CONFORMATIONAL DIVERSITY OF NON-AROMATIC HETEROCYCLIC MOLECULAR COMPOUNDS AS STUDIED BY MEANS OF MATRIX ISOLATION INFRARED SPECTROSCOPY

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Non-aromatic heterocyclic molecular compounds due to their π electron orbitals have potential to be used in the surface science as coatings with good surface adhesion properties. Such properties are even more pronounced when silicon atom is present in the ring. It is due to formation of stable covalent bonding between the coating and an inorganic substrate. The objective of this study is to elucidate conformational diversity of newly synthesized five and six membered non-aromatic cyclic compounds, namely 1-chloromethyl-1-fluorosilacyclohexane, 1-chloro-1-chloromethylsilacyclohexane, 1-chloromethyl-1-fluorosilacyclopentane and 1-chlorosilacyclopentane. In order to obtain structural parameters and to perform conformational analysis of such yet unknown molecules detailed computational and experimental studies were performed. The samples were investigated by means conventional IR and Raman spectroscopy as well as matrix isolation FTIR spectroscopy, solid nitrogen acting as matrix medium. Calculations were performed using ORCA 4.1.1 software package. Geometry of different conformers, their stability, normal vibrations and the potential barriers for the conformational interconversions were calculated using density functional theory (DFT) and utilizing augmented B3LYP hybrid functional and Dunning's augmented double zeta correlation consistent basis sets. Additionally, the Carr-Parinello Molecular Dynamics was used to mimic theoretically the matrix isolation conditions and to describe the molecular behavior in the systems with finite temperature. It was found that conformational equilibrium in the non-aromatic heterocyclic molecular compounds under study strongly depends on type of radical attached to the ring.