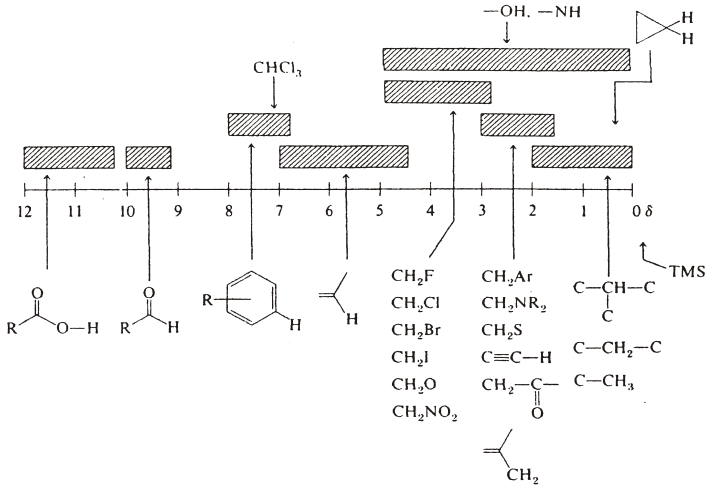
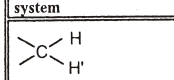
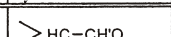
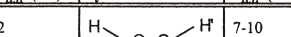
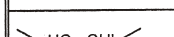
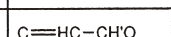
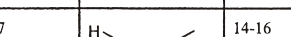
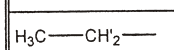
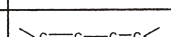
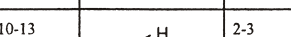
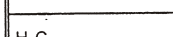
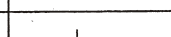
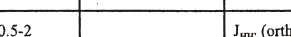
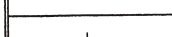
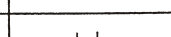
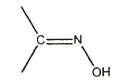
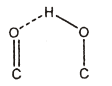
^{1}H nmr Predictions



Typical proton-proton coupling constants in some common systems

system	$J_{H,H'}$ (Hz)	system	$J_{H,H'}$ (Hz)	system	$J_{H,H'}$ (Hz)
	10-15		2		7-10
	~7		7		14-16
	~7		10-13		2-3
	~6		0.5-2		$J_{HH'}$ (ortho) 8
	0		1		$J_{HH''}$ (meta) 2
	5-7		2.5		$J_{HH'''}$ (para) 1

δ values of acidic protons*

proton	δ (ppm)	proton	δ (ppm)
ROH	0.5-4.5	$RCONH_2$, RCONHR	5-12
RNH_2, RNHR	1-5		9-12
RSH	1-2		
ArOH	4.5-6.5		
$ArNH_2$, ArNHR	3-6		7-13
ArSH	3-4		
RCOOH	9-13		

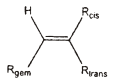
*Shifts vary widely with temperature, concentration, pH and solvent. Signals are often broadened. Low field (high δ) shifts caused by hydrogen bonding.

chemical shifts of protons in substituted benzene rings (in ppm from benzene, δ = 7.27 ppm)

substituent	Δ_{ortho}	Δ_{meta}	Δ_{para}	substituent	Δ_{ortho}	Δ_{meta}	Δ_{para}
NO_2	0.94	0.18	0.39	F	-0.30	-0.02	-0.23
CHO	0.58	0.20	0.26	Cl	0.01	-0.06	-0.08
COOH	0.80	0.16	0.25	Br	0.19	-0.12	-0.05
$COOCH_3$	0.71	0.08	0.20	I	0.39	-0.25	-0.02
COCl	0.82	0.21	0.35	NH_2	-0.76	-0.25	-0.63
CCl_3	0.8	0.2	0.2	OCH_3	-0.46	-0.10	-0.41
$COCH_3$	0.62	0.10	0.25	OH	-0.49	-0.13	-0.2
CN	0.26	0.18	0.30	OCOR	-0.2	0.1	-0.2
$CONH_2$	0.65	0.20	0.22	$NHCH_3$	-0.8	-0.3	-0.6
$^+NH_3$	0.4	0.2	0.2	$N(CH_3)_2$	-0.60	-0.10	-0.62
H_2C=CH	0.00	-0.03	-0.10	CH_3	-0.16	-0.09	-0.17
CH_2X*	0.0-0.1	0.0-0.1	0.0-0.1	CH_2CH_3	-0.15	-0.06	-0.18
*X = Cl, alkyl, OH, or NH_2				$CH(CH_3)_2$	-0.14	-0.09	-0.18
				$C(CH_3)_3$	-0.09	0.05	-0.23

Estimation of chemical shift of a proton attached to a double bond

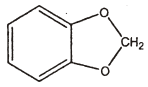
$$\delta_{C=C_H} = 5.25 + \Delta_{gem} + \Delta_{cis} + \Delta_{trans}$$



R	Δgem	Δcis	Δtrans	R	Δgem	Δcis	Δtrans
-H	0	0	0	-CHO	1.02	0.95	1.17
-alkyl	0.45	-0.22	-0.28	$-C(NR_2)=O$	1.37	0.98	0.46
-alkyl-ring	0.69	-0.25	-0.28	-C(Cl)=O	1.11	1.46	1.01
$-CH_2O$	0.64	-0.01	-0.02	-OR (R=aliphatic)	1.22	-1.07	-1.21
$-CH_2S$	0.71	-0.13	-0.22	-OR (R=conjugated)	1.21	-0.60	-1.00
$-CH_2X$	0.70	0.11	-0.04	-OCOR	2.11	-0.35	-0.64
$-CH_2NR_2$	0.58	-0.10	-0.08	$-CH_2-C=O$	0.69	-0.08	-0.06
-C=C (isolated)	1.00	-0.09	-0.23	$-CH_2-C\equiv N$	0.69	-0.08	-0.06
-C=C (conjugated)	1.24	0.02	-0.05	$-CH_2$-aromatic-ring	1.05	-0.29	-0.32
$-C\equiv N$	0.27	0.75	0.55	-Cl	1.08	0.18	0.13
$-C\equiv C-$	0.47	0.38	0.12	-Br	1.07	0.45	0.55
-C=O (isolated)	1.10	1.12	0.87	-I	1.14	0.81	0.88
-C=O (conjugated)	1.06	0.91	0.74	-NR (R=aliphatic)	0.80	-1.26	-1.21
-COOH (isolated)	0.97	1.41	0.71	-NR (R=conjugated)	1.17	-0.53	-0.99
-COOH (conjugated)	0.80	0.98	0.32	-N(C=O)R	2.08	-0.57	-0.72
-COOR (isolated)	0.80	1.18	0.55	-aromatic	1.38	0.36	-0.07
-COOR (conjugated)	0.78	1.01	0.46	$-SR_2$	1.11	-0.29	-0.13
				$-SO_2$	1.55	1.16	0.93

$X-CH_1^A-CH_2^B-CH_3^C$				$\delta CH_2 = 0.23 + C_1 + C_2$		$\delta CH = 0.23 + C_1 + C_2 + C_3$	
X	CH_3^A	CH_2^B	CH_3^C	X	C	X	C
$-CH_2CH_3$	1.3	1.3	0.9	$-CH_3$	0.5	-CO-R	1.7
-COOH	2.3	1.7	1	$-CF_3$	1.1	-I	1.8
-SH	2.5	1.6	1	>C=C<	1.3	-Ph	1.8
$-NH_2$	2.6	1.5	0.9	$-C\equiv C-R$	1.4	-Br	2.3
-Ph	2.6	1.6	0.9	-COOR	1.5	-OR	2.4
-Br	3.4	1.9	1	-NR2	1.6	-Cl	2.5
-Cl	3.5	1.8	1	$-CONR_2$	1.6	-OH	2.6
-OH	3.6	1.6	0.9	-SR	1.6	-N=C=S	2.9
$-NO_2$	4.4	2.1	1	$-C\equiv C-Ar$	1.7	-OCOR	3.1
-I	3.2	1.8	0.9	$-C\equiv N$	1.7	-OPh	3.2

chemical shifts of methyl, methylene and methine protons

methyl protons	δ (ppm)	methylene protons	δ (ppm)	methine protons	δ (ppm)
CH_3-C	0.9	$-C-CH_2-C$	1.4	C-CH-C	1.5
$CH_3-C-C=C$	1.1	$-C-CH_2-C-C=C$	1.7	C-CH-C-O	2
CH_3-C-O	1.3	$-C-CH_2-C-O$	1.9	CH-Ar	3
$CH_3-C=C$	1.6	$-C-CH_2-C=C$	2.3	C-CH-CO-R	2.7
CH_3-Ar	2.3	$-C-CH_2-Ar$	2.7	C-CH-CO-Ar	3.3
CH_3-CO-R	2.2	$-C-CH_2-CO-R$	2.4	C-CH-O-R	3.7
$CH_3-CO-Ar$	2.6	$-C-CH_2-CO-O-R$	2.2	C-CH-OH	3.9
$CH_3-CO-O-R$	2	$-C-CH_2-CO-N-R$	2.2	C-CH-O-CO-r	4.8
$CH_3-CO-O-Ar$	2.4	$-C-CH_2-O-R$	3.4	C-CH-N	2.8
$CH_3-CO-N-R$	2	$-C-CH_2-O-H$	3.6	C-CH-S	3.2
CH_3-O-R	3.3	$-C-CH_2-O-Ar$	4.3	$C-CH-NO_2$	4.7
$CH_3-O-C=C$	3.8	$-C-CH_2-O-CO-R$	4.1	C-CH-Br	4.3
CH_3-O-Ar	3.8	$-C-CH_2-N$	2.5	C-CH-I	4.3
$CH_3-O-CO-R$	3.7	$-C-CH_2-S$	2.4	$C-CH-C\equiv N$	2.7
CH_3-N	2.3	$-C-CH_2-NO_2$	4.4	C-CH-N-CO-R	4.1
CH_3-N^+	3.3	$-C-CH_2-C-NO_2$	2.1	R-CHO	9.4-10.0
CH_3-N-Ar	3	$-C-CH_2-C=C-CO$	2.4	Ar-CHO	9.7-10.5
CH_3-S	2.1	$C=C(CH_2)-CO$	2.4	H-CO-O	8.0-8.2
CH_3-C-NO_2	1.6	$-C-CH_2-Cl$	3.6	H-CO-N	8.0-8.2
$CH_3-C=C-CO$	2	$-C-CH_2-Br$	3.5	$-C\equiv C-H$	1.8-3.1
$C=C(CH_3)-CO$	1.8	$-C-CH_2-I$	3.2	Ar-H	6.0-9.0
$CH_3-N-CO-R$	2.9	$-C-CH_2-C\equiv N$	2.3	-C=CH-	4.5-6.0
			5.9	-C=CH-CO	5.8-6.7
				-CH=C-CO	6.5-8.0
				-CH=C-O	4.0-5.0
				-C=CH-O	6.0-8.1
				-CH=C-N	3.7-5.0
				-C=CH-N	5.7-8.0