

* Electron withdrawing substituents (-OH, -OCOR, -OR, -N02, halogen) cause downfield shifts of 2-4 ppm. The further the electronegative group is from 1H of interest the LESS of the effect it has on the ppm region the hydrogen peak occurs.



Common 1H chemical shift values in selected organic compounds



ICE CREAM CONE EFFECT

* The chemical shift of a nucleus can be affected by the presence its vicinity of a magnetic anisotropic group (aromatic ring or carbonyl group)
* The resonance of a nucleus which is located close to the face of an aromatic ring will be shifted to high field (towards TMS)
* A proton in which is in the plane of an aromatic ring is DE-shielded by the ice cream cone effect
* The ice cream cone effect is the main reason that protons attached to aromatic rings appear around 7-8ppm since they are in the DE shielded zone of aromatic ring





Pascals triangle summary with respect to multiplicity.



Examples ^^



**Some important concepts in IR**

Infrared adsorption spectra are calibrated in wavelengths expressed in micrometers where \_\_\_\_\_um = 10-6 m

In frequency-related wave numbers (cm^-1) which are reciprocals of wavelengths where

* Wave number

The transitions responsible for IR bands are due to molecular vibrations i.e. to periodic motions involving stretching or bending of bonds. Polar bonds are associated with STRONG IR adsorption.

Shorter and Stronger bonds have stretching vibrations at the **higher energy end** (shorter wavelength) of the IR spectrum than the longer and weaker bonds

Bonds to lighter atoms (hydrogen e.g.) vibrate at higher energy than bonds to heavier atoms

Some tables that can assist you in further knowledge.





Some important concepts in 13C NMR spectroscopy

* Since 13C nucleus is isotopically **rare** it is extremely unlikely 13C- 13C coupling is not observed. 13C can couple strong to protons that may be attached e.g. 1JC-H coupling.

**BROAD BAND**

* **IF the** 1H nucleus during 13C acquisition are irradiated so that all 1H are fully decoupled from the 13C = **BROAD BAND** where each unique 13C environment gives rise to a singlet signal

**ORD (off resonance decoupling) (also can be called SFORD)**

* distinguish by inspection whether a carbon atom is a part of a methyl group CH3 (quartet), methylene group CH2 (triplet), a methine (CH) group (doublet) or a quaternary carbon (a singlet) just as in the fully proton-coupled spectrum
* CH3-signals appear as quartets, -CH2- signals appear as triplets, -CH- groups appear as doublets and quaternary C (no attached H) appear as singlets

**DEPT (distortionless enhancement by polarization transfer)**

* Most commonly used to determine the multiplicities of 13C signals
* Quaternary carbons DO NOT APPEAR
* CH3 and CH signals point upward
* CH2 groups point downward







