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## A New Approach to the Calculation of N-15 Chemical Shifts of Cyclic Compounds

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**Abstract:** Two sets of additive parameters used previously for the calculation of C-13 chemical shifts of mono and poly six-membered cycloalkanes were applied for the prediction of N-15 chemical shifts of some methyl piperidine derivatives. These sets are based on 2 principles: the p-character (substituents electronic effect) of the atom under consideration and the steric effect that reflects the spatial arrangement of the molecule. An additional parameter, namely the ring angle of the studied atom, was added to the other parameters to define the structural distortion that is due to large steric interactions. The p-character in set (1) is represented by the number of carbon atoms; primary, secondary, tertiary, and quaternary types at $\alpha$ -position to the nitrogen, while in set (2) it is introduced as the partial electronic charge. The steric effect is expressed in terms of the actual number of the interacting proton-proton and/or proton-lone pairs in both sets. Quantum mechanical and regression analysis methods were employed for this investigation. The results showed that both sets were good for the prediction of N-15 chemical shifts. The parameters of set (2) were more consistent with the theory of nuclear magnetic resonance (NMR) spectroscopy; therefore, they are considered for further research. The study also included derivation of a common set of parameters for the calculation of C-13 and N-15 chemical shifts of cyclic systems. The derived parameters were tested by the estimation of the chemical shifts of other systems. Deviations were observed only in positions that were involved in large steric interactions.

**Key Words:** N-15 chemical shift, Additive parameters, Regression analysis

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