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TABLES DE CORRELATIONS SPECTROSCOPIQUES

IR, RMN et Spectrométrie de Masse

IUT ROBERT SCHUMAN

2024-2025

Sommaire

INFRA-ROUGE

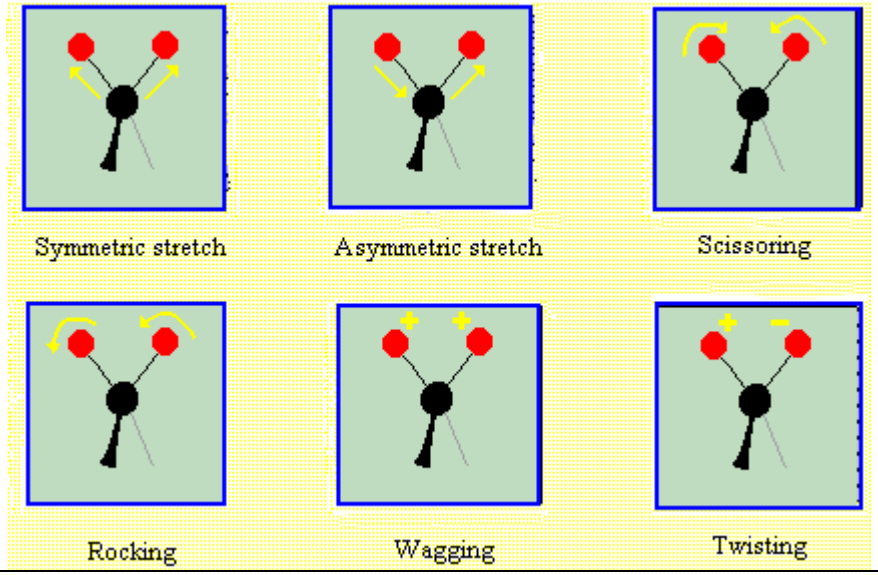
RÉSONNANCE MAGNÉTIQUE NUCLÉAIRE

RMN ^{1}H

RMN ^{13}C

SPECTROMÉTRIE DE MASSE

Fréquences Absorptions IR Caractéristiques des Principaux Groupements Fonctionnels

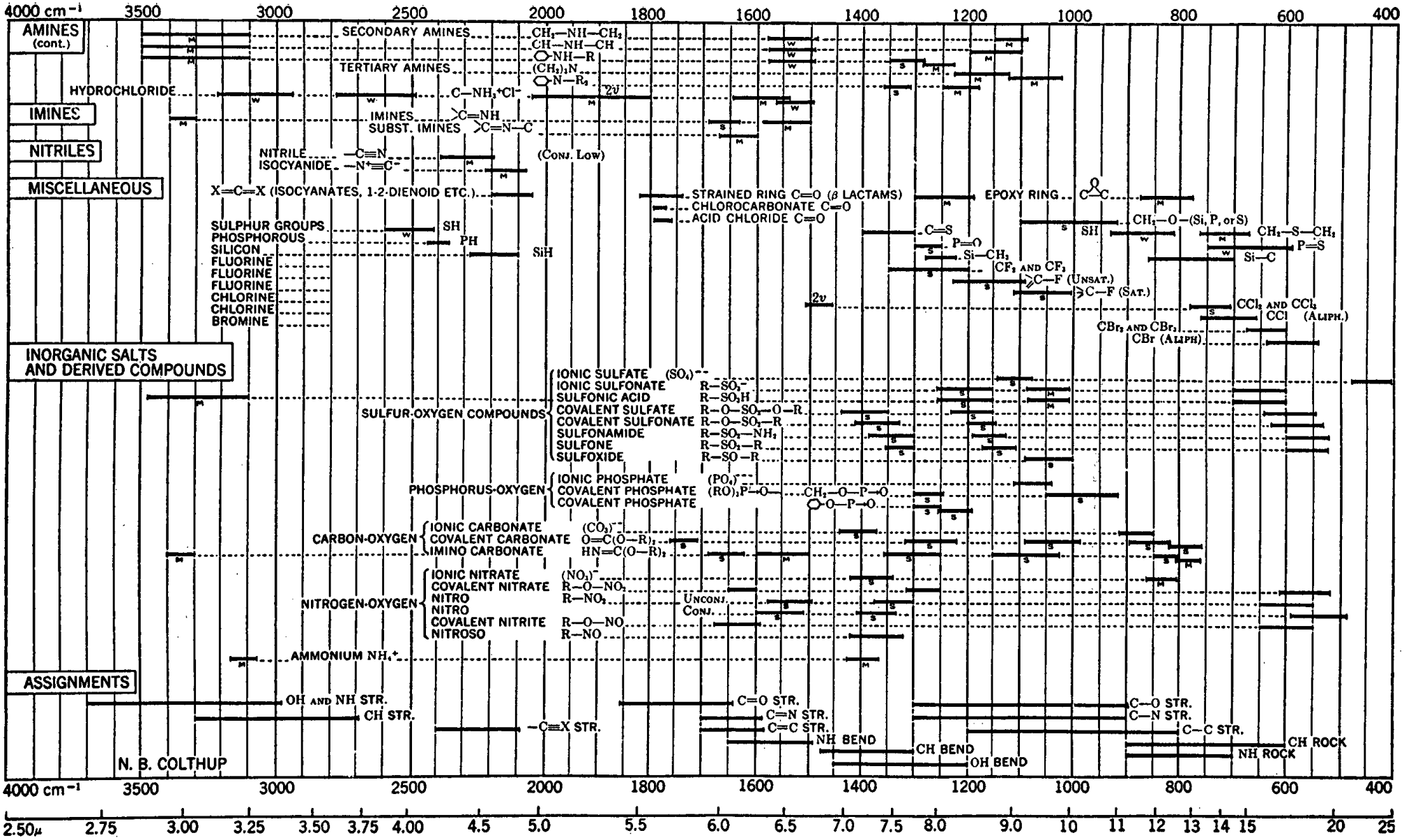


Characteristic IR Absorption Frequencies of Organic Functional Groups			
Functional Group	**Type of Vibration**	**Characteristic Absorptions (cm-1)**	**Intensity**
Alcohol			
O-H	(stretch, H-bonded)	3200-3600	strong, broad
O-H	(stretch, free)	3500-3700	strong, sharp
C-O	(stretch)	1050-1150	strong
Alkane			
C-H	stretch	2850-3000	strong
-C-H	bending	1350-1480	variable
Alkene			
=C-H	stretch	3010-3100	medium
=C-H	bending	675-1000	strong
C=C	stretch	1620-1680	variable

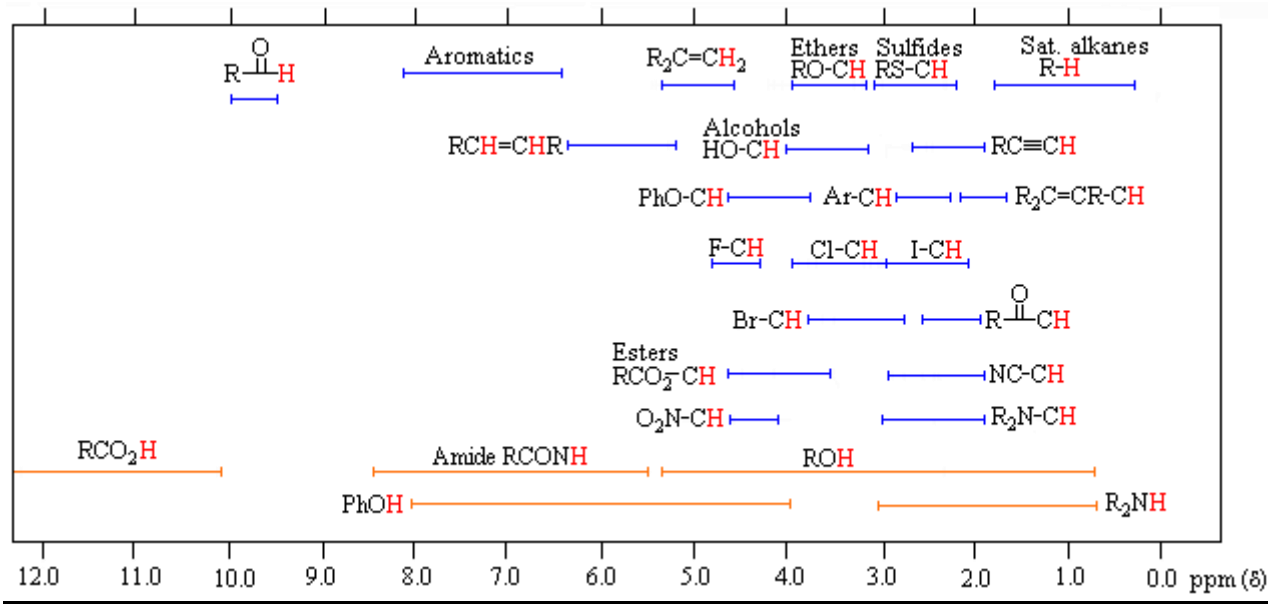
Alkyl Halide			
C-F	stretch	1000-1400	strong
C-Cl	stretch	600-800	strong
C-Br	stretch	500-600	strong
C-I	stretch	500	strong
Alkyne			
C-H	stretch	3300	strong,sharp
–C≡C–	stretch	2100-2260	variable, not present in symmetrical alkynes
Amine			
N-H	stretch	3300-3500	medium (primary amines have two bands; secondary have one band, often very weak)
C-N	stretch	1080-1360	medium-weak
N-H	bending	1600	medium
Aromatic			
C-H	stretch	3000-3100	medium
C=C	stretch	1400-1600	medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns			
Carbonyl			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
Ether			
C-O	stretch	1000-1300 (1070-1150)	strong
Nitrile			
CN	stretch	2210-2260	medium
Nitro			
N-O	stretch	1515-1560 & 1345-1385	strong, two bands

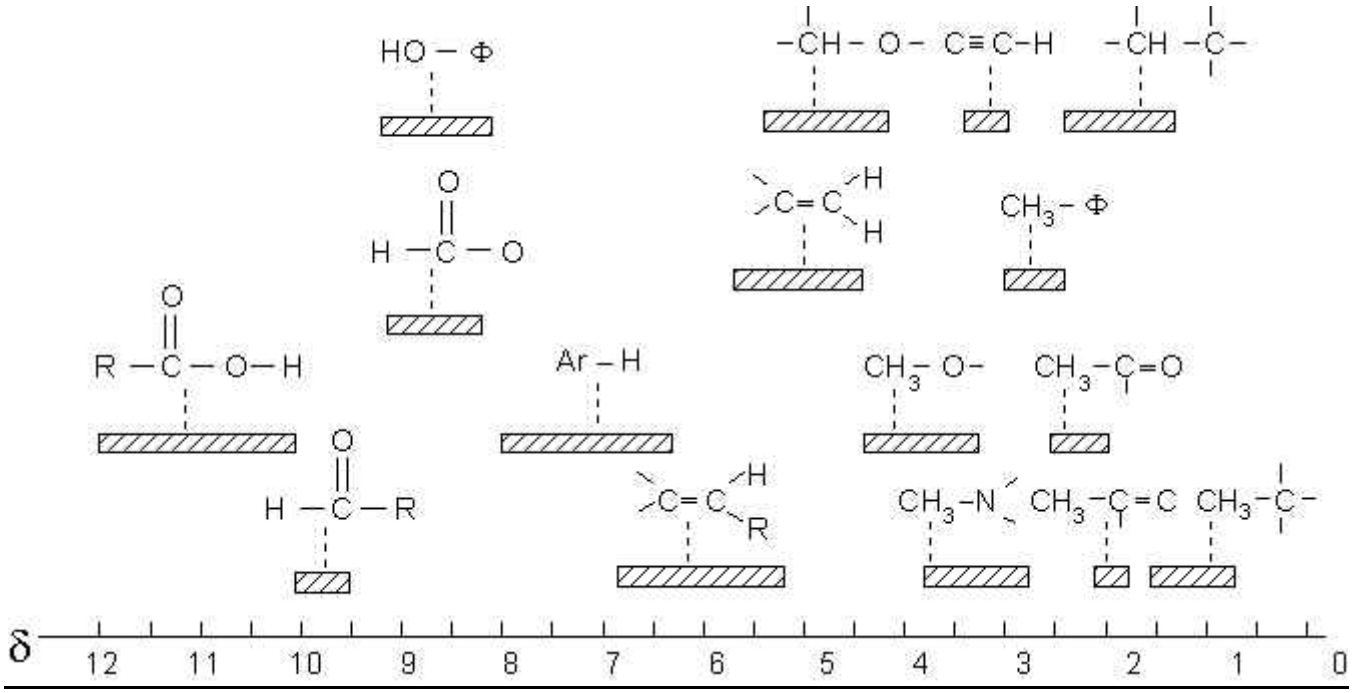
IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)			
Functional Group	**Type of Vibration**	**Characteristic Absorptions (cm^{-1})**	**Intensity**
Carbonyl			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
Acid			
C=O	stretch	1700-1725	strong
O-H	stretch	2500-3300	strong, very broad
C-O	stretch	1210-1320	strong
Aldehyde			
C=O	stretch	1740-1720	strong
=C-H	stretch	2820-2850 & 2720-2750	medium, two peaks
Amide			
C=O	stretch	1640-1690	strong
N-H	stretch	3100-3500	unsubstituted have two bands
N-H	bending	1550-1640	
Anhydride			
C=O	stretch	1800-1830 & 1740-1775	two bands
Ester			
C=O	stretch	1735-1750	strong
C-O	stretch	1000-1300	two bands or more
Ketone			
acyclic	stretch	1705-1725	strong
cyclic	stretch	4-membered - 1780 5-membered - 1745 6-membered - 1715	strong
α,β-unsaturated	stretch	1665-1685	strong
aryl ketone	stretch	1680-1700	strong

Table Infra-rouge



Echelles de déplacement chimique en RMN ^1H

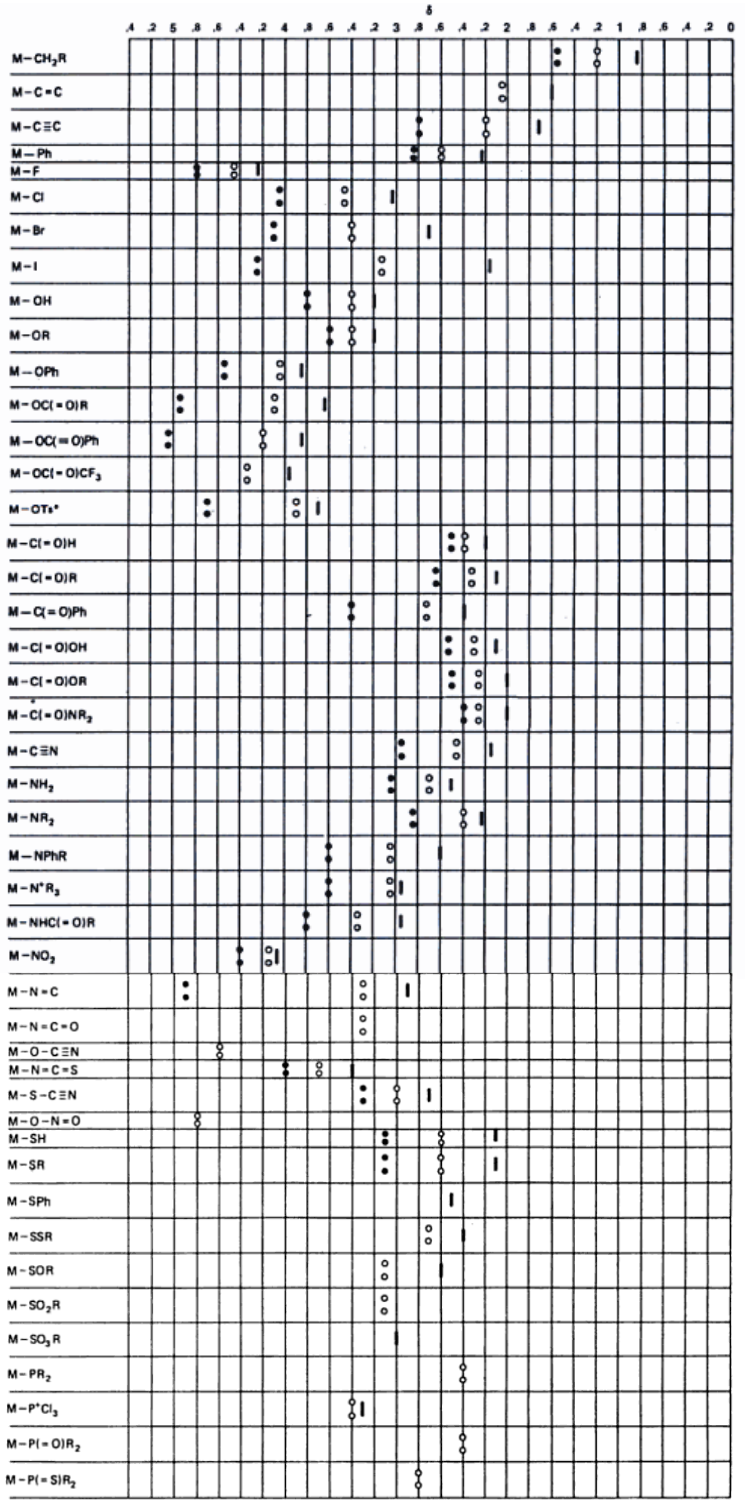


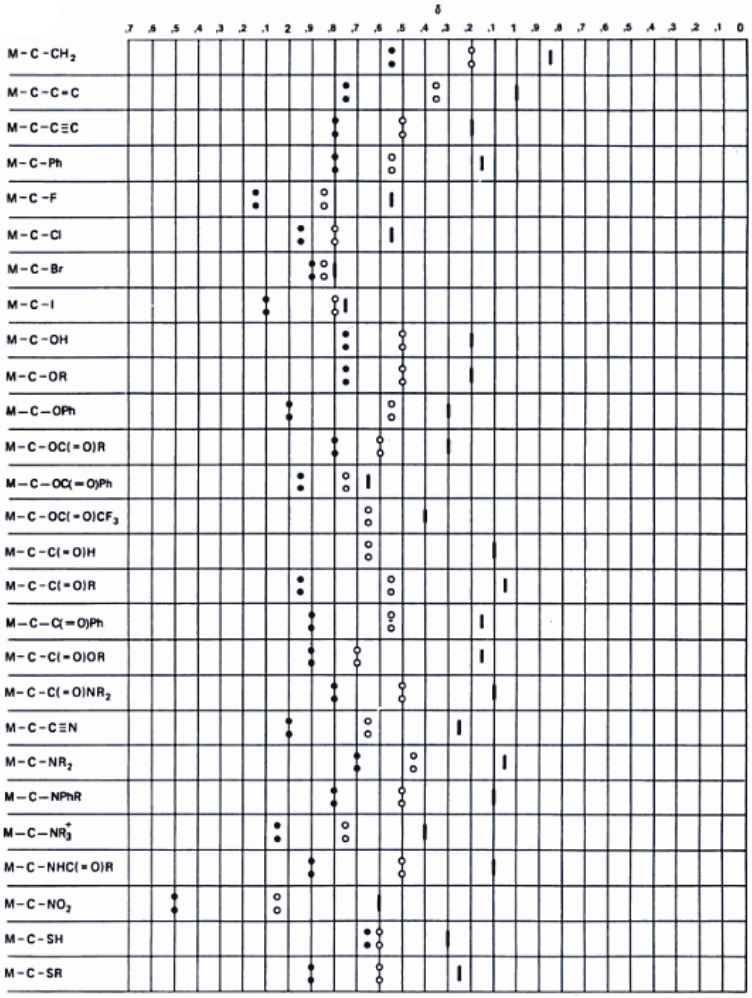


Déplacements chimiques de CH, CH_2 et CH_3 diversement substitués

CH_3		CH_2		CH	
proton	δ	**Proton**	δ	**proton**	δ
CH_3 – C	0,9	– C – CH_2 – C	1,3	– C – CH – C	1,5
CH_3 – C – C=	1,1	– C–CH_2 – C – C=C	1,7		
CH_3 – C – O	1,4	– C – CH_2 – C – O	1,9	– C – CH – C – O	2
CH_3 – C=C	1,6	– C – CH_2 – C=C	2,3		
CH_3 – Ar	2,3	– C – CH_2 – Ar	2,7	– C – CH – Ar	3
CH_3 – CO – R	2,2	– C – CH_2 – CO –R	2,4	– C – CH – CO – R	2,7
CH_3 – CO – Ar	2,6				
CH_3 – CO – OR	2,0	– C – CH_2–CO–OR	2,3		
CH_3 – OR	3,3	– C – CH_2 – OR	3,4	– C – CH – OR	3,7
CH_3 – OH	3,4	– C – CH_2 – OH	3,6	– C – CH – OH	3,9
CH_3 – O – Ar	3,8	– C – CH_2 – O – Ar	4,3		
CH_3 – O – CO – R	3,7	–C–CH_2 –O–CO–R	4,1	–C–CH –O–CO– R	4,8
CH_3 – N –	2,3	– C – CH_2 – N –	2,5	– C – CH – N –	2,8
CH_3 – C – NO_2	1,6	C–CH_2 – NO_2	4,4	C–CH – NO_2	4,7
CH_3 – C=C – CO	2,0	–C–CH_2 –C=C–CO	2,4		
CH_3 – Cl	3,0	– C – CH_2 – Cl	3,4	– C – CH – Cl	4,0
CH_3 – Br	2,7	– C – CH_2 – Br	3,3	– C – CH – Br	3,6
CH_3 – C – Br	1,7	– C – CH_2 – C – Br	1,7	– C – CH – C – Br	1,7
CH_3 – I	2,2	– C – CH_2 – I	3,1	– C – CH – I	4,2
CH_3 – C – I	1,9	– C – CH_2 – C – I	1,8	– C – CH – C – I	1,9
CH_3 – CN	2,0	– C – CH_2 – CN	2,3	– C – CH – CN	2,7

▮ = CH_3 ○ = CH_2 ⁝ = CH





$R^1R^2R^3CH$

$$\delta_H = 1.50 + \sum z_i$$

R^i	z	R^i	z	R^i	z
H—	−0.3	HC≡C—	0.9	MeO—	1.5
alkyl—	0.0	OHC—	1.2	PhO—	2.3
CH_2=$CHCH_2$—	0.2	MeCO—	1.2	AcO	2.7
$MeCOCH_2$—	0.2	RO_2C—	0.8	Cl—	2.0
$HOCH_2$—	0.3	NC—	1.2	Br—	1.9
$ClCH_2$—	0.5	H_2N—	1.0	I—	1.4
CH_2=CH—	0.8	O_2N—	3.0	MeS—	1.0
Ph—	1.3	HO—	1.7	Me_3Si—	−0.7

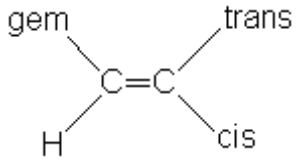
X — CH_2 — Y

$$\delta_{ppm} = 0{,}23 + \sigma_x + \sigma_y$$

Substituant (X ou Y)	**σ**	**Substituant (X ou Y)**	**σ**
–Cl	2.53	–CR=CR_2 (R = H ou alkyle)	1.32
–Br	2.33	–C_6H_5	1.85
–I	1.82	–C≡C–R (R = H ou alkyle)	1.44
–OH	2.56	–C(=O)R (R = alkyle)	1.70
–OR (Alkyle)	2.36	–C(=O)OR (R = alkyle)	1.55
–OAr (Aryle)	3.23	–C(=O)NR_2 (R = H ou alkyle)	1.59
–O(C=O)R	3.13	–C≡N	1.70
–SR	1.64	–CF_3	1.14
–NR_2 (R = H ou alkyle)	1.57	–CH_3	0.47
–NH(C=O)R	2.27	–N_3	1.97

Table de déplacement chimique d'un proton éthylénique en fonction des substituants porté par la double liaison

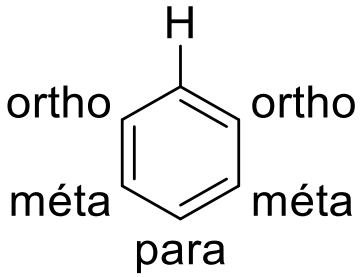
$$\delta_{ppm} = 5{,}25 + Z_{gem} + Z_{cis} + Z_{trans}$$



	R	z_{gem}	z_{cis}	z_{trans}
	H—	0	0	0
C	alkyl—	0.45	−0.22	−0.28
	ring-alkyl—	0.69	−0.25	−0.28
	CO—CH_2— or NC—CH_2—	0.69	−0.08	−0.06
	Ar—CH_2—	1.05	−0.29	−0.32
	N—CH_2—	0.58	−0.10	−0.08
	O—CH_2—	0.64	−0.10	−0.02
	Hal-CH_2—	0.70	0.11	−0.04
	S—CH_2—	0.71	−0.13	−0.22
	isolated C=C—	1.00	−0.09	−0.23
	conjugated C=C—	1.24	0.02	−0.05
	Ar—	1.38	0.36	−0.07
	OHC—	1.02	0.95	1.17
	isolated RCO—	1.10	1.12	0.87
	conjugated RCO—	1.06	0.91	0.74
	isolated HO_2C—	0.97	1.41	0.71
	conjugated HO_2C—	0.80	0.98	0.32
	isolated RO_2C—	0.80	1.18	0.55
	conjugated RO_2C—	0.78	1.01	0.46
	N—CO—	1.37	0.98	0.46
	Cl—CO—	1.11	1.46	1.01
	—C≡C—	0.47	0.38	0.12
	N≡C—	0.27	0.75	0.55
N	alkyl-N—	0.80	−1.26	−1.21
	conjugated alkyl or aryl-N—	1.17	−0.53	−0.99
	—CO—N—	2.08	−0.57	−0.72
	O_2N—	1.87	1.30	0.62
O	alkyl-O—	1.22	−1.07	−1.21
	conjugated alkyl or aryl-O—	1.21	−0.60	−1.00
	—CO—O—	2.11	−0.35	−0.64
Hal	F—	1.54	−0.40	−1.02
	Cl—	1.08	0.18	0.13
	Br—	1.07	0.45	0.55
	I—	1.14	0.81	0.88
Other	R_3Si—	0.90	0.90	0.60
	RS—	1.11	−0.29	−0.13
	RSO—	1.27	0.67	0.41
	RSO_2—	1.55	1.16	0.93

Use the 'conjugated' values when either the substituent or the double bond is further conjugated. Use the 'ring-alkyl' values when the double bond and the alkyl group are part of a five- or six-membered ring.

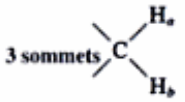
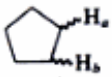
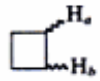
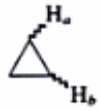
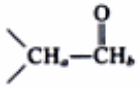
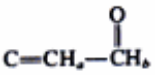
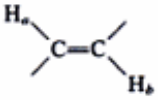
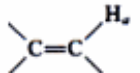
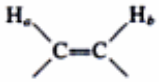
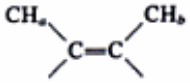
Table de déplacement chimique d'un proton aromatique en fonction des substituants porté par le cycle

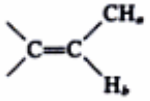
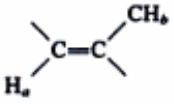
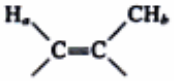
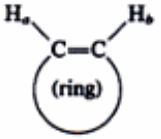
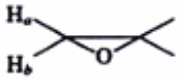
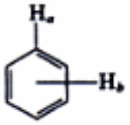
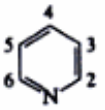
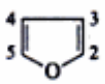
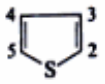


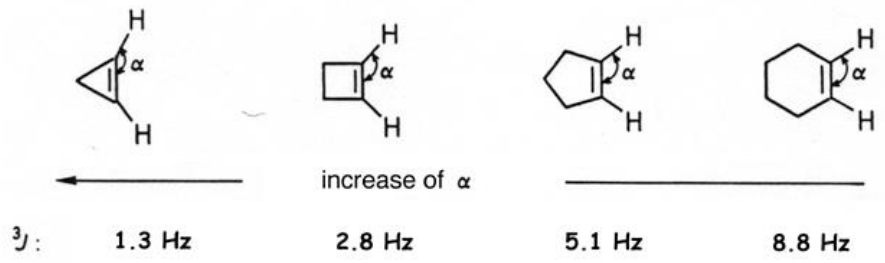
$$\delta = 7{,}26 + Z_{ortho} + Z_{méta} + Z_{para}$$

	R	Z_{ortho}	Z_{meta}	Z_{para}
	H—	0	0	0
C	Me—	−0.20	−0.12	−0.22
	Et—	−0.14	−0.06	−0.17
	Pr^i—	−0.13	−0.08	−0.18
	Bu^t—	0.02	−0.08	−0.21
	H_2NCH_2— or $HOCH_2$—	−0.07	−0.07	−0.07
	$ClCH_2$—	0.00	0.00	0.00
	F_3C—	0.32	0.14	0.20
	Cl_3C—	0.64	0.13	0.10
	CH_2=CH—	0.06	−0.03	−0.10
	Ph—	0.37	0.20	0.10
	OHC—	0.56	0.22	0.29
	MeCO—	0.62	0.14	0.21
	H_2NCO—	0.61	0.10	0.17
	HO_2C—	0.85	0.18	0.27
	MeO_2C—	0.71	0.1	0.21
	ClCO—	0.84	0.22	0.36
	HC≡C—	0.15	−0.02	−0.01
	N≡C—	0.36	0.18	0.28
N	H_2N—	−0.75	−0.25	−0.65
	Me_2N—	−0.66	−0.18	−0.67
	AcNH—	0.12	−0.07	−0.28
	O_2N—	0.95	0.26	0.38
O	HO—	−0.56	−0.12	−0.45
	MeO—	−0.48	−0.09	−0.44
	AcO—	−0.25	0.03	−0.13
Hal	F—	−0.26	0.00	−0.04
	Cl—	0.03	−0.02	−0.09
	Br—	0.18	−0.08	−0.04
	I—	0.39	−0.21	0.00
Other	Me_3Si—	0.22	−0.02	−0.02
	$(MeO)_2P(=O)$—	0.48	0.16	0.24
	MeS—	0.37	0.20	0.10

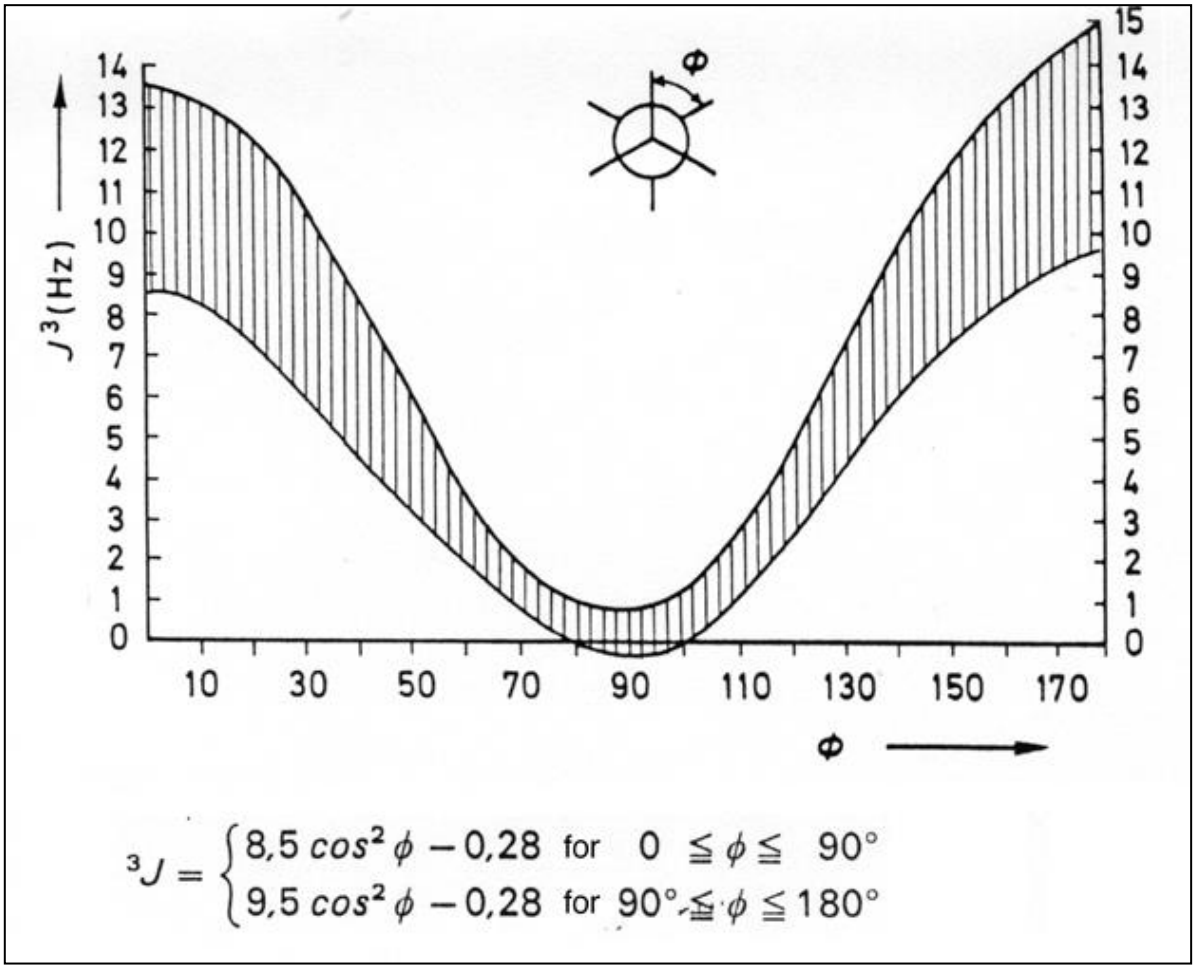
Constantes de couplage ^{1}H-^{1}H les plus fréquemment rencontrées

Type	J_{ab} (Hz)	J_{ab} typique
 3 sommets	0–30	12–15
$CH_a—CH_b$ (rotation libre)	6–8	7
	0–1	0
ax–ax	6–14	8–10
ax–eq	0–5	2–3
eq–eq	0–5	2–3
 (cis ou trans)	*cis* 5–10 *trans* 5–10	
 (cis ou trans)	*cis* 4–12 *trans* 2–10	
 (cis ou trans)	*cis* 7–13 *trans* 4–9	
$CH_a—OH_b$ (pas d'échange)	4–10	5
	1–3	2–3
	5–8	6
	12–18	17
	0–3	0–2
	6–12	10
	0–3	1–2

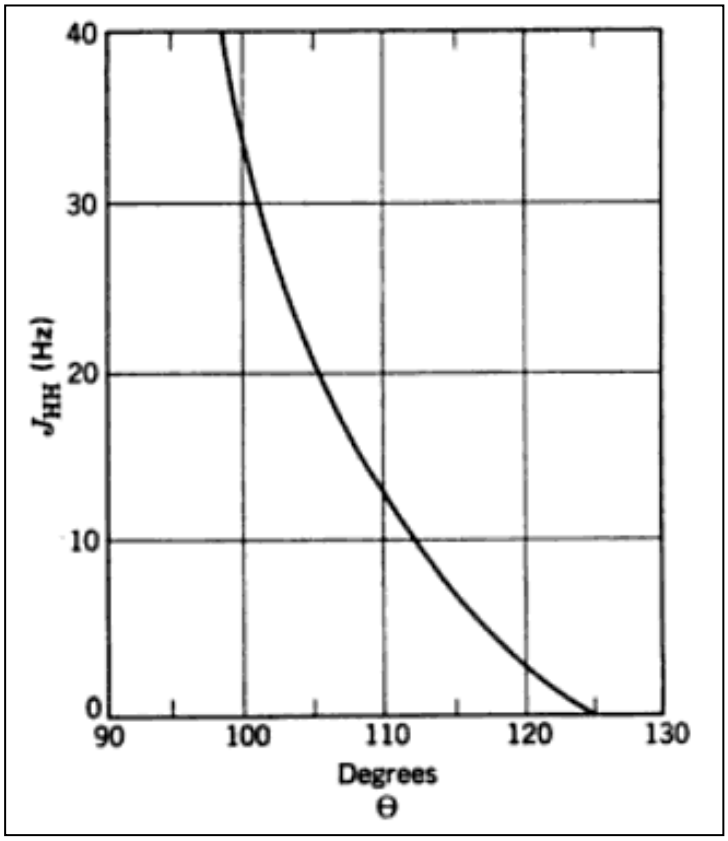
Type	J_{ab} (Hz)	J_{ab} typique
	4–10	7
	0–3	1,5
	0–3	2
$C{=}CH_a—CH_b{=}C$	9–13	10
	4 sommets 5 sommets 6 sommets sommets 8 sommets	0,5–2,0 2,5–4,0 7 5,1–7,0 8,8–11,0 9–13 10–13
$CH_a—C{\equiv}CH_b$	2–3	
$—CH_a—C{\equiv}C—CH_b—$	2–3	
		6
		4
		2,5
	*J* (ortho) 6–10 *J* (meta) 1–3 *J* (para) 0–1	9 3 ~0
	*J* (2–3) 5–6 *J* (3–4) 7–9 *J* (2–4) 1–2 *J* (3–5) 1–2 *J* (2–5) 0–1 *J* (2–6) 0–1	5 8 1,5 1,5 1 ~0
	*J* (2–3) 1,3–2,0 *J* (3–4) 3,1–3,8 *J* (2–4) 0–1 *J* (2–5) 1–2	1,8 3,6 ~0 1,5
	*J* (2–3) 4,9–6,2 *J* (3–4) 3,4–5,0 *J* (2–4) 1,2–1,7 *J* (2–5) 3,2–3,7	5,4 4,0 1,5 3,4



Courbes de Karplus



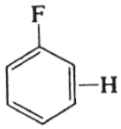
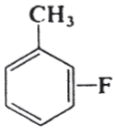
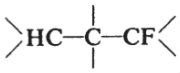
Pour les protons vicinaux (H-C-C-H)



Pour les protons géminés (H-C-H)

Constantes de couplage ^{1}H-^{19}F et ^{1}H-^{31}P

Table 3.30 ^{1}H–^{19}F coupling constants (Hz)

	Structure	J	Structure		J
$^{2}J_{HF}$		45–52		*ortho* *meta* *para*	6–11 3–9 0–4
		60–65			
		72–90			
$^{3}J_{HF}$	$CH_3—CF$	20–24			
	$CH—CF$	0–45†			
	cis-HC=CF—	3–20		*ortho* *meta* *para*	2.5 1.5 0
	trans-HC=CF—	12–53			
$^{4}J_{HF}$		0–9‡			
	cis-FC=C—CH	2–4			
	trans-FC=C—CH	0–6			

† 0–12 when gauche and 10–45 when anti-periplanar.
‡ The higher end of the range (≥ 3.5) when the atoms are held in a W conformation.

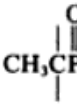
Table 3.31 ^{31}P–^{1}H coupling constants (Hz)†

Type of coupling	Class of compound		
	Phosphines	*Phosphonium salts*	*Phosphine oxides*
$^{1}J_{PH}$	(150) 185–220 (250)	400–900	200–750
$^{2}J_{PH}$	(−5) 0–15 (27) 46‡	(0) 10–18 30‡	5–25 40‡
$^{3}J_{PCCH}$	(10) 13–17 (20)	(0) 10–20 (57)	14–30
$^{3}J_{PC=CH}$	*trans* (5) 12–41 *cis*§ 6–20	*trans* 28–50 (80) *cis*§ 10–20 (35)	
		Phosphites	*Phosphates*
$^{3}J_{POCH}$		(0) 5–14 (20)	(0) 5–20 (30)
	All compounds		
$^{4}J_{PH}$	0–3 (5)¶		

† The coupling constants are often strongly dependent upon the groups attached to phosphorus, and therefore values outside the quoted ranges may occasionally be observed; values in parentheses are 'extreme' values so far reported.

‡ Values observed in P—C(=)—H systems.
§ *Trans* coupling is usually about twice that of *cis* coupling.
¶ In the system P—C=C=CH.

Proton-Phosphore

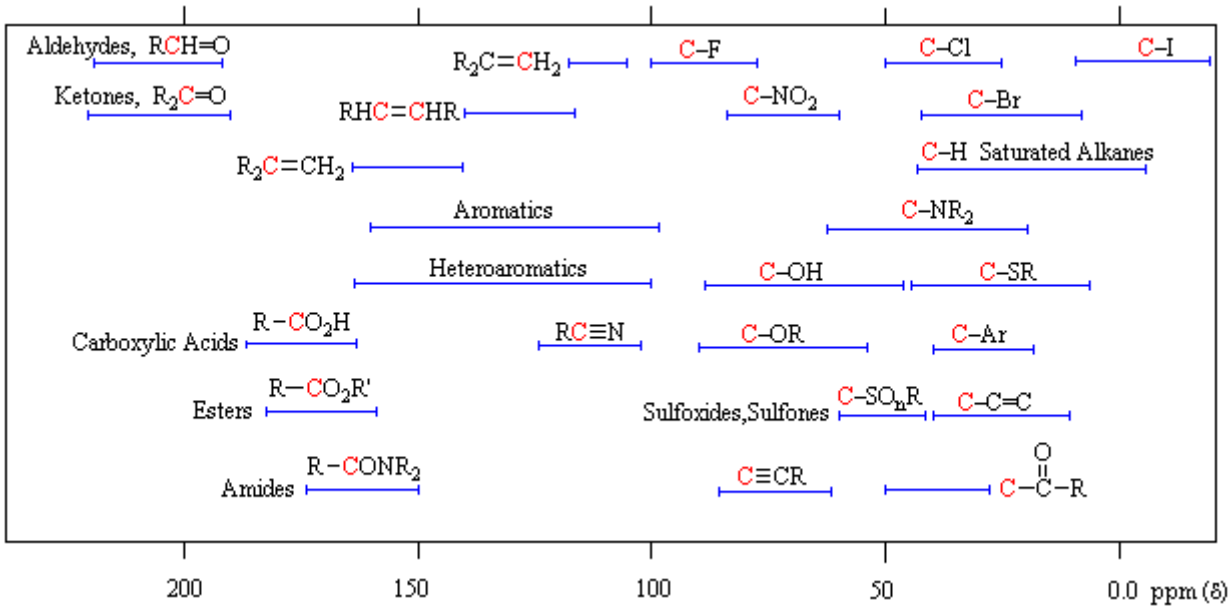
	630–707	
$(CH_3)_3P$	2,7	
$(CH_3)_3P=O$	13,4	
$(CH_3CH_2)_3P$	13,7 (HCCP)	0,5 (HCP)
$(CH_3CH_2)_3P=O$	16,3 (HCCP)	11,9 (HCP)
	10–13	
	15–20	
$CH_3OP(OR)_2$	10,5–12	
$P[N(CH_3)_2]_3$	8,8	
$O=P[N(CH_3)_2]_3$	9,5	

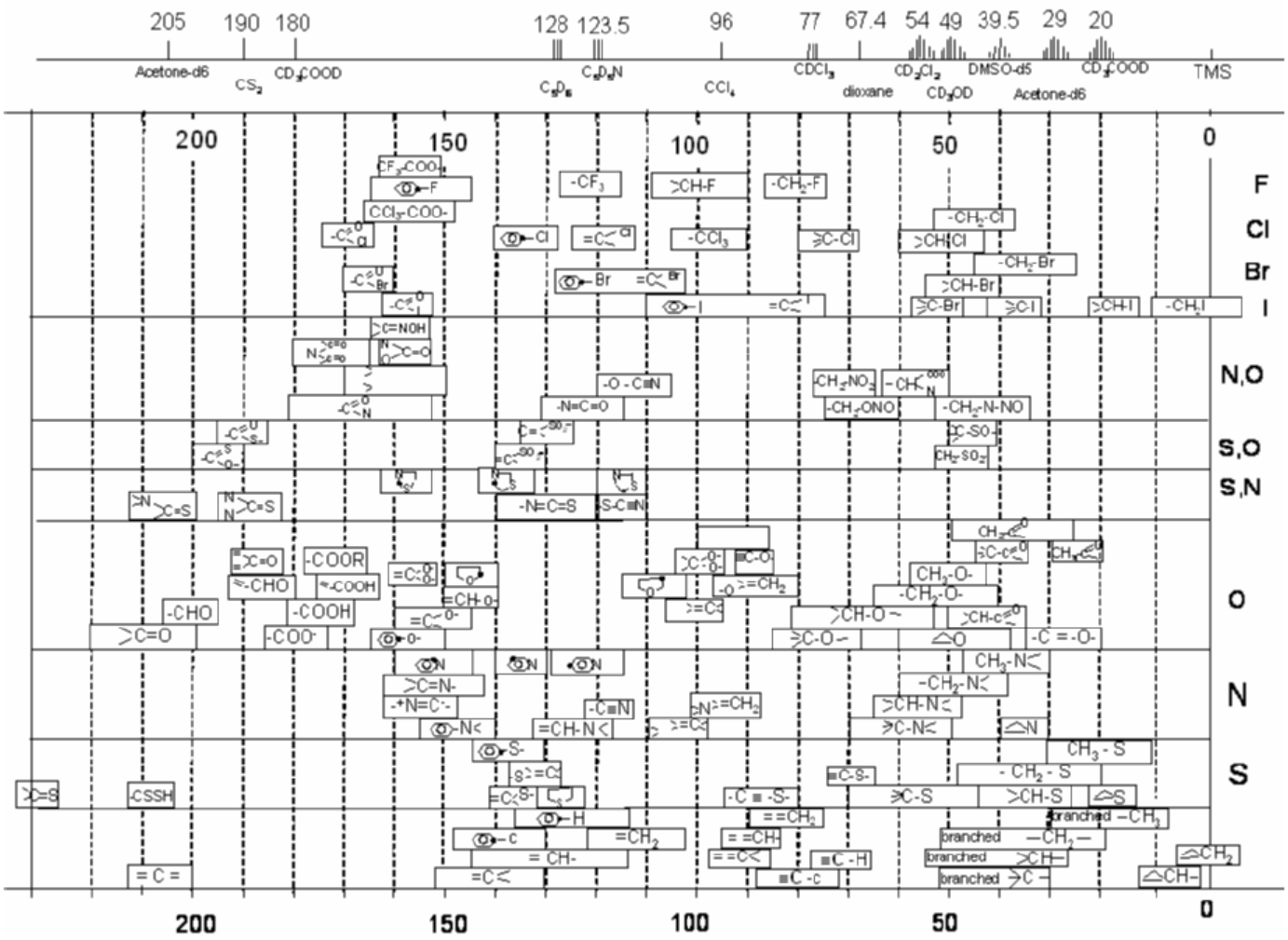
NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities (RMN ^1H)

Table 1. ^1H NMR Data

	proton	mult	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD
solvent residual peak			7.26	2.05	2.50	7.16	1.94	3.31
H_2O		s	1.56	2.84[a]	3.33[a]	0.40	2.13	4.87
acetic acid	CH_3	s	2.10	1.96	1.91	1.55	1.96	1.99
acetone	CH_3	s	2.17	2.09	2.09	1.55	2.08	2.15
acetonitrile	CH_3	s	2.10	2.05	2.07	1.55	1.96	2.03
benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33
tert-butyl alcohol	CH_3	s	1.28	1.18	1.11	1.05	1.16	1.40
	OH[c]	s			4.19	1.55	2.18	
tert-butyl methyl ether	CCH_3	s	1.19	1.13	1.11	1.07	1.14	1.15
	OCH_3	s	3.22	3.13	3.08	3.04	3.13	3.20
BHT[b]	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92
	OH[c]	s	5.01		6.65	4.79	5.20	
	$ArCH_3$	s	2.27	2.22	2.18	2.24	2.22	2.21
	$ArC(CH_3)_3$	s	1.43	1.41	1.36	1.38	1.39	1.40
chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90
cyclohexane	CH_2	s	1.43	1.43	1.40	1.40	1.44	1.45
1,2-dichloroethane	CH_2	s	3.73	3.87	3.90	2.90	3.81	3.78
dichloromethane	CH_2	s	5.30	5.63	5.76	4.27	5.44	5.49
diethyl ether	CH_3	t, 7	1.21	1.11	1.09	1.11	1.12	1.18
	CH_2	q, 7	3.48	3.41	3.38	3.26	3.42	3.49
diglyme	CH_2	m	3.65	3.56	3.51	3.46	3.53	3.61
	CH_2	m	3.57	3.47	3.38	3.34	3.45	3.58
	OCH_3	s	3.39	3.28	3.24	3.11	3.29	3.35
1,2-dimethoxyethane	CH_3	s	3.40	3.28	3.24	3.12	3.28	3.35
	CH_2	s	3.55	3.46	3.43	3.33	3.45	3.52
dimethylacetamide	CH_3CO	s	2.09	1.97	1.96	1.60	1.97	2.07
	NCH_3	s	3.02	3.00	2.94	2.57	2.96	3.31
	NCH_3	s	2.94	2.83	2.78	2.05	2.83	2.92
dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97
	CH_3	s	2.96	2.94	2.89	2.36	2.89	2.99
	CH_3	s	2.88	2.78	2.73	1.86	2.77	2.86
dimethyl sulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65
dioxane	CH_2	s	3.71	3.59	3.57	3.35	3.60	3.66
ethanol	CH_3	t, 7	1.25	1.12	1.06	0.96	1.12	1.19
	CH_2	q, 7[d]	3.72	3.57	3.44	3.34	3.54	3.60
	OH	s[c,d]	1.32	3.39	4.63		2.47	
ethyl acetate	CH_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01
	CH_2CH_3	q, 7	4.12	4.05	4.03	3.89	4.06	4.09
	CH_2CH_3	t, 7	1.26	1.20	1.17	0.92	1.20	1.24
ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12
	CH_2CH_3	q, 7	2.46	2.45	2.43	1.81	2.43	2.50
	CH_2CH_3	t, 7	1.06	0.96	0.91	0.85	0.96	1.01
ethylene glycol	CH	s[e]	3.76	3.28	3.34	3.41	3.51	3.59
"grease"[f]	CH_3	m	0.86	0.87		0.92	0.86	0.88
	CH_2	br s	1.26	1.29		1.36	1.27	1.29
n-hexane	CH_3	t	0.88	0.88	0.86	0.89	0.89	0.90
	CH_2	m	1.26	1.28	1.25	1.24	1.28	1.29
HMPA[g]	CH_3	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64
methanol	CH_3	s[h]	3.49	3.31	3.16	3.07	3.28	3.34
	OH	s[c,h]	1.09	3.12	4.01		2.16	
nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34
n-pentane	CH_3	t, 7	0.88	0.88	0.86	0.87	0.89	0.90
	CH_2	m	1.27	1.27	1.27	1.23	1.29	1.29
2-propanol	CH_3	d, 6	1.22	1.10	1.04	0.95	1.09	1.50
	CH	sep, 6	4.04	3.90	3.78	3.67	3.87	3.92
pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85
silicone grease[i]	CH_3	s	0.07	0.13		0.29	0.08	0.10
tetrahydrofuran	CH_2	m	1.85	1.79	1.76	1.40	1.80	1.87
	CH_2O	m	3.76	3.63	3.60	3.57	3.64	3.71
toluene	CH_3	s	2.36	2.32	2.30	2.11	2.33	2.32
	CH(*o*/*p*)	m	7.17	7.1–7.2	7.18	7.02	7.1–7.3	7.16
	CH(*m*)	m	7.25	7.1–7.2	7.25	7.13	7.1–7.3	7.16
triethylamine	CH_3	t,7	1.03	0.96	0.93	0.96	0.96	1.05
	CH_2	q, 7	2.53	2.45	2.43	2.40	2.45	2.58

Echelles de déplacement chimique en RMN ^{13}C



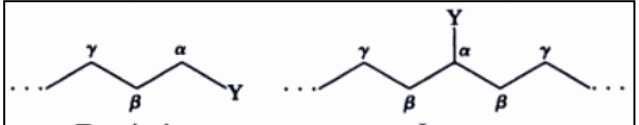


RMN ^{13}C : Alcanes

Tableau 1

Composé	C-1	C-2	C-3	C-4	C-5
Méthane	–2,3				
Éthane	5,7				
Propane	15,8	16,3	15,8		
Butane	13,4	25,2	25,2		
Pentane	13,9	22,8	34,7	22,8	13,9
Hexane	14,1	23,1	32,2	32,2	23,1
Heptane	14,1	23,2	32,6	29,7	32,6
Octane	14,2	23,2	32,6	29,9	29,9
Nonane	14,2	23,3	32,6	30,0	30,3
Décane	14,2	23,2	32,6	31,1	30,5
Isobutane	24,5	25,4			
Isopentane	22,2	31,1	32,0	11,7	
Isohexane	22,7	28,0	42,0	20,9	14,3
Néopentane	31,7	28,1			
2,2-Diméthylbutane	29,1	30,6	36,9	8,9	
3-Méthylpentane	11,5	29,5	36,9	(18,8; 3-CH_3)	
2,3-Diméthylbutane	19,5	34,3			
2,2,3-Triméthylbutane	27,4	33,1	38,3	16,1	
2,3-Diméthylpentane	7,0	25,3	36,3	(14,6; 3-CH_3)	

Tableau 2
(Incrémenter les δ du tableau 1)



	α		β		γ
Y	Terminal	Interne	Terminal	Interne	
CH_3	+9	+6	+10	+8	–2
$CH=CH_2$	+20		+6		–0,5
C≡CH	+4,5		+5,5		–3,5
COOH	+21	+16	+3	+2	–2
COO^-	+25	+20	+5	+3	–2
COOR	+20	+17	+3	+2	–2
COCl	+33	+28		+2	
$CONH_2$	+22		+2,5		–0,5
COR	+30	+24	+1	+1	–2
CHO	+31		0		–2
Phényle	+23	+17	+9	+7	–2
OH	+48	+41	+10	+8	–5
OR	+58	+51	+8	+5	–4
OCOR	+51	+45	+6	+5	–3
NH_2	+29	+24	+11	+10	–5
NH_3^+	+26	+24	+8	+6	–5
NHR	+37	+31	+8	+6	–4
NR_2	+42		+6		–3
NR_3^+	+31		+5		–7
NO_2	+63	+57	+4	+4	
CN^-	+4	+1	+3	+3	–3
SH	+11	+11	+12	+11	–4
SR	+20		+7		–3
F	+68	+63	+9	+6	–4
Cl	+31	+32	+11	+10	–4
Br	+20	+25	+11	+10	–3
I	–6	+4	+11	+12	–1

*C-C_α-C_β-C_γ $\delta = -2,3 + A + B$

-2,3 : déplacement chimique du ^{13}C du méthane

A : terme de blindage B : terme de correction stérique ou de ramification

Tableau 1 : Incréments nécessaire au calcul de A

Substituent	Increments α	β	γ	Substituent	Increments α	β	γ
—C.sp^3	9.1	9.4	−2.5	—N<	28.3	11.3	−5.1
—C≡C—	4.4	5.6	−3.4	—N<	30.7	5.4	−7.2
—C=C—	19.5	6.9	−2.1	—NO_2	61.6	3.1	−4.6
—C_6H_5	22.1	9.3	−2.6	—S—	10.6	11.4	−3.6
—Cl	31.0	10.0	−5.1	—CHO	29.9	−0.6	−2.7
—F	70.1	7.8	−6.8	—CO—	22.5	3.0	−3.0
—Br	18.9	11.0	−3.8	—COOH	20.1	2.0	−2.8
—I	−7.2	10.9	−1.5	—COO^-	24.5	3.5	−2.5
O	21.4	2.8	−2.5	—COO—	22.6	2.0	−2.8
—O—	49.0	10.1	−6.2	—CON<	22.0	2.6	−3.2
—O—CO—	56.5	6.5	−6.0	—CN	3.1	2.4	−3.3

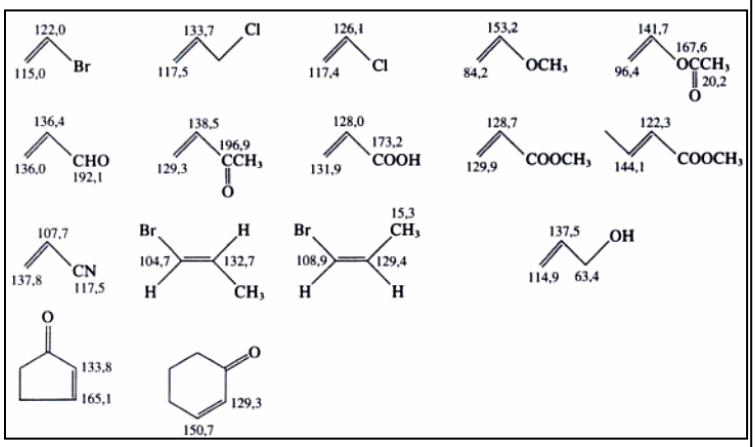
Tableau 2 : Incréments nécessaire au calcul de B

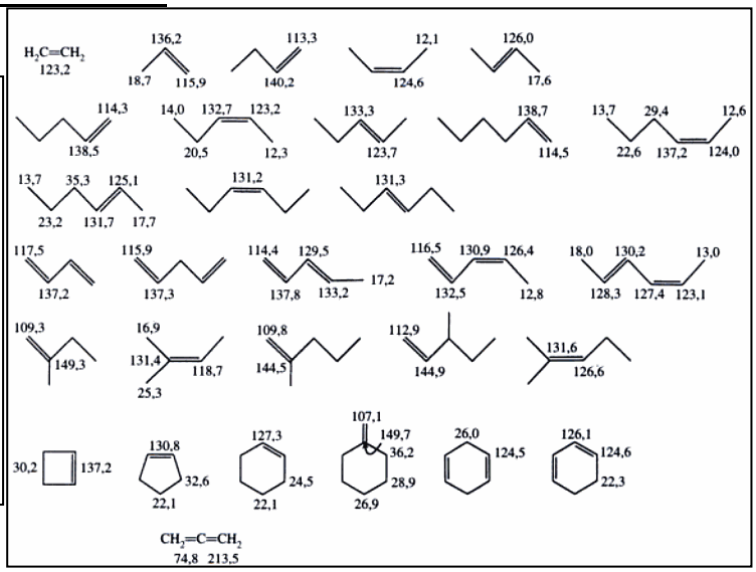
^{13}C atom observed	The number of substituents (other than H) on the α-substituents. 1	2	3	4
primary	...	...	−1.1	−3.4
secondary	...	...	−2.5	− 7.2
tertiary	...	−3.7	−9.5	−15.0
quaternary	−1.5	−8.4	−15.0	−25.0

Carbon equivalent	Functional group
primary	—CO_2H, —CO_2R, —NO_2
secondary	—C_6H_5, —CHO, —$CONH_2$, —CH_2X*
tertiary	—COR

Remarques : pour les amines et les éthers, pour déterminer B, considérer les hétéroatomes comme des carbones. Pour les esters et les amides, pour le calcul de A, le radical R (*C-CO-X-R, X = N ou O) doit être considéré comme un substituant.

RMN ^{13}C : Alcènes





$$\delta = 122{,}8 + A + B$$

122,8 : déplacement chimique des ^{13}C de l'éthène

Incréments A et B pour les alcènes alkylés de structure

C_β-C_α-*C=C-$C_{\alpha'}$-$C_{\beta'}$

Position of substitution	Increments *A*	Type of disubstitution	Increments *B*
α	10.6	α,α' cis	−1.1
β	7.2	α,α gem	−4.8
γ	−1.5	α',α' gem	+2.5
α'	−7.9	β,β gem	−2.3
β'	−1.8		
γ'	+1.5		

Incréments A pour les alcènes de structure

X-CH(α)=CH(β)

Substituent X	Increments α	Increments β	X Substituent	Increments α	Increments β
—Cl	3.3	−5.6	$—CH_2Y$*	12	−5
$—NCOR_2$	7.2	−28.5	$—CH_2CO_2H$	6.9	−4.6
$—NO_2$	22.8	−0.4	$—CH_2CN$	5.9	−2.1
$—\overset{+}{N}\equiv$	18.9	−26.2	$—C_6H_5$	13.0	−10.5
$—OCH_3$	31.0	−38.2	—C≡N	−15.6	15.1
$—OCOCH_3$	18.9	−26.4	$—CO_2R$	6.0	8.0
$—CH_3$	13.4	−6.9	$—COCH_3$	14.9	6.7
—*t*-Bu	26.9	−13.0	—CHO	15.8	14.8
			—CON<	9.6	3.1

RMN ^{13}C : Alcynes

Composé	C-1	C-2	C-3	C-4	C-5	C-6
But-1-yne	67,0	84,7				
But-2-yne		73,6				
Hex-1-yne	67,4	82,8	17,4	29,9	21,2	12,9
Hex-2-yne	1,7	73,7	76,9	19,6	21,6	12,1
Hex-3-yne	14,4	12,0	79,9			

$$\delta = 79{,}1 + A$$

$—C_\beta—C_\alpha—{}^1C\equiv C—C_{\alpha^1}—C—_{\beta^1}$

Substituents	Increments α	α'	β	β'
$—C.sp^3$	6.9	−5.7	4.8	2.3
$—CH_2OH$	11.1	1.9		
$—COCH_3$	31.4	4.0		
$—C_6H_5$	12.7	6.4		
$—CH=CH_2$	10.0	11.0		

RMN ^{13}C : Halogénures d'alkyle

Composé	C-1	C-2	C-3
CH_4	−2,3		
CH_3F	75,4		
CH_3Cl	24,9		
CH_2Cl_2	54,0		
$CHCl_3$	77,5		
CCl_4	96,5		
CH_3Br	10,0		
CH_2Br_2	21,4		
$CHBr_3$	12,1		
CBr_4	−28,5		
CH_3I	−20,7		
CH_2I_2	−54,0		
CHI_3	−139,9		
CI_4	−292,5		
CH_3CH_2F	79,3	14,6	
CH_3CH_2Cl	39,9	18,7	
CH_3CH_2Br	28,3	20,3	
CH_3CH_2I	−0,2	21,6	
$CH_3CH_2CH_2Cl$	46,7	26,5	11,5
$CH_3CH_2CH_2Br$	35,7	26,8	13,2
$CH_3CH_2CH_2I$	10,0	27,6	16,2

RMN ^{13}C : Hétéroaromatiques

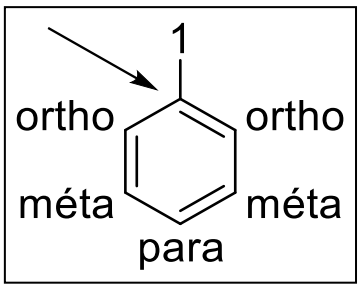
Composé	C-2	C-3	C-4	C-5	C-6	Substituant
Furane	142,7	109,6				
2-Méthylfurane	152,2	106,2	110,9	141,2		13,4
2-Carboxaldéhydfurane	153,3	121,7	112,9	148,5		178,2
2-Méthylfuroate	144,8	117,9	111,9	146,4		159,1 (C=O) 51,8 (CH_3)
Pyrrole	118,4	108,0				
2-Méthylpyrrole	127,2	105,9	108,1	116,7		12,4
2-Carboxaldéhydpyrrole	134,0	123,0	112,0	129,0		178,9
Thiophène	124,4	126,2				
2-Méthylthiophène	139,0	124,7	126,4	122,6		14,8
2-Carboxaldéhydthiophène	143,3	136,4	128,1	134,6		182,8
Thiazole	152,2		142,4	118,5		
Imidazole	136,2		122,3	122,3		
Pyridine	150,2	123,9	135,9			
Pyrimidine	159,5		157,4	122,1	157,4	
Pyrazine	145,6					
2-Méthylpyrazine	154,0	141,8[a]	143,8[a]	144,7[a]		21,6

[a] Attributions incertaines

RMN ^{13}C : Amines

Composé	C-1	C-2	C-3	C-4	
CH_3NH_2	26,9				
$CH_3CH_2NH_2$	35,9	17,7			
$CH_3CH_2CH_2NH_2$	44,9	27,3	11,2		
$CH_3CH_2CH_2CH_2NH_2$	42,3	36,7	20,4	14,0	
$(CH_3)_3N$	47,5				
$CH_3CH_2N(CH_3)_2$	58,2	13,8			
Cyclohexylamine	50,4	36,7	25,7	25,1	
N-Méthylcyclohexylamine	58,6	33,3	25,1	26,3	($N-CH_3$ 33,5)

RMN ^{13}C : Aromatiques



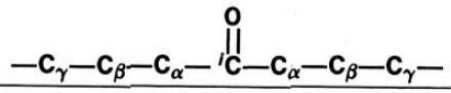
$$\delta = 128.5 + \Sigma AS_i$$

R_i	C-1	*ortho*	*meta*	*para*
H	0	0	0	0
CH_3	+ 9.3	+ 0.8	0	- 2.9
CH_2-CH_3	+15.6	- 0.4	0	- 2.6
$CH(Me)_2$	+20.2	- 2.5	+0.1	- 2.4
$C(Me)_3$	+22.4	- 3.1	-0.1	- 2.9
CF_3	- 9.0	- 2.2	+0.3	+ 3.2
C_6H_5	+13	- 1	+0.4	- 1
$CH=CH_2$	+ 9.5	- 2.0	+0.2	- 0.5
$C\equiv CH$	- 6.1	+ 3.8	+0.4	- 0.2
CH_2OH	+12	- 1	0	- 1
COOH	+ 2.1	+ 1.5	0	+ 5.1
COO^-	+ 8	+ 1	0	+ 3
$COOCH_3$	+ 2.1	+ 1.1	+0.1	+ 4.5
COCl	+ 5	+ 3	+1	+ 7
CHO	+ 8.6	+ 1.3	+0.6	+ 5.5
$COCH_3$	+ 9.1	+ 0.1	0	+ 4.2
$COCF_3$	- 5.6	+ 1.8	+0.7	+ 6.7
COC_6H_5	+ 9.4	+ 1.7	-0.2	+ 3.6
CN	-15.4	+ 3.6	+0.6	+ 3.9
OH	+26.9	-12.7	+1.4	- 7.3
OCH_3	+31.4	-14.4	+1.0	- 7.7
$OCOCH_3$	+23	- 6	+1	- 2
OC_6H_5	+29	- 9	+2	- 5
NH_2	+18	-13.3	+0.9	- 9.8
$N(Me)_2$	+23	-16	+1	-12
$N(Ph)_2$	+19	- 4	+1	- 6
$NHCOCH_3$	+11	-10	0	- 6
NO_2	+20	- 4.8	+0.9	+ 5.8
NCO	+ 5.7	- 3.6	+1.2	- 2.8
F	+34.8	-12.9	+1.4	- 4.5
Cl	+ 6.2	+ 0.4	+1.3	- 1.9
Br	- 5.5	+ 3.4	+1.7	- 1.6
I	-32	+10	+3	+ 1

RMN ^{13}C : Aldéhydes et cétones

$\delta = 193 + A$

A = somme des incréments

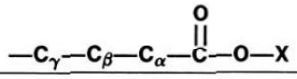


Substituent	Increments A_α	A_β	A_γ *
—C.sp^3	6.5	2.6	1.0
—C_6H_5	−1.2	0.0	...
—CH═CH_2	−0.8	0.0	...
—2-furanyl	−12.0	...	...

* When $C_\alpha C_\beta$ = CH═CH—

RMN ^{13}C : Acides carboxyliques et esters

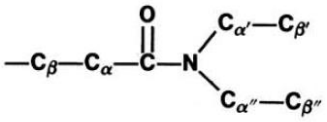
$\delta = 166 + A$



Substituents	Increments α	β	γ	X
—C.sp^3	11	3	−1	−5
—C_6H_5	6	1	...	−8
—CH═CH_2	5	...	...	−9

RMN ^{13}C : Amides

$\delta = 165 + A$



Substituents	α	β	γ	α'	β'
—C.sp^3	7.7	4.5	−0.7	−1.5	−0.3
—C_6H_5	4.7	...	...	−4.5	...
—vinyl	3.3	...	...	...	...

RMN ^{13}C : Nitriles

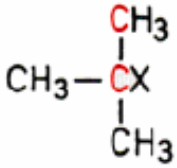
R-**C**≡N

Substituent	δ value	Substituent	δ value	Substituent	δ value
—Me	117.7	—CH_2Cl	115.7	—p-$C_6H_4NO_2$	112.2
—Et	120.8	—vinyl	117.2	—2-furanyl	111.7
—*i*-Pr	123.7	—C_6H_5	118.7	—cinnamyl	118.3

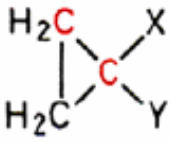
Constantes de couplage J_{CC}, J_{CH}, J_{CF} et J_{CX}

$^1J(C,C)$

H_3C-CH_3	34.6
$H_2C=CH_2$	67.6
$HC\equiv CH$	171.5
$C_6H_5-H_2C-CH_3$	34
$C_6H_5-HC=CH_2$	70
$C_6H_5-C(=O)-CH_3$	43
$H_3C-C\equiv N$	57.3



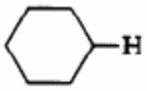
X = CH_3	36.9
= NH_2	37.1
= OH	39.5
= Cl	40.0
= Br	40.2



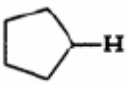
X	Y	
Br	H	13.3
I	H	12.9
Cl	Cl	15.5

$^1J(C,H)$

*sp*³	
CH_3CH_3	124.9
$CH_3CH_2CH_3$	119.2
$(CH_3)_3CH$	114.2
CH_3NH_2	133.0
CH_3OH	141.0
CH_3Cl	150.0
CH_2Cl_2	178.0
$CHCl_3$	209.0



123.0



128.0

134.0

161.0

205.0

*sp*²	
$CH_2=CH_2$	156.2
$CH_3CH=C(CH_3)_2$	148.4
$CH_3CH=O$	172.4
$NH_2CH=O$	188.3
C_6H_6	159.0
sp	
$CH\equiv CH$	249.0
$C_6H_5C\equiv CH$	251.0
$HC\equiv N$	269.0

$^2J(C,H)$

*sp*³	
CH_3CH_3	−4.5
CH_3CCl_3	5.9
$CH_3CH=O$	26.7
*sp*²	
$CH_2=CH_2$	−2.4
$(CH_3)_2C=O$	5.5
$CH_2=CHCH=O$	26.9
*C_6H_6	1.0
sp	
$CH\equiv CH$	49.3
$C_6H_5OC\equiv CH$	61.0

* ^2J = 7.6 (>^2J)

$^1J_{CX}$

$^1J_{CD}$ = 20 Hz
$^1J_{CF}$ = -160 Hz
$^1J_{CN}$ = 6-8 Hz
$^1J_{P-H}$ = >600 Hz

J_{CF}

$|J|_{FC}$ values (Hz)

NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities (RMN ^{13}C)

Table 2. ^{13}C NMR Data[a]

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD
solvent signals		77.16 ± 0.06	29.84 ± 0.01 206.26 ± 0.13	39.52 ± 0.06	128.06 ± 0.02	1.32 ± 0.02 118.26 ± 0.02	49.00±0.01
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34
tert-butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91
tert-butyl methyl ether	OCH_3	49.45	49.35	48.70	49.19	49.52	49.66
	C	72.87	72.81	72.04	72.40	73.17	74.32
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11
	CH_3Ar	21.20	21.31	20.97	21.40	21.23	21.38
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15
	C	34.25	35.00	34.33	34.35	35.05	35.36
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96
1,2-dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11
dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88
diglyme	CH_3	59.01	58.77	57.98	58.66	58.90	59.06
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32
	CO	171.07	170.61	169.54	169.95	171.31	173.32
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.50
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45
dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11
ethanol	CH_3	18.41	18.89	18.51	18.72	18.80	18.40
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88
	CO	171.36	170.96	170.31	170.44	171.68	172.89
	CH_2	60.49	60.56	59.74	60.21	60.98	61.50
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39
	CO	209.56	208.30	208.72	206.55	209.88	212.16
	CH_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34
	CH_2CH_3	7.86	8.03	7.61	7.91	8.14	8.09
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29
n-hexane	CH_3	14.14	14.34	13.88	14.32	14.43	14.45
	$CH_2(2)$	22.70	23.28	22.05	23.04	23.40	23.68
	$CH_2(3)$	31.64	32.30	30.95	31.96	32.36	32.73
HMPA[b]	CH_3	36.87	37.04	36.42	36.88	37.10	37.00
methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86
nitromethane	CH_3	62.50	63.21	63.28	61.16	63.66	63.08
n-pentane	CH_3	14.08	14.29	13.28	14.25	14.37	14.39
	$CH_2(2)$	22.38	22.98	21.70	22.72	23.08	23.38
	$CH_2(3)$	34.16	34.83	33.48	34.45	34.89	35.30
2-propanol	CH_3	25.14	25.67	25.43	25.18	25.55	25.27
	CH	64.50	63.85	64.92	64.23	64.30	64.71
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35
silicone grease	CH_3	1.04	1.40		1.38		2.10
tetrahydrofuran	CH_2	25.62	26.15	25.14	25.72	26.27	26.48
	CH_2O	67.97	68.07	67.03	67.80	68.33	68.83
toluene	CH_3	21.46	21.46	20.99	21.10	21.50	21.50
	C(*i*)	137.89	138.48	137.35	137.91	138.90	138.85
	CH(*o*)	129.07	129.76	128.88	129.33	129.94	129.91
	CH(*m*)	128.26	129.03	128.18	128.56	129.23	129.20
	CH(*p*)	125.33	126.12	125.29	125.68	126.28	126.29
triethylamine	CH_3	11.61	12.49	11.74	12.35	12.38	11.09
	CH_2	46.25	47.07	45.74	46.77	47.10	46.96

Abondance isotopique de différents éléments

Element	Isotope	Accurate Mass	Natural Abundance
Bromine	79Br	78.918336	50.69%
	81Br	80.916289	49.31%
Carbon	12C	12.000000	98.90%
	13C	13.003355	1.10%
Chlorine	35Cl	34.968852	75.77%
	37Cl	36.965903	24.23%
Fluorine	19F	18.998403	100.00%
Hydrogen	1H	1.007825	99.985%
	2H	2.014102	0.015%
Iodine	127I	126.904473	100.00%
Iron	54Fe	53.93961	5.80%
	56Fe	55.93494	91.72%
	75Fe	56.93540	2.20%
Nitrogen	14N	14.003074	99.63%
	15N	15.000108	0.37%
Oxygen	16O	15.994915	99.76%
	17O	16.999131	0.04%
	18O	17.999160	0.20%
Phosphorus	31P	30.973762	100.00%
Silicon	28Si	27.976927	92.23%
	29Si	28.976495	4.67%
	30Si	29.973770	3.10%
Sodium	23Na	22.989767	100.00%
Sulfur	32S	31.972070	95.02%
	33S	32.971456	0.75%
	34S	33.967866	4.21%

Les fragmentations les plus courantes en spectrométrie de masse

- ***Alcanes*** :
  Perte d'un méthyle : $M^{+\bullet} \rightarrow M^+ + CH_3^{\cdot}$ (**15**)
  Suivi d'une perte d'un éthylène : $M^+ \rightarrow M^+ + CH_2{=}CH_2$ (**28**)

- ***Alcènes*** :
  Obtention d'un carbocation allylique : $R\text{-}CH_2\text{-}CH{=}CH_2^{+\bullet} \rightarrow {}^+CH_2\text{-}CH{=}CH_2$ (**41**) + $R^{\cdot}$

- ***Alcools*** :
  Primaire : $R\text{-}CH_2\text{-}OH^{+\bullet} \rightarrow R^{\bullet} + CH_2{=}OH^+$ (**31**)

- ***Ethers*** :
  Rupture en α : $R\text{-}O\text{-}CH_2\text{-}R^{+\bullet} \rightarrow R\text{-}O{=}CH_2^+ + R^{\bullet}$

- ***Amines*** :
  Rupture en α : $R\text{-}NH\text{-}CH_2\text{-}R^{+\bullet} \rightarrow R\text{-}NH{=}CH_2^+ + R^{\bullet}$

- ***Aldéhydes*** :
  Perte d'un radical hydrogène : $R\text{-}CO\text{-}H^{+\bullet} \rightarrow R\text{-}C{\equiv}O^+ + H^{\bullet}$ (**1**)
  suivi d'un perte de CO : $R\text{-}C{\equiv}O^+ \rightarrow R^+ + CO$ (**28**)
  Perte de la chaîne principale : $R\text{-}CO\text{-}H^{+\bullet} \rightarrow R^{\bullet} + HC{\equiv}O^+$ (**29**)
  Rupture en β : $R\text{-}CH_2\text{-}CO\text{-}H^{+\bullet} \rightarrow R^+ + CH_2{=}CHO^{\bullet}$ (**43**)
  Réarrangement de McLafferty : $RCH_2CH_2CH_2CHO^{+\bullet} \rightarrow RCH{=}CH_2 + CH_2{=}CHOH^{+\bullet}$ (**44**)

- ***Cétones*** :
  Rupture en α : $R\text{-}CO\text{-}R'^{+\bullet} \rightarrow R^{\bullet} + R'C{\equiv}O^+$
  Réarrangement de McLafferty (voir aldéhydes)

- ***Acides, esters et amides*** :
  Réarrangement de McLafferty (voir aldéhydes)
  Rupture en α (voir cétones)

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