

## Scalar couplings among common nuclei

Generally speaking, the scalar coupling is larger if the nuclei have higher gyromagnetic ratio and closer through bond. For example, one bond  $^1\text{H}$ - $^1\text{H}$  coupling is about six times of  $^2\text{H}$ - $^1\text{H}$  (take a close look at the residual solvent peak for d6-DMSO!). The sign of J coupling is not stressed in this document as conventional experiments cannot distinguish positive from negative.

### $^1\text{H}$ - $^1\text{H}$ :

$^2\text{J}$  has been found from -12.5 Hz (cyclohexane) to 16.5 Hz.

$^3\text{J}$  depends on the dihedral angle. It typically ranges from a couple of Hertz (furan) to 8 Hz (benzene).

$^4\text{J}$  is about 0 to 3 Hz. It is about 2 Hz in benzene.

$^5\text{J}$  is about 1 Hz (benzene).

### $^1\text{H}$ - $^{13}\text{C}$ :

$^1\text{J}$  depends on  $^{13}\text{C}$  hybridization, electronegativity of adjacent atoms and ring size. Typical values are 125 Hz for  $\text{sp}^3$ , 160 Hz for  $\text{sp}^2$  and 250 Hz for  $\text{sp}$ . It is 209 Hz for  $\text{CHCl}_3$ .

$^2\text{J}$  is about several to more than 10 Hz (that's why a HMBC is typically set up for about 10Hz coupling). In extreme cases,  $^2\text{J}$  can be as large as 50 Hz (alkyne).

$^3\text{J}$  ranges from several to more than 10 Hz (12.5 Hz for  $\text{trans CH}_2=\text{CHCH}_2$  vicinal coupling, and 7.5 Hz for cis).

### $^1\text{H}$ - $^{19}\text{F}$ :

$^2\text{J}$  is about 50 Hz ( $-\text{CHF}_2$ ).

$^3\text{J}$  ranges from several to more than 10 Hz, somewhat similar to proton-proton  $^3\text{J}$  (estimate of coupling constant involving fluorine can be treated similarly to that of a proton: while the lower gyromagnetic ratio tends to make the  $^{19}\text{F}$  coupling constant smaller, the richer electronic environment (9 vs. 1 and much stronger electronegativity) makes it larger than capable of reaching further-away nuclei (non-zero  $^4\text{J}$  and  $^4\text{J}$ )

### $^1\text{H}$ - $^{31}\text{P}$ :

$^1J$  and  $^3J$  depends on the solvent. They have been found between 670 Hz to 740 Hz for  $^1J$  and 6.5 to 12 Hz for  $^3J$ .

Indirect  $^2J$  is about several Hertz (P-O...H-C in DNA, Sychrovsk et al. JACS 2006, 128 (21), 6823-6828).

$^1H$ - $^{15}N$ :

$^1J$  depends on  $^{15}N$  hybridization etc. About -70Hz for sp<sup>3</sup>, -90 Hz for sp<sup>2</sup> and -140 Hz for sp<sup>3</sup>.

$^2J$  ranges from several to more than 10 Hz.

$^3J$  is generally several Hz.

$^1H$ - $^{29}Si$ :

$^1J$  is 367 Hz for SiHCl<sub>3</sub>, and 200 Hz for C<sub>6</sub>H<sub>5</sub>SiH<sub>3</sub>.

$^2J$  is 6.6 Hz for TMS.

$^{13}C$ - $^{13}C$ :

$^1J$  are 35 Hz (sp<sup>3</sup>-sp<sup>3</sup>), 55 Hz (sp<sup>2</sup>-sp<sup>3</sup>) and up to 75 Hz (sp<sup>2</sup>-sp<sup>2</sup>) in amino acids.

$^{13}C$ - $^{31}P$ :

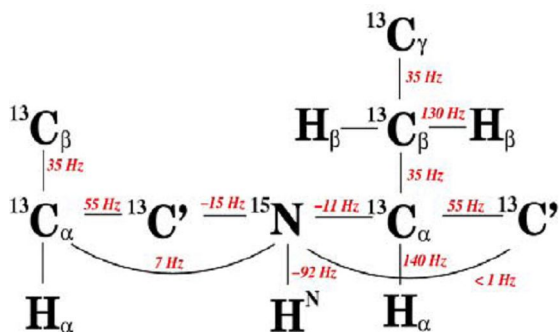
Depending on the carbon hybridization,  $^1J$  is ranges from -34 Hz (MeP(O)(OEt)<sub>2</sub>) to 476 Hz (P(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>).

$^2J$  is reported as 5.2 Hz by Rodrigues et al. J Bacteriol. 2007, 189: 5405–5412, and 19.6 Hz by Appel et al. Angewandte Chemie International Edition in English Volume 24 Issue 7, Pages 589 - 590

$^{13}C$ - $^{15}N$ :

$^1J$  is about 11 (sp<sup>3</sup>) to 15 Hz (sp<sup>2</sup>) in peptides.

$^2J$  ranges from less than 1 Hz to 7 Hz in peptides.



$^{13}\text{C}$ - $^{29}\text{Si}$ :

$^1\text{J}$  is 51 Hz in TMS

$^{13}\text{C}$ - $^{19}\text{F}$ :

Typical  $^1\text{J}$  is 185 Hz and  $^2\text{J}$  is 20 Hz. Again  $^{19}\text{F}$  is behaving somewhat like  $^1\text{H}$ , with corresponding coupling constant slight larger.

$^{19}\text{F}$ - $^{19}\text{F}$ :

$^2\text{J}$  ranges from less than 100 Hz to more than 300 Hz.

$^3\text{J}$  is about 10 Hz ( $-\text{CF}_2\text{COCF}_3$ )

$^4\text{J}$  or  $^5\text{J}$  is expected to be several Hz at most.

## References

1. Kolio Dimov Troev, "Chemistry and application of H-phosphonates", Elsevier, New York, 2006
2. M. Sattler et al. Prog. NMR Spectrosc. (1999) 34, 93-158