Tabla 1. Desplazamientos químicos (δ) de protones de metilos, metilenos y metinos de alcanos monosustituídos con sustituyentes X en posición α .

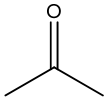
	X	CH_3X	$—CH_2X$	$—\overset{|}{C}HX$
C	$—CH_3$ $—CH_2—$	0.86—0.91	1.25—1.33	1.50
	$—CH=CH_2$	1.71	2.00—2.30	2.60
	—CH=CH	1.80	2.10—2.16	2.59
	—Fenilo	2.35	2.59—2.63	2.89
Halógenos	—F	4.27	4.36	—
	—Cl	3.06	3.47	4.14
	—Br	2.69	3.35—3.37	4.21
	—I	2.16	3.16	4.24
O	—OH	3.39	3.49—3.59	3.94
	—O—Alquilo	3.24	3.27—3.37	3.55
	—O—C=C	3.50	3.70	—
	—O—fenilo	3.73	3.86—3.98	4.51
	$—O—COCH_3$	3.67	3.98—4.05	4.94
	$—O—COCF_3$	4.10	4.30	—
	—O-CO-fenilo	3.88	4.25—4.37	5.22
	$—O-SO_2$-fenilo	3.70	3.94—4.07	4.70
N	$—NH_2$	2.47	2.61—2.74	3.07
	$—N—(Alquilo)_2$	2.19	2.50	2.88
	$—NCH_3—$Fenilo	2.91	—	—
	$—N(CH_3)CHO$	2.88-2.97	—	4.12
	$—\overset{+}{N}—(Alquilo)_3$	3.33	3.40	3.50
	$—NHCOCH_3$	2.71	3.18—3.21	4.01
	$—NO_2$	4.29	4.28—4.37	4.44
	—NCS	3.37	3.64	3.98
S	—SH	2.00	2.44—2.46	3.16
	—S—Alquilo	2.09	2.43—2.49	2.93
	—S—S—alquilo	2.30	2.63—2.67	—
	$—SO_2R$	2.80-3.00	2.94	—
	$—SOCH_3$	2.50	—	—
	—SCN	2.61	2.98	3.48
	—CHO	2.20	2.42—2.46	2.39
	$—COCH_3$	2.09	2.32—2.47	2.54
	—CO-fenilo	2.55	2.86—2.92	3.58
	—COOH	2.08	2.31—2.36	2.56
	$—COOCH_3$	2.01	2.22—2.28	2.48
	$—CONH_2$	2.02	2.19—2.23	2.44
	—COCl	2.80	—	— —
	—COBr	2.70	—	—
	—COSH	2.40	—	—
	—C=N—OH	1.90	—	—
	—CN	1.98	2.29—2.35	2.67

Tabla 2. Desplazamientos químicos de protones de metilos, metilenos y metinos de alcanos monosustituídos con sustituyentes X en posición β o γ.

δ_{CH_3} = 0.9 + desplazamiento
δ_{CH_2} = 1.25 + desplazamiento
δ_{CH} = 1.5 + desplazamiento

Los desplazamientos están dados en la tabla, en ppm.

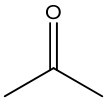
	X	CH_3-C-X	$-CH_2-C-X$	$>CH-C-X$	$H_3C-C-C-X$
C	—CH=CH$_2$	0.10—0.12	.05	—	—
	—CH=CH	0.25—0.32	0.25	—	0.07
	—Fenilo	0.31—0.42	0.40	—	0.05
Halógenos	—F	0.34—0.44	0.17	0.02	—
	—Cl	0.43—0.70	0.56	0.24	0.16
	—Br	0.76—0.86	0.64	0.43	0.16
	—I	0.98—1.05	0.63	—	0.13
O	—OH	0.26—0.32	0.28	—	0.03
	—O—Alquilo	0.18—0.34	0.30	—	0.03
	—O—C=C	0.40	-	—	—
	—O—fenilo	0.41—0.48	0.45	—	0.15
	—O—COCH$_3$	0.31—0.55	0.31	—	0.07
	—O-CO-fenilo	0.47—0.68	0.51	—	0.17
	—O-SO$_2$-fenilo	0.35—0.40	0.35	—	0.05
N	—NH$_2$	0.13—0.25	0.18	—	0.03
	—N(CH$_3$)CHO	0.20—0.29	—	—	—
	—N(Alquilo)$_3$	0.35	—	—	—
	—NHCOCH$_3$	0.22—0.38	0.30	—	0.06
	—NO$_2$	0.63—0.69	0.76	—	0.13
	—NCS	0.50	—	—	—
S	—SH	0.41—0.53	0.32	—	0.12
	—S—Alquilo	0.35—0.49	0.34	—	0.08
	—S—S—alquilo	0.42—0.45	0.46	—	0.13
	—SO$_2$R	0.57	—	—	—
	—SCN	0.62	—	—	—
	—CHO	0.17—0.23	0.42	—	0.07
	—COCH$_3$	0.15—0.22	0.31	—	0.03
	—CO-fenilo	0.18—0.22	0.47	—	0.12
	—COOH	0.26—0.33	0.43	—	0.10
	—COOCH$_3$	0.22—0.26	0.40	—	0.08
	—CONH$_2$	0.23—0.32	0.43	—	0.09
	—CN	0.41—0.47	0.46	—	0.11

Tabla 3. Valores de d para metilenos disustituidos X—CH_2—Y

Sust.	Br—	Cl—	I—	R_2N—	HO—	RO—	PhO—	RCOO—	RS—	CH3—	C=C—	C≡C	Ph—	F_3C—	CN—	RCO—	ROOC—	R_2NOC—
Br—	4.92	5.13	4.38	4.13	5.12	4.92	5.79	5.69	4.20	3.72	3.88	4.00	4.41	3.70	4.26	4.26	4.11	4.15
	Cl—	5.31	4.80	4.37	5.32	5.12	5.99	5.89	4.40	3.41	4.08	4.20	4.61	3.90	4.26	4.46	4.12	4.25
		I—	3.87	3.62	4.61	4.41	5.16	5.06	3.69	2.85	3.62	3.49	3.90	3.19	3.70	3.75	3.60	3.64
			R_2N—	3.37	4.35	4.15	5.03	4.93	3.44	2.44	3.20	3.16	3.56	2.94	3.50	3.50	3.35	3.40
				HO—	5.35	5.15	6.02	5.92	4.43	3.53	4.13	4.28	4.58	3.93	4.49	4.49	4.34	4.38
					RO—	4.95	5.82	5.72	4.23	3.23	3.91	4.03	4.44	3.73	4.24	4.29	4.22	4.26
						PhO—	6.69	6.59	5.10	3.93	4.78	4.90	5.31	4.60	5.16	5.16	5.09	5.13
							RCOO—	6.46	5.00	4.04	4.68	4.80	5.21	4.54	5.10	5.10	4.91	4.35
								RS—	3.51	2.43	3.14	3.31	3.72	3.01	3.57	3.57	3.42	3.46
									CH3—	1.17	2.02	2.14	2.55	1.84	2.40	2.43	2.25	2.26
										C=C—	2.87	2.99	3.32	2.69	3.20	3.25	3.10	3.14
											C≡C	3.11	3.52	2.81	3.37	3.37	3.22	3.26
												Ph—	3.95	3.22	3.72	3.78	3.63	3.66
													F_3C—	2.51	3.07	3.07	2.92	2.96
														F_3C—	3.63	3.63	3.48	3.52
															RCO—	3.63	3.48	3.52
																ROOC—	3.33	3.37
																	R_2NOC—	3.41

Tabla 4. Desplazamientos químicos (δ) de protones en alcanos monosustituidos.

Sustituyente	Metilo	Etilo		n-Propilo			Isopropilo		t-Butilo
	—CH_3	—CH_2	—CH_3	—CH_2	—CH_2	—CH_3	—CH_2	—CH_3	—CH_3
——H	0.23	0.86	0.86	0.91	1.33	0.91	1.33	0.91	0.89
——$CH{=}CH_2$	1.71	2.00	1.00	—	—	—	—	—	1.02
——C≡C	1.80	2.16	1.15	2.10	1.50	0.97	2.59	1.15	1.22
——Fenilo	2.35	2.63	1.21	2.59	1.65	0.95	2.89	1.25	1.32
——F	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	1.60
——Br	2.69	3.37	1.66	3.35	1.89	1.06	4.21	1.73	1.76
——I	2.16	3.16	1.88	3.16	1.88	1.03	4.24	1.89	1.95
——OH	3.39	3.59	1.18	3.49	1.53	0.93	3.94	1.16	1.22
——O—Alquilo	3.24	3.37	1.15	3.27	1.55	0.93	3.55	1.08	1.24
——O—C≡C	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—$COCH_3$	3.67	4.05	1.21	3.98	1.56	0.97	4.94	1.22	1.45
——O-CO-fenilo	3.88	4.37	1.38	4.25	1.76	1.07	5.22	1.37	1.58
——NH_2	2.47	2.74	1.10	2.61	1.43	0.93	3.07	1.03	1.15
——$NHCOCH_3$	2.71	3.21	1.12	3.18	1.55	0.96	4.01	1.13	1.28
——NO_2	4.29	4.37	1.58	4.28	2.01	1.03	4.44	1.53	1.59
——SH	2.00	2.44	1.31	2.46	1.57	1.02	3.16	1.34	1.43
——S—Alquilo	2.09	2.49	1.25	2.43	1.59	0.98	2.93	1.25	1.39
——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	1.07
——$COCH_3$	2.09	2.47	1.05	2.32	1.56	0.93	2.54	1.08	1.12
——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	1.23
——$COOCH_3$	2.01	2.28	1.12	2.22	1.65	0.98	2.48	1.15	1.16
——$CONH_2$	2.02	2.23	1.13	2.19	1.68	0.99	2.44	1.18	1.22
——CN	1.98	2.35	1.31	2.29	1.71	1.11	2.67	1.35	1.37

RMN ^{1}H

Estimación de los desplazamientos químicos de ^{1}H de grupos metileno $R_1CH_2R_2$

(δ en ppm respecto del TMS; véase H. M. Bell, L. K. Berry, E. A. Madigan, *Org. Magn. Reson.* 22, 693 [1984])

$$\delta_{CH_2R_1R_2} = 0.23 + z_{R_1} + z_{R_2}$$

	Sustituyente R	z_R
	-alquilo	véase H17
	-C≡C-	1.33
	-C≡CH	1.52
C	-C≡C-alquilo	1.52
	-C≡C-fenilo	1.77
	-fenilo	1.85
	-F	3.15
H	-Cl	2.48
A	-Br	2.29
L	-OH	2.46
	-O-alquilo	2.27
O	-O-fenilo	2.89
	-OCO-alquilo	2.98
	-OCO-fenilo	3.23
	$-NH_2$	1.69
	-NH-alquilo	1.60
	$-N(alquilo)_2$	1.41
	-NH-fenilo	2.15
N	-N(alquilo)fenilo	2.39
	$-NH_3^+$	2.31 para D_2O [a]
	$-NH_2^+$-alquilo	2.31
	$-NH^+(alquilo)_2$	2.46
	$-N^+(alquilo)_3$	2.56 para D_2O [b]
	-NHCO-alquilo	2.23
	-N(alquilo)CO-alquilo	2.23
	-NHCO-fenilo	2.33
	-SH	1.63
S	-S-alquilo	1.63
	-S-fenilo	1.92
	-CO-alquilo	1.58
	-CO-fenilo	2.08
O	-COOH	1.49
=	-COO-alquilo	1.49
C	-COO-fenilo	1.74
/	$-CONH_2$	1.39
\	-CON(alquilo)$_2$	1.39
	-CONH-fenilo	1.59
	-C≡N	1.73

[a] Para CD_3SOCD_3 o CD_3SOCD_3/$CDCl_3$ como disolventes, se deben emplear valores 0.2-0.3 ppm inferiores.

[b] Para $CDCl_3$ como disolvente, se deben emplear valores 0.3-0.5 ppm superiores.

Estimación de los desplazamientos químicos en alcanos polisustituidos

(δ en ppm respecto del TMS)

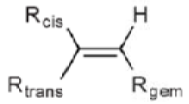
$$\delta_{CH_2R_1R_2} = 1.25 + \sum_1^2 z_i \qquad \delta_{CHR_1R_2R_3} = 1.50 + \sum_1^3 z_i$$

	Sustituyente	z_i
	-alquilo	0.0
C	-C≡C-	0.8
	-C≡C-	0.9
	-fenilo	1.3
H	-Cl	2.0
A	-Br	1.9
L	-I	1.4
	-OH	1.7
	-O-alquilo	1.5
O	-O-fenilo	2.3
	-OCO-alquilo	2.7
	-OCO-fenilo	2.9
	$-NH_2$	1.0
N	$-N(alquilo)_2$	1.0
	$-NO_2$	3.0
S	-S-alquilo	1.0
	-CHO	1.2
O	-CO-alquilo	1.2
=	-COOH	0.8
C	-COO-alquilo	0.7
/	-CN	1.2
\		

Ejemplo:

Valor básico:	1.5
-O-alquilo:	1.5
-COOH:	0.8
-fenilo:	1.3
Estimado:	5.1
Experimental:	4.8

Estimation of ^{1}H Chemical Shifts of Substituted Ethylenes (δ in ppm)



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

	Substituent R	Z_{gem}	Z_{cis}	Z_{trans}
	–H	0.00	0.00	0.00
C	–alkyl	0.45	-0.22	-0.28
	–alkyl ring[1]	0.69	-0.25	-0.28
	$-CH_2$–aromatic	1.05	-0.29	-0.32
	$-CH_2X$, 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
	$-CH_2O$–	0.64	-0.01	-0.02
	$-CH_2N<$	0.58	-0.10	-0.08
	$-CH_2CN$	0.69	-0.08	-0.06
	$-CH_2S$–	0.71	-0.13	-0.22
	$-CH_2CO$–	0.69	-0.08	-0.06
	–C=C<	1.00	-0.09	-0.23
	–C=C< conjugated[2]	1.24	0.02	-0.05
	–C≡C–	0.47	0.38	0.12
	–aromatic	1.38	0.36	-0.07
	–aromatic, fixed[3]	1.60	–	-0.05
	–aromatic, *o*-substituted	1.65	0.19	0.09
X	–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

	Substituent R	Z_{gem}	Z_{cis}	Z_{trans}
O	$-OC\lesssim (sp^3)$	1.22	-1.07	-1.21
	$-OC= (sp^2)$	1.21	-0.60	-1.00
	–OCO–	2.11	-0.35	-0.64
	$-OP(O)(OCH_2CH_3)_2$	1.33	-0.34	-0.66
N	$-NR_2$; R: H, $C\lesssim (sp^3)$	0.80	-1.26	-1.21
	–NR–; R: $C= (sp^2)$	1.17	-0.53	-0.99
	–NCO–R	2.08	-0.57	-0.72
	–N=N–phenyl	2.39	1.11	0.67
	$-NO_2$	1.87	1.30	0.62
	–C≡N	0.27	0.75	0.55
S	–S–	1.11	-0.29	-0.13
	–S(O)–	1.27	0.67	0.41
	$-S(O)_2$–	1.55	1.16	0.93
	–SCO–	1.41	0.06	0.02
	–SCN	0.94	0.45	0.41
	–SF	1.68	0.61	0.49
O ‖ C	–CHO	1.02	0.95	1.17
	–CO–	1.10	1.12	0.87
	–CO– conjugated[2]	1.06	0.91	0.74
	–COOH	0.97	1.41	0.71
	–COOH conjugated[2]	0.80	0.98	0.32
	–COOR	0.80	1.18	0.55
	–COOR conjugated[2]	0.78	1.01	0.46
	$-CON<$	1.37	0.98	0.46
	–COCl	1.11	1.46	1.01
	$-P(O)(OCH_2CH_3)_2$	0.66	0.88	0.67

1) The increment "alkyl ring" is to be used if the substituent and the double bond are part of a cyclic structure.
2) The increment "conjugated" is to be used if either the double bond or the substituent is conjugated to other substituents.
3) The increment "aromatic, fixed" is to be used if the double bond conjugated to an aromatic ring is part of a fused ring (such as in 1,2-dihydronaphthalene).

RMN ^{1}H

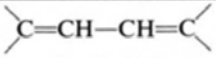
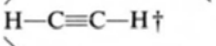
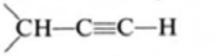
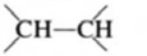
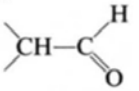
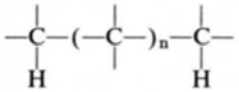
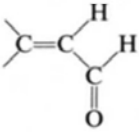
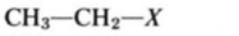
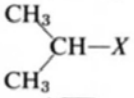
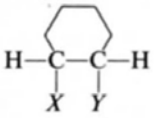
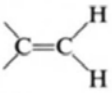
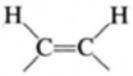
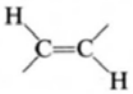
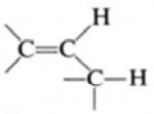
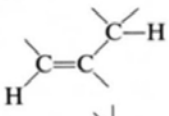
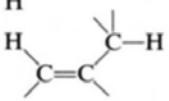
Effect of Substituents on ^{1}H Chemical Shifts of Monosubstituted Benzene (ppm)

$$\delta_{H_i} = 7.34 + Z_i$$

	Substituent R	Z_2	Z_3	Z_4
C	$-CH_3$	-0.17	-0.09	-0.17
	$-CH_2CH_3$	-0.14	-0.05	-0.18
	$-CH(CH_3)_2$	-0.13	-0.08	-0.18
	$-C(CH_3)_3$	0.05	-0.04	-0.18
	$-CF_3$	0.19	-0.07	0.00
	$-CCl_3$	0.55	-0.07	-0.09
	$-CH_2OH$	-0.07	-0.07	-0.07
	$-CH=CH_2$	0.08	-0.02	-0.09
	–CH=CH–phenyl (*trans*)	0.16	0.00	-0.15
	$-C\equiv CH$	0.16	-0.01	-0.01
	$-C\equiv C$–phenyl	0.20	-0.04	-0.07
	–phenyl	0.22	0.06	-0.04
	–2-pyridyl	0.73	0.09	0.02
X	–F	-0.31	-0.03	-0.21
	–Cl	-0.01	-0.06	-0.12
	–Br	0.15	-0.12	-0.06
	–I	0.36	-0.24	-0.02
O	–OH	-0.51	-0.10	-0.41
	$-OCH_3$	-0.44	-0.05	-0.40
	$-OCH_2CH=CH_2$	-0.45	-0.13	-0.43
	–O–phenyl	-0.33	-0.02	-0.25
	$-OCOCH_3$	-0.26	0.03	-0.12
	–OCO–phenyl	-0.12	0.10	-0.06
	$-OS(O)_2CH_3$	-0.05	0.07	-0.01
N	$-NH_2$	-0.67	-0.20	-0.59
	$-NHCH_3$	-0.73	-0.16	-0.64
	$-N(CH_3)_2$	-0.60	-0.10	-0.62
	–N(phenyl)$_2$	-0.26	-0.10	-0.34
	$-N^+(CH_3)_3\,I^-$	0.72	0.40	0.34
	–NHCHO (*trans* to O)	-0.25	0.03	-0.13
	–NHCHO (*cis* to O)	-0.20	0.21	-0.01
	$-N(CH_3)CHO$	-0.16	0.07	-0.05
	$-NHCOCH_3$	0.15	-0.02	-0.23
	$-NHCSNH_2$	0.14	0.07	-0.14
	$-NHNH_2$	-0.60	-0.08	-0.55
	–N=N–phenyl	0.67	0.20	0.20
	–NO	0.55	0.29	0.35
	$-NO_2$	0.93	0.26	0.39
	$-C\equiv N$	0.32	0.14	0.28
	–NCS	-0.11	0.04	-0.02
S	–SH	-0.08	-0.16	-0.22
	$-SCH_3$	-0.08	-0.10	-0.24
	–S–phenyl	-0.06	-0.20	-0.26
	–S–S–phenyl	0.13	-0.05	-0.10
	$-S(O)-CH=CH_2$	0.28	0.15	0.15
	–S(O)–phenyl	0.29	0.09	0.13
	$-S(O)_2CH_3$	0.70	0.37	0.41
	$-S(O)_2OCH_3$	0.60	0.26	0.28
	$-S(O)_2Cl$	0.68	0.27	0.37
	$-S(O)_2NH_2$	0.51	0.28	0.24
O ‖ C	–CHO	0.54	0.19	0.29
	$-COCH_3$	0.62	0.12	0.22
	$-COCH_2CH_3$	0.61	0.11	0.21
	–CO–phenyl	0.56	0.12	0.23
	–CO–(2-pyridyl)	0.86	0.11	0.20
	–COOH	0.79	0.14	0.28
	$-COOCH_3$	0.70	0.09	0.21
	$-COOCH(CH_3)_2$	0.73	0.11	0.20
	–COO–phenyl	0.87	0.18	0.30
	$-CONH_2$	0.48	0.11	0.19
	–COF	0.71	0.21	0.38
	–COCl	0.77	0.15	0.35
	–COBr	0.70	0.15	0.32
	–CH=N–phenyl	0.64	0.24	0.24

RMN ^{1}H

SPIN-SPIN COUPLING CONSTANTS

Type	J, cps	Type	J, cps
H_2†	280		9–13
CH_4†	12.4		9.1
	12–15		2–3
	2–9		1–3
	~0		6–8
	6.5–7.5		
	5.5–7.0		*o*– 6–9 *m*– 1–3 *p*– 0–1
	a,a 5–10 a,e 2–4 e,e 2–4		$\alpha\beta$ 1.6–2.0 $\alpha\beta'$ 0.6–1.0 $\alpha\alpha'$ 1.3–1.8 $\beta\beta'$ 3.2–3.8
	0.5–3		
	7–12		$\alpha\beta$ 2.0–2.6 $\alpha\beta'$ 1.5–2.2 $\alpha\alpha'$ 1.8–2.3 $\beta\beta'$ 2.8–4.0
	13–18		
	4–10		$\alpha\beta$ 4.6–5.8 $\alpha\beta'$ 1.0–1.8 $\alpha\alpha'$ 2.1–3.3 $\beta\beta'$ 3.0–4.2
	0.5–2.5		$\alpha\beta$ 4.9–5.7 $\alpha\gamma$ 1.6–2.6 $\alpha\beta'$ 0.7–1.1 $\alpha\alpha'$ 0.2–0.5 $\beta\gamma$ 7.2–8.5 $\beta\beta'$ 1.4–1.9
	~0		

† The coupling constant for these molecules, which contain only equivalent protons, has been determined from the spectra of the partially deuterated substances.

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