Tables

For

Organic Structure Analysis

Magnetic properties of commonly studied species.

Nucleus	*Natural abundance (%)*	*Approximate sensitivity at constant B_O for natural abundance*[1]	*Resonance frequency at 2.35 T (100 MHz)*	*Relative magnetic moment (μ)*	*Relative quadrupole moment (Q)*
I = 1/2 [2]					
*^{1}H	99.98	**1.0**	100.0	**1.0**	–
^{3}H	–	0.0	106.7	1.07	–
*^{13}C	1.1	1.8×10^{-4}	25.3	0.25	–
^{15}N[a]	0.4	3.8×10^{-6}	10.1	-0.10	–
*^{19}F	100.0	0.83	94.1	0.94	–
^{29}Si[a]	4.7	3.6×10^{-3}	19.9	-0.20	–
*^{31}P	100.0	0.07	40.5	0.41	–
Free electron[a]	–	–	65,820.0	-657.4	–
I = 0 [0]					
^{12}C	98.9	–	–	–	–
^{16}O	99.9	–	–	–	–
^{28}Si	92.3	–	–	–	–
^{30}Si	3.1	–	–	–	–
^{32}S	94.8	–	–	–	–
^{34}S	4.4	–	–	–	–
I = 1 [3]					
^{2}H	0.02	1.5×10^{-6}	15.4	0.31	0.17
^{14}N	99.6	1.0×10^{-3}	7.2	0.14	1.0
I = 3/2 [4]					
^{11}B	80.4	0.13	32.1	0.96	2.2
^{23}Na	100.0	0.09	26.5	0.79	9.3
^{33}S	0.8	1.7×10^{-5}	7.7	0.23	-4.0
^{35}Cl	75.5	3.6×10^{-3}	9.8	0.23	5.0
^{37}Cl	24.5	6.7×10^{-4}	8.2	0.25	-4.0
^{79}Br	50.5	0.04	25.1	0.75	20.7
^{81}Br	49.5	0.05	27.0	0.81	17.6
I = 5/2 [6]					
^{17}O[a]	0.04	1.1×10^{-5}	13.5	-0.68	-1.6
^{127}I	100.0	0.09	20.0	1.00	37.5
I = 3 [7]					
^{10}B	19.7	3.7×10^{-3}	10.7	0.64	4.6

[ ] Number of energy levels.
a Negative magnetic moment.
* Most useful.
[1] Data from *Bruker Almanac* adjusted for natural abundance

Some useful NMR solvents

Solvent	δ ^{1}H (ppm) (mult.)	δ ^{13}C (ppm) (mult.)	Liquid Range (°C)	Dielectric Constant	δ HOD (ppm) in ^{1}H NMR
Acetic Acid-d_4	11.65 (1) 2.04 (5)	179.0 (1) 20.0 (7)	17 – 118	6.1	11.6
Acetone-d_6	2.05 (5)	206.7 (13) 29.9 (7)	-94 – 57	20.7	2.0
Acetonitrile-d_3	1.94 (5)	118.7 (1) 1.4 (7)	-45 – 82	37.5	2.1
Benzene-d_6	7.16 (1)	128.4 (3)	5 – 80	2.3	0.4
Chloroform-d	7.27 (1)	77.2 (3)	-64 – 62	4.8	1.5
Cyclohexane-d_{12}	1.38 (1)	26.4 (5)	6 – 81	2.0	–
D_2O	4.80		4 – 101	78.5	4.8
Dichloromethane-d_2	5.32 (3)	54.0 (5)	-95 – 40	8.9	1.5
p-Dioxane-d_8	3.53 (m)	66.7 (5)	12 – 101	2.2	2.4
DMF-d_7	8.03 (1) 2.92 (5) 2.75 (5)	163.2 (3) 34.9 (7) 29.8 (7)	-61 – 153	36.7	3.5
DMSO-d_6	2.50 (5)	39.5 (7)	18 – 189	46.7	3.3
Methanol-d_4	4.87 (1) 3.31 (5)	49.2 (7)	-98 – 65	32.7	5.0
Pyridine-d_5	8.74 (1) 7.58 (1) 7.22 (1)	150.4 (3) 135.9 (3) 123.9 (5)	-42 – 116	12.4	5.0
THF-d_8	3.58 (1) 1.73 (1)	67.6 (5) 25.4 (1)	-109 – 66	7.6	2.5
Toluene-d_8	7.09 (m) 7.00 (1) 6.98 (m) 2.09 (5)	137.9 (1) 129.2 (3) 128.3 (3) 125.5 (3) 20.4 (7)	-95 – 111	2.4	0.4
TFA-d	11.50 (1)	164.2 (4) 116.6 (4)	-15 – 72	39.5	11.5

^{1}H NMR shifts of common impurities in various solvents (δ ppm (mult))

Impurity	Chloroform-d	DMSO-d_6	Pyridine-d_5	Benzene-d_6	D_2O
Acetic Acid	2.13 (s)	1.95 (s)	2.13 (s)	1.63 (s)	2.16 (s)
Acetone	2.17 (s)	2.12 (s)	2.00 (s)	1.62 (s)	2.22 (s)
Acetonitrile	1.98 (s)	2.09 (s)	1.85 (s)	0.67 (s)	2.05 (s)
Benzene	7.37 (s)	7.40 (s)	7.33 (s)	7.30 (s)	7.44 (s)
t-Butanol	1.28 (s)	1.14 (s)	1.37 (s)	1.06 (s)	1.23 (s)
Chloroform	7.27 (s)	8.35 (s)	8.41 (s)	6.41 (s)	ns
Cyclohexane	1.43 (s)	1.42 (s)	1.38 (s)	1.40 (s)	ns
Dichloromethane	5.30 (s)	5.79 (s)	5.62 (s)	4.46 (s)	ns
Diethyl Ether	3.48 (q)	3.42 (q)	3.38 (q)	3.27 (q)	3.56 (q)
	1.20 (t)	1.13 (t)	1.12 (t)	1.10 (t)	1.17 (t)
DMF	8.01 (s)	7.98 (s)			7.91 (s)
	2.95 (s)	2.92 (s)	2.72 (s)	2.40 (s)	3.00 (s)
	2.88 (s)	2.76 (s)	2.66 (s)	1.98 (s)	2.86 (s)
DMSO	2.62 (s)	2.52 (s)	2.49 (s)	1.91 (s)	2.70 (s)
p-Dioxane	3.70 (s)	3.61 (s)	3.61 (s)	3.38 (s)	3.75 (s)
Ethanol	3.72 (q)	3.49 (q)	3.86 (q)	3.39 (q)	3.64 (q)
	1.24 (t)	1.09 (t)	1.29 (t)	0. 97 (t)	1.16 (t)
Ethyl Acetate	4.12 (q)	4.08 (q)	4.06 (q)	3.91 (q)	4.14 (q)
	2.04 (s)	2.02 (s)	1.94 (s)	1.68 (s)	2.08 (s)
	1.25 (t)	1.21 (t)	1.10 (t)	0.94 (t)	1.23 (t)
Methanol	3.48 (s)	3.20 (s)	3.57 (s)	3.09 (s)	3.35 (s)
Petroleum Ether	1.28 (bs)	1.28 (bs)	1.20 (bs)	1.22 (s)	ns
	0.90 (t)	0.89 (t)	0.86 (t)	0.89 (t)	
i-Propanol	4.03 (m)		4.16 (m)	3.76 (m)	
	1.22 (d)	1.06 (d)	1.29 (d)	1.01 (d)	1.18 (d)
n-Propanol	3.60 (t)		3.75 (t)	3.76 (t)	3.61 (t)
	1.60 (m)	1.45 (m)	1.70 (m)	1.40 (m)	1.57 (m)
	0.93 (t)	0.87 (t)	0.97 (t)	0.80 (t)	0.89 (t)
Pyridine	8.60 (m)	8.61 (m)	8.71 (m)	8.50 (m)	8.50 (m)
	7.69 (m)	7.83 (m)	7.58 (m)	7.05 (m)	7.90 (m)
	7.28 (m)	7.21 (m)	7.21 (m)	6.70 (m)	7.47 (m)
THF	3.74 (m)	3.63 (m)	3.67 (m)	3.01 (m)	3.75 (m)
	1.85 (m)	1.78 (m)	1.64 (m)	0.87 (m)	1.88 (m)
Toluene	7.19 (m)	7.22 (m)	7.22 (m)	7.10 (m)	ns
	2.34 (s)	2.32 (s)	2.22 (s)	2.13 (s)	
Triethylamine	2.56 (q)	2.47 (q)	2.43 (q)	2.40 (q)	2.59 (q)
	1.03 (t)	0.99 (t)	0.96 (t)	0.95 (t)	1.02 (t)

ns=not soluble

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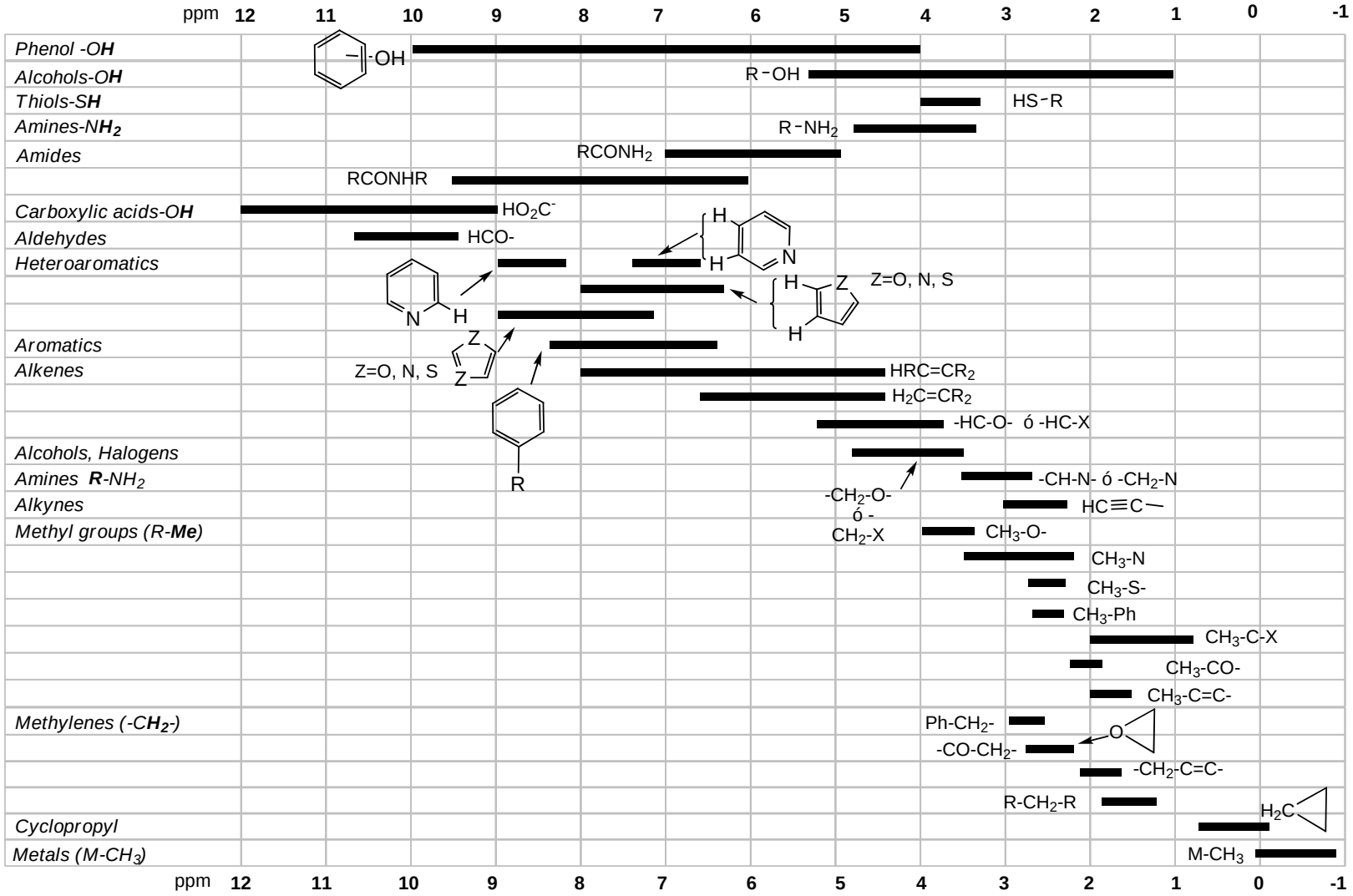
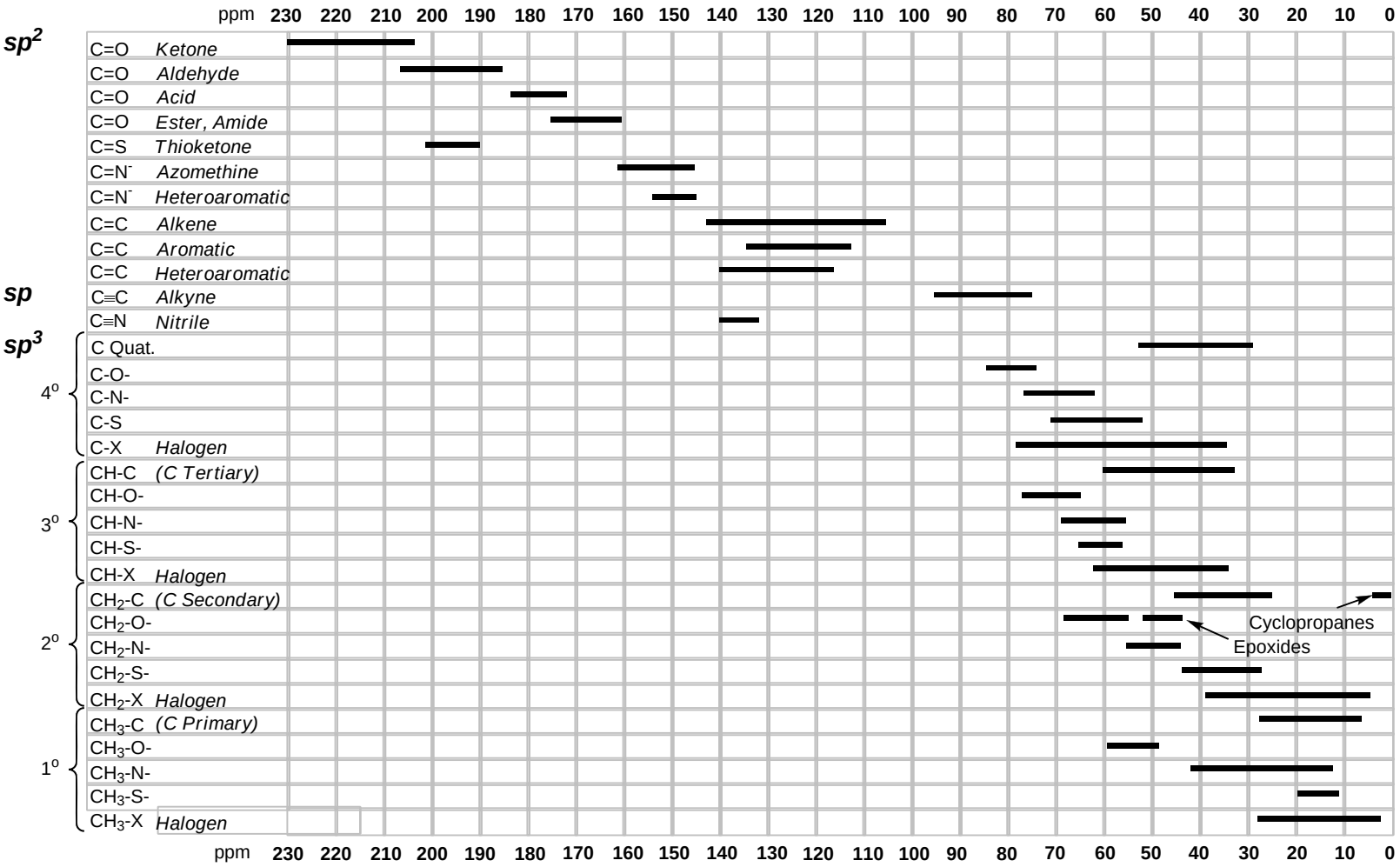
^{1}H NMR Chemical Shifts in Organic Compounds



Relative to TMS (0 ppm)

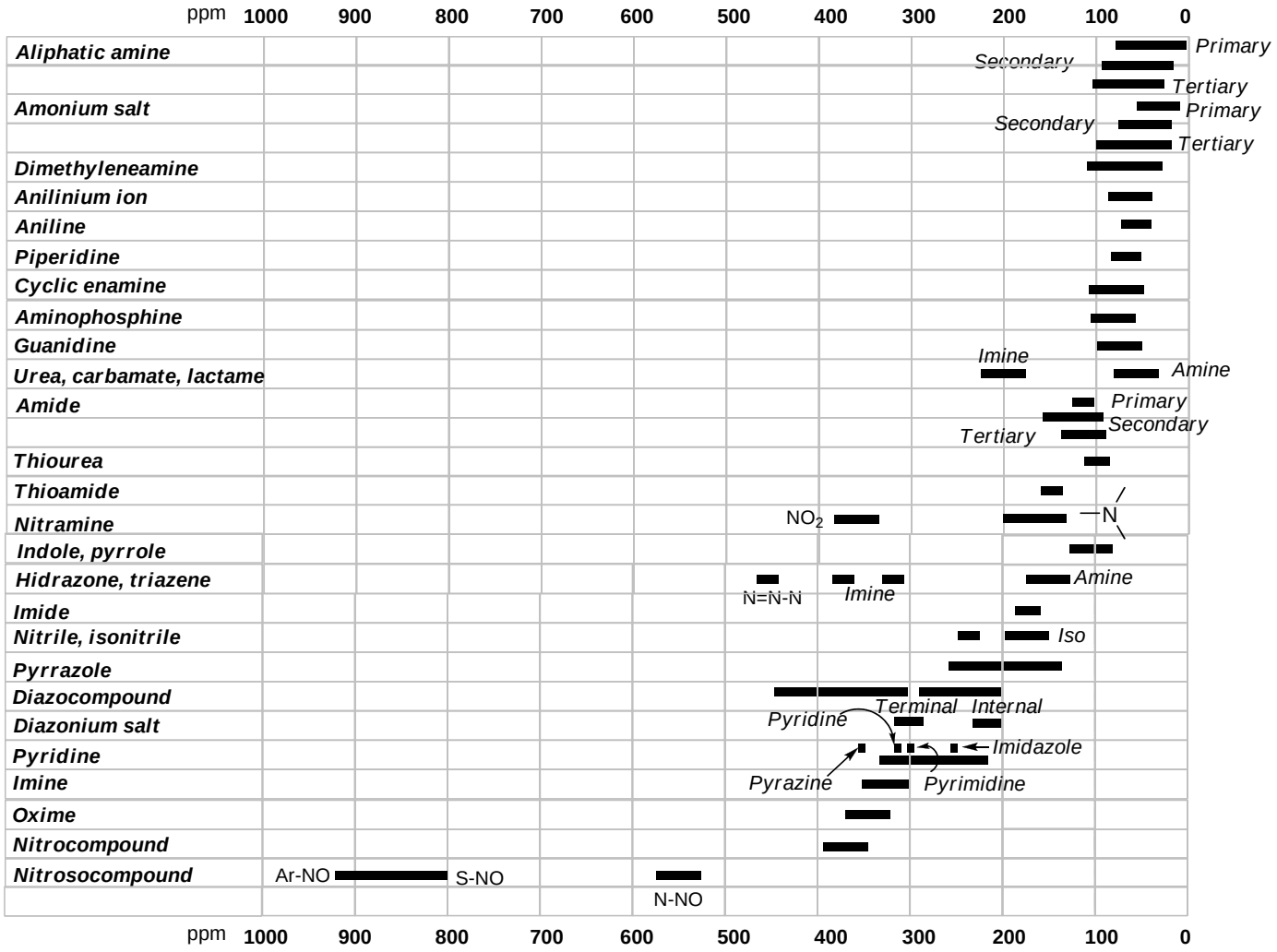
^{13}C NMR Chemical Shifts in Organic Compounds



*Relative to TMS (0 ppm)

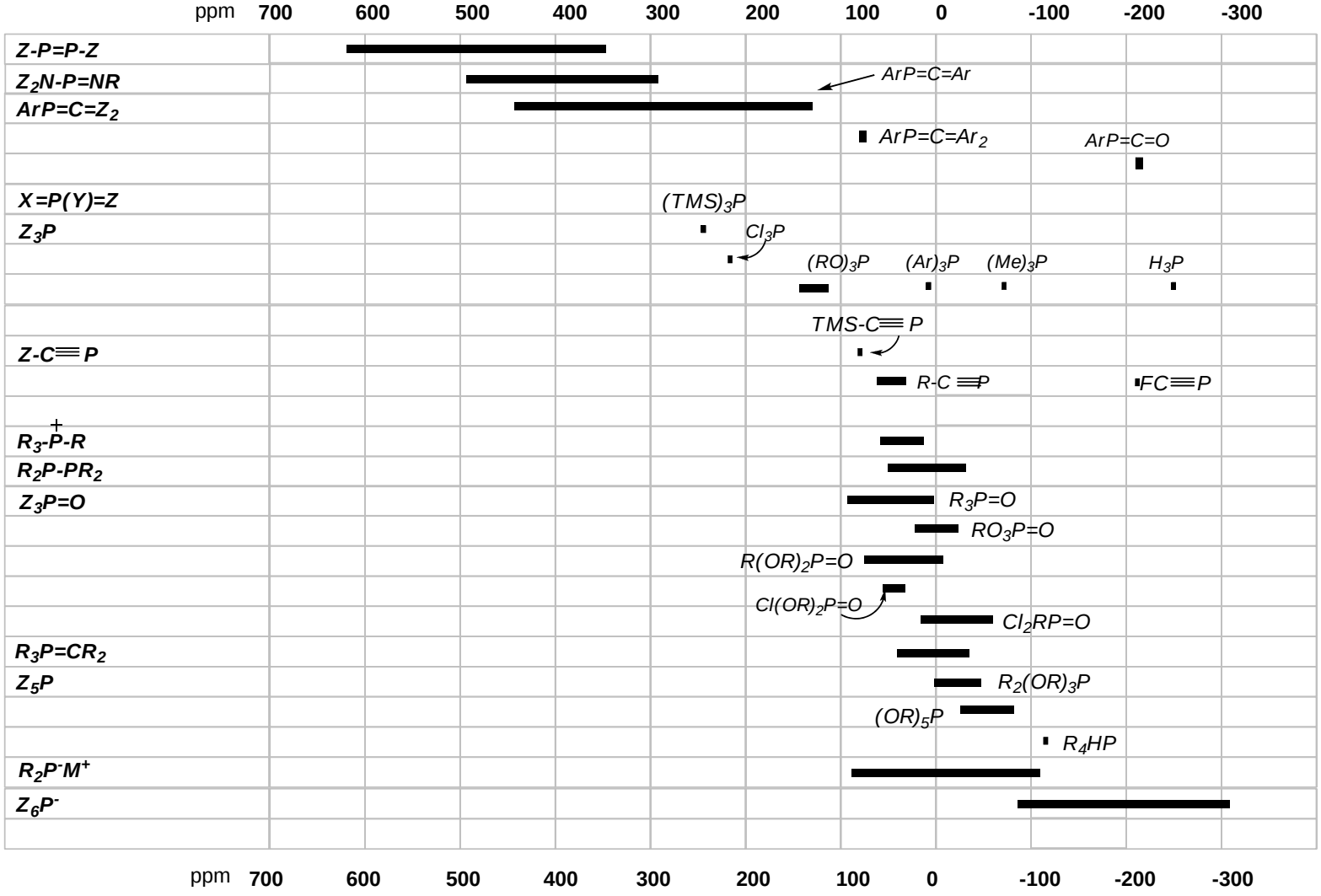
4° Quaternary, 3° Tertiary, 2° Secondary, 1° Primary

^{15}N NMR Chemical Shifts in Organic Compounds



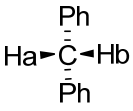
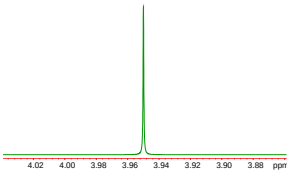
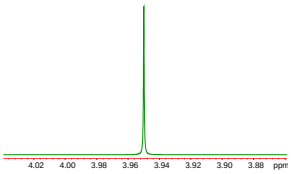
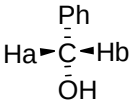
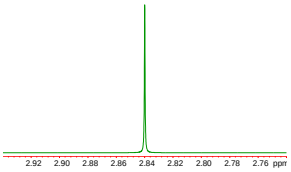
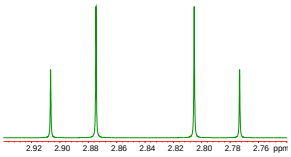
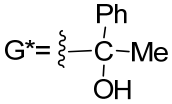
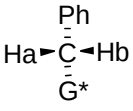
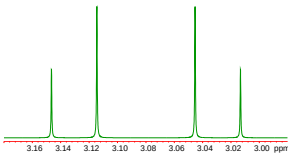
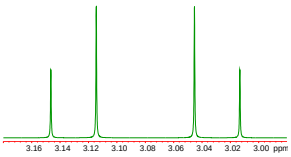
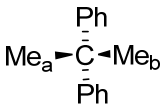
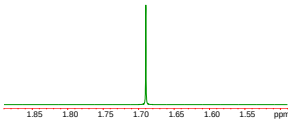
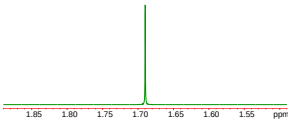
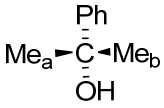
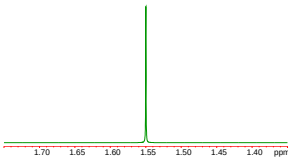
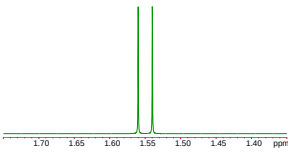
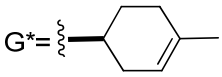
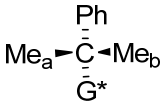
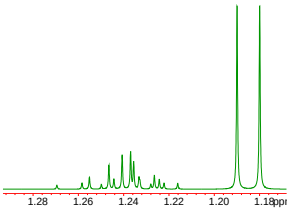
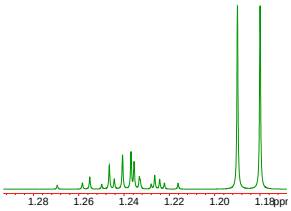
*Nitrometane as reference (380 ppm)

^{31}P NMR Chemical Shifts in Organic Compounds

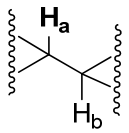
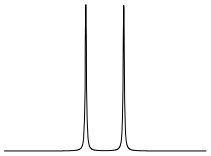
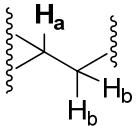
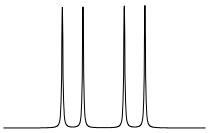
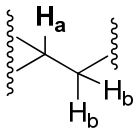
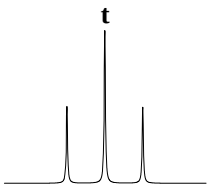
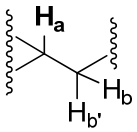
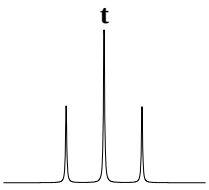
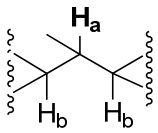
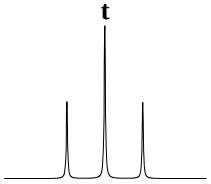
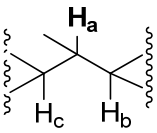
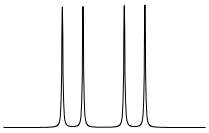
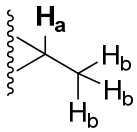
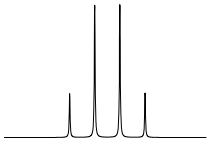
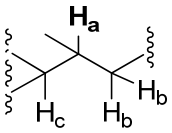
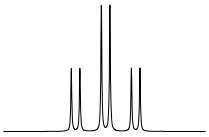
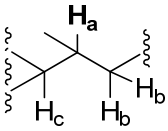
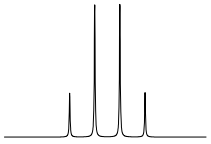
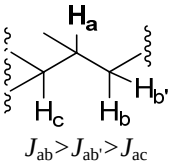
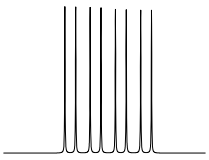
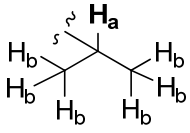
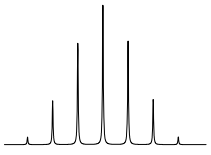
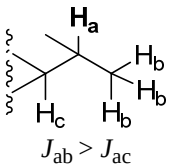
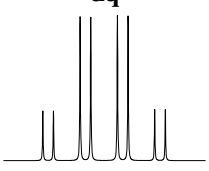


*Reference H_3PO_4 85%. Adapted from A Complete Introduction to Modern NMR Spectroscopy. R. S. Macomber. J. Wiley and Sons. 1998.

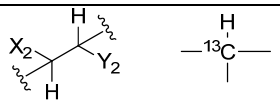
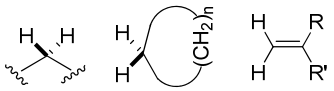
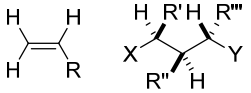
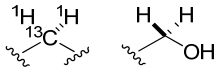
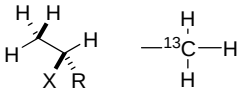
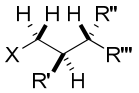
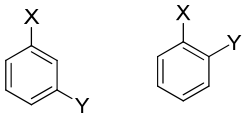
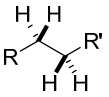
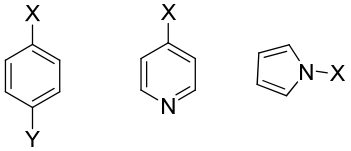
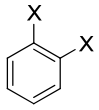
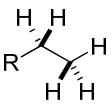
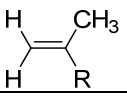
Symmetry Effects for Homotopic; Enantiotopic, and Diasterotopic Groups

GROUP *A/B Relationships*	*Example*	*Appearance ^{1}H RMN* *Achiral solvent*	*Appearance ^{1}H RMN* *Chiral solvent*
Methylenes			
Homotopic			
Enantiotopic			
Diastereotopic				
Methyls			
Homotopic			
Enantiotopic			
Diastereotopic				

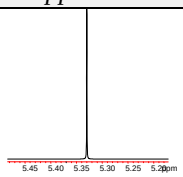
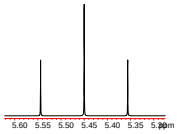
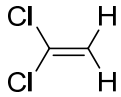
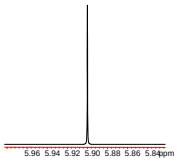
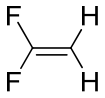
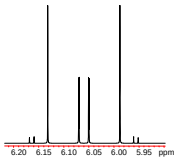
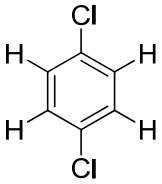
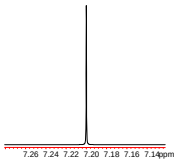
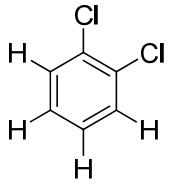
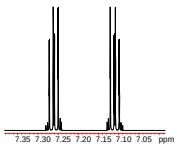
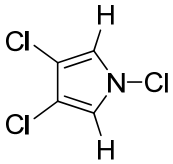
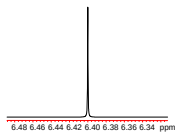
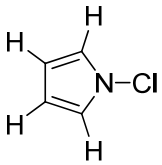
First-order Splitting Patterns of Some Common Spin Systems.

Entry	*Structure*	*Notation and Pattern for* ***Ha*** $J_{ab}=J_{ac}$	*Entry*	*Structure*	***Ha*** *multiplets*
1		**d** 	**7**	 $\nu_b \neq \nu_{b'}$ $J_{ab} > J_{ab'}$	**dd** 
2		**t** 	**8**	 **$\Delta\nu_{ab}$> 0;$\nu_b = \nu_{b'}$** $J_{ab} = J_{ab'}$	**t** 
3		**t** 	**9**	 $J_{ac} > J_{ab}$	**dd** 
4		**q** 	**10**	 $J_{ab} > J_{ac}$	**dt** 
5		**q** 	**11**	 $J_{ab} > J_{ab'} > J_{ac}$	**ddd** 
6		**sp** 	**12**	 $J_{ab} > J_{ac}$	**dq** 

Common Coupled Spin Systems

Entry	*No. spins*	*Spin Type*	*J values by inspection*	*Examples*
1	2	AX	Yes	
2	2	AB	Yes	
3	3	AMX ABX ABC	Yes J_{AB} and $J_{(AX+BX)}$ None	
4	3	A_2X	Yes	
5	3	A_2B	Yes	
6	4	A_3X A_3B	Yes Yes	
7	4	AMX_2	Yes	
8	4	ABX_2 ABCX ABCD	J_{AB} None None	rare 
9	4	A_2X_2 A_2B_2	Yes No	
10	4	AA'XX'	J_{AX} when $J_{AA'}$ or $J_{XX'}$ is small No when large	
11	4	AA'BB'	No	
12	5	A_3X_2 A_3B_2	Yes Yes	
13	5	A_3MX A_3XY	Yes J_{XY}	

Examples of Magnetic and Chemical Equivalence.

Type	*^1H Group Symmetry*	*Chemical Equivalence*	*Magnetic Equivalence*	*Spectral Type*	*^1H Spectral Appearance*
CH_2Cl_2	Homotopic	Yes	Yes	A_2	
CH_2F_2	Homotopic	Yes	Yes	A_2X_2	
	Homotopic	Yes	Yes	A_2	
	Homotopic	Yes	No	AA'XX'	
	Homotopic	Yes	Yes	A_4	
	Two homotopic sets	Yes	No	AA'BB'	
	Homotopic vinyl Hs	Yes	Yes	A_2X	
	Two homotopic sets	Yes	No	AA'BB'