

Tabla 1. Propiedades magnéticas de núcleos seleccionados

Isótopo	% ^b	Z	N	A	I	γ^c	ν^d	μ^e	Q ^f	S ^g
n	—	0	1	1	1/2	-183.26	29.167	-1.91315	0	0.322
¹ H	99.985	1	0	1	1/2	267.512	42.5759	2.79268	0	1.00
² H	0.015	1	1	2	1	41.0648	6.53566	0.857387	2.73×10^{-3}	9.65×10^{-3}
⁷ Li	92.58	3	4	7	3/2	103.96	16.546	3.2560	-3×10^{-2}	0.293
¹⁰ B	19.58	5	5	10	3	28.748	4.5754	1.8007	7.4×10^{-2}	1.99×10^{-2}
¹¹ B	80.42	5	6	11	3/2	85.828	13.660	2.6880	3.55×10^{-2}	0.165
¹³ C	1.108	6	7	13	1/2	67.2640	10.7054	0.702199	0	1.59×10^{-2}
¹⁴ N	99.63	7	7	14	1	19.325	3.0756	0.40347	1.6×10^{-2}	1.01×10^{-3}
¹⁵ N	0.37	7	8	15	1/2	-27.107	4.3142	-0.28298	0	1.04×10^{-3}
¹⁷ O	0.037	8	9	17	5/2	-36.27	5.772	-1.8930	-2.6×10^{-2}	2.91×10^{-2}
¹⁹ F	100	9	10	19	1/2	251.667	40.0541	2.62727	0	0.833
²³ Na	100	11	12	23	3/2	70.761	11.262	2.2161	0.14	9.25×10^{-2}
²⁷ Al	100	13	14	27	5/2	69.706	11.094	3.6385	0.149	0.206
²⁹ Si	4.70	14	15	29	1/2	-53.142	8.4578	-0.55477	0	7.84×10^{-3}
³¹ P	100	15	16	31	1/2	108.29	17.235	1.1305	0	6.63×10^{-2}
³³ S	0.76	16	17	33	3/2	20.517	3.2654	0.64257	-6.4×10^{-2}	2.26×10^{-3}
³⁵ Cl	75.53	17	18	35	3/2	26.212	4.1717	0.82091	-7.89×10^{-2}	4.70×10^{-3}
³⁷ Cl	24.47	17	20	37	3/2	21.82	3.472	0.6833	-6.21×10^{-2}	2.71×10^{-3}

a) Recogido de "The 64th CRC Handbook of Chemistry and Physics", CRC Press, Boca Raton, FL, 1984.

b) Abundancia natural

c) Cte. Giromagnética ($10^6 \text{ rad T}^{-1}\text{s}^{-1}$)

d) Frecuencia de resonancia en MHz en un campo de 1T

e) Momento magnético en magnetones nucleares

f) Momento cuadrupolar eléctrico en barns

g) Sensibilidad (relativa al protón) para igual no. de núcleos a campo constante

Tabla 2. Disolventes utilizados en Resonancia Magnética Nuclear

Solvent	¹ H NMR shift δ	Mpt.* (°C)	Bpt- ₇₆₀ * (°C)
Carbon tetrachloride (CCl ₄)	—	— 23	77
Carbon disulfide (CS ₂)	—	— 112 T	46
Hexachloro-1,3-butadiene (C ₄ Cl ₆)	—	— 21	215 H
Dichlorofluoromethane (CCl ₂ F ₂)	—	— 160 T	— 30
[D ₁] Chloroform (CDCl ₃)	7.24	— 64	61
[D ₄] Methanol (CD ₃ OD)	3.35 4.78	— 98 T	64
[D ₆] Acetone (CD ₃ COCD ₃)	2.04	— 95 T	56
[D ₆] Benzene (C ₆ D ₆)	7.27	6	80
[D ₁₂] Cyclohexane (C ₆ D ₁₂)	1.42	7	81
[D ₈] Toluene (C ₆ D ₅ CD ₃)	2.30 7.19	— 95	111
[D ₅] Nitrobenzene (C ₆ D ₅ NO ₂)	7.50 7.67 8.11	6	211 H
[D ₂] Dichloromethane (CD ₂ Cl ₂)	5.32	— 97 T	40
[D ₁] Bromoform (CDBr ₃)	6.83	8	150 H
[D ₂] 1,1,2,2-Tetrachloroethane (C ₂ D ₂ Cl ₄)	6.00	— 44	146 H
[D ₃] Acetonitrile (CD ₃ CN)	1.93	— 45	82
[D ₁₀] Diethyl ether (C ₄ D ₁₀ O)	1.07 3.34	— 116 T	35
[D ₈] Tetrahydrofuran (C ₄ D ₈ O)	1.73 3.58	— 108 T	66
[D ₈] Dioxane (C ₄ D ₈ O ₂)	3.58	12	102
[D ₆] Dimethyl-sulfoxide (CD ₃ SOCD ₃)	2.49	19	189 H
[D ₅] Pyridine (C ₅ D ₅ N)	7.19 7.55 8.71	— 42	115
[D ₂] Water (D ₂ O)	4.65	0	100
[D ₄] Acetic acid (CD ₃ COOD)	2.03 11.53	17	118
[D ₁] Trifluoroacetic acid (CF ₃ COOD)	11.5	— 15	72
[D ₁₈] Hexamethylphosphoric triamide (HMPT) [(CD ₃) ₂ N] ₃ PO	2.53	7	233 H

Tabla 3. Desplazamientos químicos en RMN-¹H de diferentes tipos de compuestos orgánicos

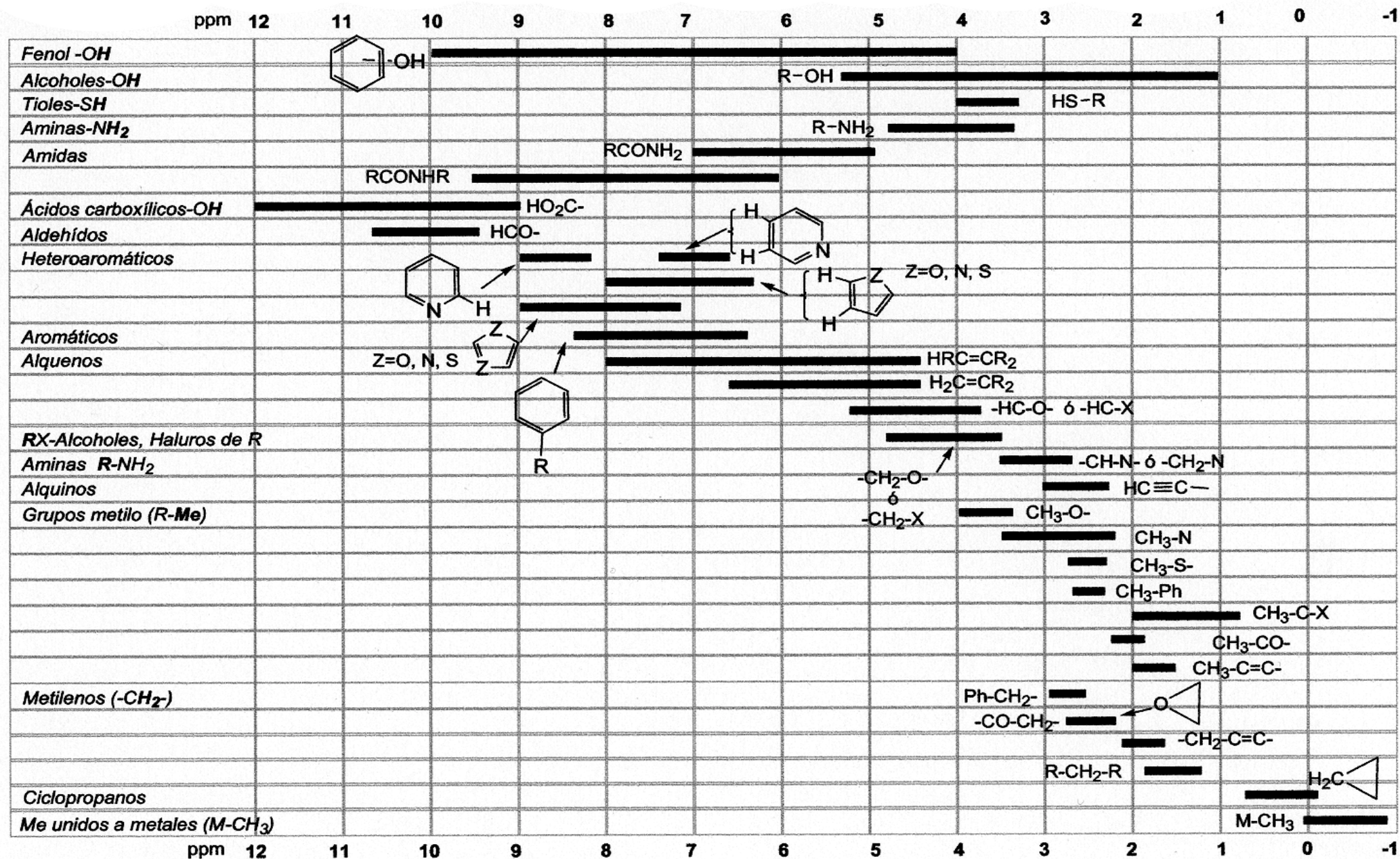
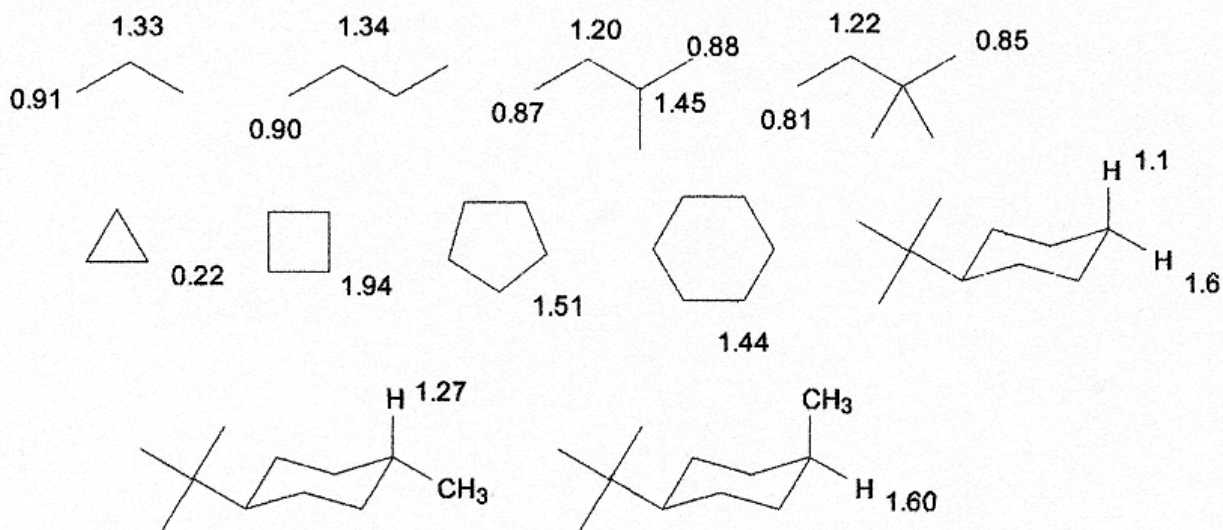


Tabla 4. Desplazamientos Químicos en RMN-¹H en alcanos monosustituídos

Sustituyente	Metilo	Etilo		n-Propilo			Isopropilo		t-Butilo
	-CH ₃	-CH ₂	-CH ₃	-CH ₂	-CH ₂	-CH ₃	-CH	-CH ₃	-CH ₃
C	-H	0.23	0.86	0.86	0.91	1.33	0.91	1.33	0.89
	-CH=CH ₂	1.71	2.00	1.00					1.02
H A L	-C≡CH	1.80	2.16	1.15	2.10	1.50	0.97	2.59	1.15
	-fenilo	2.35	2.63	1.21	2.59	1.65	0.95	2.89	1.25
	-F 1)	4.27	4.36	1.24					1.34
	-Cl	3.06	3.47	1.33	3.47	1.81	1.06	4.14	1.55
	-Br	2.69	3.37	1.66	3.35	1.89	1.06	4.21	1.73
	-I	2.16	3.16	1.88	3.16	1.88	1.03	4.24	1.89
	-OH	3.39	3.59	1.18	3.49	1.53	0.93	3.94	1.16
	-O-alquilo	3.24	3.37	1.15	3.27	1.55	0.93	3.55	1.08
	-OCH=CH ₂	3.5	3.66	1.21					
	-O-fenilo	3.73	3.98	1.38	3.86	1.70	1.05	4.51	1.31
O	-OCOCH ₃	3.67	4.05	1.21	3.98	1.56	0.97	4.94	1.22
	-OCO-fenilo	3.88	4.37	1.38	4.25	1.76	1.07	5.22	1.37
	-OSO ₂ -p-tolilo	3.70	4.07	1.30	3.94	1.60	0.95	4.70	1.25
	-NH ₂	2.47	2.74	1.10	2.61	1.43	0.93	3.07	1.03
	-NHCOCCH ₃	2.71	3.21	1.12	3.18	1.55	0.96	4.01	1.13
N	-NO ₂	4.29	4.37	1.58	4.28	2.01	1.03	4.44	1.53
	-SH	2.00	2.44	1.31	2.46	1.57	1.02	3.16	1.34
S	-S-alquilo	2.09	2.49	1.25	2.43	1.59	0.98	2.93	1.25
	-S-S-alquilo	2.30	2.67	1.35	2.63	1.71	1.03		1.32
	-CHO	2.20	2.46	1.13	2.42	1.67	0.97	2.39	1.13
O C / \	-COCH ₃	2.09	2.47	1.05	2.32	1.56	0.93	2.54	1.08
	-CO-fenilo	2.55	2.92	1.18	2.86	1.72	1.02	3.58	1.22
	-COOH	2.08	2.36	1.16	2.31	1.68	1.00	2.56	1.21
	-COOCH ₃	2.01	2.28	1.12	2.22	1.65	0.98	2.48	1.15
	-CONH ₂	2.02	2.23	1.13	2.19	1.68	0.99	2.44	1.18
-C(CH ₃)=NOH	1.9	2.22; 2.40	1.09	2.25	1.56	0.91			
-CN	1.98	2.35	1.31	2.29	1.71	1.11	2.67	1.35	

Tabla 5. Desplazamientos Químicos de protones unidos a carbonos sp^3

Alcanos



Alcanos sustituidos

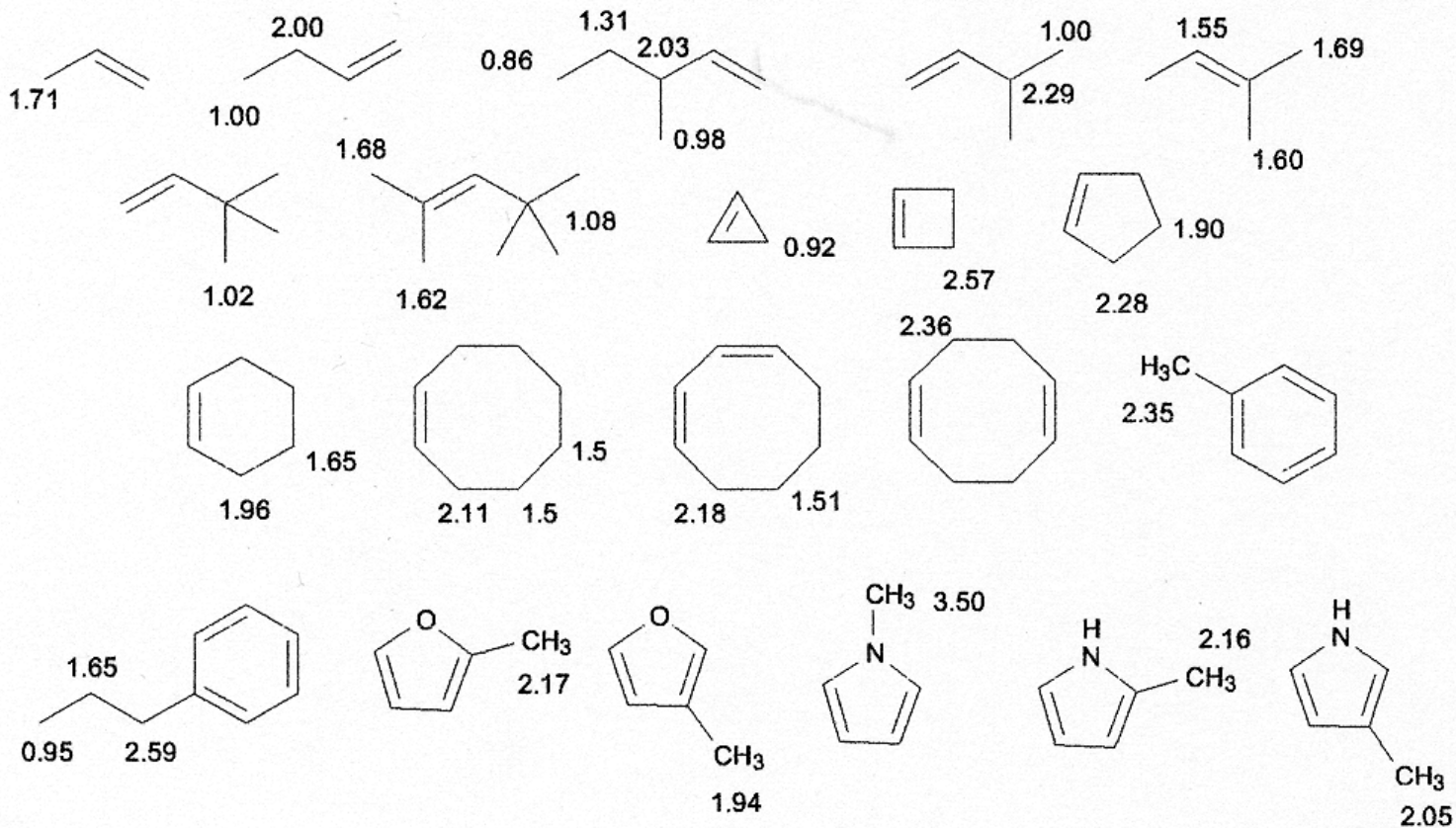
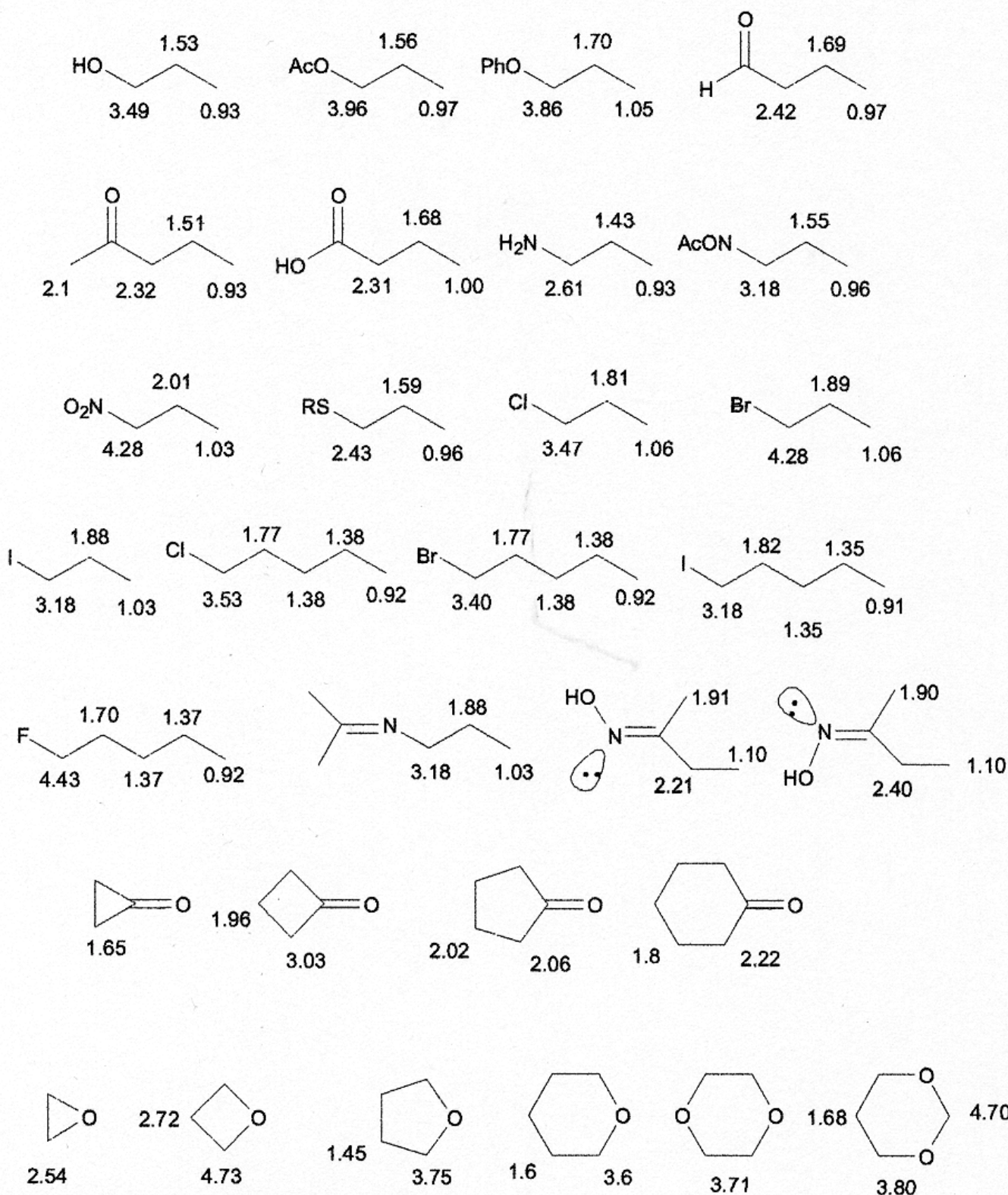


Tabla 6 . Desplazamientos Químicos de protones unidos a carbonos sp^3 (cont.)

Alcanos funcionalizados



Alquinos y grupos $C\equiv M$ funcionalizados

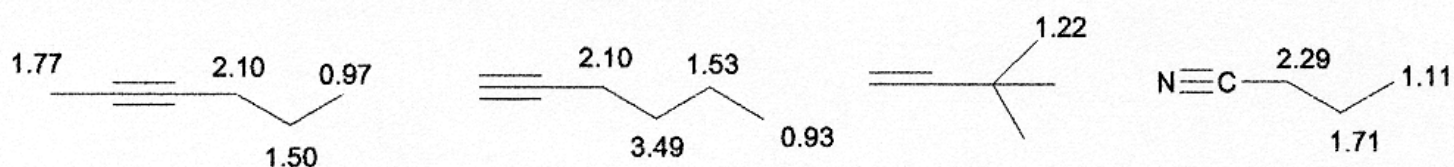


Tabla 7. Desplazamientos químicos de protones unidos a carbonos sp^2

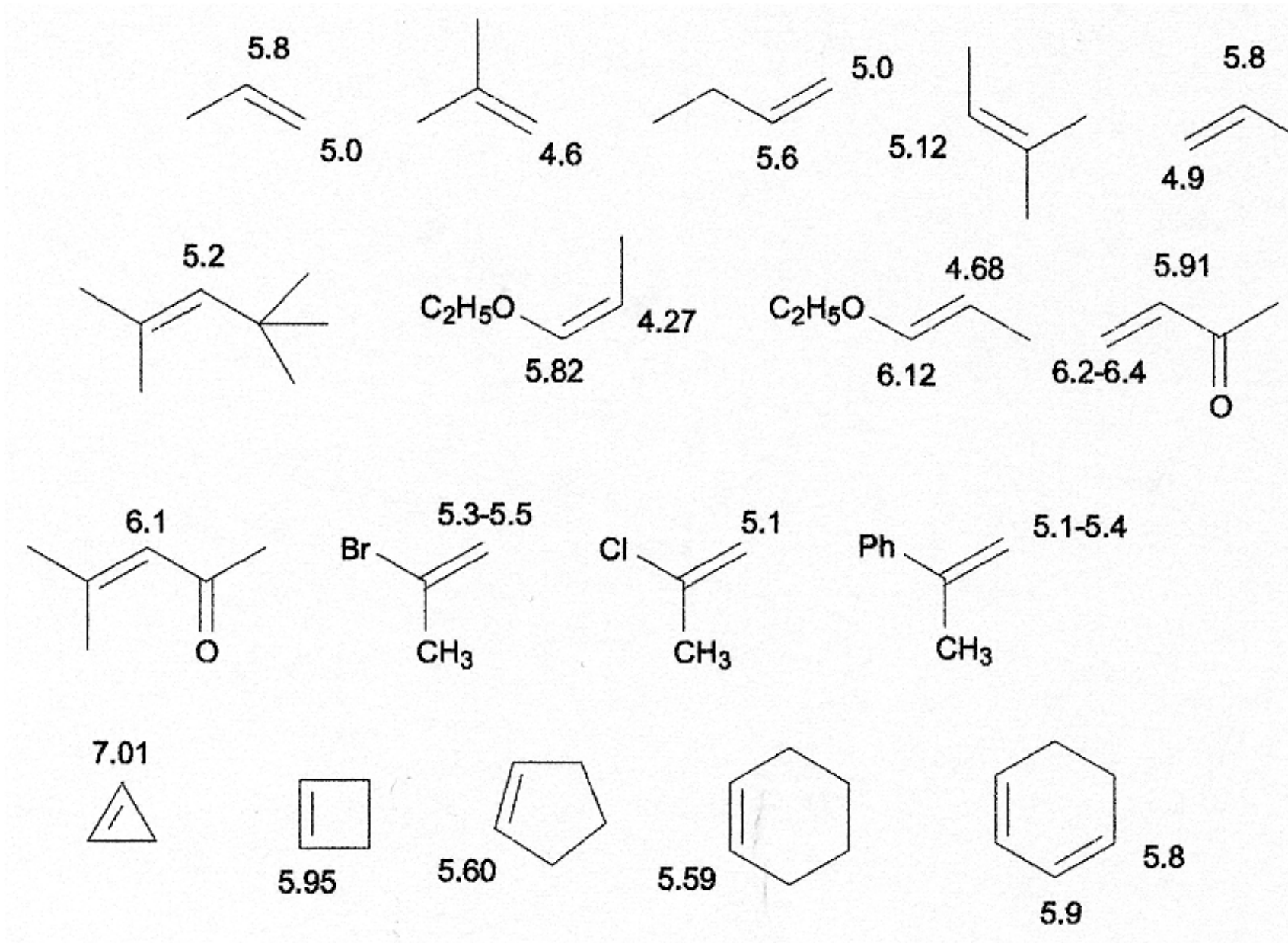


Tabla 8. Desplazamientos químicos de protones unidos a carbonos sp^2 (cont.)

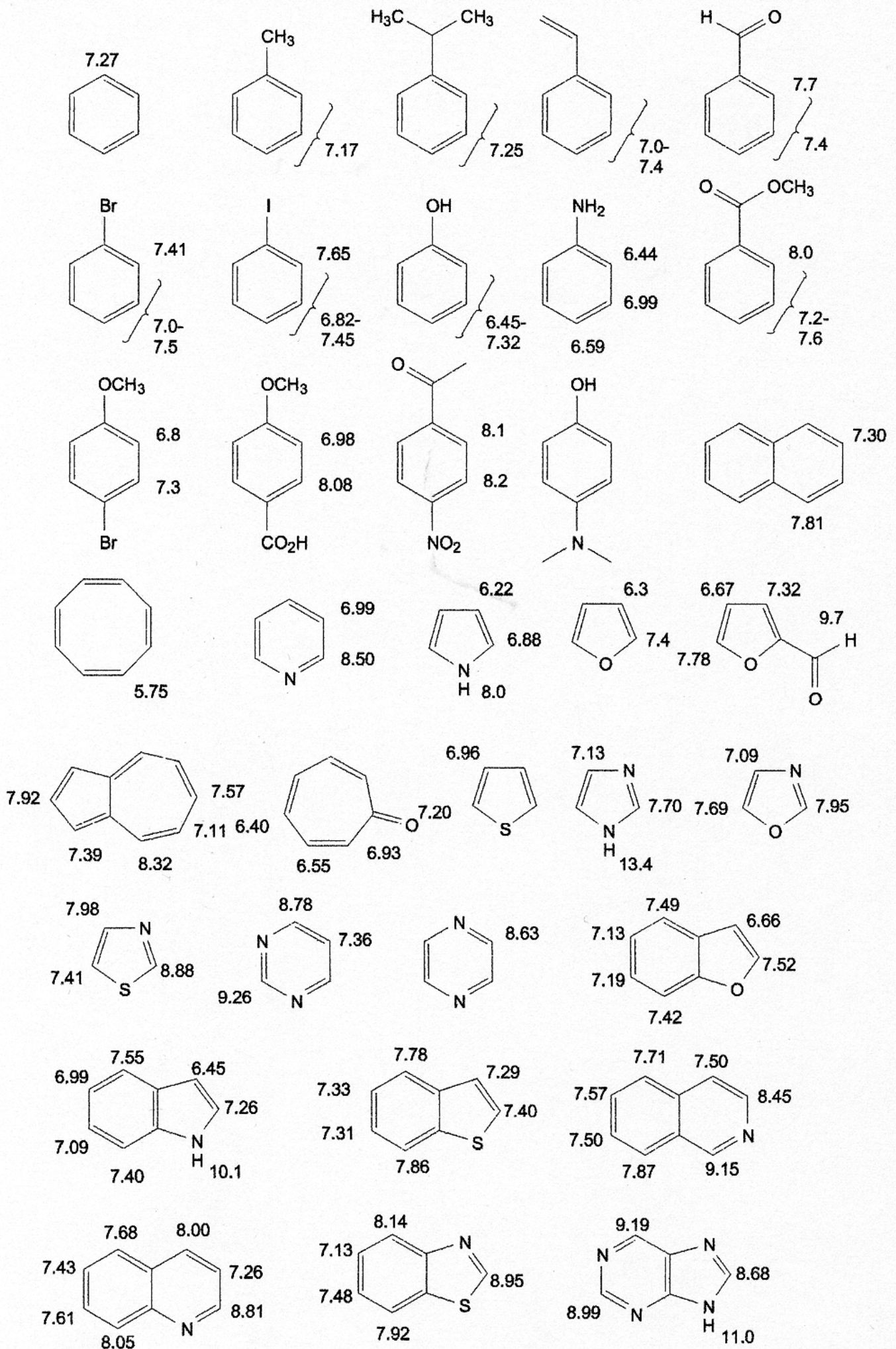


Tabla 9

Desplazamientos químicos de ^1H (δ en ppm respecto del TMS) y constantes de acoplamiento (J en Hz) en derivados acetilénicos

$\text{H}-\text{C}\equiv\text{C}-\text{H}$	1.80	$\overset{\text{a}}{\text{CH}_3}-\text{C}\equiv\text{C}-\overset{\text{b}}{\text{H}}$	(a) 1.80
$\text{H}-\text{C}\equiv\text{C}-\text{alquilo}$	1.7-1.9		(b) 1.80
$\text{H}-\text{C}\equiv\text{C}-\text{C}=\text{C}$	2.6-3.1	$\overset{\text{b}}{\text{CH}_3}\overset{\text{a}}{\text{CH}_2}-\text{C}\equiv\text{CH}$	(a) 2.16
$\text{H}-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}$	1.7-2.4		(b) 1.15
$\text{H}-\text{C}\equiv\text{C}-\text{C}_6\text{H}_5$	2.7-3.4	$(\overset{\text{b}}{\text{CH}_3})_2\overset{\text{a}}{\text{CH}}-\text{C}\equiv\text{CH}$	(a) 2.59
			(b) 1.15
$\text{H}-\text{C}\equiv\text{C}-\text{O}-\text{alquilo}$	1.3	$\text{C}_6\text{H}_5-\text{SO}_3\overset{\text{a}}{\text{CH}_2}-\overset{\text{b}}{\text{C}\equiv\text{CH}}$	(a) ~ 4.7
$\text{H}-\text{C}\equiv\text{C}-\text{CO}$	2.1-3.3		(b) 2.55
$\text{CH}_3-\text{C}\equiv\text{C}-\text{H}$	$ J = 2.9$	$\text{CH}_3\text{CONH}\overset{\text{a}}{\text{CH}_2}-\overset{\text{b}}{\text{C}\equiv\text{CH}}$	(a) 4.06
$\text{CH}_3-\text{C}\equiv\text{C}-\text{CH}_3$	$ J = 2.7$		(b) 2.25
$\text{H}-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-\text{H}$	$ J = 2.2$		

Desplazamientos químicos en RMN- ^1H para alquinos $\text{Z}-\text{C}\equiv\text{C}-\text{H}$

Substituyente Z	^1H RMN (δ)
H	1.80
CH_2R	1.79
CR_3	1.91
Ring	2.03
$\text{C}=\text{C}$	2.60 - 3.10
$\text{C}\equiv\text{C}$	1.70 - 2.40
Ph	3.08
CH_2Ph	2.18
OR	1.30
CH_2OH	2.50
$\text{CH}(\text{OH})\text{CH}_3$	2.39
CH_2NH_2	2.27
CH_2NR_2	2.23
CH_2Cl	2.42
COCH_3	3.30
COOH	3.10
COOR	2.95
CO	2.10 - 3.30

Tabla 10 Desplazamientos Químicos (CCl_4 ó CDCl_3) de protones OH, NH y SH

← δ

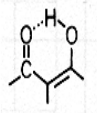
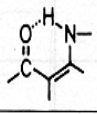







δ	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1	0			
														3.5 - 5.5					Alkyl-OH	OH	
									8.5 - 10.5										Aryl-OH		
				12.5 - 14.5															Heteroaryl-OH		
	6.5 - 13.5																				
				12.5 - 14.5															R-CO-OH		
							9.5 - 10.5												$\text{R}_2\text{C}=\text{N}-\text{OH}$		
																2.5 - 3.5			Alkyl-SH	SH	
														4.5 - 6.5					Aryl-SH		
												5.5 - 6.5							R-CO-SH		
																	2.5 - 3.5			Alkyl-NH ₍₂₎	NH ₍₂₎
													5.5 - 7.5							Aryl-NH ₍₂₎	
									8.5 - 10.5											Heteroaryl-NH ₍₂₎	
	6.5 - 13.5																				
									9.5 - 10.5											RNH_3^+	
						8.5 - 10.5														R_2NH_2^+	
						8.5 - 10.5														R_3NH^+	
								9.5 - 10.5												R-CO-NH ₍₂₎	
								9.5 - 10.5												R-SO ₂ -NH ₍₂₎	
								9.5 - 10.5												$\text{R}_2\text{C}=\text{N}-\text{NH}_{(2)}$	
																					
																					
																					
																					
																					
																					
																					
																				Heteroaromatics	

Tabla 11

Estimación de los desplazamientos químicos en alcanos polisustituídos

(δ en ppm respecto del TMS)

$$\delta_{\text{CH}_2\text{R}_1\text{R}_2} = 1.25 + \sum_1^2 z_i \qquad \delta_{\text{CHR}_1\text{R}_2\text{R}_3} = 1.50 + \sum_1^3 z_i$$



Sustituyente		z_i
C	-alquilo	0.0
	-C=C-	0.8
	-C≡C-	0.9
H A L	-fenilo	1.3
	-Cl	2.0
	-Br	1.9
O	-I	1.4
	-OH	1.7
	-O-alquilo	1.5
N	-O-fenilo	2.3
	-OCO-alquilo	2.7
	-OCO-fenilo	2.9
	-NH ₂	1.0
S	-N(alquilo) ₂	1.0
	-NO ₂	3.0
	-S-alquilo	1.0
O C / \	-CHO	1.2
	-CO-alquilo	1.2
	-COOH	0.8
	-COO-alquilo	0.7
	-CN	1.2

Tabla 12

Estimación de los desplazamientos químicos de ¹H de grupos metilo y metileno en alcanos sustituidos*

(δ en ppm respecto del TMS^a; véase E. C. Friedrich, K. G. Runkle, *J. Chem. Educ.* **61**(9), 830 [1984])

$$\delta\text{CH}_2\text{R}_1\text{R}_2 = 0.23 + \text{ZR}_1 + \text{ZR}_2$$

Sustituyente R	Z _R	Sustituyente R	Z _R	Sustituyente R	Z _R
-H	0.34	-OH	2.56	-S-alquilo(H)	1.64
-CH ₃	0.68	-O-alquilo	2.36	-S-arilo	1.90
-alquilo	0.58	-O-fenilo	2.94	-SS-alquilo	1.72
ZCH ₂ Z; Z=Cl,Br....	0.91	-OCO-alquilo(H)	3.01	-SCOCH ₃	1.94
	0.66	-OCO-fenilo	3.27	-SCO-fenilo	2.16
	0.77	-OCO-NH alquilo(arilo)	3.16	-SCON alquilo ₂	1.97
		-OCO-CF ₃	3.35	-S-C≡N	2.04
-CF ₃	1.14	-OSO ₂ alquilo	3.13	-SO-alquilo(arilo)	1.74
-CF ₂ H	1.12	-OSO ₂ arilo	3.06	-SO ₂ -alquilo(arilo)	2.45
-CCl ₃	1.55	-O-C≡N	3.57	-SO ₂ NH ₂	2.29
-CBr ₃	1.92	-N alquilo ₂ (H ₂)	1.57	-SO ₂ Cl	2.86
		-NH fenilo	2.04	-PO-alquilo ₂	0.98
-CO-alquilo(H)	1.50	-N ⁺ alquilo ₃	2.55	-PO(O-alquilo) ₂	1.09
-CO-O alquilo(H)	1.46	-NH-CO-alquilo(H)	2.27	-PS alquilo ₂	0.83
-CO-fenilo	1.90	-NH-CO-fenilo	2.43		
-CO-O fenilo	1.50	-NH-COO-alquilo	2.25	-F	3.30
-CO-N alquilo ₂ (H ₂)	1.47	-NH-COS-alquilo	2.55	-Cl	2.53
-CO-NH-fenilo	1.45	-NH-SO ₂ -arilo	1.98	-Br	2.33
-CO-Cl	1.84	-NO ₂	3.36	-I	2.19
-fenilo	1.83	-N=C=O	2.36		
-C-alquilo(H)=C-alquilo ₂ (H ₂)	1.32	-N=C=S	2.62	-Si(CH ₃) ₃	0.03
-C≡C-alquilo(H)	1.44	-N ₃	1.97	-Sn(alquilo) ₃	-0.45
-C≡N	1.59				

^a En disoluciones diluidas de CCl₄ o de CDCl₃ como disolvente.

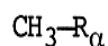
* Nota: Los traductores de la presente versión española consideran conveniente añadir esta tabla H11 (no incluida en la 3.^a edición alemana) por su gran utilidad. Estas tablas tipo Shoolery permiten el cálculo del desplazamiento químico de metilos y metilenos con una aproximación que oscila entre ±0.1 y ±0.5 ppm, entre los valores estimado y observado, para el 62% y el 99% respectivamente, de los cerca de 400 casos estudiados.

Tabla 13

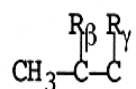
Estimación de los desplazamientos químicos de ^1H de grupos metilo y metileno en alcanos sustituidos*

(δ en ppm respecto del TMS^a; véase P. S. Beauchamp, R. M. Márquez, *J. Chem. Educ.* **74**(12), 1483 [1997])

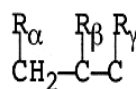
Sustituyente R	$Z_{R\alpha}$	$Z_{R\beta}$	$Z_{R\gamma}$
-alquilo	0.0	0.0	0.0
-C-alquilo=C alquilo ₂	0.8	0.2	0.1
-C=C-alquilo	0.9	0.3	0.1
-arilo	1.4	0.4	0.1
-F	3.2	0.5	0.2
-Cl	2.2	0.5	0.2
-Br	2.1	0.7	0.2
-I	2.0	0.9	0.1
-OH	2.3	0.3	0.1
-O-alquilo	2.1	0.3	0.1
-OC-alquilo=C alquilo ₂	2.5	0.4	0.2
-O-arilo	2.8	0.5	0.3
-OCO-alquilo	2.8	0.5	0.1
-OCO-arilo	3.1	0.5	0.2
-OSO ₂ -arilo	2.8	0.4	0.0
-NH ₂	1.5	0.2	0.1
-NHCO-alquilo	2.1	0.3	0.1
-NO	3.2	0.8	0.1
-SH	1.3	0.4	0.1
-S-alquilo	1.3	0.4	0.1
-CHO	1.1	0.4	0.1
-CO-alquilo	1.2	0.3	0.0
-CO-arilo	1.7	0.3	0.1
-COOH	1.1	0.3	0.1
-COO-alquilo	1.1	0.3	0.1
-CONH ₂	1.0	0.3	0.1
-COCl	1.8	0.4	0.1
-C≡N	1.1	0.4	0.2
-SO-alquilo	1.6	0.5	0.3
-SO ₂ -alquilo	1.8	0.5	0.3



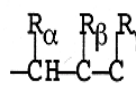
$$\delta_{\text{CH}_3} = 0.9 + Z_{R\alpha}$$



$$\delta_{\text{CH}_3} = 0.9 + \sum (Z_{R\beta} + Z_{R\gamma})$$



$$\delta_{\text{CH}_2} = 1.2 + \sum (Z_{R\alpha} + Z_{R\beta} + Z_{R\gamma})$$



$$\delta_{\text{CH}} = 1.5 + \sum (Z_{R\alpha} + Z_{R\beta} + Z_{R\gamma})$$

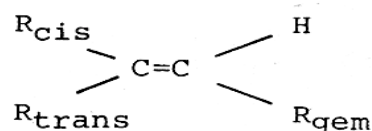
* Nota: Los traductores de la presente versión española consideran conveniente añadir esta tabla H12 (no incluida en la 3.^a edición alemana) por su gran utilidad. Estas tablas unificadas tipo Shoolery tienen en cuenta los efectos producidos por los sustituyentes en las posiciones α , β e incluso γ , y permiten el cálculo del desplazamiento químico de metilos, metilenos y metinos.

Tabla 14

Estimación del desplazamiento químico de ^1H para protones unidos a un doble enlace

(δ en ppm respecto del TMS)

$$\delta_{\text{C=CH}} = 5.25 + Z_{\text{gem}} + Z_{\text{cis}} + Z_{\text{trans}}$$

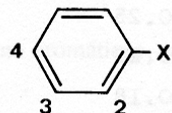


Sustituyente R	Z_{gem}	Z_{cis}	Z_{trans}
C			
-H ⁻	0	0	0
-alquilo	0.45	-0.22	-0.28
-alquilo-anillo ¹⁾	0.69	-0.25	-0.28
-CH ₂ -aromático	1.05	-0.29	-0.32
-CH ₂ X, X: F, Cl, Br	0.70	0.11	-0.04
-CHF ₂	0.66	0.32	0.21
-CF ₃	0.66	0.61	0.32
-CH ₂ O	0.64	-0.01	-0.02
-CH ₂ N	0.58	-0.10	-0.08
-CH ₂ S	0.71	-0.13	-0.22
-CH ₂ CO, CH ₂ CN	0.69	-0.08	-0.06
-C=C aislado	1.00	-0.09	-0.23
-C=C conjugado ²⁾	1.24	0.02	-0.05
-C≡C	0.47	0.38	0.12
-aromático con giro libre	1.38	0.36	-0.07
-aromático fijo ³⁾	1.60	-	-0.05
-aromático sustituido en o	1.65	0.19	0.09
H			
-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
L			
O			
-OR, R alifático	1.22	-1.07	-1.21
-OR, R insaturado	1.21	-0.60	-1.00
-OCOR	2.11	-0.35	-0.64
-NH ₂	0.80	-1.26	-1.21
-NHR, R alifático	0.80	-1.26	-1.21
-NR ₂ , R alifático	0.80	-1.26	-1.21
N			
-NHR, R insaturado	1.17	-0.53	-0.99
-NRR', R insaturado R' cualquier sust. }	1.17	-0.53	-0.99
-NCOR	2.08	-0.57	-0.72
-N=N-fenilo	2.39	1.11	0.67
-NO ₂	1.87	1.30	0.62
-SR	1.11	-0.29	-0.13
-SOR	1.27	0.67	0.41
S			
-SO ₂ R	1.55	1.16	0.93
-SCOR	1.41	0.06	0.02
-SCN	0.80	1.17	1.11
-SF ₅	1.68	0.61	0.49
-CHO	1.02	0.95	1.17
-CO aislado	1.10	1.12	0.87
-CO conjugado ¹⁾	1.06	0.91	0.74
O=C\			
-COOH aislado	0.97	1.41	0.71
-COOH conjugado ¹⁾	0.80	0.98	0.32
-COOR aislado	0.80	1.18	0.55
-COOR conjugado ¹⁾	0.78	1.01	0.46
-CONR ₂	1.37	0.98	0.46
-COCl	1.11	1.46	1.01
-CN	0.27	0.75	0.55
-PO (OCH ₂ CH ₃) ₂	0.66	0.88	0.67
-OPO (OCH ₂ CH ₃) ₂	1.33	-0.34	-0.66

Tabla 15

Influencia del sustituyente sobre el desplazamiento químico de los protones del anillo benzénico

(δ en ppm respecto del TMS)



$$\delta_{H_i} = 7.26 + Z_i$$

Sustituyente X	Z ₂	Z ₃	Z ₄
-H	0	0	0
-CH ₃	-0.20	-0.12	-0.22
-CH ₂ CH ₃	-0.14	-0.06	-0.17
-CH(CH ₃) ₂	-0.13	-0.08	-0.18
-C(CH ₃) ₃	0.02	-0.08	-0.21
-CH ₂ Cl	0.00	0.00	0.00
-CF ₃	0.32	0.14	0.20
C -CCl ₃	0.64	0.13	0.10
-CH ₂ OH	-0.07	-0.07	-0.07
-CH=CH ₂	0.06	-0.03	-0.10
-CH=CH-fenilo	0.15	-0.01	-0.16
-C≡CH	0.15	-0.02	-0.01
-C≡C-fenilo	0.19	0.02	0.00
-fenilo	0.37	0.20	0.10
H -F	-0.26	0.00	-0.20
-Cl	0.03	-0.02	-0.09
A -Br	0.18	-0.08	-0.04
-I	0.39	-0.21	0.00
-OH	-0.56	-0.12	-0.45
-OCH ₃	-0.48	-0.09	-0.44
-OCH ₂ CH ₃	-0.46	-0.10	-0.43
O -O-fenilo	-0.29	-0.05	-0.23
-OCOCH ₃	-0.25	0.03	-0.13
-OCO-fenilo	-0.09	0.09	-0.08
-OSO ₂ CH ₃	-0.05	0.07	-0.01

Sustituyente X	Z ₂	Z ₃	Z ₄
-NH ₂	-0.75	-0.25	-0.65
-NHCH ₃	-0.80	-0.22	-0.68
-N(CH ₃) ₂	-0.66	-0.18	-0.67
-NH-fenilo	-0.30	-0.06	-0.43
-N ⁺ (CH ₃) ₃ I ⁻	0.69	0.36	0.31
N -NHCOCH ₃	0.12	-0.07	-0.28
-N(CH ₃)COCH ₃	-0.16	0.05	-0.02
-NHNH ₂	-0.60	-0.08	-0.55
-N=N-fenilo	0.67	0.20	0.20
-NO	0.58	0.31	0.37
-NO ₂	0.95	0.26	0.38
-SH	-0.08	-0.16	-0.22
-SCH ₃	-0.08	-0.10	-0.24
S -S-fenilo	0.06	-0.09	-0.15
-SO ₃ CH ₃	0.60	0.26	0.33
-SO ₂ Cl	0.76	0.35	0.45
-CHO	0.56	0.22	0.29
-COCH ₃	0.62	0.14	0.21
-COCH ₂ CH ₃	0.63	0.13	0.20
-COC(CH ₃) ₃	0.44	0.05	0.05
O=C -CO-fenilo	0.47	0.13	0.22
-COOH	0.85	0.18	0.27
-COOCH ₃	0.71	0.11	0.21
-COOCH(CH ₃) ₂	0.70	0.09	0.19
-COO-fenilo	0.90	0.17	0.27
-CONH ₂	0.61	0.10	0.17
-COCl	0.84	0.22	0.36
-COBr	0.80	0.21	0.37
-CH=N-fenilo	~0.6	~0.2	~0.2
-CN	0.36	0.18	0.28
-Si(CH ₃) ₃	0.22	-0.02	-0.02
-PO(OCH ₃) ₂	0.48	0.16	0.24

Tabla 16. Constantes de acoplamiento protón-protón

Type	J_{ab} (Hz)	J_{ab} Typical	Type	J_{ab} (Hz)	J_{ab} Typical
	0-30	12-15		4-10	7
CH_a-CH_b (free rotation)	6-8	7		0-3	1.5
	0-1	0		0-3	2
			$C=CH_a-CH_b=C$	9-13	10
ax-ax	6-14	8-10		3 member	0.5-2.0
ax-eq	0-5	2-3		4 member	2.5-4.0
eq-eq	0-5	2-3		5 member	5.1-7.0
	<i>cis</i> 5-10			6 member	8.8-11.0
(<i>cis</i> or <i>trans</i>)	<i>trans</i> 5-10		$CH_a-C\equiv CH_b$	2-3	
	<i>cis</i> 4-12		$-CH_a-C\equiv C-CH_b-$	2-3	
(<i>cis</i> or <i>trans</i>)	<i>trans</i> 2-10				6
	<i>cis</i> 7-13				4
(<i>cis</i> or <i>trans</i>)	<i>trans</i> 4-9				2.5
CH_a-OH_b (no exchange)	4-10	5		J (ortho)	6-10
	1-3	2-3		J (meta)	1-3
$C=CH_a-CH_b$	5-8	6		J (para)	0-1
	12-18	17		J (2-3)	5-6
	0-3	0-2		J (3-4)	7-9
	6-12	10		J (2-4)	1-2
$CH_a-C=CH_b$	0-3	1-2		J (3-5)	1-2
				J (2-5)	0-1
				J (2-3)	1.3-2.0
				J (3-4)	3.1-3.8
				J (2-4)	0-1
				J (2-5)	1-2
				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
				J (1-2)	2-3
				J (1-3)	2-3
				J (2-3)	2-3
				J (3-4)	3-4
				J (2-4)	1-2
				J (2-5)	1.5-2.5
				J (4-5)	4-6
				J (2-5)	1-2
				J (2-4)	0-1
				J (4-6)	2-3
				J (4-5)	3-4
				J (2-5)	1-2
				J (2-4)	~0

Tabla 17. Constantes de acoplamiento protón-flúor y protón-fósforo

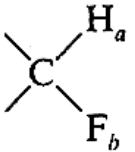
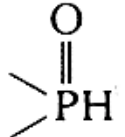
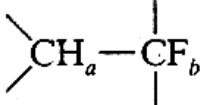
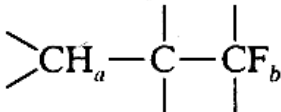
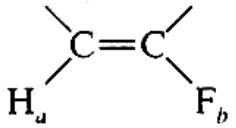
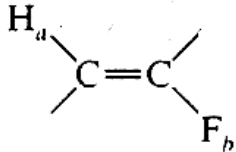
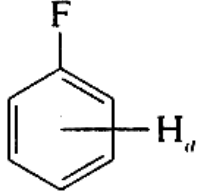
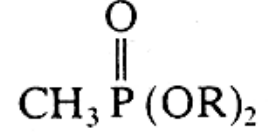
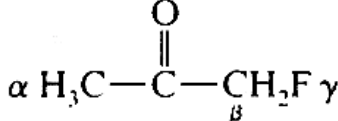
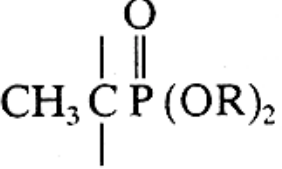
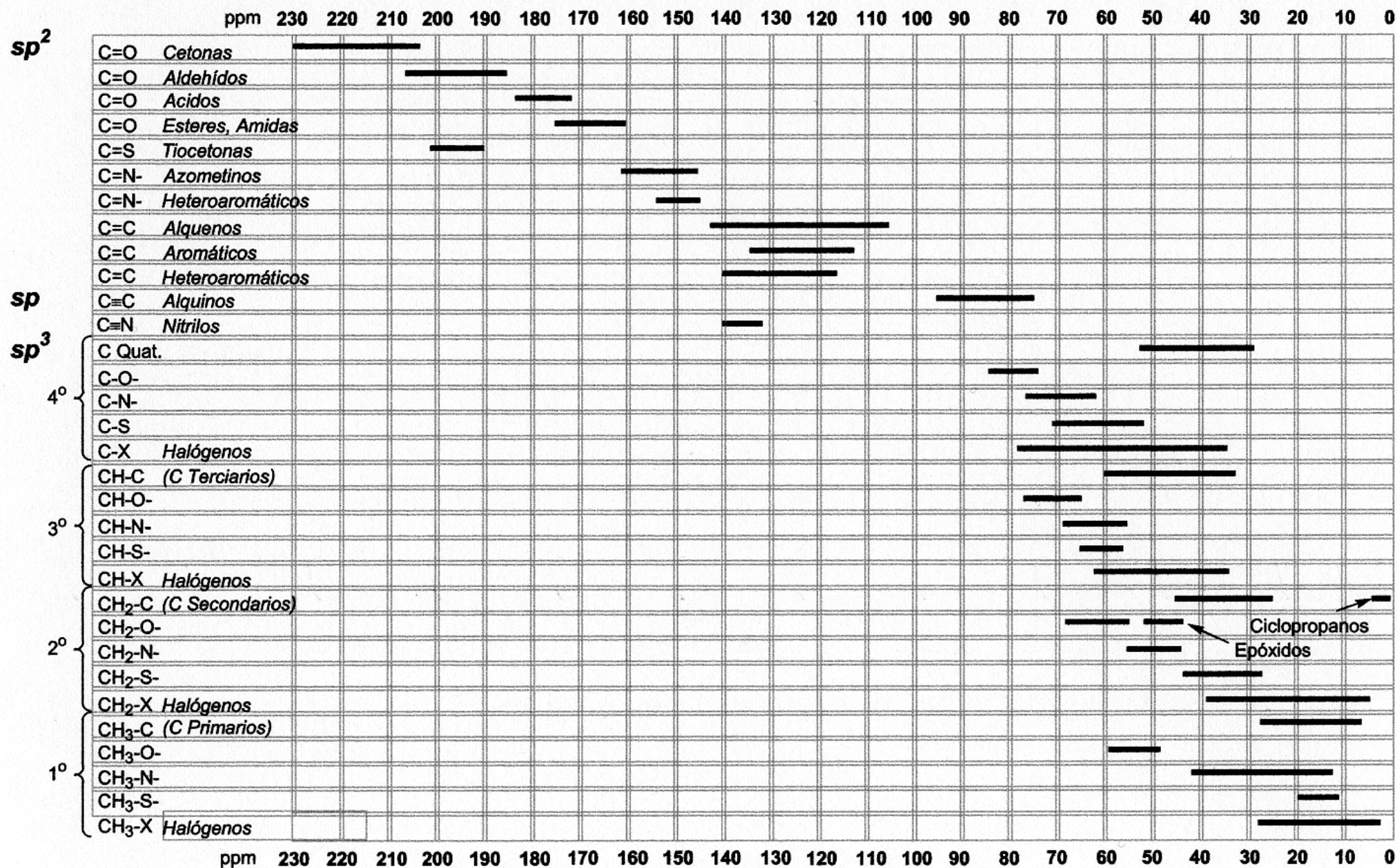
Type	J_{ab} (Hz)	J_{ab} Typical	Type	J_{ab} (Hz)	J_{ab} Typical
Proton-Fluorine			Proton-Phosphorus		
		44-81		630-707	
		3-25	(CH ₃) ₃ P	2.7	
		0-4	(CH ₃) ₃ P=O	13.4	
		1-8	(CH ₃ CH ₂) ₃ P	13.7 (HCCP)	0.5 (HCP)
		12-40	(CH ₃ CH ₂) ₃ P=O	16.3 (HCCP)	11.9 (HCP)
		<i>o</i> 6-10 <i>m</i> 5-6 <i>p</i> 2		10-13	
		$\alpha\gamma$ 4.3 $\beta\gamma$ 48		15-20	
			CH ₃ OP (OR) ₂	10.5-12	
			P[N(CH ₃) ₂] ₃	8.8	
			O=P[N(CH ₃) ₂] ₃	9.5	

Tabla 18. Desplazamientos químicos y multiplicidades en RMN-¹H de disolventes deuterados

<i>Solvent</i>	δ^1H (ppm) (mult.)	<i>Liquid</i> <i>Range</i> (°C)	<i>Dielectric</i> <i>Constant</i>	δ HOD (ppm) in ¹ H NMR
Acetic Acid-d ₄	11.65 (1) 2.04 (5)	17 – 118	6.1	11.6
Acetone-d ₆	2.05 (5)	-94 – 57	20.7	2.0
Acetonitrile-d ₃	1.94 (5)	-45 – 82	37.5	2.1
Benzene-d ₆	7.16 (1)	5 – 80	2.3	0.4
Chloroform-d	7.27 (1)	-64 – 62	4.8	1.5
Cyclohexane-d ₁₂	1.38 (1)	6 – 81	2.0	–
D ₂ O	4.80	4 – 101	78.5	4.8
Dichloromethane-d ₂	5.32 (3)	-95 – 40	8.9	1.5
<i>p</i> -Dioxane-d ₈	3.53 (m)	12 – 101	2.2	2.4
DMF-d ₇	8.03 (1) 2.92 (5) 2.75 (5)	-61 – 153	36.7	3.5
DMSO-d ₆	2.50 (5)	18 – 189	46.7	3.3
Methanol-d ₄	4.87 (1) 3.31 (5)	-98 – 65	32.7	5.0
Pyridine-d ₅	8.74 (1) 7.58 (1) 7.22 (1)	-42 – 116	12.4	5.0
THF-d ₈	3.58 (1) 1.73 (1)	-109 – 66	7.6	2.5
Toluene-d ₈	7.09 (m) 7.00 (1) 6.98 (m) 2.09 (5)	-95 – 111	2.4	0.4
TFA-d	11.50 (1)	-15 – 72	39.5	11.5

Tabla 19. Desplazamientos químicos en RMN-¹³C de diferentes tipos de compuestos orgánicos



*Relativo al TMS (0 ppm)

4° Cuaternario, 3° Terciario, 2° Secundario, 1° Primario

Tabla 20. Desplazamientos químicos en RMN-¹³C para carbonos sp³

Alcanos y cicloalcanos

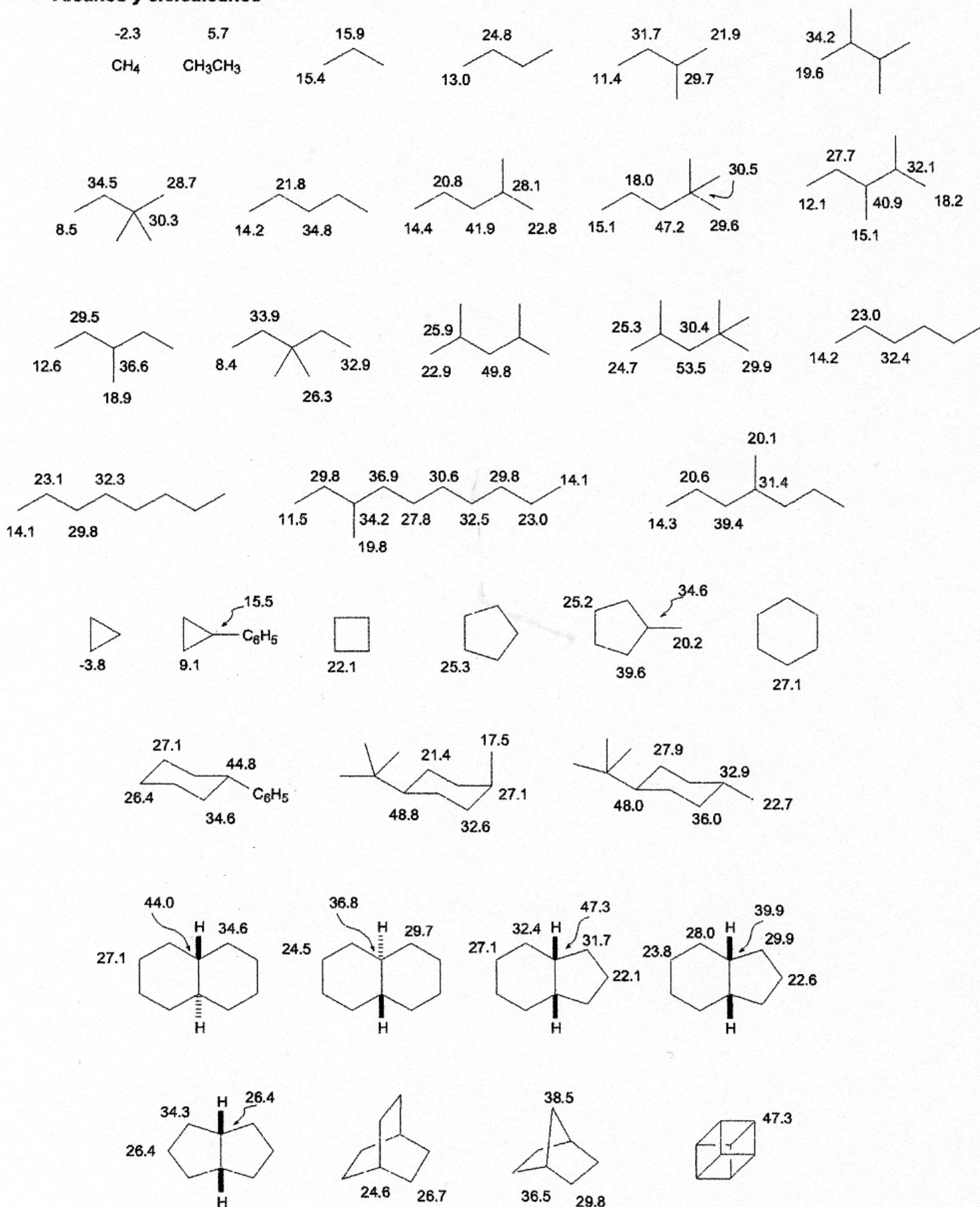


Tabla 21. Desplazamientos químicos en RMN-¹³C para carbonos sp³ (cont.)

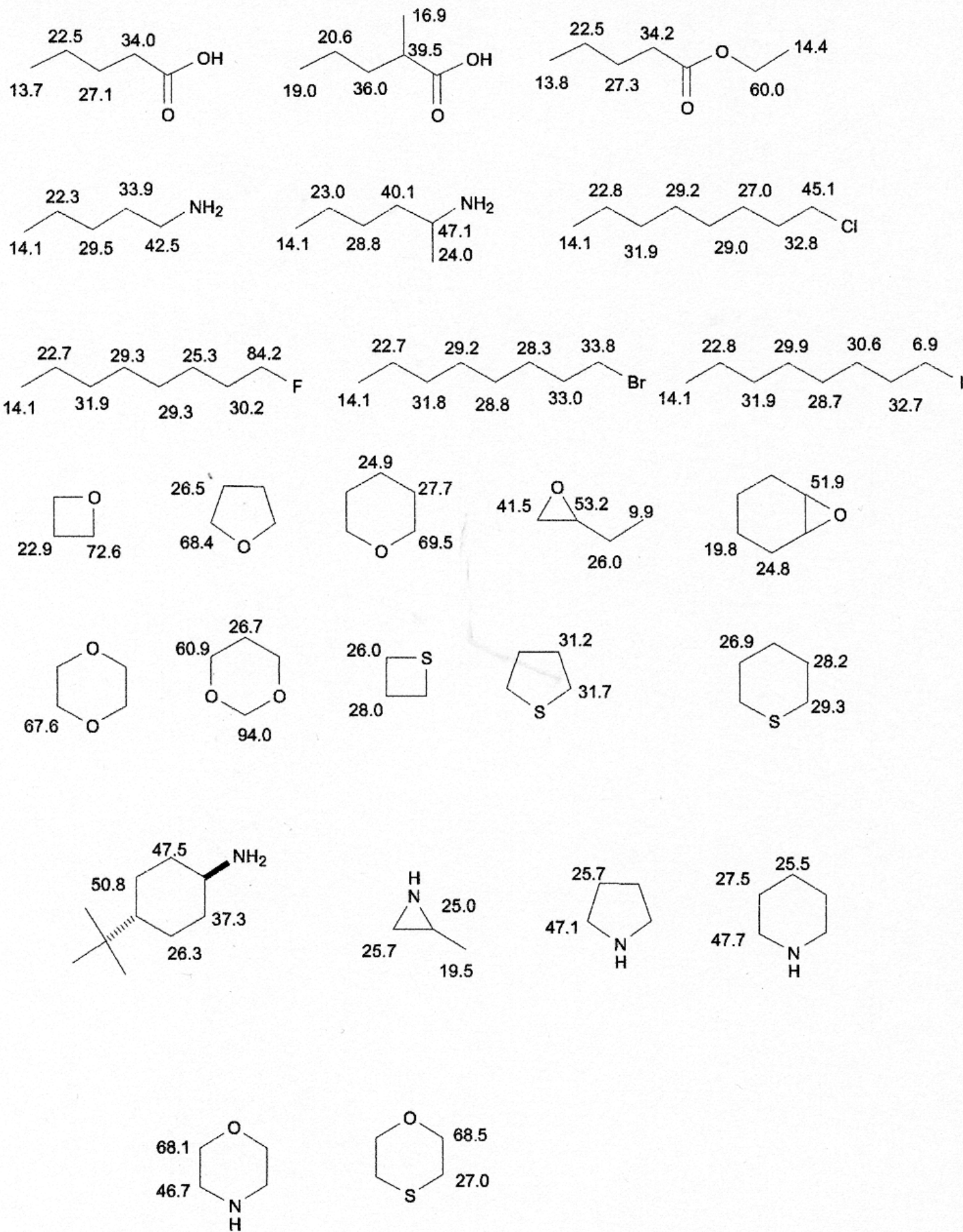
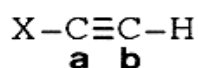


Tabla 22

Desplazamientos químicos de ^{13}C en algunos alquinos

(δ en ppm respecto del TMS)



X	a	b
-H	71.9	71.9
-CH ₃	80.4	68.3
-CH ₂ CH ₃	85.5	67.1
-CH ₂ CH ₂ CH ₃	84.0	68.7
-CH ₂ CH ₂ CH ₂ CH ₃	83.0	66.0
-CH(CH ₃) ₂	89.2	67.6
-C(CH ₃) ₃	92.6	66.8
-ciclohexilo	88.7	68.3
-CH ₂ OH	83.0	73.8
-CH=CH ₂	82.8	80.0
-C≡C-CH ₃	68.8	64.7
-fenilo	84.6	78.3
-OCH ₂ CH ₃	88.2	22.0
-SCH ₂ CH ₃	72.6	81.4
-CHO	81.8	83.1
-COCH ₃	81.9	78.1
-COOH	74.0	78.6
-COOCH ₃	74.8	75.6

Tabla 23. Desplazamientos químicos en RMN-¹³C para carbonos sp²

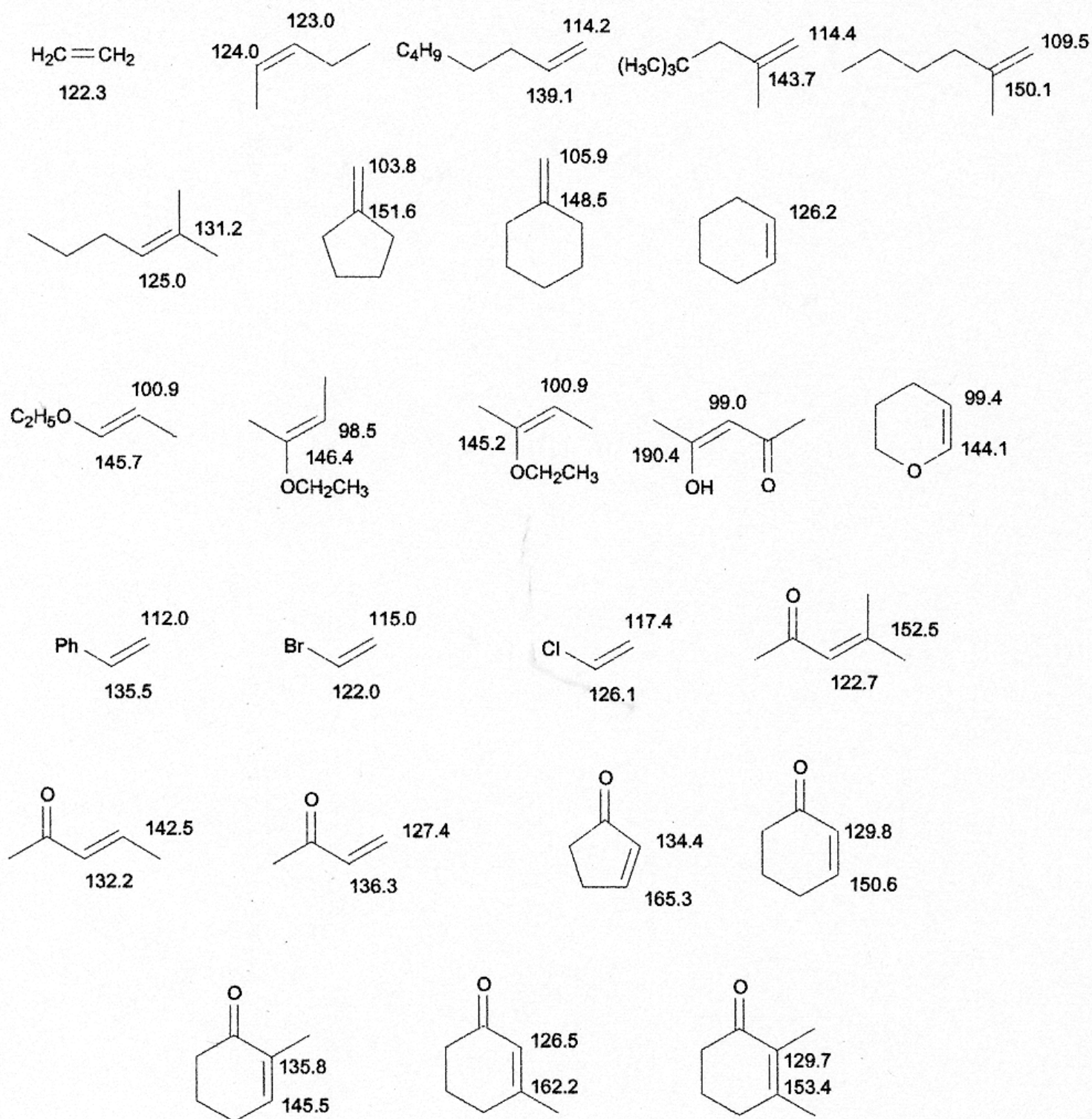


Tabla 24. Desplazamientos químicos en RMN-¹³C para carbonos sp² (compuestos aromáticos)

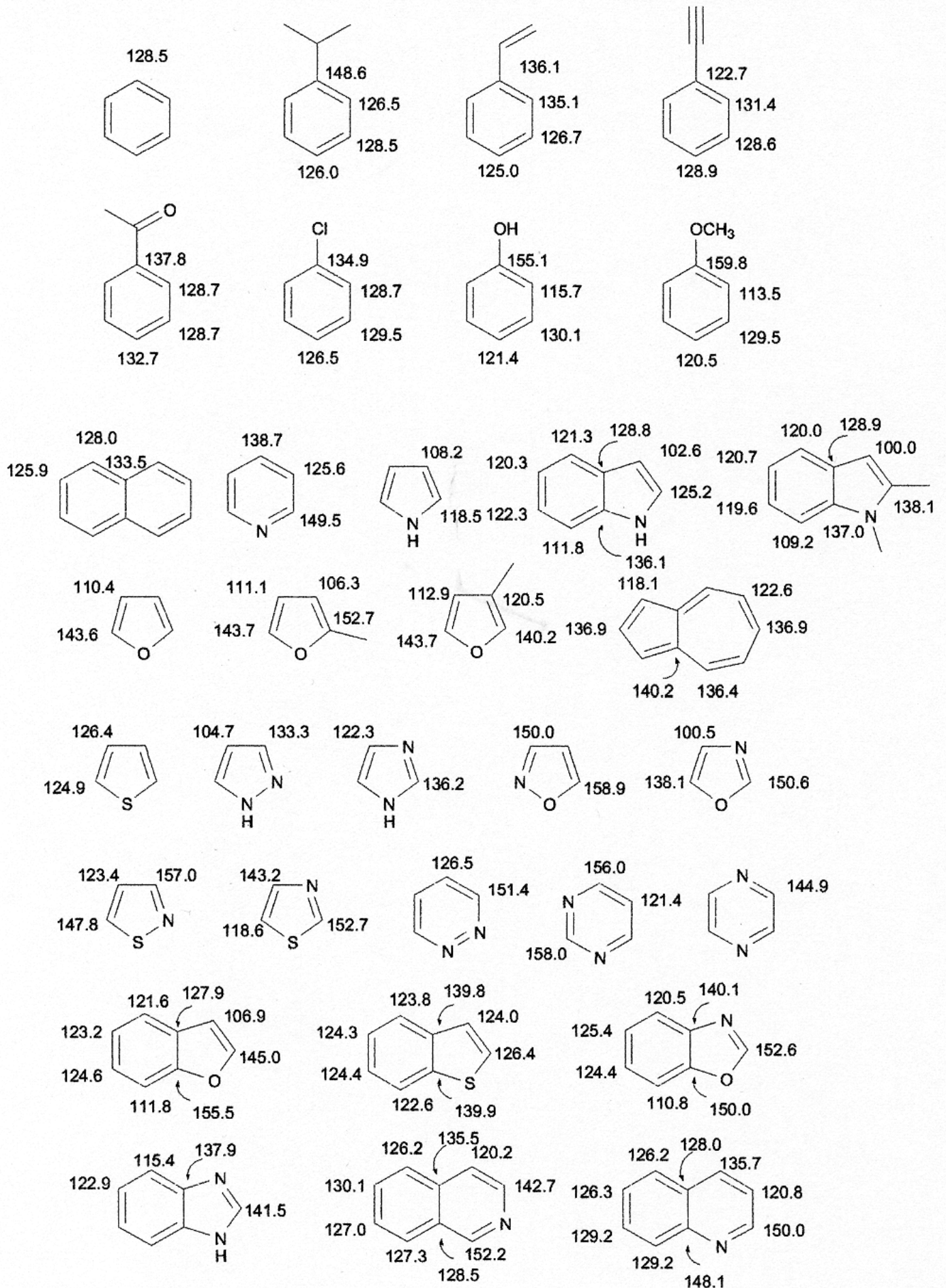


Tabla 25

Desplazamientos químicos de ^{13}C para grupos carbonilo

(δ en ppm respecto del TMS)


R	R-CHO	R-COCH ₃	R-COOH	R-COO ⁻	R-COOCH ₃	R-CONH ₂	R-COOCOR	R-COCl
-H	197.0	199.7	166.3	171.3	161.6	167.6	158.5	
-CH ₃	200.5	206.7	176.9	182.6	171.3	173.4	167.4	170.4
-CH ₂ CH ₃	202.7	207.6	180.4	185.1	173.3	177.2	170.3	174.7
-CH(CH ₃) ₂	204.6	211.8	184.1		177.4		172.8	178.0
-C(CH ₃) ₃	205.6	213.5	185.9	188.6	178.8	180.9	173.9	180.3
-n-C ₈ H ₁₇	202.6	207.9	180.7	183.1	174.4	176.3	169.4	173.8
-CH ₂ Cl	193.3	200.1	173.8	175.9	167.8	168.3	162.1	167.7
-CHCl ₂		193.6	170.3	171.8	165.1		157.6	165.5
-CCl ₃	176.9	186.3	167.1	167.6	162.5		154.1	
-ciclohexilo	204.7	209.4	182.1	185.4	175.3	177.3		176.3
-CH=CH ₂	194.4	197.5	171.7	174.5	166.5	168.3		165.6
-C \equiv CH	176.8		156.5		153.4			
-fenilo	192.0	196.9	172.6	177.6	166.8	169.7	162.8	168.0

Tabla 26

Estimación de los desplazamientos químicos de ¹³C en compuestos alifáticos

(δ en ppm respecto del TMS)

$$\delta = -2.3 + \sum_i Z_i + \sum_j S_j + \sum_k K_k$$

Sustituyente	Incrementos Z _i para sustituyentes en posición			
	α	β	γ	δ
C				
-H	0.0	0.0	0.0	0.0
-C≡ (*)	9.1	9.4	-2.5	0.3
 (*)	21.4	2.8	-2.5	0.3
-C=C- (*)	19.5	6.9	-2.1	0.4
-C≡C-	4.4	5.6	-3.4	-0.6
-fenilo	22.1	9.3	-2.6	0.3
HAL				
-F	70.1	7.8	-6.8	0.0
-Cl	31.0	10.0	-5.1	-0.5
-Br	18.9	11.0	-3.8	-0.7
-I	-7.2	10.9	-1.5	-0.9
O				
-O- (*)	49.0	10.1	-6.2	0.3
-O-CO-	56.5	6.5	-6.0	0.0
-O-NO	54.3	6.1	-6.5	-0.5
N				
-N< (*)	28.3	11.3	-5.1	0.0
-N+≡ (*)	30.7	5.4	-7.2	-1.4
-NH ₃ ⁺	26.0	7.5	-4.6	0.0
-NO ₂	61.6	3.1	-4.6	-1.0
-NC	31.5	7.6	-3.0	0.0
S				
-S- (*)	10.6	11.4	-3.6	-0.4
-S-CO-	17.0	6.5	-3.1	0.0
-SO- (*)	31.1	7.0	-3.5	0.5
-SO ₂ - (*)	30.3	7.0	-3.7	0.3
-SO ₂ Cl	54.5	3.4	-3.0	0.0
-SCN	23.0	9.7	-3.0	0.0
-CHO	29.9	-0.6	-2.7	0.0
-CO-	22.5	3.0	-3.0	0.0
O=C				
-COOH	20.1	2.0	-2.8	0.0
-COO ⁻	24.5	3.5	-2.5	0.0
-COO-	22.6	2.0	-2.8	0.0
-CON<	22.0	2.6	-3.2	-0.4
-COCl	33.1	2.3	-3.6	0.0
-CS-N<	33.1	7.7	-2.5	0.6
-C=NOH sin	11.7	0.6	-1.8	0.0
-C=NOH anti	16.1	4.3	-1.5	0.0
-CN	3.1	2.4	-3.3	-0.5
-Sn<	-5.2	4.0	-0.3	0.0

Correcciones estéricas S

Núcleo de ¹³ C considerado	Número de sustituyentes diferentes de H unidos al átomo en posición α (sólo para aquellos sustituyentes en α señalados con (*) en la pág. C10)			
	1	2	3	4
Primario (CH ₃)	0.0	0.0	-1.1	-3.4
Secundario (CH ₂)	0.0	0.0	-2.5	-6.0
Terciario (CH)	0.0	-3.7	-8.5	-10.0
Cuaternario (C)	-1.5	-8.0	-10.0	-12.5

Correcciones de conformación K para sustituyentes en posición γ

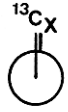
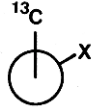
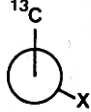
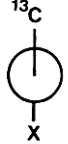
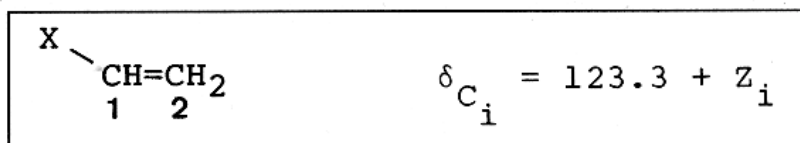
Conformación	K
Sinperiplanar 	-4.0
Sinclinal 	-1.0
Anticlinal 	0.0
Antiperiplanar 	2.0
Libre rotación	0.0

Tabla 27

**Influencia del sustituyente sobre los desplazamientos químicos de ^{13}C
en compuestos vinílicos
(δ en ppm respecto del TMS)**

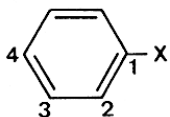


Sustituyente X	Z_1	Z_2
-H	0.0	0.0
-CH ₃	12.9	- 7.4
-CH ₂ CH ₃	17.2	- 9.8
C -CH ₂ CH ₂ CH ₃	15.7	- 8.8
-CH(CH ₃) ₂	22.7	-12.0
-CH ₂ CH ₂ CH ₂ CH ₃	14.6	- 8.9
-C(CH ₃) ₃	26.0	-14.8
-CH ₂ Cl	10.2	- 6.0
-CH ₂ Br	10.9	- 4.5
-CH ₂ I	14.2	- 4.0
-CH ₂ OH	14.2	- 8.4
-CH ₂ OCH ₂ CH ₃	12.3	- 8.8
-CH=CH ₂	13.6	- 7.0
-C \equiv CH	- 6.0	5.9
-fenilo	12.5	-11.0
H -F	24.9	-34.3
A -Cl	2.8	- 6.1
L -Br	- 8.6	- 0.9
-I	-38.1	7.0
-OCH ₃	29.4	-38.9
O -OCH ₂ CH ₃	28.8	-37.1
-OCH ₂ CH ₂ CH ₂ CH ₃	28.1	-40.4
-OCOCH ₃	18.4	-26.7
-N(CH ₃) ₂	28.0*	-32.0*
-N ⁺ (CH ₃) ₃	19.8	-10.6
N -N-pirrolidonilo	6.5	-29.2
-NO ₂	22.3	- 0.9
-NC	- 3.9	- 2.7
S -SCH ₂ -fenilo	18.5	-16.4
-SO ₂ CH=CH ₂	14.3	7.9
-CHO	15.3	14.5
O -COCH ₃	13.8	4.7
= -COOH	5.0	9.8
C -COOCH ₂ CH ₃	6.3	7.0
-COCl	8.1	14.0
-CN	-15.1	14.2
-Si(CH ₃) ₃	16.9	6.7
-SiCl ₃	8.7	16.1

Tabla 28

Influencia del sustituyente sobre los desplazamientos químicos de ¹³C en bencenos monosustituídos

(δ en ppm respecto del TMS; véase también D. F. Ewing, *Org. Magn. Res.* **12**, 499 [1979])



$$\delta_{C_i} = 128.5 + Z_i$$

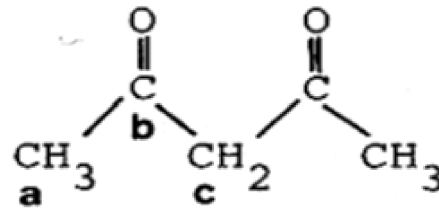
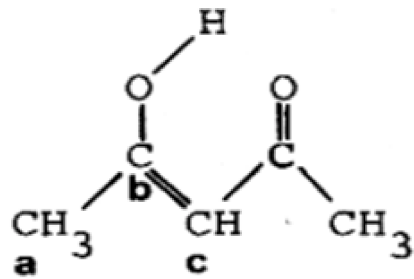
Sustituyente	Z ₁	Z ₂	Z ₃	Z ₄
-H	0.0	0.0	0.0	0.0
-CH ₃	9.2	0.7	-0.1	-3.0
-CH ₂ CH ₃	15.7	-0.6	-0.1	-2.8
-CH(CH ₃) ₂	20.2	-2.2	-0.3	-2.8
-CH ₂ CH ₂ CH ₂ CH ₃	14.2	-0.2	-0.2	-2.8
-C(CH ₃) ₃	22.4	-3.3	-0.4	-3.1
-ciclopropilo	15.1	-3.3	-0.6	-3.6
-CH ₂ Cl	9.3	0.3	0.2	0.0
-CH ₂ Br	9.5	0.7	0.3	0.2
C -CF ₃	2.5	-3.2	0.3	3.3
-CCl ₃	16.3	-1.7	-0.1	1.8
-CH ₂ OH	12.4	-1.2	0.2	-1.1
-CHOCH ₂	9.2	-3.1	-0.1	-0.5
-CH ₂ NH ₂	14.9	-1.4	-0.2	-2.0
-CH ₂ SCH ₃	9.8	0.4	-0.1	-1.6
-CH ₂ SOCH ₃	0.8	1.5	0.4	-0.2
-CH ₂ CN	1.6	0.5	-0.8	-0.7
-CH=CH ₂	8.9	-2.3	-0.1	-0.8
-C≡CH	-6.2	3.6	-0.4	-0.3
-fenilo	13.1	-1.1	0.5	-1.1
H -F	34.8	-13.0	1.6	-4.4
A -Cl	6.3	0.4	1.4	-1.9
L -Br	-5.8	3.2	1.6	-1.6
-I	-34.1	8.9	1.6	-1.1
-OH	26.9	-12.8	1.4	-7.4
-ONa	39.6	-8.2	1.9	-13.6
-OCH ₃	31.4	-14.4	1.0	-7.7
O -OCH=CH ₂	28.2	-11.5	0.7	-5.8
-O-fenilo	27.6	-11.2	-0.3	-6.9
-OCOCH ₃	22.4	-7.1	0.4	-3.2
-OSi(CH ₃) ₃	26.8	-8.4	0.9	-7.1
-OPO(O-fenilo) ₂	21.9	-8.4	1.2	-3.0
-OCN	25.0	-12.7	2.6	-1.0

Sustituyente X	Z ₁	Z ₂	Z ₃	Z ₄
-NH ₂	18.2	-13.4	0.8	-10.0
-NHCH ₃	21.4	-16.2	0.8	-11.6
-N(CH ₃) ₂	22.5	-15.4	0.9	-11.5
-NH-fenilo	14.7	-10.6	0.9	-10.5
-N(fenilo) ₂	19.8	-7.0	0.9	-5.6
-NH ₃ ⁺	0.1	-5.8	2.2	2.2
N -N ⁺ (CH ₃) ₃	19.5	-7.3	2.5	2.4
-NHCOCH ₃	9.7	-8.1	0.2	-4.4
-NHNH ₂	22.8	-16.5	0.5	-9.6
-N(CH ₃)NO	23.7	-9.5	0.8	-1.4
-N=N-fenilo	24.0	-5.8	0.3	2.2
-N ⁺ ≡N	-12.7	6.0	5.7	16.0
-NC	-1.8	-2.2	1.4	0.9
-NCO	5.1	-3.7	1.1	-2.8
-NCS	3.0	-2.7	1.3	-1.0
-NO	37.4	-7.7	0.8	7.0
-NO ₂	19.9	-4.9	0.9	6.1
-SH	2.1	0.7	0.3	-3.2
-SCH ₃	10.0	-1.9	0.2	-3.6
-SC(CH ₃) ₃	4.5	9.0	-0.3	0.0
S -S-fenilo	7.3	2.5	0.6	-1.5
-SOCH ₃	17.6	-5.0	1.1	2.4
-SO ₂ CH ₃	12.3	-1.4	0.8	5.1
-SO ₂ Cl	15.6	-1.7	1.2	6.8
-SO ₃ H	15.0	-2.2	1.3	3.8
-SO ₂ OCH ₃	6.4	-0.6	1.5	5.9
-SCN	-3.7	2.5	2.2	2.2
-CHO	8.2	1.2	0.5	5.8
-COCH ₃	8.9	0.1	-0.1	4.4
-COCF ₃	-5.6	1.8	0.7	6.7
-CO-fenilo	9.3	1.6	-0.3	3.7
-COOH	2.1	1.6	-0.1	5.2
-COO ⁻	9.7	4.6	2.2	4.6
-COOCH ₃	2.0	1.2	-0.1	4.3
-CONH ₂	5.0	-1.2	0.1	3.4
-CON(CH ₃) ₂	8.0	-1.5	-0.2	1.0
-COCl	4.7	2.7	0.3	6.6
-CS-fenilo	18.7	1.0	-0.6	2.4
-CN	-15.7	3.6	0.7	4.3
-P(CH ₃) ₂	13.6	1.6	-0.6	-1.0
-P(fenilo) ₂	8.9	5.2	0.0	0.1
-PO(OCH ₂ CH ₃) ₂	1.6	3.6	-0.2	3.4
-PS(OCH ₂ CH ₃) ₂	6.1	2.8	-0.4	3.4
-SiH ₃	-0.5	7.3	-0.4	1.3
-Si(CH ₃) ₃	11.6	4.9	-0.7	0.4
-Sn(CH ₃) ₃	13.4	7.4	-0.2	-0.3
-Pb(CH ₃) ₃	20.1	8.0	-0.1	-1.0

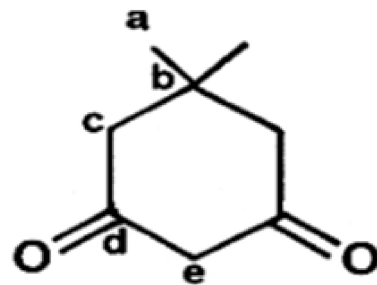
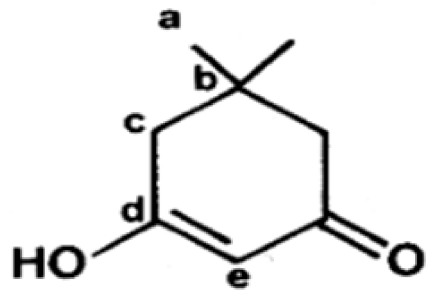
Tabla 29

Desplazamientos químicos de ^{13}C en algunos enoles

(δ en ppm respecto del TMS)



	Enol	Cetona
(a)	22.5	28.5
(b)	190.5	201.1
(c)	99.0	56.6



	Enol	Cetona
(a)	28.3	28.3
(b)	32.8	31.0
(c)	46.2	54.2
(d)	191.1	203.6
(e)	103.3	57.3

Tabla 30. Desplazamientos químicos y multiplicidades en RMN-¹³C de disolventes deuterados

Solvent	¹³ C NMR shift δ	Multiplicity	$J(^{13}\text{C},\text{D})$ (Hz)
[D ₁] Chloroform	77.0	triplet	32
[D ₄] Methanol	49.3	septet	21
[D ₆] Acetone	29.3	septet	20
	206.3	multiplet	<1
[D ₆] Benzene	128.0	triplet	24
[D ₂] Dichloromethane	53.5	quintet	27
[D ₃] Acetonitrile	1.3	septet	21
	117.7	multiplet	<1
[D ₁] Bromoform	10.2	triplet	31.5
[D ₂] 1,1,2,3-Tetrachloroethane	74.0	triplet	
[D ₈] Tetrahydrofuran	25.5	quintet	21
	67.7	quintet	22
[D ₈] Dioxane	66.5	quintet	22
[D ₆] Dimethyl sulfoxide	39.7	septet	21
[D ₅] Pyridine	123.5	triplet	25
	135.5	triplet	24
	149.5	triplet	27
[D ₂] Water	-	-	-
[D ₄] Acetic acid	20.0	septet	20
	178.4	multiplet	<1
[D _{1,8}] Hexamethylphosphoric-triamide (HMPT)	35.8	septet	21
Carbon tetrachloride	96.0	singlet	-
Carbon disulfide	192.8	singlet	-
Trichlorofluoromethane	117.6	doublet	(¹ J(C,F) = 337
[D ₁] Trifluoroacetic acid	116.5	quartet	(¹ J(C,F) = 283)
	164.4	quartet	(² J(C,F) = 44)

Tabla 31. Datos útiles de RMN para diferentes núcleos magnéticamente activos

Isotope	Spin	Natural Abundance (%)	Sensitivity		MHz at T of 7.0463	Reference Compound	Determined Range (ppm)
			Relative ^a	Absolute ^b			
¹ H	1/2	99.98	1.00	1.00	300.000	Si(CH ₃) ₄	10 to 0
² H	1	1.5 × 10 ⁻²	9.65 × 10 ⁻³	1.45 × 10 ⁻⁶	46.051	Si(CD ₃) ₄	10 to 0
³ H	1/2	0	1.21	0	319.990	Si(CT ₃) ₄	10 to 0
³ He	1/2	1.3 × 10 ⁻⁴	0.44	5.75 × 10 ⁻⁷	228.533		
⁶ Li	1	7.42	8.50 × 10 ⁻³	6.31 × 10 ⁻⁴	44.146	⁶ LiCl ₂ /D ₂ O	2 to -10
⁷ Li	3/2	92.58	0.29	0.27	116.590	⁷ LiCl ₂ /D ₂ O	2 to -10
⁹ Be	3/2	100	1.39 × 10 ⁻²	1.39 × 10 ⁻²	42.160		
¹⁰ B	3	19.58	1.99 × 10 ⁻²	3.90 × 10 ⁻³	32.239	¹⁰ BF ₃ /(C ₂ H ₅) ₂ O	65 to -130
¹¹ B	3/2	80.42	0.17	0.13	96.251	¹¹ BF ₃ /(C ₂ H ₅) ₂ O	65 to -130
¹³ C	1/2	1.108	1.59 × 10 ⁻²	1.76 × 10 ⁻⁴	75.432	Si(CH ₃) ₄	0 to 220
¹⁴ N	1	99.63	1.01 × 10 ⁻³	1.01 × 10 ⁻³	21.671	¹⁴ NH ₃ (l) ^c	900 to 0
¹⁵ N	1/2	0.37	1.04 × 10 ⁻³	3.85 × 10 ⁻⁶	30.398	¹⁵ NH ₃ (l) ^c	900 to 0
¹⁷ O	5/2	3.7 × 10 ⁻²	2.91 × 10 ⁻²	1.08 × 10 ⁻⁵	40.670	H ₂ O	1700 to -50
¹⁹ F	1/2	100	0.83	0.83	282.231	CFCl ₃	276 to -280
²¹ Ne	3/2	0.257	2.50 × 10 ⁻³	6.43 × 10 ⁻⁶	23.683		
²³ Na	3/2	100	9.25 × 10 ⁻²	9.25 × 10 ⁻²	79.353	1M NaCl/H ₂ O	10 to -65
²⁵ Mg	5/2	10.13	2.67 × 10 ⁻³	2.71 × 10 ⁻⁴	18.358	MgCl ₂ /H ₂ O	50 to -25
²⁷ Al	5/2	100	0.21	0.21	78.172	Al(NO ₃) ₃	240 to -240
²⁹ Si	1/2	4.7	7.84 × 10 ⁻³	3.69 × 10 ⁻⁴	59.595	Si(CH ₃) ₄	80 to -380
³¹ P	1/2	100	6.63 × 10 ⁻²	6.63 × 10 ⁻²	121.442	85% H ₃ PO ₄	270 to -480
³³ S	3/2	0.76	2.26 × 10 ⁻³	1.72 × 10 ⁻⁵	23.009		
³⁵ Cl	3/2	75.53	4.70 × 10 ⁻³	3.55 × 10 ⁻³	29.395	³⁵ NaCl in H ₂ O	1200 to -100
³⁷ Cl	3/2	24.47	2.71 × 10 ⁻³	6.63 × 10 ⁻⁴	24.467	³⁷ NaCl in H ₂ O	1200 to -100

^a At constant field for equal number of nuclei.

^b Product of relative sensitivity and natural abundance.

^c At 25°C.