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Blechta, Vratislav  
2012

Dostupný z <http://www.nusl.cz/ntk/nusl-155593>

Dílo je chráněno podle autorského zákona č. 121/2000 Sb.

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Datum stažení: 06.05.2024

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## APPLICATION OF HCSE PULSE SEQUENCE TO DETECTION OF SMALL SIGNED CARBON-CARBON COUPLING CONSTANTS.

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The HCSE pulse sequence [1] presented at previous Valtice conference aimed to detection of small ( $J > 0.5$  Hz) homonuclear couplings. Originally this sequence was designed for silicon-silicon couplings.

The ability of HCSE to detect signed  $^nJ(\text{C},\text{C})$  couplings,  $n > 1$ , is demonstrated on a set of 9 mono-substituted benzenes  $\text{X}-\text{C}_6\text{H}_5$  with  $\text{X} = \text{F}, \text{NO}_2, \text{MeO}, \text{Cl}, \text{Br}, \text{NO}, \text{N}\equiv\text{C}, \text{Me}$  and  $\text{Me}_3\text{Si}$ . All 36  $^2J(\text{C},\text{C})$  and  $^3J(\text{C},\text{C})$  couplings in these compounds were calculated and compared with 26 experimental values in the paper by Witanowski et al. [2]. With the exception of one signed value all the reported [2] experimental values were absolute values only. The HCSE pulse sequence applied on these compounds yielded 34 signed values, 2 constants were not observed being probably very close to zero and therefore undetectable. The absolute values agree with the experimental ones given in ref. [2]. and all the detected signs agree with the computed ones. Influence of relaxations and coupling magnitudes on the signal intensities are discussed.

*Financial support provided by The TACR (grant no. TA01010646) are gratefully acknowledged.*

### References

- [1] V. Blechta and J. Schraml, *Magn. Reson. Chem.*, **2012**, accepted DOI 10.1002/mrc.2869
- [2] M. Witanowski, K. Kamińska-Trela, Z. Biedrzycka, *J. Mol. Struct.*, **2007**, 844.