Estimation of the ^{35}Cl NQR Frequencies of Some Organic and Organometallic Molecules Using *ab initio* Calculations at Different Levels and Basis Sets

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Ab initio calculations of organic and organometallic molecules at RHF, B3LYP and MP2 levels and 6-31G(d), 6-31+G(d), 6-311G(d) and 6-311+G(d) basis sets were executed. They were used to estimate the ^{35}Cl NQR frequencies of these molecules. A satisfactory agreement between experimental and estimated NQR frequencies was obtained for the populations of the less diffuse 3p-components of the Cl atom valence p-orbitals obtained from the RHF, B3LYP and MP2 calculations with the split valence basis sets 6-31G(d) and 6-31+G(d). An analogous conformity was not obtained using the 6-311G(d) and 6-311+G(d) basis sets.

Key words: Ab initio Calculations; p-orbital Populations; ^{35}Cl NQR Frequency; Chloro-containing Organic and Organometallic Molecules.