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

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\textit{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 $631+G(d)$ 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.

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