1-chloromethyl-1-fluorosilacyclohexane conformations and its rearrangements analysis by means of computational and vibrational study

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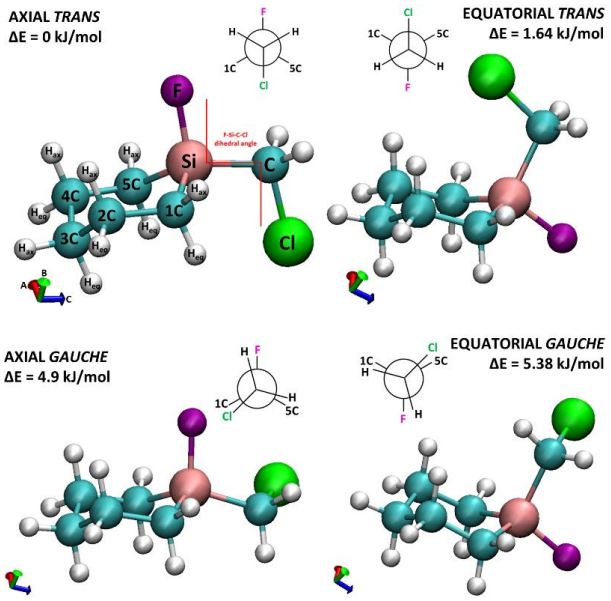
Organosilicon compounds can be very useful in the field of surface science. Cyclic hydrocarbon films have good surface adhesion properties which are mostly related to a π electron orbital[1]. Substituting one carbon atom in the ring with a silicon atom enhances adhesion since it acts as hydrolytically sensitive center that can react with inorganic substrates such as glass to form stable covalent bonds[2]. 1-chloromethyl-1-fluorosilacyclohexane is a newly synthesized molecular compound with unknown structural parameters and conformational diversity.



Fiqure 1 Structures of four lowest energy conformers of 1-chloromethyl-1-fluorosilacyclohexane and the respective DFT/B3LYP relative energies. The F-Si-C-Cl dihedral angle change is shown as Newman projection. Internal axes are marked as: A (red), B (green), C (blue).

Several different vibrational spectroscopy methods were employed to analyse the properties of this molecule. Infrared and Raman spectra were recorded for the sample in liquid phase. Additionally, IR spectra were registered in gaseous phase and after isolating the molecule in argon and nitrogen matrices with and without a usage of hot nozzle technique. DFT calculations were performed utilizing B3LYP functional and augmented Dunning correlation-consistent valence double zeta basis set. The 1-fluoro-1-chlormethyl-silacyclohexane molecule can reveal twelve conformations out of which the chair-axial-trans one has the lowest energy. However, there are also three more chair type conformers that are stable enough to possibly be observed in experimental spectra.

keywords: IR, Raman, matrix isolation, conformational analysis, DFT

Literature

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