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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 $^nJ(\text{C,C})$ couplings, $n > 1$, is demonstrated on a set of 9 mono-substituted benzenes $\text{X-C}_6\text{H}_5$ with $\text{X} = \text{F}, \text{NO}_2, \text{MeO}, \text{Cl}, \text{Br}, \text{NO}, \text{N}\equiv\text{C}, \text{Me}$ and Me_3Si . All 36 $^2J(\text{C,C})$ and $^3J(\text{C,C})$ 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.

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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.