Ab initio Study of Nitrogen-14 Nuclear Quadrupole Coupling and NMR Signal Linewidths in Some Azoles*

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Ab initio values of Nitrogen ^{14}N Nuclear Quadrupole Coupling Constants (NQCC's) are calculated for a series of methyl-substituted azoles in the Multiconfigurational SCF (MCSCF) approximation. The four triazoles and two tetrazoles studied here are all isoelectronic. This enabled us to use the same level of approximation – basis set and active space – for all the molecules. The computed NQCC's are used to estimate the relative widths of the ^{14}N NMR signals, assuming an identical effect of molecular tumbling for all the nuclei in a molecule and neglecting solvent effects. The linewidths for the unsubstituted N atoms are, in agreement with experiment, much larger than for the methyl-substituted N atom. For the 1-methyl-tetrazole we present also the NMR shielding and spin-spin coupling constants and discuss in some more detail the dependence of all calculated NMR properties on the basis set and correlation effects.

Key words: ^{14}N NQCC, Azoles, MCSCF, *Ab initio*, Electron Correlation.

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