

Accoppiamenti $^{13}\text{C-H}$

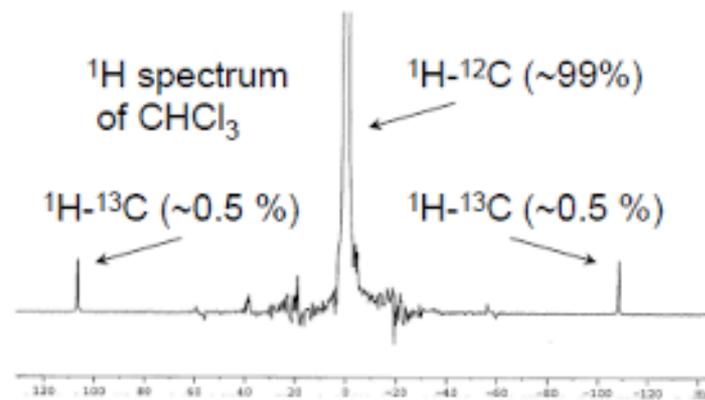
Accoppiamenti ^{13}C -H

$^1J_{\text{CH}}$ 125-300 Hz (Si ricava anche dai picchi satelliti nello spettro ^1H NMR)

$^2J_{\text{CH}}, ^3J_{\text{CH}} = 0-60$ Hz

Per C sp³: $^2J_{\text{CH}} \approx ^3J_{\text{CH}}$

Per C sp²: $^2J_{\text{CH}} < ^3J_{\text{CH}}$



$^1J_{\text{CH}}$

Dipende da:

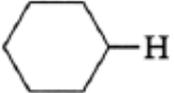
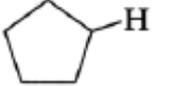
- 1) Ibridazione del C
- 2) Elettronegatività dei sostituenti

1) Ibridazione:

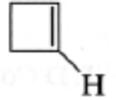
$^1J_{\text{CH}} = 5 \times \%s$ carattere s (Hz) per C non sostituiti 125 -250 Hz

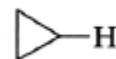
Accoppiamenti $^1J_{C-H}$

sp³

CH ₄	125.0
CH ₃ CH ₃	124.9
CH ₃ CH ₂ CH ₃	119.2
(CH ₃) ₃ CH	114.2
	123.0
	128.0
PhCH ₃	129.0

sp²

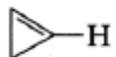
CH ₂ CH=C(CH ₃) ₂	148.4
CH ₂ =CH ₂	156.2
C ₆ H ₆	159.0
	160.0
C=C=C-H	168.0
	170.0



161.0

NB

sp

CH≡CH	249.0
C ₆ H ₅ C≡CH	251.0
	238.0

NB

Si utilizzano i valori di 1J per avere informazioni sulla natura dell'ibrido

Accoppiamenti $^1J_{C-H}$

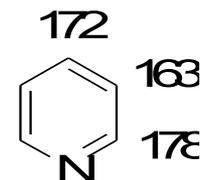
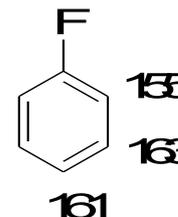
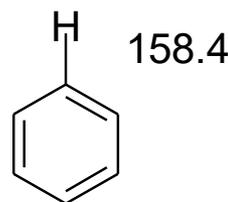
1) Sostituenti elettronegativi aumentano la 1J

$(CH_3)_4Si$	118.0
CH_4	125.0
CH_3F	149.0
CH_3OH	141.0
CH_3Cl	150.0
CH_3Br	151.0
$(CH_3O)_2CH_2$	162.0
CH_2Cl_2	178.0
$CHCl_3$	209.0

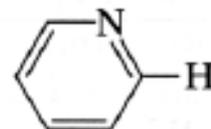
sp³

sp²

$CH_2=CH_2$	156.2
$ \begin{array}{c} a \quad c \\ CH_2=CHF \\ b \end{array} $	159.2, 162.2, 200.2



$CH_3CH=O$	172.4
------------	-------



178.0

$NH_2CH=O$	188.3
$=COH(OR)$	195.0
$CH_3CHX, X=halogen$	198.0

Accoppiamenti $^n J_{C-X}$ con eteronuclei

1J ^{13}C - ^{19}F 150 - 400 Hz

2J ^{13}C - ^{19}F ≈ 50 Hz

1J ^{13}C - ^{31}P 10-300 Hz

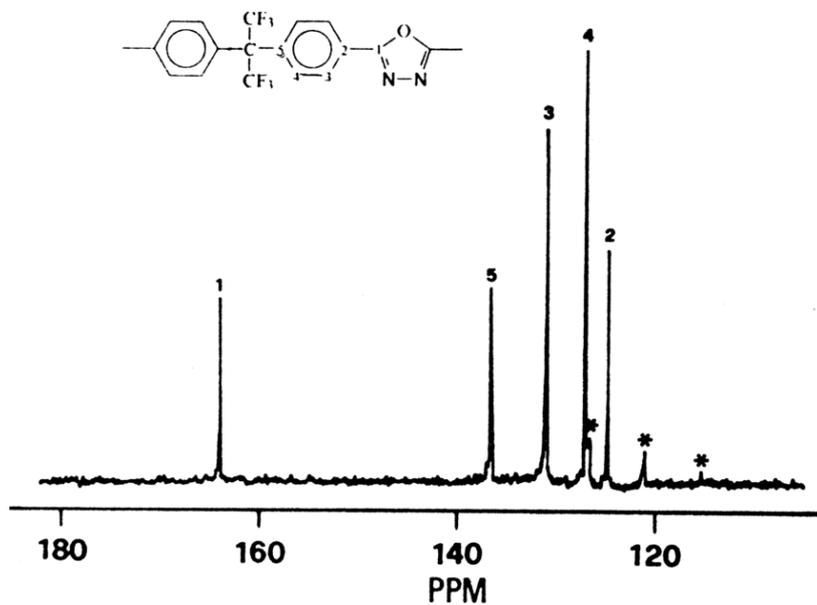
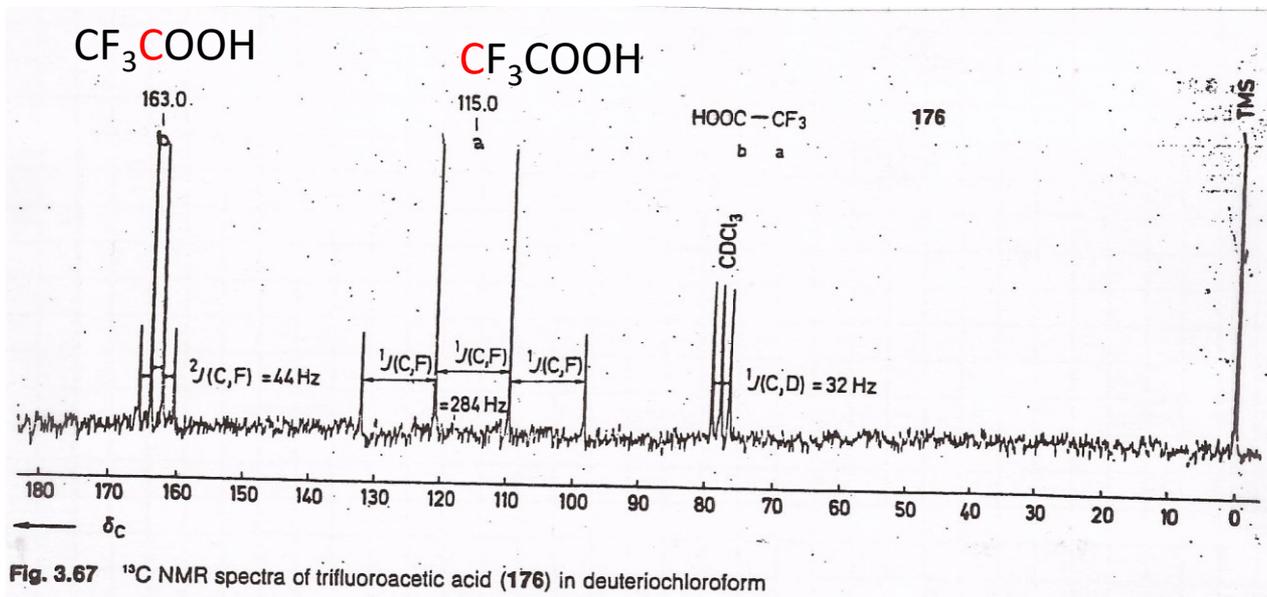
2J ^{13}C - ^{31}P 10-20 Hz

1J ^{13}C - ^{14}N ($I = 1$) difficilmente rilevabile

1J ^{13}C - ^{15}N ($I = 1/2$) difficilmente rilevabile

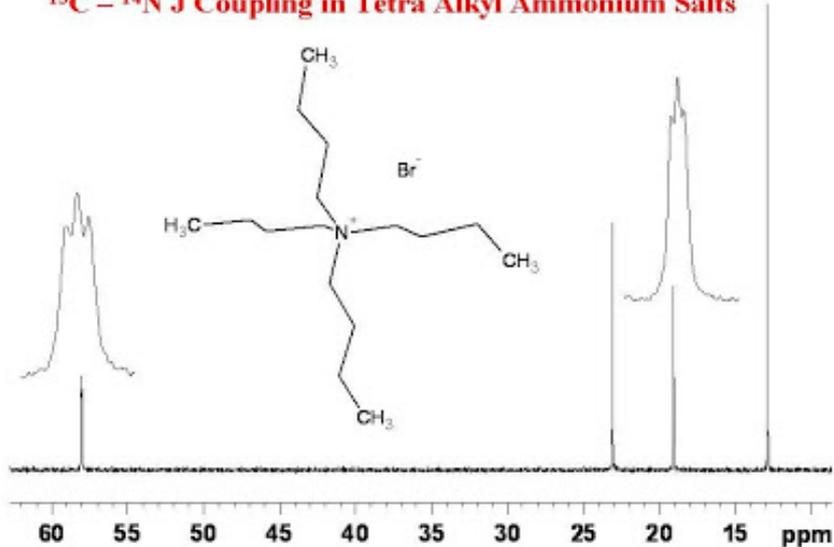
Compound	1J (Hz)	2J (Hz)	3J (Hz)	4J (Hz)
CH ₃ CF ₃	271			
CF ₂ H ₂	235			
CF ₃ CO ₂ H	284	43.7		
C ₆ H ₅ F	245	21.0	7.7	3.3
(C ₄ H ₉) ₃ P	10.9	11.7	12.5	
(CH ₃ CH ₂) ₄ P ⁺ Br ⁻	49.0	4.3		
(C ₆ H ₅) ₃ P ⁺ CH ₃ I ⁻	88.0	10.9		
	1J (Hz) of CH ₃ = 52			
C ₂ H ₅ (P=O)(OC ₂ H ₅) ₂	143	7.1 (J_{COP})	6.9 (J_{CCOP})	
(C ₆ H ₅) ₃ P	12.4	19.6	6.7	
CDCl ₃	31.5			
CD ₃ (C=O)CD ₃	19.5			
(CD ₃) ₂ SO	22.0			
C ₆ D ₆	25.5			

Accoppiamenti $^n J_{C-X}$ con eteronuclei

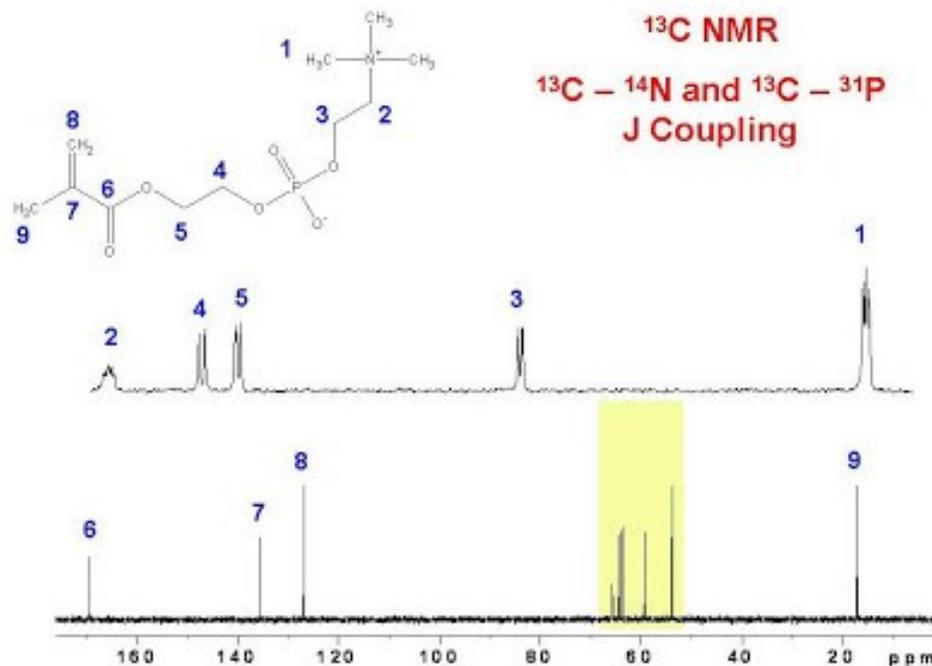


Accoppiamenti ${}^n J_{C-x}$ con eteronuclei

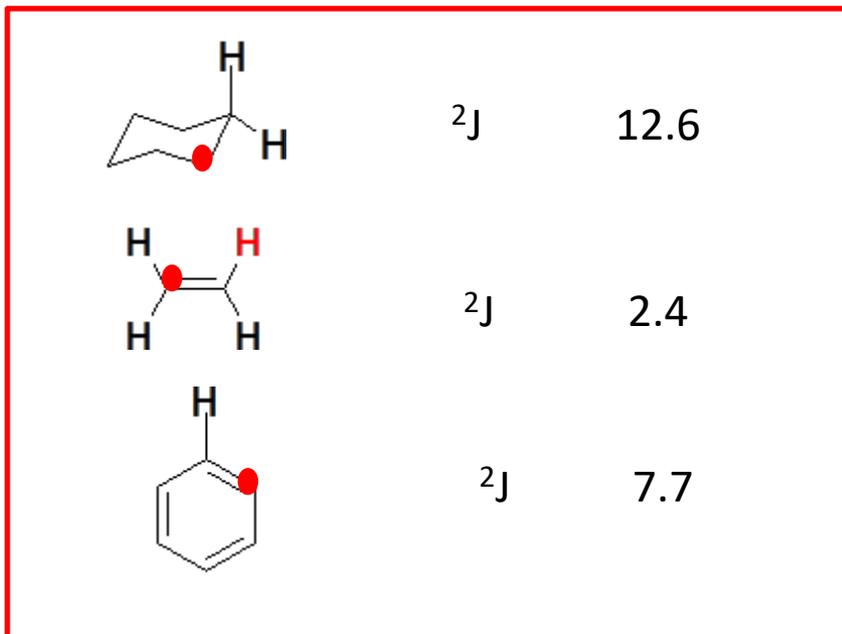
${}^{13}\text{C} - {}^{14}\text{N}$ J Coupling in Tetra Alkyl Ammonium Salts



$$I({}^{14}\text{N}) = 1$$



Accoppiamenti



Tipici valori per ${}^2J_{\text{C-H}}$

Compound	$J(\text{Hz})$
<i>sp</i> ³	
CH_3CH_3	-4.5
CH_3CCl_3	5.9
$\text{RC}(=\text{O})\text{CH}_3$	6.0
$\text{CH}_3\text{CH}=\text{O}$	26.7
<i>sp</i> ²	
* C_6H_6	1.0
$\text{CH}_2=\text{CH}_2$	2.4
$\text{C}=\text{C}(\text{CH}_3)\text{H}$	5.0
$(\text{CH}_3)_2\text{C}=\text{O}$	5.5
$\text{CH}_2=\text{CHCH}=\text{O}$	26.9
<i>sp</i>	
$\text{CH}\equiv\text{CH}$	49.3
$\text{C}_6\text{H}_5\text{OC}\equiv\text{CH}$	61.0

* ${}^3J = 7.6 \text{ Hz } (>{}^2J)$.

CH_3CR	CR	CH ₃	CH ₂ I	CCl ₃	CHO	CO ₂ Me
	2J	-4.5	-5.0	-5.9	-6.6	-6.9
$\text{CHR}_2\text{-CH}_3$	CR ₂	CH ₂	CHCl	CCl ₂	C=O	
	2J	-4.5	-2.6	<1	+26.7	