Turkish Journal of Chemistry

Turkish Journal

of

Chemistry

Development of a New Set of Additive Parameters for the Estimation of Geometrical Distortion of Cycloalkanes from C-13 NMR Chemical Shifts

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Abstract: A previous model for the calculation of C-13 chemical shifts is modified by replacement of 3 parameters representing the p-character of carbon atom in cyclic systems with a single parameter aiming for the development of a new set of parameters with a wide range of application for the calculation of C-13 NMR chemical shifts. The considered systems are cyclohexanes, trans decalins, and a number of hypothetical polycyclic 6-member ring hydrocarbons. The developed parameters include a combination of quantum mechanical and statistical methods. They are based on 2 factors: through bond (electronic) effect represented by the partial electronic charge on the tested carbon, and long-range (steric) effect expressed in terms of proton-proton interactions. The results of this study are compared to those of previous studies and sometimes are preferable.

Key Words: Additivity parameters, C-13 NMR chemical shifts, geometrical distortion, cycloalkanes

Keywords
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Turk. J. Chem., **31**, (2007), 479-490.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.31,iss.4.