

Revised July 2005



DATA FOR ORGANIC TOPIC 5 TEST & EXAM

- IR Data

Bond	Functional Group	Frequency Range cm^{-1}
C-H	Alkanes	2850 - 3000
=C-H	Alkenes and aromatics	3030 - 3140
$\equiv\text{C-H}$	Alkynes	3300
O-H	Alcohols	3500 - 3700 (non hydrogen bonded) 3200 - 3500 (Hydrogen bonded)
O-H	Carboxylic acids	2500 - 3000
N-H	Amines	3200 - 3600
C=C	Alkenes	1600 - 1680
C=O	Aldehydes, ketones, esters, acids	1650 - 1780
C \equiv C	Alkynes	2100 - 2260
C \equiv N	Nitriles	2200 - 2400

- H NMR Data

Typical shifts of hydrogen atoms in certain environments are shown below. These peaks are relative to TMS and should only be used as a guide.

Type of H	δ (ppm)
C-CH ₃	0.85 - 0.95
C-CH ₂ -C	1.20 - 1.35
C-C(C)H-C	1.40 - 1.65
CH ₃ -C=C	1.6 - 1.9
CH ₃ -Aromatic Ring	2.2 - 2.5
CH ₃ -C=O	2.1 - 2.6
CH ₃ -N-	2.1 - 3.0
CH ₃ -O-	3.5 - 3.8
-CH ₂ -Cl	3.6 - 3.8
CHCl ₂	5.8 - 5.9
CH ₂ F	4.3 - 4.4
CH ₂ Br	3.4 - 3.6
CH ₂ I	3.1 - 3.3
CH ₂ =C-	4.6 - 5.0
-CH=C-	5.2 - 5.7
-C \equiv C-H	2.4 - 2.7
-CHO	9.5 - 9.7
-COOH	10 - 13
-OH	0.5 - 5.5
Aromatic Ring-OH	4 - 8

Factors affecting chemical shift.

1. Electronegativity causes a downfield shift.
2. Hydrogen's attached to a carbon atom that is part of a multiple bond or aromatic ring appear downfield of those that are attached to saturated C atoms.