

TABELLA 4.4 Parametri empirici di spostamento chimico ^{13}C per alcuni idrocarburi lineari e ramificati.

Atomi ^{13}C	Spostamento (ppm) (A)
α	9.1
β	9.4
γ	-2.5
δ	0.3
ε	0.1
$1^\circ(3^\circ)^a$	-1.1
$1^\circ(4^\circ)^a$	-3.4
$2^\circ(3^\circ)^a$	-2.5
$2^\circ(4^\circ)$	-7.2
$3^\circ(2^\circ)$	-3.7
$3^\circ(3^\circ)$	-9.5
$4^\circ(1^\circ)$	-1.5
$4^\circ(2^\circ)$	-8.4

^a Le notazioni $1^\circ(3^\circ)$ e $1^\circ(4^\circ)$ si riferiscono a un gruppo CH_3 legato rispettivamente a un gruppo R_2CH e a un gruppo R_3C . La notazione $2^\circ(3^\circ)$ si riferisce a un gruppo RCH_2 legato a un gruppo R_2CH , e così via.

$$\delta = -2.5 + \sum nA$$

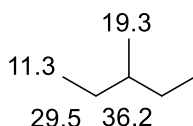


TABELLA 4.5 Spostamenti chimici ^{13}C per alcuni alcani lineari e ramificati (ppm relativi a TMS).

Composto	C-1	C-2	C-3	C-4	C-5
Metano	-2.5				
Etano	5.7				
Propano	15.8	16.3			
Butano	13.4	25.2			
Pentano	13.9	22.8	34.7		
Esano	14.1	23.1	32.2		
Eptano	14.1	23.2	32.6	29.7	
Ottano	14.2	23.2	32.6	29.9	
Nonano	14.2	23.3	32.6	30.0	30.3
Decano	14.2	23.2	32.6	31.1	30.5
Isobutano	24.5	25.4			
Isopentano	22.2	31.1	32.0	11.7	
Isoesano	22.7	28.0	42.0	20.9	14.3
Neopentano	31.7	28.1			
2,2-dimetilbutano	29.1	30.6	36.9	8.9	
3-metilpentano	11.5	29.5	36.9	(18.8, 3-CH ₃)	
2,3-dimetilbutano	19.5	34.3			
2,2,3-trimetilbutano	27.4	33.1	38.3	16.1	
2,3-dimetilpentano	7.0	25.3	36.3	(14.6, 3-CH ₃)	

TABELLA 4.6 Effetti incrementali del sostituito Y (ppm) negli alcani dovuti alla sostituzione di H con Y. Y può essere terminale o interno.^a

$\dots - \overset{\gamma}{\text{C}} - \underset{\beta}{\text{C}} - \overset{\alpha}{\text{C}} - \text{Y}$ Terminale $\dots - \overset{\gamma}{\text{C}} - \underset{\beta}{\text{C}} - \overset{\alpha}{\text{C}}(\text{Y}) - \underset{\beta}{\text{C}} - \overset{\gamma}{\text{C}} - \dots$ Interno					
Y	α		β		γ
	Terminale	Interno	Terminale	Interno	
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				-2
Fenile	23	17	9	7	-2
OH	48	41	10	8	-5
OR	58	51	8	5	-4
OCOR	51	24	6	5	-3
NH ₂	29	24	11	10	
NH ₃ ⁺	26	31	8	6	-5
NHR	37		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

^a Si aggiungono questi incrementi ai valori di spostamento chimico dell'appropriato atomo di carbonio riportati in tabella 4.5 o ai valori di spostamento chimico calcolati in base alla tabella 4.4.

Fonte: Wehrli, F.W. *et al.* (1983).

TABELLA 4.7 Spostamenti chimici ¹³C dei cicloalcani (ppm riferiti a TMS).

C ₃ H ₆	-2.9	C ₇ H ₁₄	28.4
C ₄ H ₈	22.4	C ₈ H ₁₆	26.9
C ₅ H ₁₀	25.6	C ₉ H ₁₈	26.1
C ₆ H ₁₂	26.9	C ₁₀ H ₂₀	25.3

TABELLA 4.8 Spostamenti chimici di eterocicli saturi (ppm riferiti a TMS, campione puro).

Non sostituiti

 40.6	 18.1	 18.2
 22.9 72.6	 28.1 26.1	 19.0 48.1
 25.8 67.9	 31.2 31.7	 25.7 47.1
 24.9 27.7 69.5	 26.6 27.8 29.1	 25.9 27.8 47.9

Sostituiti

 47.3 47.6 18.1	 21.8 32.4 36.5	 24.4 56.7 48.0
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TABELLA 4.9 Spostamenti chimici ^{13}C di alcheni e cicloalcheni (ppm riferiti a TMS).

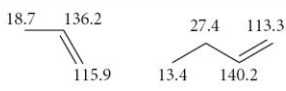
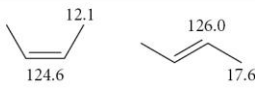
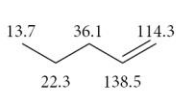
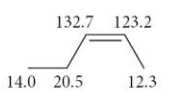
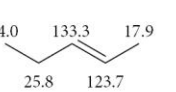
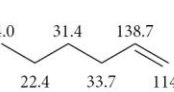
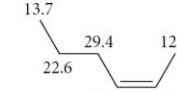
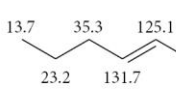
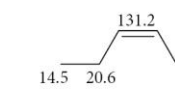
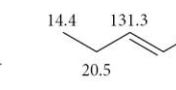
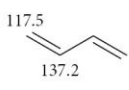
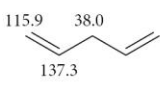
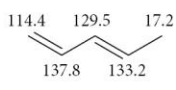
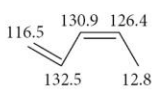
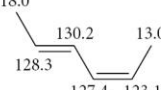
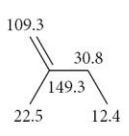
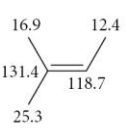
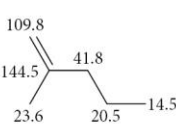
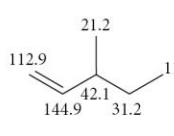
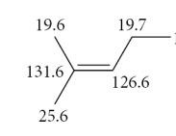
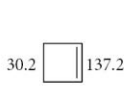
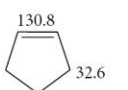
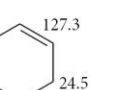
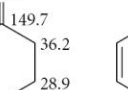
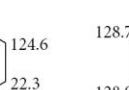
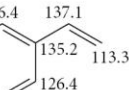
$\text{H}_2\text{C}=\text{CH}_2$ 123.2						
						
			$\text{CH}_2=\text{C}=\text{CH}_2$ 74.8 213.5			
						
						
						

TABELLA 4.10 Spostamenti chimici ^{13}C di alcheni sostituiti (ppm riferiti a TMS).

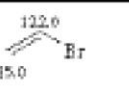
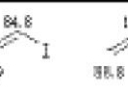
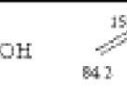
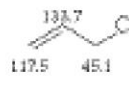
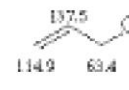
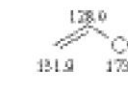
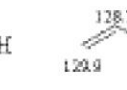
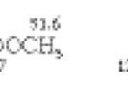
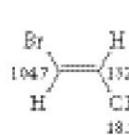
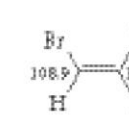
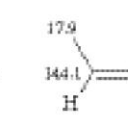
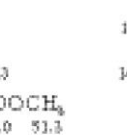
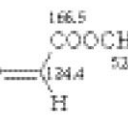
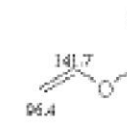
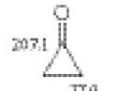
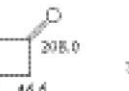
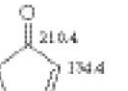
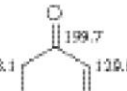
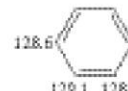
						
						
						
						

TABELLA 4.11 Spostamenti chimici ^{13}C di alchini (ppm riferiti a TMS).

Composto	C-1	C-2	C-3	C-4	C-5	C-6
1-butino	71.9	86.0	12.3	13.8		
2-butino	3.3	73.6				
1-esino	68.1	84.5	18.1	30.7	21.9	13.5
2-esino	2.7	73.7	76.9	19.6	21.6	12.1
3-esino	15.4	13.0	80.9			

TABELLA 4.12 Variazioni incrementali di spostamento chimico per atomi di carbonio aromatici in benzeni monosostituiti (ppm rispetto al benzene a 128.5 ppm). Spostamenti chimici dell'atomo di carbonio dei sostituenti (ppm rispetto a TMS)^a.

Sostituente	C-1 (sito di legame)	C-2	C-3	C-4	C del sostituente (ppm riferiti a TMS)
H	0.0	0.0	0.0	0.0	
CH ₃	9.3	0.7	-0.1	-2.9	2.3
CH ₂ CH ₃	15.6	-0.5	0.0	-2.6	29.2 (CH ₂), 15.8 (CH ₃)
CH(CH ₃) ₂	20.1	-2.0	0.0	-2.5	34.4 (CH), 24.1 (CH ₃)
C(CH ₃) ₃	22.2	-3.4	-0.4	-3.1	34.5 (C), 31.4 (CH ₃)
CH=CH ₂	9.1	-2.4	0.2	-0.5	137.1 (CH), 113.3 (CH ₂)
C≡CH	-5.8	6.9	0.1	0.4	84.0 (C), 77.8 (CH)
C ₆ H ₆	12.1	-1.8	-0.1	-1.6	
CH ₂ OH	13.3	-0.8	-0.6	-0.4	64.5
CH ₂ O(C=O)CH ₃	7.7	-0.0	-0.0	-0.0	20.7 (CH ₃), 169.7 (C=O)
OH	26.6	-12.7	1.6	-7.3	
OCH ₃	31.4	-14.4	1.0	-7.7	54.1
OC ₆ H ₅	29.0	-9.4	1.6	-5.3	
O(C=O)CH ₃	22.4	-7.1	-0.4	-3.2	23.9 (CH ₃), 169.7 (C=O)
(C=O)H	8.2	1.2	0.6	5.8	192
(C=O)CH ₃	7.8	-0.4	-0.4	2.8	24.6 (CH ₃), 195.7 (C=O)
(C=O)C ₆ H ₅	9.1	1.5	-0.2	3.8	196.4 (C=O)
(C=O)CF ₃	-5.6	1.8	0.7	6.7	
(C=O)OH	2.9	1.3	0.4	4.3	168
(C=O)OCH ₃	2.0	1.2	-0.1	4.8	51.0 (CH ₃), 166.8 (C=O)
(C=O)Cl	4.6	2.9	0.6	7.0	168.5
(C=O)NH ₂	5.0	-1.2	0.0	3.4	
C≡N	-16	3.6	0.6	4.3	119.5
NH ₂	19.2	-12.4	1.3	-9.5	
N(CH ₃) ₂	22.4	-15.7	0.8	-11.8	40.3
NH(C=O)CH ₃	11.1	-9.9	0.2	-5.6	
NO ₂	19.6	-5.3	0.9	6.0	
N=C=O	5.7	-3.6	1.2	-2.8	129.5
F	35.1	-14.3	0.9	-4.5	
Cl	6.4	0.2	1.0	-2.0	
Br	-5.4	3.4	2.2	-1.0	
I	-32.2	9.9	2.6	-7.3	
CF ₃	2.6	-3.1	0.4	3.4	
SH	2.3	0.6	0.2	-3.3	
SCH ₃	10.2	-1.8	0.4	-3.6	15.9
SO ₂ NH ₂	15.3	-2.9	0.4	3.3	
Si(CH ₃) ₃	13.4	4.4	-1.1	-1.1	

^a Vedi Ewing, D.E. (1979), *Org. Magn. Reson.*, **12**, p. 499. Sono riportati 709 valori di spostamento chimico di benzeni monosostituiti.

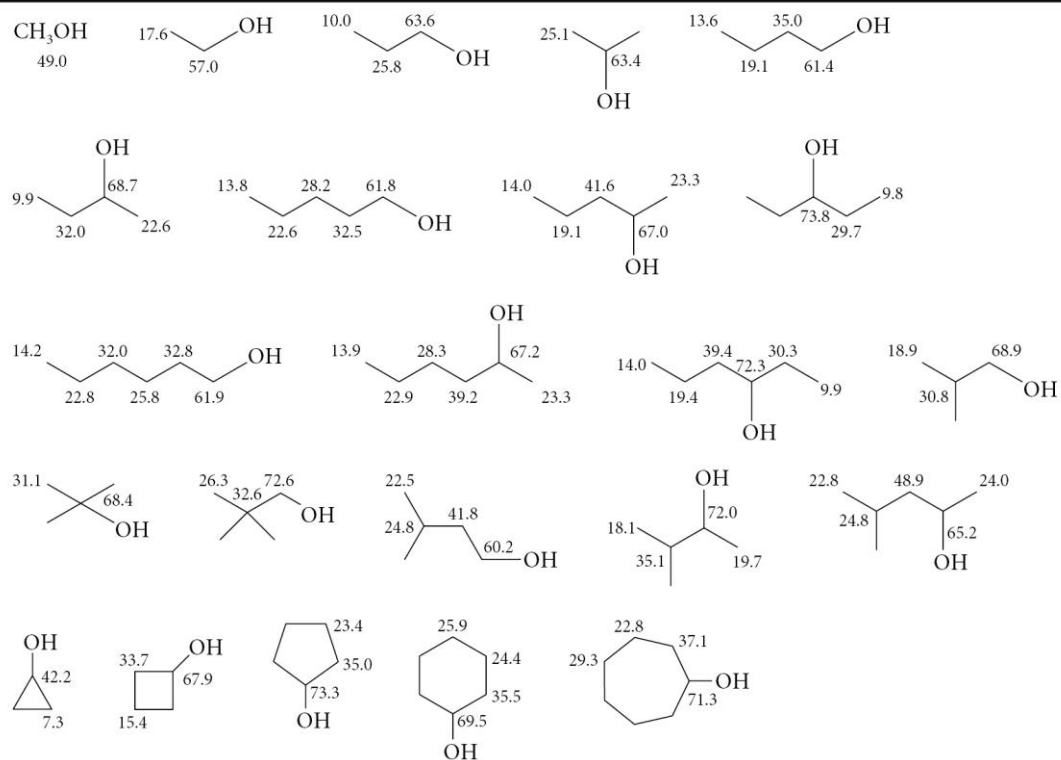
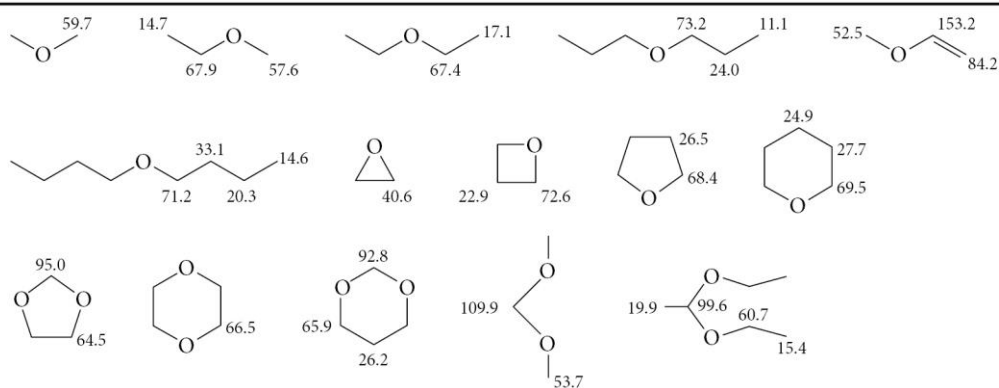
TABELLA 4.14 Spostamenti chimici di atomi di carbonio di alcoli (ppm riferiti a TMS).**TABELLA 4.15** Spostamenti chimici di atomi di carbonio di eteri, acetali ed epossidi (ppm riferiti a TMS).

TABELLA 4.16 Spostamenti chimici di atomi di carbonio di alogenuri alchilici (composti puri, ppm riferiti a TMS).

Composto	C-1	C-2	C-3
CH ₄	-2.5		
CH ₃ F	75.4		
CH ₃ Cl	24.9		
CH ₂ Cl ₂	54.0		
CHCl ₃	77.5		
CCl ₄	96.5		
CH ₃ Br	10.0		
CH ₂ Br ₂	21.4		
CHBr ₃	12.31		
CBr ₄	-28.5		
CH ₃ I	-20.7		
CH ₂ I ₂	-54.0		
CHI ₃	-139.9		
CI ₄	-292.5		
CH ₃ CH ₂ F	79.3	14.6	
CH ₃ CH ₂ Cl	39.9	18.7	
CH ₃ CH ₂ Br	28.3	20.3	
CH ₃ CH ₂ I	-0.2	21.6	
CH ₃ CH ₂ CH ₂ Cl	46.7	26.5	11.5
CH ₃ CH ₂ CH ₂ Br	35.7	26.8	13.2
CH ₃ CH ₂ CH ₂ I	10.0	27.6	16.2

TABELLA 4.17 Spostamenti chimici ^{13}C di ammine acicliche e alicicliche (in CDCl_3 , ppm riferiti a TMS).

$\text{H}_3\text{C}-\text{NH}_2$ 26.9	 36.7 18.8	 27.1 11.4 44.4	 26.2 42.8	 47.5 20.1 42.0 13.9 36.1
 20.0 31.6 50.2	 45.1 53.6 13.0	 33.0 10.7 48.6 23.5	 47.4 32.6	 44.1 15.5
 22.7 14.1 29.3 42.4	 32.2 36.6 52.0 14.1 20.6	 44.3 52.0 11.9 23.5 15.5	 24.1 14.2 42.7 46.8 19.7	
 17.1 11.4 26.9 48.2	 10.5 30.3 54.3	 43.2 40.3 25.8 22.7	 36.8 28.3 60.6 20.7	 41.8 15.7 48.8 23.1
 32.1 54.7 26.9	 18.6 35.3 52.3 18.1 20.6	 29.9 8.7 37.5 49.5	 55.0 18.5 41.2 18.5	 41.0 51.1 12.4
 22.8 14.1 26.7 34.1 42.4	 23.4 52.0 11.8	 11.8 45.5	 11.0 23.6 44.4 44.1	
 48.9 34.3 14.0	 53.4 36.4 24.0	 50.6 37.0 25.3 25.8	 33.6 58.6 33.3 25.1 26.3	 41.6 63.8 29.0 25.8 26.4
 52.8 38.6 28.2 24.2	 22.6 32.0 46.0 50.7 36.7	 21.3 26.7 42.4 46.0 34.7	 45.2 63.0 117.3 136.0	 56.4 116.9 136.2 46.7 11.8

TABELLA 4.19 Spostamenti chimici ^{13}C del gruppo $\text{C}=\text{O}$ e di altri atomi di carbonio di chetoni e aldeidi (ppm riferiti a TMS).

 30.6 206.7	 34.5 211.0 7.9	 47.8 9.9 208.2	 22.7 37.9 219.6	 24.6 26.6 41.8 209.7	 30.6 24.4 43.9 215.0
 128.4 128.2 132.9 137.1 26.3	 137.5 196.9 128.6 30.7 199.7	 15.8 13.8 45.9 202.5	 136.4 192.1 136.0	 175.3	
 129.5 128.5 134.2 192.4 136.4	 203.5 58.7 30.9 58.7	 24.8 192.6 101.1 192.6	 22.4 197.1	 29.6 206.9 37.0 206.9	

TABELLA 4.20 Spostamenti chimici ^{13}C del gruppo $\text{C}=\text{O}$ e di altri atomi di carbonio di acidi carbossilici, esteri, lattoni, cloruri, anidridi, carbammati e nitrili (ppm riferiti a TMS).

$\text{H}_3\text{C}-\text{COOH}$ 178.1 20.6	$\text{Cl}_3\text{C}-\text{COOH}$ 168.0 89.1	$\text{O}=\text{C}-\text{Cl}$ 169.5 33.8	$(\text{CH}_3)_2\text{CH}-\text{COOH}$ 34.1 18.8 184.8	$\text{CH}_2=\text{CH}-\text{COOH}$ 128.0 131.9 173.2
$\text{F}_3\text{C}-\text{COOH}$ 163.0 115.0	$\text{H}_3\text{C}-\text{COO}^-\text{Na}^+$ 181.5 in D_2O			
$\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$ 17.2 51.5 176.5	$\text{CH}_3\text{CH}_2\text{COOCH}_3$ 20.0 170.3 60.0 13.8	$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3$ 9.2 27.2 173.3 50.8	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOCH}_3$ 14.3 23.4 32.2 25.5 33.9 172.1 51.1	
$\text{CH}_3\text{CH}_2\text{COOCH}_3$ 21.4 170.0 66.8 20.4	$\text{CH}_2=\text{CHCOOCH}_3$ 129.9 128.7 164.5 52.0	$\text{CH}_3\text{COOCH}_2\text{CH}_3$ 20.8 168.0 142.4 97.4	$\text{F}_3\text{CCOOCH}_3$ 158.1 114.1 61.0 14.1	$\text{Cyclopentadiene-1-COOCH}_3$ 167.2 132.8 52.3 133.0 39.5
$\text{Cyclohexadiene-1-COOCH}_3$ 166.0 130.2 129.9 128.7 133.1	$\text{Cyclohexadiene-1-COOH}$ 169.4 130.3 130.3 128.7 134.0	$\text{Cyclohexadiene-1-COCl}$ 167.9 133.3 131.4 129.1 135.4	$\text{CH}_3\text{COOCH}_2\text{COOCH}_3$ 167.3 20.2	$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{COOCH}_3$ 8.4 27.1 170.3
Cyclopentanone 28.4 171.7	Cyclopentanone 136.7 164.3	Cyclohexanone 125.3 131.1 165.5	Cyclopentanone 27.7 177.9 22.2 68.6	Cyclohexanone 29.8 171.2 19.1 69.4 22.7
CH_3CONH_2 25.5 174.3	$\text{CH}_3\text{N}(\text{CH}_3)\text{CONH}_2$ 31.1 36.2 162.4	$\text{CH}_3\text{C}(=\text{O})\text{NH}_2$ 18.3 141.3 171.0 124.0	$\text{N,N-Dimethylbenzamide}$ 127.2 135.2 169.5 127.2 128.6 37.6 37.6	$\text{H}_2\text{NCONHCH}_3$ 157.8 60.9 14.5
$\text{C}\equiv\text{N}$ 1.3 117.7	CH_2CN 10.8 10.6 120.8	$\text{CH}_2=\text{CHCN}$ 18.8 149.3 101.2 117.6	$\text{CH}_2=\text{CHCN}$ 150.2 100.9 116.0 17.3	$\text{Cyclohexadiene-1-CN}$ 118.7 112.3 132.7 129.1 132.0