# Correlation between the $^{35}$Cl NQR Parameters of Chloro-containing Organic and Organometallic Compounds and the Results of *ab initio* Calculations*

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The results of comparison of experimental $^{35}$Cl NQR parameters for a great number of organic and organometallic compounds and estimated ones using *ab initio* calculations at the RHF/6-31G(d) level were systematized. The NQR frequency changes on going from one compound to another depend, in general, on the changes of populations of the Cl atom $p_\sigma$-orbitals in these compounds and, first of all, of populations of their less diffuse parts.

*Key words: ab initio* Calculations; p-orbital Populations; $^{35}$Cl NQR Frequency; Asymmetry Parameter; Chloro-containing Organic and Organometallic Compounds.