Estimation of the ^{79}Br NQR Frequencies of Bromo-Containing Molecules Using *ab initio* Calculations at Different Levels

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Ab initio calculations of bromo-containing molecules on the RHF, B3LYP and MP2 levels and 6−31G(d), 6−31+G(d), 6−311G(d) and 6311+G(d) basis sets were executed. They were used to estimate the ^{79}Br NQR frequencies of these molecules. A satisfactory agreement between experimental and estimated NQR frequencies is obtained for the sum of populations of 13p- and 14p-components of the Br atom valence p-orbitals obtained from the RHF, B3LYP and MP2 calculations (particularly from RHF calculations) with the split valence basis sets 6−311G(d) and 6−311+G(d). The agreement between the experimental and estimated NQR frequencies is worse for the populations of the 9p-components of the Br atom valence p-orbitals obtained from these calculations with the basis sets 6−31G(d) and 6−31+G(d). An analogous conformity was not obtained using the populations of other components of the Br atom valence p-orbitals or their total populations obtained from all above-mentioned calculations.

Key words: ab initio Calculations; Valence p-orbital Populations; ^{79}Br NQR Frequency; Bromo-containing Molecules.