

## ANEXO TABLAS

Tomadas de: ORGANIC STRUCTURES FROM SPECTRA L D Field, S Sternhell, J R Kalman. Fourth Edition. 2008. John Wiley & Sons Ltd.

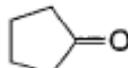
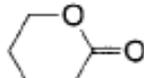
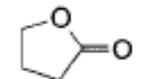
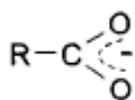
Tabla 1-Bandas típicas de estiramiento **-O-H**

-O-H no puenteado (libre)	3600 cm <sup>-1</sup>
-O-H en puente de hidrógeno	3100 - 3200 cm <sup>-1</sup>

Tabla 2- Frecuencias de absorción al IR de diversos grupos funcionales

Functional group	Structure	$\bar{\nu}$ (cm <sup>-1</sup> )	Intensity
Amine		3300 - 3500	
Terminal acetylenes		3300	strong
Imines		1480 - 1690	
Enol ethers		1600 - 1660	strong
Alkenes		1640 - 1680	weak to medium
Nitro groups		1500 - 1650	strong
		1250 - 1400	medium
Sulfoxides		1010 - 1070	strong
Sulfones		1300 - 1350	strong
		1100 - 1150	strong
Sulfonamides and Sulfonate esters		1140 - 1180	strong
		1300 - 1370	strong
Alcohols		1000 - 1260	strong
Ethers		1085 - 1150	strong
Alkyl fluorides		1000 - 1400	strong
Alkyl chlorides		580 - 780	strong
Alkyl bromides		560 - 800	strong
Alkyl iodides		500 - 600	strong

Tabla 3: Frecuencias de absorción al IR de grupos carbonilos

Carbonyl group	Structure	$\bar{\nu}$ (cm <sup>-1</sup> )
Ketones	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}'$	1700 - 1725
Aldehydes	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$	1720 - 1740
Aryl aldehydes or ketones, $\alpha$ , $\beta$ -unsaturated aldehydes or ketones	$\text{Ar}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}'$ $\text{R}-\text{CH}=\text{CH}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}'$ $\text{R}' = \text{alkyl, aryl, or H}$	1660 - 1715
Cyclopentanones		1740 - 1750
Cyclobutanones		1760 - 1780
Carboxylic acids	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	1700 - 1725
$\alpha$ , $\beta$ -unsaturated and aryl carboxylic acids	$\text{Ar}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$ $\text{R}-\text{CH}=\text{CH}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	1680 - 1715
Esters <sup>§</sup>	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OR}'$	1735 - 1750
Phenolic Esters <sup>§</sup>	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OAr}$	1760 - 1800
Aryl or $\alpha$ , $\beta$ -unsaturated Esters <sup>§</sup>	$\text{R}-\text{CH}=\text{CH}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OR}'$ $\text{Ar}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OR}'$	1715 - 1730
$\delta$ -Lactones <sup>§</sup>		1735 - 1750
$\gamma$ -Lactones <sup>§</sup>		1760 - 1780
Amides	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{NR}'\text{R}''$	1630 - 1690
Acid chlorides	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{Cl}$	1785 - 1815
Acid anhydrides (two bands)	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}$	1740 - 1850
Carboxylates		1550 - 1610 1300 - 1450

Esters and lactones also exhibit a strong C-O stretch in the range 1160 - 1250 cm<sup>-1</sup>

Tabla 4: Masas exactas de isótopos

seleccionados

Isótopo	Abundancia	Masa
$^1\text{H}$	99.98	1.00783
$^{12}\text{C}$	98.9	12.0000
$^{13}\text{C}$	1.1	13.00336
$^{14}\text{N}$	99.6	14.0031
$^{16}\text{O}$	99.8	15.9949
$^{19}\text{F}$	100.0	18.99840
$^{31}\text{P}$	100.0	30.97376
$^{32}\text{S}$	95.0	31.9721
$^{33}\text{S}$	0.75	32.9715
$^{34}\text{S}$	4.2	33.9679
$^{35}\text{Cl}$	75.8	34.9689
$^{37}\text{Cl}$	24.2	36.9659
$^{79}\text{Br}$	50.7	78.9183
$^{81}\text{Br}$	49.3	80.9163

Tabla 5: Masas de fragmentos comunes

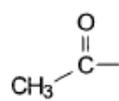
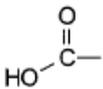
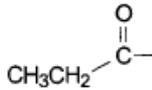
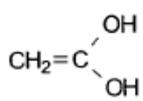
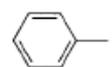
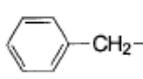
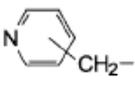
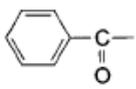
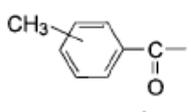
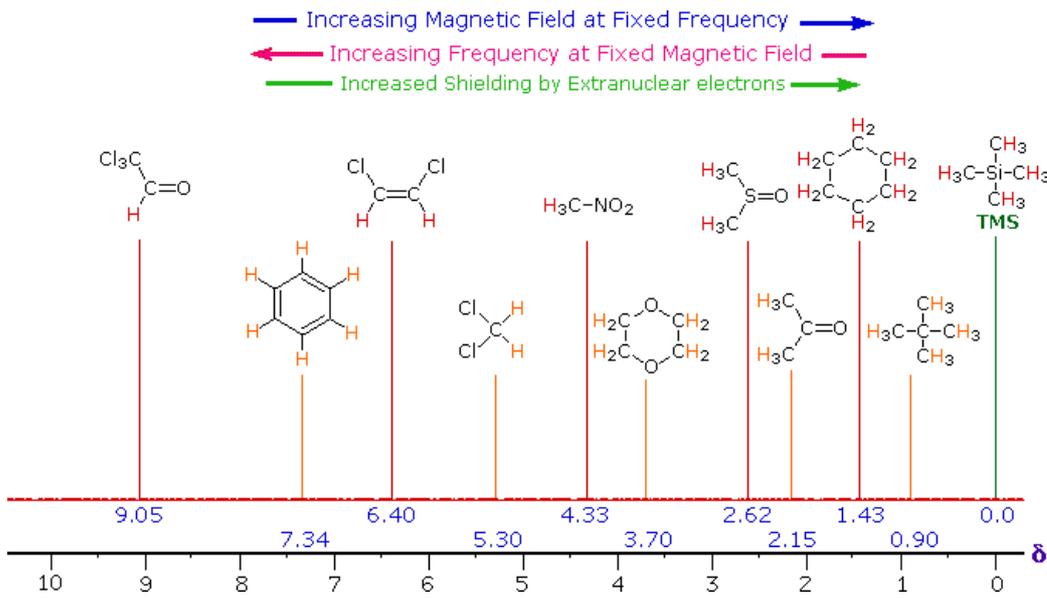
$\text{CH}_3^-$	15	$\text{CH}_3\text{CH}_2^-$	29		29
$\text{NO}$	30	$-\text{CH}_2\text{OH}$	31	$\text{CH}_2=\text{CH}-\text{CH}_2$	41
	43		45	$-\text{NO}_2$	46
$\text{C}_4\text{H}_7$	55	$\text{C}_4\text{H}_9$	57		57
	60	$\text{C}_5\text{H}_5$	65		77
	91		92		105
	119	$\text{I}-$	127		

Tabla 6:  
Despl

azamientos típicos en  $^1\text{H}$ -RMN (en ppm)



Group	$\delta$ $^1\text{H}$ (ppm from TMS)
Tetramethylsilane $(\text{CH}_3)_4\text{Si}$	0
Methyl groups attached to $sp^3$ hybridised carbon atoms	0.8 - 1.2
Methylene groups attached to $sp^3$ hybridised carbon atoms	1.0 - 1.5
Methine groups attached to $sp^3$ hybridised carbon atoms	1.2 - 1.8
Acetylenic protons	2 - 3.5
Olefinic protons	5 - 8
Aromatic and heterocyclic protons	6 - 9
Aldehydic protons	9 - 10

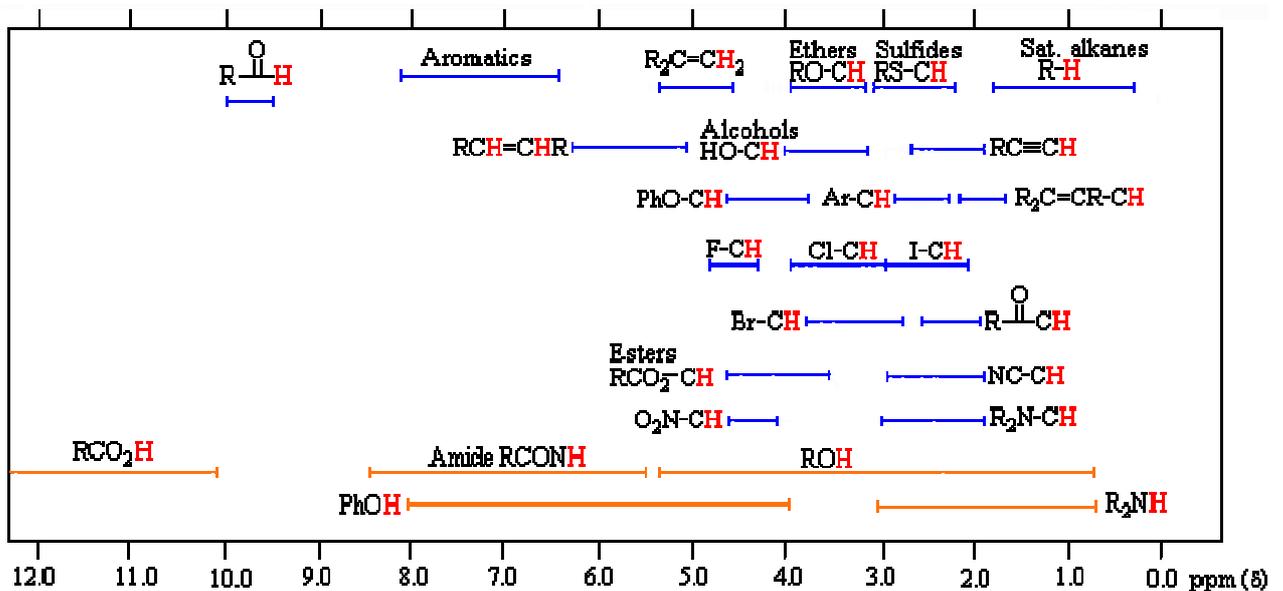


Tabla 7: Desplazamientos típicos en  $^1\text{H}$ -RMN (en ppm) de protones de grupos alquílicos

X	CH <sub>3</sub> —X	CH <sub>3</sub> CH <sub>2</sub> —X		(CH <sub>3</sub> ) <sub>2</sub> CH—X	
	—CH <sub>3</sub>	—CH <sub>3</sub>	—CH <sub>2</sub> —	—CH <sub>3</sub>	>CH—
—H	0.23	0.86	0.86	0.91	1.33
—CH=CH <sub>2</sub>	1.71	1.00	2.00	1.00	1.73
—Ph	2.35	1.21	2.63	1.25	2.89
—Cl	3.06	1.33	3.47	1.55	4.14
—Br	2.69	1.66	3.37	1.73	4.21
—I	2.16	1.88	3.16	1.89	4.24
—OH	3.39	1.18	3.59	1.16	3.94
—OCH <sub>3</sub>	3.24	1.15	3.37	1.08	3.55
—O—Ph	3.73	1.38	3.98	1.31	4.51
—OCO—CH <sub>3</sub>	3.67	1.21	4.05	1.22	4.94
—OCO—Ph	3.89	1.38	4.37	1.36	5.30
—CO—CH <sub>3</sub>	2.09	1.05	2.47	1.08	2.54
—CO—Ph	2.55	1.18	2.92	1.22	3.58
—CO—OCH <sub>3</sub>	2.01	1.12	2.28	1.15	2.48
—NH <sub>2</sub>	2.47	1.10	2.74	1.03	3.07
—NH—COCH <sub>3</sub>	2.71	1.12	3.21	1.13	4.01
—C≡N	1.98	1.31	2.35	1.35	2.67
—NO <sub>2</sub>	4.29	1.58	4.37	1.53	4.44

Tabla 8: Desplazamientos típicos en  $^1\text{H}$ -RMN (en ppm) de protones olefinicos



X	$\sigma_{\text{gem}}$	$\sigma_{\text{cis}}$	$\sigma_{\text{trans}}$
—H	0.0	0.0	0.0
—alkyl	0.45	-0.22	-0.28
—aryl	1.38	0.36	-0.07
—CH=CH <sub>2</sub>	1.00	-0.09	-0.23
—CH=CH—conjugated	1.24	0.02	-0.05
—C≡C—H	0.47	0.38	0.12
—CO—R	1.10	1.12	0.87
—CO—OH	0.80	0.98	0.32
—CO—OR	0.78	1.01	0.46
—C≡N	0.27	0.75	0.55
—Cl	1.08	0.18	0.13
—Br	1.07	0.45	0.55
—OR	1.22	-1.07	-1.21
—NR <sub>2</sub>	0.80	-1.26	-1.21

Tabla 9: Desplazamientos típicos en  $^1\text{H}$ -RMN (en ppm) de protones aromáticos en derivados de benceno en relación a benceno:  $\delta$  7,26 ppm (el signo positivo corresponde a desplazamientos a campos bajos y negativo a campos altos)

X	<i>ortho</i>	<i>meta</i>	<i>para</i>
—H	0.0	0.0	0.0
—CH <sub>3</sub>	-0.20	-0.12	-0.22
—C(CH <sub>3</sub> ) <sub>3</sub>	-0.03	-0.08	0.20
—CH=CH <sub>2</sub>	0.06	-0.03	-0.10
—C≡C—H	0.16	-0.04	-0.02
—CO—OR	0.71	0.11	0.21
—CO—R	0.62	0.14	0.21
—OCO—R	-0.25	0.03	-0.13
—OCH <sub>3</sub>	-0.48	-0.09	-0.44
—OH	-0.56	-0.12	-0.45
—Cl	0.03	-0.02	-0.09
—Br	0.18	-0.08	-0.04
—C≡N	0.36	0.18	0.28
—NO <sub>2</sub>	0.95	0.26	0.38
—NR <sub>2</sub>	-0.66	-0.18	-0.67
—NH <sub>2</sub>	-0.75	-0.25	-0.65

Tabla 10: Desplazamientos típicos en  $^1\text{H}$ -RMN (en ppm) de protones aromáticos en derivados aromáticos polinucleares y heterocíclicos

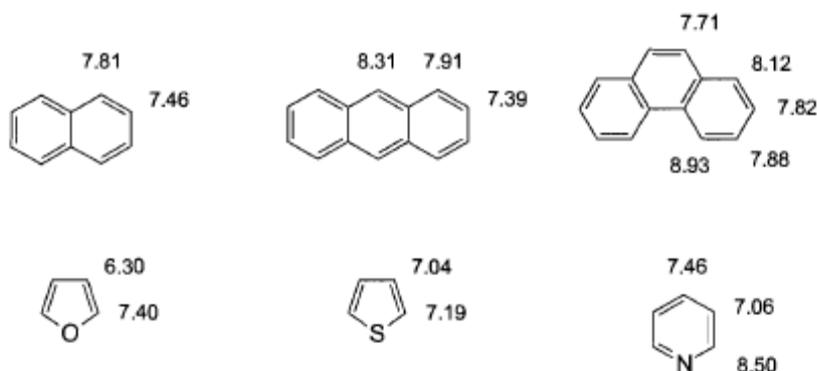
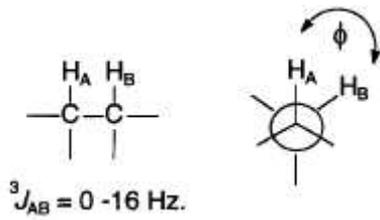
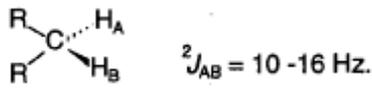


Tabla 11: Constantes de acoplamiento  $^1\text{H}$ - $^1\text{H}$  (en Hz)



$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	${}^3J_{\text{HH}} = 7.2$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	${}^3J_{\text{HH}} = 7.2$
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	${}^4J_{\text{HH}} = 0.3$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	${}^4J_{\text{HH}} = 0.3$
$\text{H}_2\text{C}=\text{C}=\text{C}=\text{CH}_2$	${}^5J_{\text{HH}} = 7$	$\text{H}_2\text{C}=\text{C}=\text{C}=\text{CH}_2$	${}^5J_{\text{HH}} = 7$
$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$	${}^5J_{\text{HH}} = 1.3$	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$	${}^5J_{\text{HH}} = 1.3$
	${}^4J_{\text{HH}} = 1.5$		${}^4J_{\text{HH}} = 1.5$

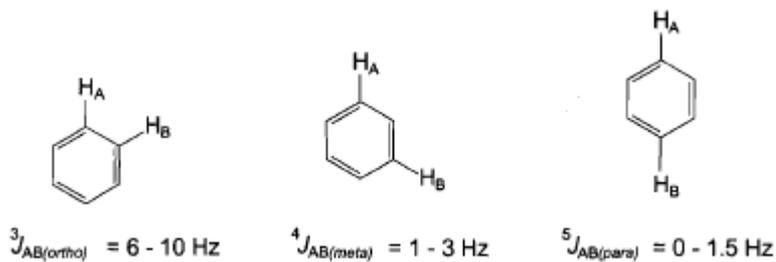
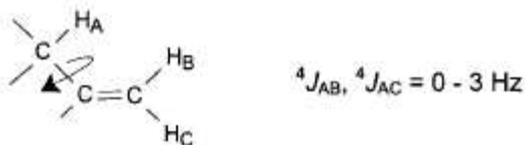
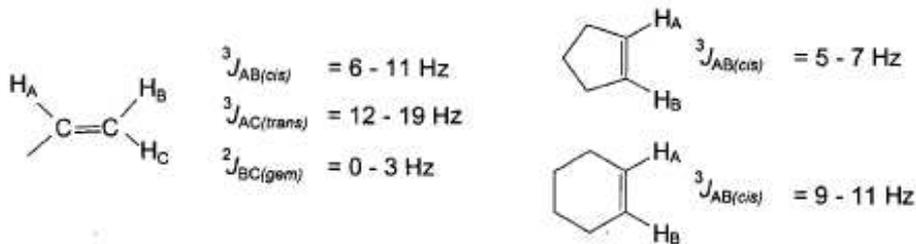


Tabla 12: Desplazamientos típicos en  $^{13}\text{C}$ -RMN (en ppm)

Group	$^{13}\text{C}$ shift (ppm)
TMS	0.0
$-\text{CH}_3$ (with only $-\text{H}$ or $-\text{R}$ at $\text{C}_\alpha$ and $\text{C}_\beta$ )	0 - 30
$-\text{CH}_2$ (with only $-\text{H}$ or $-\text{R}$ at $\text{C}_\alpha$ and $\text{C}_\beta$ )	20 - 45
$-\text{CH}$ (with only $-\text{H}$ or $-\text{R}$ at $\text{C}_\alpha$ and $\text{C}_\beta$ )	30 - 60
C quaternary (with only $-\text{H}$ or $-\text{R}$ at $\text{C}_\alpha$ and $\text{C}_\beta$ )	30 - 50
$\text{O}-\text{CH}_3$	50 - 60
$\text{N}-\text{CH}_3$	15 - 45
$\text{C}=\text{C}$	70 - 95
$\text{C}=\text{C}$	105 - 145
C (aromatic)	110 - 155
C (heteroaromatic)	105 - 165
$-\text{C}\equiv\text{N}$	115 - 125
$\text{C}=\text{O}$ (acids, acyl halides, esters, amides)	155 - 185
$\text{C}=\text{O}$ (aldehydes, ketones)	185 - 225

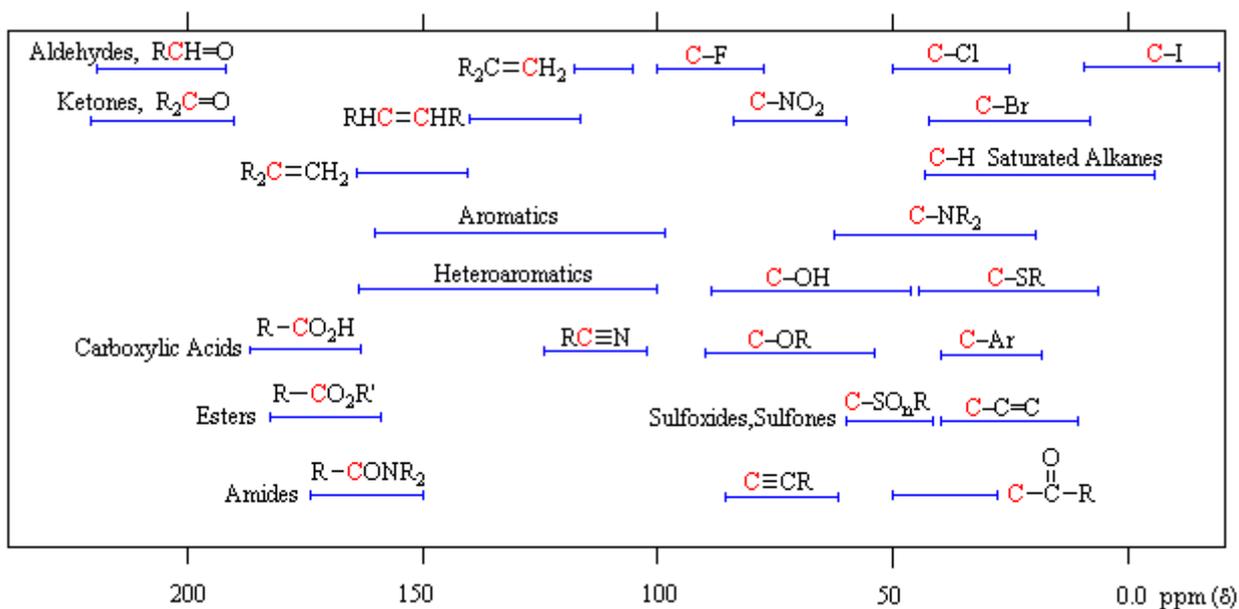


Tabla 13: Desplazamientos típicos en  $^{13}\text{C}$ -RMN para carbonos  $sp^3$  en alquil derivados (en ppm)

X	CH <sub>3</sub> -X	CH <sub>3</sub> CH <sub>2</sub> -X		(CH <sub>3</sub> ) <sub>2</sub> CH-X	
	-CH <sub>3</sub>	-CH <sub>3</sub>	-CH <sub>2</sub> -	-CH <sub>3</sub>	>CH-
-H	-2.3	7.3	7.3	15.4	15.9
-CH=CH <sub>2</sub>	18.7	13.4	27.4	22.1	32.3
-Ph	21.4	15.8	29.1	24.0	34.3
-Cl	25.6	18.9	39.9	27.3	53.7
-OH	50.2	18.2	57.8	25.3	64.0
-OCH <sub>3</sub>	60.9	14.7	67.7	21.4	72.6
-OCO-CH <sub>3</sub>	51.5	14.4	60.4	21.9	67.5
-CO-CH <sub>3</sub>	30.7	7.0	35.2	18.2	41.6
-CO-OCH <sub>3</sub>	20.6	9.2	27.2	19.1	34.1
-NH <sub>2</sub>	28.3	19.0	36.9	26.5	43.0
-NH-COCH <sub>3</sub>	26.1	14.6	34.1	22.3	40.5
-C≡N	1.7	10.6	10.8	19.9	19.8
-NO <sub>2</sub>	61.2	12.3	70.8	20.8	78.8

Tabla 14: Desplazamientos típicos en  $^{13}\text{C}$ -RMN para carbonos  $sp^2$  en vinil derivados CH<sub>2</sub>=CH-X (en ppm)

X	CH <sub>2</sub> =	=CH-X
-H	123.3	123.3
-CH <sub>3</sub>	115.9	136.2
-C(CH <sub>3</sub> ) <sub>3</sub>	108.9	149.8
-Ph	112.3	135.8
-CH=CH <sub>2</sub>	116.3	136.9
-C≡C-H	129.2	117.3
-CO-CH <sub>3</sub>	128.0	137.1
-CO-OCH <sub>3</sub>	130.3	129.6
-Cl	117.2	126.1
-OCH <sub>3</sub>	84.4	152.7
-OCO-CH <sub>3</sub>	96.6	141.7
-C≡N	137.5	108.2
-NO <sub>2</sub>	122.4	145.6
-N(CH <sub>3</sub> ) <sub>2</sub>	91.3	151.3

Tabla 15: Desplazamientos típicos en  $^{13}\text{C}$ -RMN (en ppm) de carbonos en derivados de benceno en relación a benceno:  $\delta$  128,5 ppm (el signo positivo corresponde a desplazamientos a campos bajos y negativo a campos altos)

X	<i>ipso</i>	<i>ortho</i>	<i>meta</i>	<i>para</i>
—H	0.0	0.0	0.0	0.0
—NO <sub>2</sub>	19.9	-4.9	0.9	6.1
—CO—OCH <sub>3</sub>	2.0	1.2	-0.1	4.3
—CO—NH <sub>2</sub>	5.0	-1.2	0.1	3.4
—CO—CH <sub>3</sub>	8.9	0.1	-0.1	4.4
—C≡N	-16.0	3.5	0.7	4.3
—Br	-5.4	3.3	2.2	-1.0
—CH=CH <sub>2</sub>	8.9	-2.3	-0.1	-0.8
—Cl	5.3	0.4	1.4	-1.9
—CH <sub>3</sub>	9.2	0.7	-0.1	-3.0
—OCO—CH <sub>3</sub>	22.4	-7.1	0.4	-3.2
—OCH <sub>3</sub>	33.5	-14.4	1.0	-7.7
—NH <sub>2</sub>	18.2	-13.4	0.8	-10.0

Tabla 6: Desplazamientos típicos en  $^{13}\text{C}$ -RMN (en ppm) de carbonos aromáticos en derivados aromáticos polinucleares y heterocíclicos

