Summary of Coupling in Multinuclear NMR

Two spin ½ 100% abundant nuclei (^{1}H, ^{19}F, ^{31}P, ^{103}Rh, ^{89}Y)

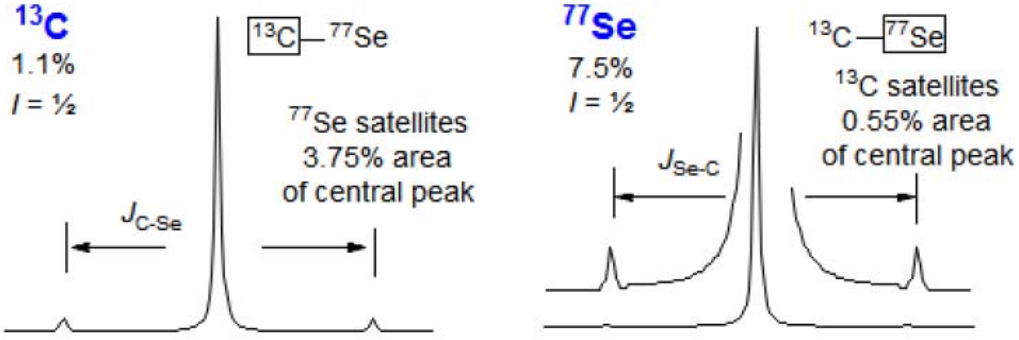
Both nuclei will show full coupling, just as in proton-proton coupling

One spin ½ 100% abundant nucleus and one low abundance nucleus

The low abundance nucleus will show full coupling, the 100% abundant nucleus will show *satellites*.

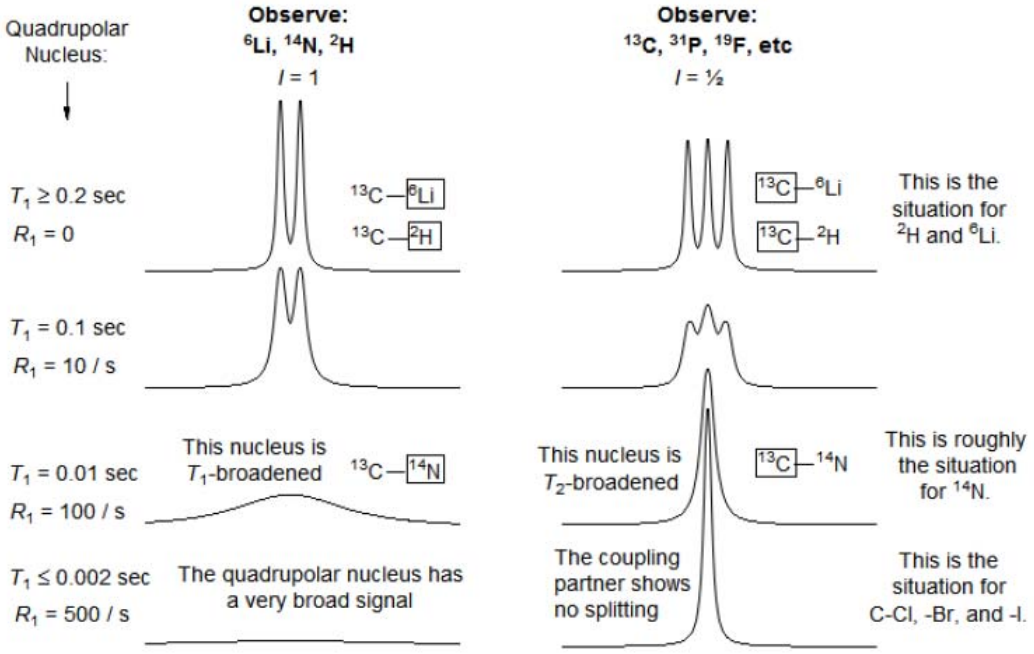
Two spin ½ low abundance nuclei

Both nuclei will show *satellites*. Homonuclear coupling only seen as satellites.



One spin ½ nucleus and one quadrupolar nucleus

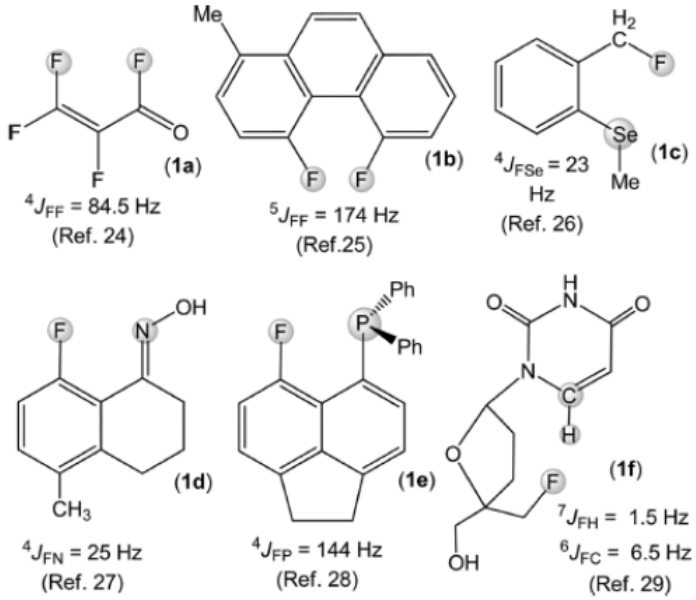
The appearance of both signals will depend on the the T_1 of the quadrupolar nucleus (we can assume that the spin ½ nucleus will always have relatively long T_1).



جفت شدنها از طریق فضا

با جفت شدن اسپین-اسپین مستقیم متفاوت است و متوسط آن در محلول صفر نمی شود

Scheme 1. Molecular Structures of Small Organics with ^{1}H, ^{13}C, ^{14}N, ^{19}F, ^{31}P, and ^{77}Se Spin-Active Nuclei[a]



Chem. Rev. 2014, 114, 4838−4867

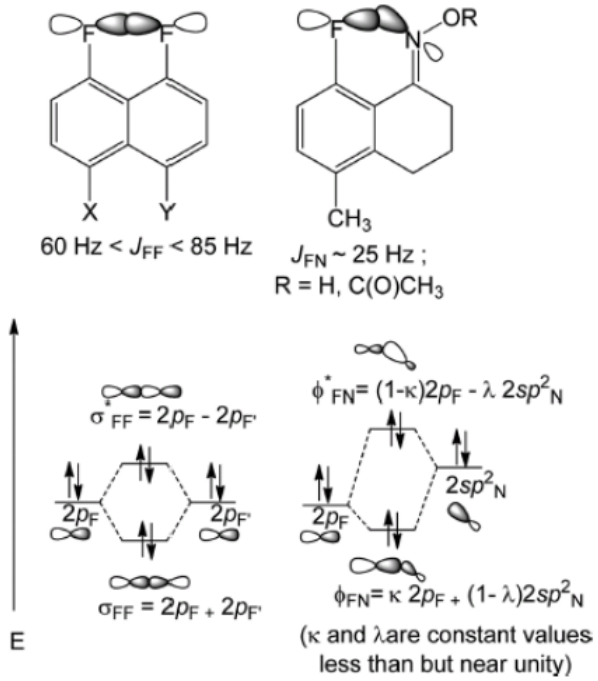
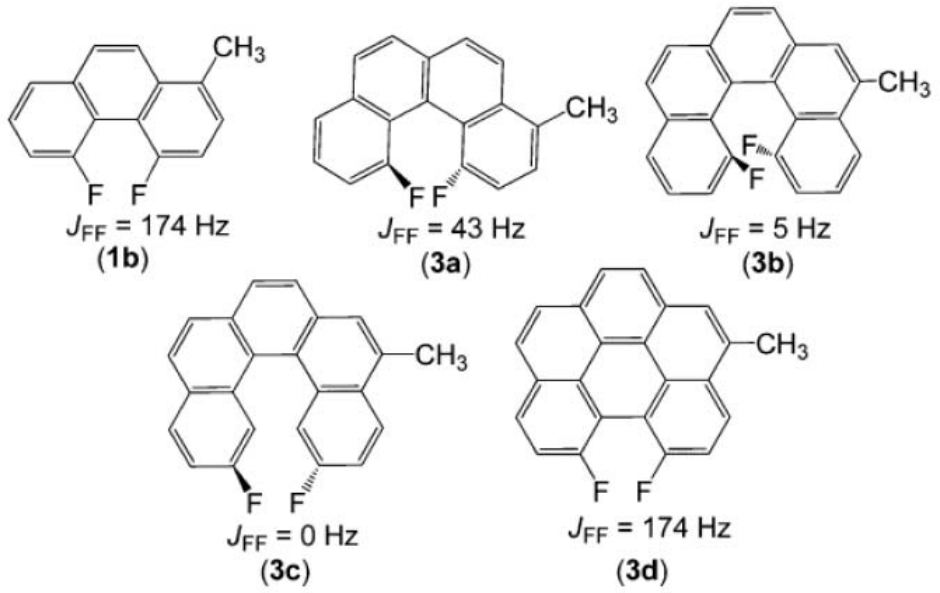


Figure 2. Orbitals generated by the overlap of two lone-pair orbitals on intramolecularly crowded nitrogen- and fluorine-containing compounds according to Mallory's model.

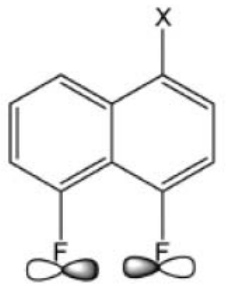
Chem. Rev. 2014, 114, 4838−4867

Scheme 3. J_{FF} TS Couplings Decrease in the Series of Difluoro Benzenoid Fused Rings 3a−3c with the Increase of Helical Character of the Structure



Chem. Rev. 2014, 114, 4838−4867

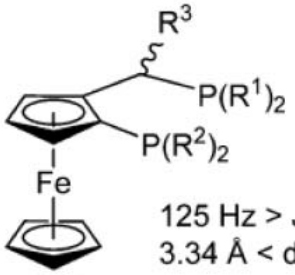
Scheme 4. 1,8-Difluoronaphthalene Molecules with SSCCs $J_{FF} = 68 \pm 8$ Hz



(in-plane σ overlap)

X = H, **4a**, *J* 59.0 Hz *d* 2.533 Å
CN, **4b**, *J* 66.1 Hz *d* 2.517 Å
CH_3, **4c**, *J* 65.6 Hz *d* 2.516 Å
Br, **4d**, *J* 67.4 Hz *d* 2.512 Å
Cl, **4e**, *J* 66.5 Hz *d* 2.511 Å
$NHCOCH_3$, **4f**, *J* 65.9 Hz *d* 2.509 Å
NO_2, **4g**, *J* 76.4 Hz *d* 2.479 Å

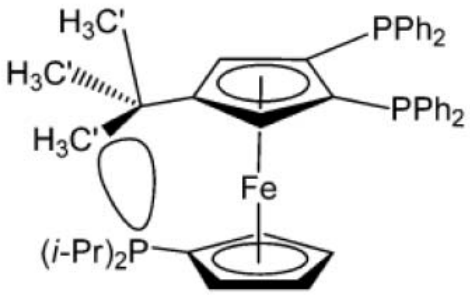
Scheme 20. Ferrocenyl Homoannular Diphosphines (R^1, R^2, R^3 = aryl or alkyl)



(20a)

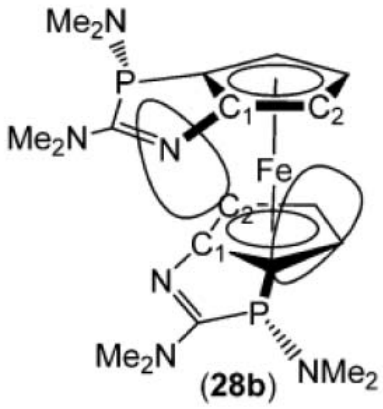
125 Hz > *J*(P,P) > 0 Hz
3.34 Å < d(P,P) < 4.83 Å

Scheme 28. $^{TS}J_{PC}$ Couplings within Ferrocenyl Phosphine



(**28a**)

^{5TS}J(P,C') 5.5 Hz
d(P...C') 3.64 Å

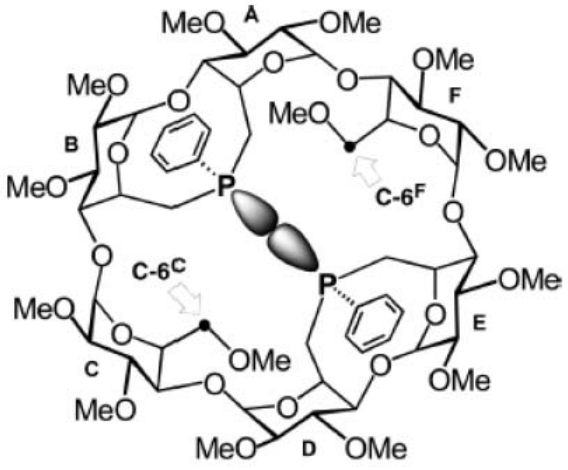


(**28b**)

δC^1 123.2 ppm δC^2 65.8 ppm

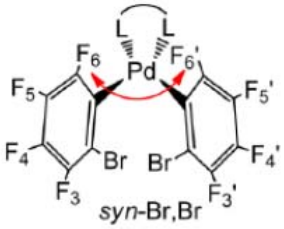
$J(P,C_2)$ 7.5 Hz $d(P...C_2)$ 3.68 Å
$J(P,C_1)$ 2.5 Hz $d(P...C_1)$ 3.80 Å

Scheme 29. $^{8TS}J_{PC}$ in a Cyclodextrin-Based Diphosphine[a]



(**29a**)

Scheme 35. $^{19}F-^{19}F$ Inter-ring SSCCs for Palladium Complexes Bearing the Asymmetric Fluorinated Aryl Groups *m*-C_6BrF_4 and *o*-C_6BrF_4

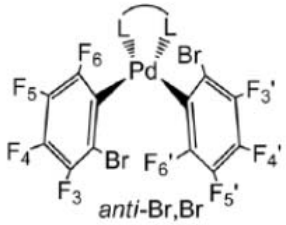


syn-Br,Br

(35a)

$^{6TS}J(F_6,F_{6'})$ 9.9-52.0 Hz

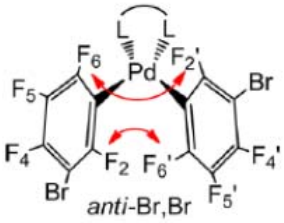
$d(F_6...F_{6'})$ 3.20-2.65 Å



anti-Br,Br

(35a')

L L = PhP(=O)(2-pyridyl)$_2$

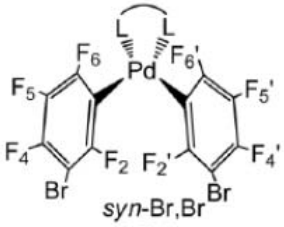


anti-Br,Br

(35b)

$^{6TS}J(F_6,F_{2'})$ 11.9 Hz

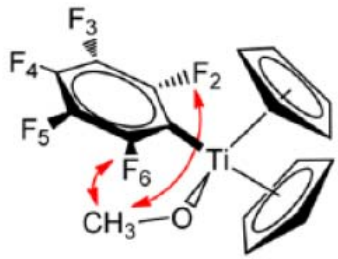
$^{6TS}J(F_2,F_{6'})$ 25.5 Hz



syn-Br,Br

(35b')

Scheme 34. $^{TS}J_{FH}$ and $^{TS}J_{PP}$ in Titanium Complexes



(34a)

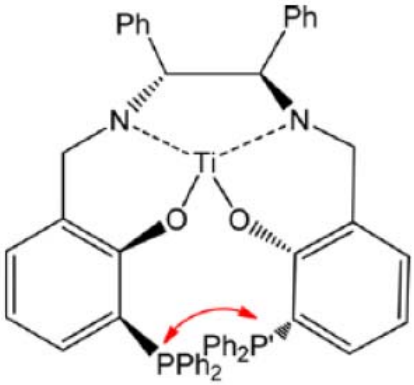
$\delta F_2 = -112$ ppm

$\delta F_6 = -114$ ppm

$\delta F_{3-5} = -160$ ppm

$^{6TS}J(F_2,H)$, 0.9 Hz (m)

$^{6TS}J(F_6,H)$, 0.9 Hz (dt)



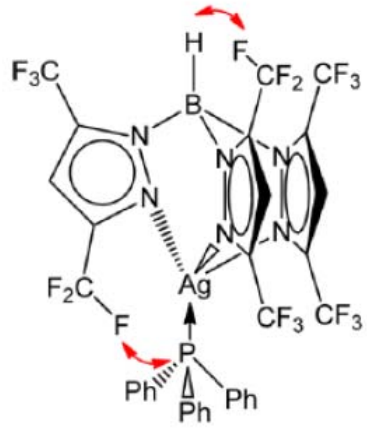
(34b)

$\delta P = -16.2$ ppm

$\delta P' = -16.4$ ppm

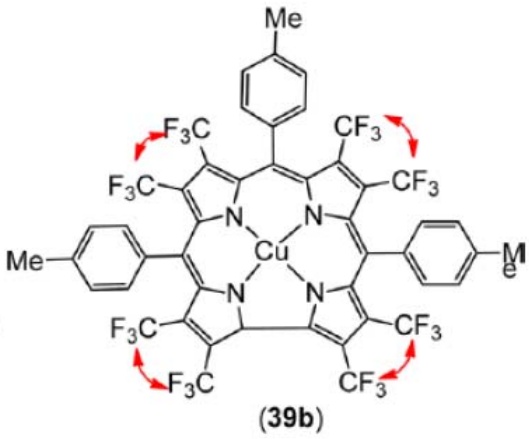
$^{8TS}J(P,P')$, 12.4 Hz (d)

Scheme 39. Trifluoromethylated Tris(pyrazolyl)borato and Corrole Complexes of Ag and Cu



(39a)

^{5TS}J(F,P) 8.1 Hz
^{4TS}J(F,Ag) 1.4 Hz
^{5TS}J(F,H) 2.5 Hz



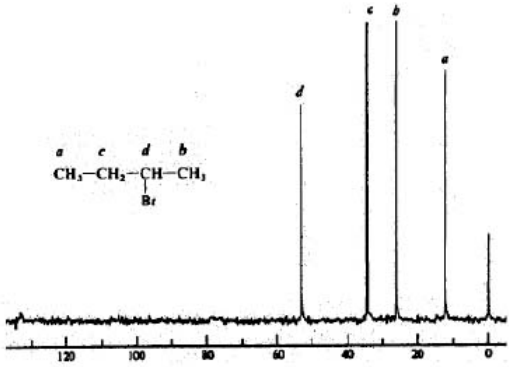
(39b)

^{5TS}J(F,F) 9.0-14.0 Hz

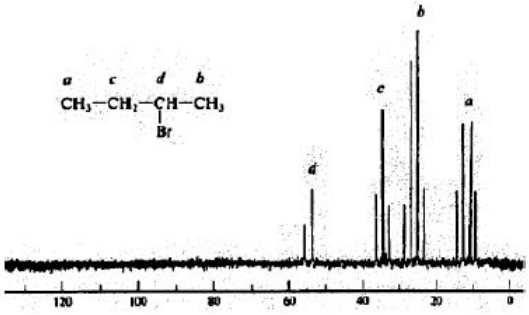
جفت شدنهای سایر هسته ها
Heteronuclear Couplings

Review: Carbon-Proton Coupling (Ch. 4.3 & 4.4)

H-decoupled



H-coupled



Carbon-Deuterium Coupling (Ch. 4.13)

For I = 1 : 2n+1 lines

n	2nI+1 Lines	Relative Intensities											
0	1	1											
1	3	1	1	1									
2	5	1	2	3	2	1							
3	7	1	3	6	7	6	3	1					
4	9	1	4	10	16	19	16	10	4	1			
5	11	1	5	15	30	45	51	45	30	15	5	1	
6	13	1	6	21	50	90	126	141	126	90	50	21	6	1

FIGURE 4.17 An intensity triangle for deuterium multiplets (n = number of deuterium atoms).

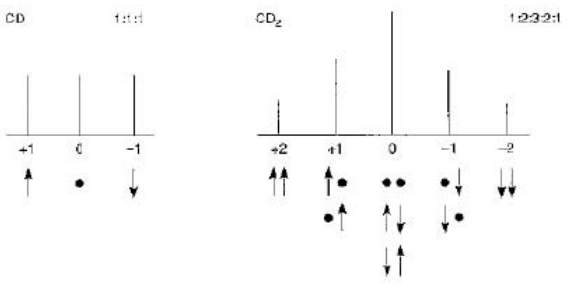


FIGURE 4.18 An intensity analysis of three- and five-line deuterium multiplets.

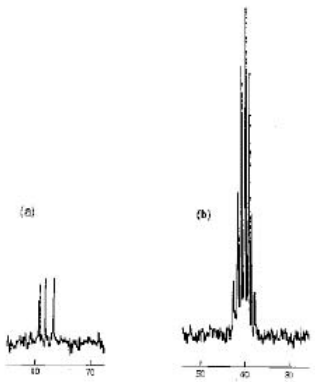
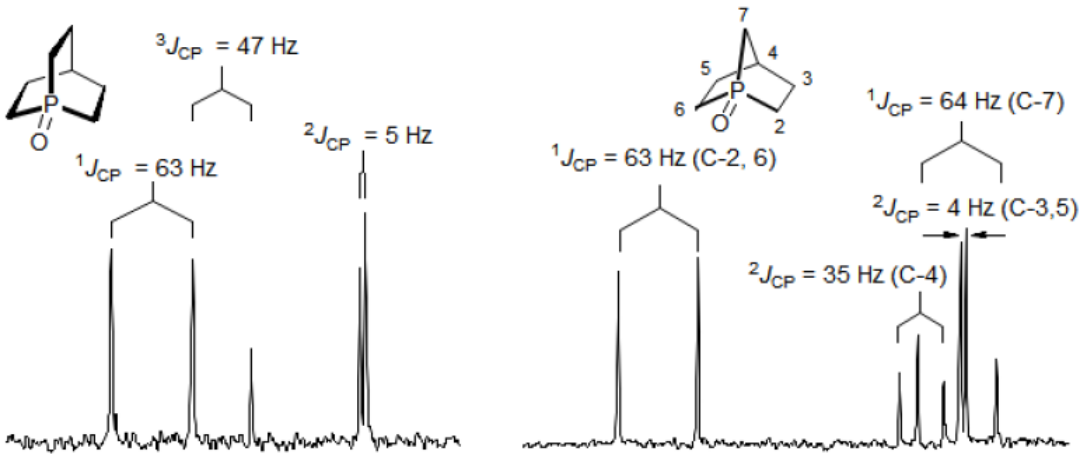
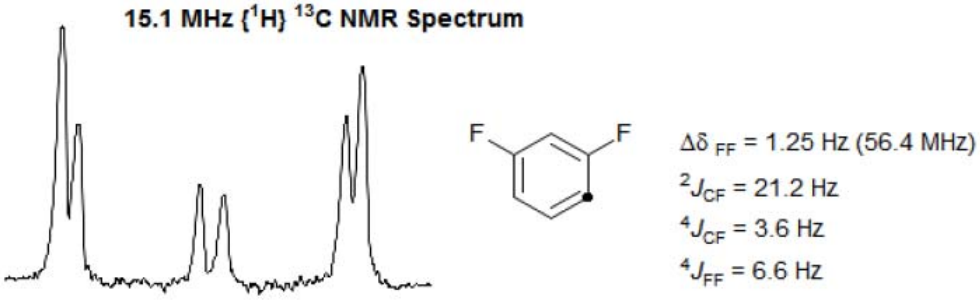


FIGURE 4.16 The ^{13}C NMR peaks of two common solvents. (a) Chloroform-d. (b) Dimethylsulfoxide-d_6.



25 MHz ^{13}C NMR spectra of two bicyclic phosphine oxides (Wetzel, Kenyon *J. Am. Chem. Soc.* 1974, *96*, 5189).



^{13}C NMR signal of C-4 of 1,3-difluorobenzene (Weigert, F. J.; Roberts, J. D. *J. Am. Chem. Soc.* **1971**, *93*, 2361).