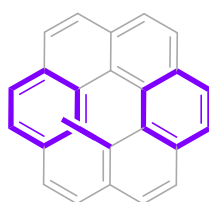


Química Orgánica

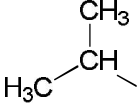
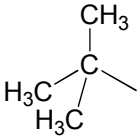
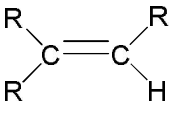
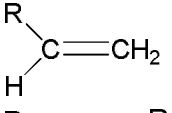
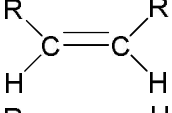
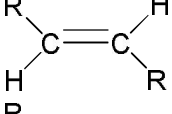
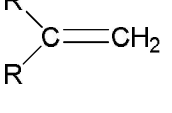
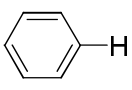
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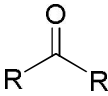
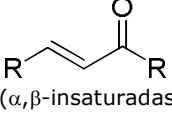
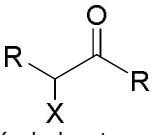
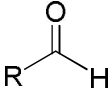
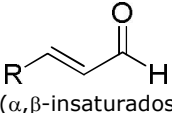
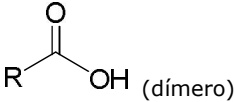
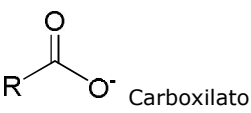
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Espectroscopía*

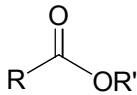
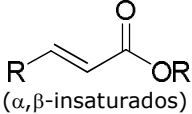
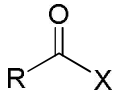
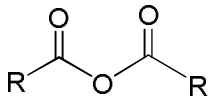
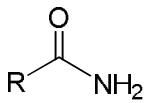
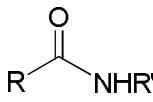
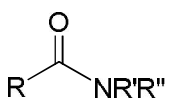


Cátedra de Química Orgánica

Tablas de IR

Compuesto	Grupo Funcional	Banda (cm ⁻¹)	Asignación
Alcanos	-CH ₃ , -CH ₂ , -CH	2880-2975	ν C-H
	-CH ₃	1435-1470 1370-1385	δ C-H asim δ C-H sim
		1380-1385 1365-1370	δ C-H sim
		1385-1395 1365	δ C-H sim
	(CH ₂) _n (n ≥ 4)	720-750	δ C-H en el plano
Olefinas	C=C-H	3010-3095	ν =C-H
	C=C (no conjugada)	1650	ν C=C
	C=C (conjugada)	1600	ν C=C
		820 ± 30	δ =C-H fuera del plano
		990 ± 5	δ =C-H fuera del plano
		700 ± 30	δ =C-H fuera del plano
	970 ± 10	δ =C-H fuera del plano	
	890 ± 5	δ =C-H fuera del plano	
Alquinos	C≡C-H	3300-3310	ν C≡C-H
	C≡C	2100-220 (d)	ν C≡C
Aromáticos		3030-3080 1600(1580) y 1500 (1450)	ν =C-H ν C=C
	Monosustituídos	690-710 (f) 730-770 (f)	δ =C-H fuera del plano δ =C-H fuera del plano
	<i>o</i> -Disustituídos	735-770 (f) 680-725 (m)	δ =C-H fuera del plano
	<i>m</i> -Disustituídos	750-810 (f) 860-900 (m)	δ =C-H fuera del plano
	<i>p</i> -Disustituídos	800-860 (f)	δ =C-H fuera del plano

Compuesto	Grupo Funcional	Banda (cm ⁻¹)	Asignación
Alcoholes y Fenoles	O-H (libre)	3580-3670 (aguda)	v O-H
	O-H (asociación intramolecular)	3400-3600 (aguda)	v O-H
	O-H (asociación intermolecular - Dímeros)	3400-3500 (aguda)	v O-H
	O-H (asociación intermolecular - Polímeros)	3200-3400 (ancha)	v O-H
	R-OH (primarios)	1050	v C-O
	R-OH (secundarios)	1100	v C-O
	R-OH (terciarios)	1150	v C-O
	=C-OH (fenoles)	1180	v C-O
	RO-H y =CO-H (fenoles)	1200-1400	δ O-H
Eteres	C-O-C (alifáticos)	1070-1150	v C-O asim.
	=C-O-C (aromáticos y no saturados)	1200-1270	v C-O asim.
		1020-1070	v C-O sim.
Cetonas		1715	v C=O
	 (α,β-insaturadas)	1685	v C=O
	 (α-halocetonas)	1730	v C=O
	Cíclicas		
	4 miembros	1770	v C=O
	5 miembros	1750	v C=O
	6 miembros	1715	v C=O
Aldehídos		2720 y 2820	v =C-H
		1725	v C=O
	 (α,β-insaturados)	1690	v C=O
Acidos		2500-3000	v O-H
		1710 (<i>f</i>)	v C=O
		930 (<i>m</i>)	δ O-H fuera del plano
	Asociación Intramolecular	1670	v C=O
	 Carboxilato	1550-1610 (dos bandas)	v C=O sim. y asim.

Compuesto	Grupo Funcional	Banda (cm ⁻¹)	Asignación
Esteres		1735	v C=O
	 (α,β -insaturados)	1720	v C=O
	Todos	1050 y 1300 (dos bandas)	v C-O sim. y asim.
Halogenuros de ácido		1800	v C=O
Anhídridos		1820 y 1760 (dos bandas)	v C=O
		1050-1300 (1 o 2 bandas f)	v C-O
Amidas		3500 y 3400 (dos bandas) Amida Libre	v N-H
		3050-3200 Asociada	
		1690 libre	v C=O (Banda Amida I)
		1650 asociada	
		1600 libre	δ N-H (Banda Amida II)
		1640 asociada	
	1400 libre	v C-N (Banda Amida III)	
	1420 asociada		
		3440 libre	v N-H
	3300 asociada		
	1680 libre	v C=O (Banda Amida I)	
	1655 asociada		
	1530 libre	δ N-H (Banda Amida II)	
	1550 asociada		
	1260 libre	v C-N (Banda Amida III)	
	1300 asociada		
		1650	v C=O (Banda Amida I)
Aminas	R-NH ₂ ; =C-NH ₂	3300 y 3500 (f) (dos bandas)	v N-H
		1580-1650 (m-f)	δ N-H
	R-NH ₂ (fase líquida)	800-900 (banda ancha)	δ N-H fuera del plano

Compuesto	Grupo Funcional	Banda (cm ⁻¹)	Asignación
Aminas (cont)	RR'NH	3300-3500 (<i>d</i>) (una banda)	ν N-H
	Asociadas	3100-3400 (<i>m</i>) 1550-1650 (<i>δ</i>)	ν N-H δ N-H
	Todas	1000-1200	ν C-N
Nitrilos	-C≡N	2240-2260 (<i>d-m</i>)	ν C≡N
	-C=N-C≡N	2215-2235 (<i>f</i>)	ν C≡N
		2220-2240 (<i>m-f</i>)	ν C≡N
Nitrocompuestos	R-NO ₂	1560 (<i>f</i>)	ν NO (asim)
		1380 (<i>f</i>)	ν NO (sim)
	Ar-NO ₂	1530	ν NO (asim)
		1340	ν NO (sim)
		870 610	ν C-N δ C-N-O

Tablas de RMN-¹H

Tabla 1


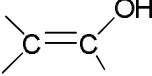
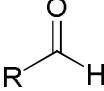
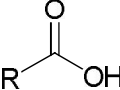
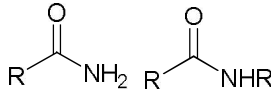
Tipos de Compuesto	Grupo Funcional	δ (ppm)
Ciclopropanos		0.2
Vinílicos	-C=C-H	4.6-5.9
Acetilénicos	-C≡C-H	2.0-3.0
Aromáticos	Ar-H	6.0-8.5
Alcoholes	RO-H	1.0-5.5
Fenoles	ArO-H	4-12
Enoles		15-17
Aldehídos		9-10
Acidos		10.5-12.0
Aminas	RNH ₂	1-5
Amidas		5-9.5

Tabla 2

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

	X	CH ₃ -X	-CH ₂ -X	-CH-X
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
	-C≡CH	1.80	2.10-2.16	2.59
	-Ph	2.35	2.59-2.63	2.89
Halog.	-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-R	3.24	3.27-3.37	3.55
	-O-C=C	3.50	3.37	-
	-O-Ph	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-COPh	3.88	4.25-4.37	5.22
-O-SO ₂ -Ph	3.70	3.94-4.07	4.70	
N	-NH ₂	2.47	2.61-2.74	3.07
	-NR ₂	2.19	2.50	2.88
	-NRPh	2.91	-	-
	-NRCHO	2.88 y 2.97	-	4.12
	-N ⁺ R ₃	3.33	3.40	3.50
	-NHCOCH ₃	2.17	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-R	2.09	2.43-2.49	2.93
	-S-S-R	2.30	2.63-2.67	-
	-SO ₂ R	2.80-3.00	2.94	-
	-SOCH ₃	2.50	-	-
	-SCN	2.61	2.98	3.48
C=O	-CHO	2.20	2.42-2.46	2.39
	-COCH ₃	2.09	2.32-2.47	2.54
	-COPh	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	-C=NOH	1.90	-	-
	-C≡N	1.98	2.29-2.35	2.67

Tabla 3

Desplazamientos químicos (δ) de los protones de metilos, metilenos y metinos de alcanos monosustituídos con sustituyentes **X** en la posición β o γ .

$$\delta \text{CH}_3 = 0.90 + \text{desplazamiento}$$

$$\delta \text{CH}_2 = 1.25 + \text{desplazamiento}$$

$$\delta \text{CH} = 1.50 + \text{desplazamiento}$$

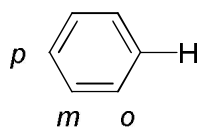
	X	CH ₃ -C-X	-CH ₂ -C-X	-CH-C-X	CH ₃ -C-C-X
C	-CH=CH ₂	0.10-0.12	0.05	-	-
	-C≡CH	0.25-0.32	0.25	-	0.07
	-Ph	0.31-0.42	0.40	-	0.05
Halog.	-F	0.34-0.44	0.17	-	-
	-Cl	0.43-0.70	0.56	0.02	0.16
	-Br	0.76-0.86	0.64	0.24	0.16
	-I	0.98-1.05	0.63	0.43	0.13
O	-OH	0.26-0.32	0.28	-	0.03
	-O-R	0.18-0.34	0.30	-	0.03
	-O-C=C	0.40	-	-	-
	-O-Ph	0.41-0.48	0.45	-	0.15
	-O-COCH ₃	0.31-0.55	0.31	-	0.07
	-O-COPh	0.47-0.68	0.51	-	0.17
	-O-SO ₂ -Ph	0.35-0.40	0.35	-	0.05
N	-NH ₂	0.13-0.25	0.18	-	0.03
	-NRCHO	0.20-0.28	-	-	-
	-N ⁺ R 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-R	0.35-0.49	0.34	-	0.08
	-S-S-R	0.42-0.45	0.46	-	0.13
	-SO _{2R}	0.57	-	-	-
	-SCN	0.62	-	-	-
C=O	-CHO	0.17-0.23	0.42	-	0.07
	-COCH ₃	0.15-0.22	0.31	-	0.03
	-COPh	0.28-0.32	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
C-N	-C≡N	0.41-0.47	0.46	-	0.11

Tabla 4: Valores de δ para metilenos disustituídos (**X-CH₂-Y**)

Sust	Br-	Cl-	I-	R ₂ N-	HO-	RO-	PhO-	RCOO-	RS-	CH ₃ -	C=C-	C≡C	Ph-	F ₃ C-	CN-	RCO-	ROOC-	R ₂ NOC-
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 ₂ N-	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	4.43	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
									CH ₃ -	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 ₃ C-	2.51	3.07	3.07	2.92	2.96
														CN-	3.63	3.63	3.48	3.52
															RCO-	3.63	3.48	3.52
																ROOC-	3.33	3.37
																	R ₂ NOC-	3.41

Tabla 5

Influencia del sustituyente sobre el desplazamiento químico de los protones de un anillo aromático.

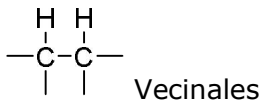

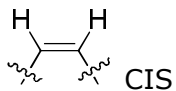
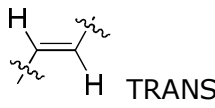
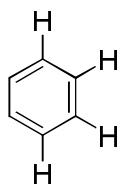


	Sustituyente	Z_o	Z_m	Z_p
C	-H	0	0	0
	-CH ₃	-0.20	-0.12	-0.22
	-CH ₂ CH ₃	-0.14	-0.06	-0.17
	-CH(CH ₃) ₂	-0.13	-0.08	-0.18
	-C(CH ₃) ₃	0.02	-0.08	-0.21
	-CH ₂ Cl	0	0	0
	-CF ₃	0.32	0.14	0.20
	-CCl ₃	0.64	0.13	0.10
	-CH ₂ OH	-0.07	-0.07	-0.07
	-CH=CH ₂	0.06	-0.03	-0.10
	-CH=CHPh	0.15	-0.01	-0.16
	-C≡CH	0.15	-0.02	-0.01
	-C≡CPh	0.19	0.02	0
	-Ph	0.37	0.20	0.10
	Hal.	-F	-0.26	0
-Cl		0.03	-0.02	-0.09
-Br		0.18	-0.08	-0.04
-I		0.39	-0.21	0
O	-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
	-OPh	-0.29	-0.05	-0.23
	-OCOCH ₃	-0.25	0.03	-0.13
	-OCOPh	-0.09	0.09	-0.08
	-OSO ₂ CH ₃	-0.05	0.07	-0.01
N	-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
	-NHPh	-0.30	-0.06	-0.43
	-N ⁺ (CH ₃) ₃	0.69	0.36	0.31
	-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=NPh	0.67	0.20	0.20
	-NO ₂	0.95	0.26	0.38

	Sustituyente	Z_o	Z_m	Z_p
S	-SH	-0.08	-0.16	-0.22
	-SCH ₃	-0.08	-0.10	-0.24
	-SPh	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
C=O	-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
	-COPh	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
	-COOPh	0.09	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
Var.	-CH=NPh	≈ 0.6	≈ 0.2	≈ 0.2
	-C≡N	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 6

Constantes de Acoplamiento H-H.

Estructura	Rango de $J_{H,H}$ en Hz
 Vecinales	0-9
 Geminales	1 - 3.5
 CIS	6 - 14
 TRANS	11 - 18
	ORTO 7 - 10 META 2 - 3 PARA ~1