Tables

For

Organic Structure Analysis

Nucleus	Natural abundance (%)	Approximate sensitivity at constant B ₀ for natural abundance ¹	Resonance frequency at 2.35 T (100 MHz)	Relative magnetic moment (µ)	Relative quadrupole moment (Q)
I = 1/2 [2]					
*1H	99.98	1.0	100.0	1.0	_
³ H	-	0.0	106.7	1.07	-
*13C	1.1	1.8 x 10 ⁻⁴	25.3	0.25	_
15Na	0.4	3.8 x 10 ⁻⁶	10.1	-0.10	_
*19F	100.0	0.83	94.1	0.94	_
²⁹ Si ^a	4.7	3.6 x 10 ⁻³	19.9	-0.20	-
* ³¹ P	100.0	0.07	40.5	0.41	_
Free electron ^a $I = 0 [0]$	_	_	65,820.0	-657.4	_
¹² C	98.9	_	_	_	_
16 O	99.9	-	-	—	_
28Si	92.3	-	-	-	_
30Si	3.1	-	-	_	-
32S	94.8	-	-	-	-
34S	4.4	-	-	-	-
I = I [3]	0.02	6	15 4	0.21	0.17
2 H	0.02	1.5 x 10 ⁻⁶	15.4	0.31	0.17
¹⁴ N	99.6	1.0 x 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
338	0.8	1.7 x 10 ⁻⁵	7.7	0.23	-4.0
35Cl	75.5	3.6 x 10 ⁻³	9.8	0.23	5.0
37Cl	24.5	6.7 x 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]					
17Oa	0.04	1.1 x 10 ⁻⁵	13.5	-0.68	-1.6
127I	100.0	0.09	20.0	1.00	37.5
I = 3 [7] ¹⁰ B	19.7	3.7 x 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

11.65 (1)	170.0 (1)			
2.04(5)	179.0(1)	17 - 118	6.1	11.6
2.04 (5)	20.0 (7)			
2.05 (5)	206.7 (13)	-94 - 57	20.7	2.0
	29.9 (7)			
1.94 (5)	118.7 (1)	-45 - 82	37.5	2.1
	1.4 (7)	- 00	2.2	0.4
7.16(1)	128.4 (3)	5 - 80	2.3	0.4
7.27 (1)	77.2 (3)	-64 - 62	4.8	1.5
1.38 (1)	26.4 (5)	6 – 81	2.0	-
4.80		4 - 101	78.5	4.8
5.32 (3)	54.0 (5)	-95 - 40	8.9	1.5
3.53 (m)	66.7 (5)	12 - 101	2.2	2.4
8.03 (1)	163.2 (3)	-61 - 153	36.7	3.5
2.92 (5)	34.9 (7)			
2.75 (5)	29.8 (7)			
2.50 (5)	39.5 (7)	18 - 189	46.7	3.3
4.87(1)	49.2 (7)	-98 – 65	32.7	5.0
3.31 (5)				
8.74 (1)	150.4 (3)	-42 - 116	12.4	5.0
7.58 (1)	135.9 (3)			
7.22(1)	123.9 (5)			
3.58 (1)	67.6 (5)	-109 - 66	7.6	2.5
1.73 (1)	25.4 (1)			
7.09 (m)	137.9 (1)	-95 – 111	2.4	0.4
7.00(1)	129.2 (3)			
6.98 (m)	128.3 (3)			
2.09 (5)	125.5 (3)			
11.50 (1)	20.4 (7)	15 70	20.5	11.7
11.50(1)	164.2 (4)	-15 - 72	39.5	11.5
	2.05 (5) 2.05 (5) 1.94 (5) 7.16 (1) 7.27 (1) 1.38 (1) 4.80 5.32 (3) 3.53 (m) 8.03 (1) 2.92 (5) 2.75 (5) 2.50 (5) 4.87 (1) 3.31 (5) 8.74 (1) 7.22 (1) 3.58 (1) 1.73 (1) 7.09 (m) 7.00 (1) 6.98 (m) 2.09 (5) 11.50 (1)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Impurity	Chloroform-d	DMSO-d ₆	Pyridine-d5	Benzene-d ₆	D20
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)
<i>p</i> -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>i</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)
<i>n</i> -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)

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

ns=not soluble From: J. Org. Chem. **1997**, 62, 7512-7515

¹H NMR Chemical Shifts in Organic Compounds

ppm 12	11 10	9 8	7 6	5 4	3 2	1	0
Phenol -O H	🗍 - Л-ОН 💳						
Alcohols-O H			R-OH 🚃				
Thiols-S H					HS-R		
Amines-N H 2			R-NH ₂	2			
Amides	RCONHR -	RCOI	NH ₂				
Carboxylic acids-0 H		HO ₂ C ⁻	<u>ر اا</u> ا				
Aldehydes		HCO-					
Heteroaromatics				Z Z=O, N, S			
Aromatics		z /		4			
Alkenes	Z=O, N, S			HRC= CR_2			
				-HC-	O- ó -HC-X		
Alcohols, Halogens		Ŷ					
Amines R -NH ₂		R			-CH-N- ó -C	H ₂ -N	
Alkynes			-(GH ₂ -O-	HC≡(<u> </u>	
Methyl groups (R- Me)				СН ₂ -Х — (CH ₃ -O-		
					CH ₃ -	Ν	
					СН3-8	3-	
					CH ₃ -Ph		
						CH ₃	-C-X
					-	CH ₃ -CO-	
						CH ₃ -C=C-	
Methylenes (-CH ₂ -)				Ph-CH ₂ ·	0		
				-CO-C	H ₂ -	·CH₂-C=C-	
					R-CH ₂ -R		H ₂ C
Cyclopropyl							
Metals (M-CH ₃)						M-CH ₃	,

Relative to TMS (0 ppm)

¹³C NMR Chemical Shifts in Organic Compounds



*Relative to TMS (0 ppm)

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

¹⁵N NMR Chemical Shifts in Organic Compounds

ppm	1000	900	800	700	600	500	400	300	200	100	0
Aliphatic amine									Seconda	rv 📃	Prin
											Tertial
Amonium salt									Secon	darv	Prim
									0000//		T ertia
Dimethyleneamine											
nilinium ion											•
niline											
Piperidine										-	
yclic enamine										_	
minophosphine											
luanidine									Imine		
lrea, carbamate, lacta	me										Amine
mide										Prii	nary
									Tertiary	Sec	ondary
hiourea							_			-	
hioamide										• /	
litramine						NC	D ₂			■N	
ndole, pyrrole											
lidrazone, triazene							Imi	ne		Amine	
nide						IN=IN-IN			_		
itrile, isonitrile										Iso	
yrrazole										•	
iazocompound								Terminal	Internal		
iazonium salt						Pyri	dinê		_		
yridine									🗕 Imidaz	oie	
nine						Pyraz	iné 🗖	Pyr	imidine		
xime											
itrocompound											
itrosocompound	Ar-N	10	S-NO			1					
					N-NC)					

*Nitrometane as reference (380 ppm)



shere $H_3 = O_4 \circ 3\%$. Adapted from A complete introduction to would find which spectroscopy. R. S. Macomber, J. Wiley and Sons.

GROUP A/B Relationships	Example	Appearance ¹ H RMN	Appearance ¹ H RMN Chiral solvent		
Mothylanas		Achirdi soiveni	Chirai solveni		
<u>Meinvienes</u> Homotopic	Ph Ha►Ç̄≺Hb Ph				
Enantiotopic	Ph	4.02 4.00 3.98 3.36 3.94 3.92 3.90 3.88 ppr	4.02 4.00 3.98 3.96 3.94 3.92 3.90 3.88 ppm		
	Ha ► Ç̄́ ≺ Hb ŌH				
Diastereotonic		2.92 2.90 2.88 2.86 2.84 2.82 2.80 2.78 2.76 ppr	2.92 2.90 2.88 2.86 2.84 2.82 2.80 2.78 2.76 ppm		
Ph G*= §Me OH	Ph Ha►Ç̄◄Hb Ğ*	3.16 3.14 3.12 3.10 3.06 3.04 3.02 3.00 ppr	3.16 3.14 3.12 3.10 3.08 3.06 3.04 3.02 3.00 ppm		
Methyls					
Homotopic	Ph Me _a ►Ç≺Me _b Ph				
Enantiotopic	Ph Me _a ►⊄⊂Me _b ŌH	1.86 1.80 1.75 1.70 1.86 1.80 1.56 ppr	1.80 1.80 1.75 1.70 1.85 1.80 1.55 ppm		
Diastereotopic	Ph Me _a ►Ç̄-Me _b	1/20 1.85 1.80 1.55 1.50 1.45 1.40 ppr	1.70 1.85 1.60 1.55 1.50 1.45 1.40 ppm		
G*= \$	G	1.28 1.26 1.24 1.22 1.20 1.18pp	1.28 1.26 1.24 1.22 1.20 1.18ppr		

Symmetry Effects for Homotopic; Enantiotopic, and Diasterotopic Groups

Entry	Structure	Notation and Pattern for Ha $J_{ab}=J_{ac}$	Entry	Structure	Ha multiplets
1	H _a H _b	d	7	H_{a} H_{b} H_{b} H_{b} $V_{b} \neq V_{b'}$ $J_{ab} > J_{ab'}$	dd
2	H _a H _b		8	$\mathbf{\Delta v}_{ab} > 0; \mathbf{v}_{b} = \mathbf{v}_{b'}$	
3	Ha Hb Hb	t	9	H_a H_c H_b $J_{ac} > J_{ab}$	dd
4	H_{a} H_{b} H_{b}	q	10	H_a	dt
5	H _a H _c H _b	q	11	H_{a}	ddd
6	$H_{b} \xrightarrow{2} H_{a} H_{b} H_{b} H_{b}$	sp	12	H_a H_b H_c H_b H_b H_b H_b	dq

First-order Splitting Patterns of Some Common Spin Systems.

Common Coupled	l Spin Systems
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Entry	No. spins	Spin Type	J values by inspection	Examples
1	2	AX	Yes	$\begin{array}{c} H \\ X_2 \\ Y_2 \\ Y_2 \\ Y_2 \\ H \end{array} \begin{array}{c} H \\ -13 \\ H \\ -13 \\ H \\ H \end{array}$
2	2	AB	Yes	
3	3	AMX ABX ABC	Yes J_{AB} and $J_{(AX+BX)}$ None	$\begin{array}{c} H \\ H \\ H \\ H \\ R \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ R \\ R \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ R \\ R \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ H \\ H \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ R \\ R \\ H \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ R \\ H \\ H \end{array} \xrightarrow{H} \begin{array}{c} H \\ R \\ R \\ H \\$
4	3	A_2X	Yes	¹ H ¹ H ^H ^H ^H ^H ^H ^H ^O H
5	3	A_2B	Yes	R'H R'H
6	4	$\begin{array}{c} A_3 X \\ A_3 B \end{array}$	Yes Yes	
7	4	AMX ₂	Yes	
8	4	ABX ₂ ABCX ABCD	J_{AB} None None	$x \qquad x \qquad x \qquad x \qquad y \qquad y \qquad y \qquad y \qquad y \qquad y \qquad $
9	4	$\begin{array}{c} A_2 X_2 \\ A_2 B_2 \end{array}$	Yes No	
10	4	AA'XX'	J_{AX} when $J_{AA'}$ or $J_{XX'}$ is small No when large	$\begin{array}{ccc} X & X \\ \hline \\ \downarrow \\ Y \end{array} \qquad \begin{array}{c} X \\ \hline \\ \downarrow \\ N \end{array} \qquad \begin{array}{c} X \\ \hline \\ X \\ \end{array} \qquad \begin{array}{c} X \\ \hline \\ N \end{array} \qquad \begin{array}{c} X \\ \hline \\ X \\ \end{array} \qquad \begin{array}{c} X \\ \end{array} \end{array} \qquad \begin{array}{c} X \\ \end{array} \qquad \begin{array}{c} X \\ \end{array} \end{array} \qquad \begin{array}{c} X \\ \end{array} \qquad \begin{array}{c} X \\ \end{array} \end{array} \end{array} \end{array} $ \qquad \begin{array}{c} X \\ \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array} \end{array}
11	4	AA'BB'	No	x x
12	5	$\begin{array}{c} A_3 X_2 \\ A_3 B_2 \end{array}$	Yes Yes	
13	5	A ₃ MX A ₃ XY	Yes $J_{\rm XY}$	$H = CH_3$

Type	¹ H Group Symmetry	Chemical Equivalence	Magnetic Equivalence	Spectral Type	¹ H Spectral Appearance
CH ₂ Cl ₂	Homotopic	Yes	Yes	A2	5.45 5.40 5.35 5.30 5.25 5.20m
CH ₂ F ₂	Homotopic	Yes	Yes	A ₂ X ₂	660 555 550 546 540 535 5 30 m
	Homotopic	Yes	Yes	A ₂	
F F H	Homotopic	Yes	No	AA'XX'	420 615 610 605 600 595 pm
	Homotopic	Yes	Yes	A ₄	726 724 722 720 718 718 718 pm
	Two homotopic sets	Yes	No	AA'BB'	7.36 7.30 7.26 7.20 7.16 7.10 7.06 ppm
	Homotopic vinyl Hs	Yes	Yes	A ₂ X	
	Two homotopic sets	Yes	No	AA'BB'	68 65 64 63 62 61 60 ppm

Examples of Magnetic and Chemical Equivalence.