Conformational Structure of Chloromethyldichlorophosphines

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The ^{35}Cl nuclear quadrupole resonances (77 K) and ab initio calculations of trichloromethyldichlorophosphine (**I**) show that it exists in the chess conformation form. The barrier to internal rotation about the P-C bond in **I** at the RHF/6-31^{++} G(d,p) level equals to 38.1 kJ mol^{-1}. In chloromethyldichlorophosphine (**II**) the extension of the basis set up to the RHF/6-31^{++}G(df, pd) level does not improve the description of the most preferable gauche-conformation; only if electron correlation (at the MP2 level) is taken into account the results are in a good agreement with experimental data.

Key words: Chloromethyl- and Trichloromethyldichlorophosphine; Conformations; ^{35} Cl NQR Frequencies; *ab initio* and MNDO-PM3 Calculations.