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QUANTUM CHEMICAL INVESTIGATION OF CARBON-CARBON SPIN-SPIN COUPLING CONSTANTS

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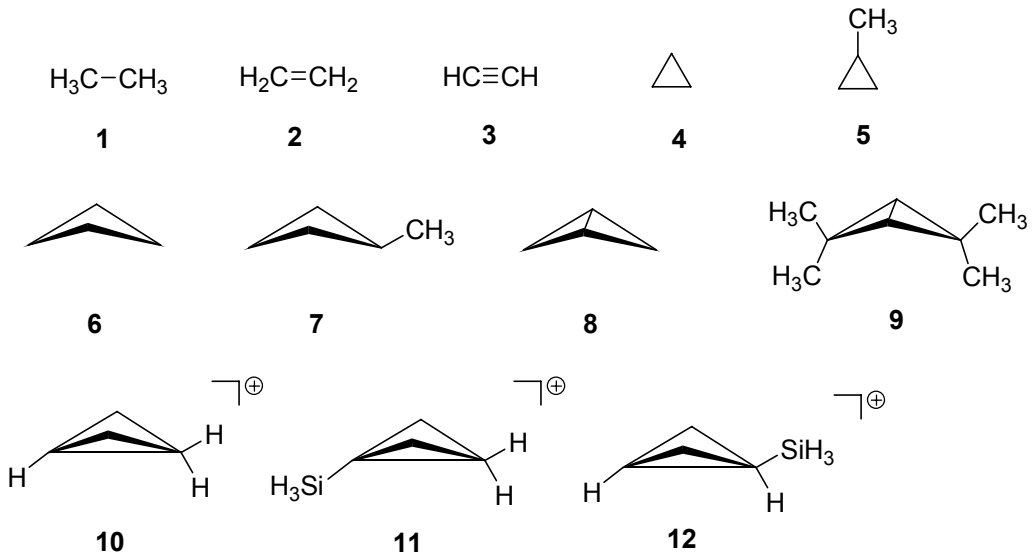
The experimental determination of Nuclear spin spin coupling constants is a well known fruitful and straightforward tool for elucidating details of chemical bonding. In addition to the most often measured *J*(H,H) and *J*(C,H) couplings, *J*(C,C) coupling constants are highly diagnostic and characteristic for particular C-C-bonds. On the other hand, several studies have demonstrated that spin-spin coupling constants are among the most difficult parameters to predict quantitatively.[1]

We will present preliminary results of calculations of carbon-carbon coupling constants for simple organic molecules and some carbocations **1** – **12** and show a comparison with available experimental data.[2] Similar to recent benchmark studies[3] the Lee-Yang-Parr (B3LYP) hybrid functional has been used for modelling the n-electron space. It is shown that reliable data are obtained if appropriate models for the one-electron space (basis sets) are used.



1 **2** **3** **4** **5** **6** **7** **8** **9** **10** **11** **12**

References

(1) Helgaker, T., Jaszunski,M., Ruud, K. Chem. Rev. 1999, 99, 293-352.
(2) I. R. Elanov, H.-U. Siehl, manuscript in preparation.
(3) Deng, W., Cheseman,J.R.; Frisch, M.J. J. Chem. Theor. Comput. 2006, 2, 1028-1037.

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