Solid State Effects in 4,6-Dichloropyrimidine Studied by ^{35}Cl-NQR Spectroscopy and ab initio Calculations

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Quantum chemistry methods – ab initio – have been used for the assignment of the ^{35}Cl-NQR resonance frequencies to particular chlorine atoms substituted in positions 4 and 6 of pyrimidine. The so-called solid state effect, that is the influence of intermolecular interactions, in particular hydrogen bond formation, on the NQR parameters has also been studied.

Key words: ^{35}Cl-NQR; 4,6-Dichloropyrimidine; Electronic Structure; B3LYP/6-31G*.