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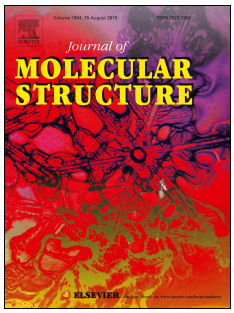

1-Dimethylamino-1-silacyclohexane: Synthesis, molecular structure and conformational behavior by gas-phase electron diffraction, Raman spectroscopy and detailed quantum chemical calculations

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1-Dimethylamino-1-silacyclohexane: synthesis, molecular structure and conformational behavior by gas-phase electron diffraction, Raman spectroscopy and detailed quantum chemical calculations

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Abstract

1-(N,N-dimethylamino)-1-silacyclohexane **1** was synthesized. Contributions of the conformers of **1,** Eq-*trans*: Eq-*gauche*: Ax-*trans*, were found to be 55(15):15(15):30(15) mol.% in gas phase at 288 K from gas electron diffraction. The enthalpy ΔH=0.29(15) kcal/mol for Ax-to-Eq transition was measured by temperature dependent Raman spectroscopy of liquid **1** and its solutions. Geometry, conformational properties and intramolecular conversion were explored by theoretical calculations. The nitrogen bond configurations for **1** was found to be close to planar, with a sum of the bond angles of ca. 350-355^{o} that is quite different from those analogs in which the N atom is connected to a carbon atom rather than to a silicon atom.

Keywords: 1-dimethylamino-1-silacyclohexane, synthesis, gas electron diffraction, quantum chemical calculations, Raman spectroscopy, potential energy surface

1. Introduction

Silacyclohexanes reveal specific properties as compared with carbon analogs [1]. Most evident for silacyclohexane derivatives is existence, and even preference, of conformers with axial position of a substituent attached to a silicon atom. For the cyclohexane derivatives, essential domination of equatorial forms is in general intrinsic. Probably, the most noticeable contribution of axial conformer for both, silacyclohexane and cyclohexane, was observed in case of a cyano group as a substituent [2,3]. A separate problem in conformational analysis