Conformational Stability and Structural Determination of Vinyldichlorosilane by *ab initio* Calculations

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The Conformational stability and barriers of interconversion between the cis and gauche conformers of vinyldichlorosilane, $CH_2CHSiHCl_2$, have been studied using *ab initio* calculations employing the RHF/3-21G* and RHF/6-31G* basis sets. The cis conformer was found to be more stable than the gauche one by 45 cm^{-1} (539 J/mol) and 140 cm^{-1} (1.68 kJ/mol) from the RHF/3-21G* and RHF/6-31G* basis sets, respectively. Additionally, the structural parameters of both rotamers have been calculated. These results are compared with results of related molecules.

Key words: Conformational Stability; *ab initio* Calculations; Vinyldichlorosilane.