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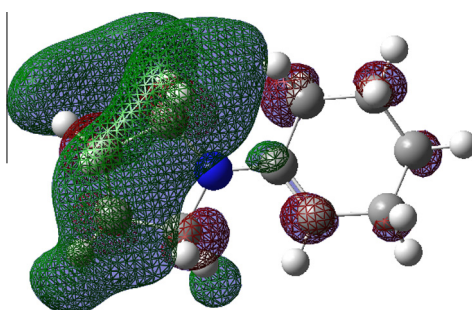
Vibrational spectroscopic investigation of 1-pyrrolidino-1-cyclohexene: A comparative density functional study

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HIGHLIGHTS

- Infrared, Raman and quantum chemical calculations of 1pych.
- Potential energy surface of 1pych.
- Mixture of envelope and twist forms of 1pych is supposed to be the most stable form.
- B3-LYP method is provides satisfactory results for the prediction vibrational data.

GRAPHICAL ABSTRACT



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ABSTRACT

Infrared and Raman spectra of 1-pyrrolidino-1-cyclohexene (1pych) have experimentally been reported in the region of 4000–100 cm⁻¹. The conformational analysis, optimized geometric parameters, normal mode frequencies and corresponding vibrational assignments of 1pych (C₁₀H₁₇N) have theoretically been examined by means of the Becke-3-Lee-Yang-Parr (B3-LYP) density functional theory (DFT) method together with the 6-31++G(d,p) basis set. Furthermore, reliable vibrational assignments have been made the basis of potential energy distribution (PED) and the thermodynamics functions, highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) of 1pych have been predicted. Angular distribution of the probability density of populations of its conformational isomers is determined by analysis of the potential energy surface (PES). Comparison between the experimental and theoretical results indicates that B3-LYP method is provides satisfactory results for the prediction vibrational wavenumbers and structural parameters and the mixture of envelope and twist conformers is supposed to be the most stable form of 1pych.

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Introduction

It has been reported that many pyrrolidine derivatives are of great interest in medicinal and pharmaceutical chemistry [1–6]. 1-Pyrrolidino-1-cyclohexene (1pych) is a pyrrolidine derivative and referred to in the literature by different synonyms such as 1-(1-cyclohexen-1-yl)pyrrolidine, N-cyclohexenylpyrroli-

dine, N-(1-cyclohexen-1-yl)pyrrolidine. 1pych has been used for the recyclisation of carbo- and heterocyclic compounds involving malononitrile and its derivatives [7], in the reduction of enamines [8], for analysis of the transition metal catalyzed hydroboration of enamines [9], and for expedient synthesis of a novel class of pseudo-aromatic amino acids [10].

Vibrational spectroscopy has widely been used as a standard tool for structural characterization of molecular systems together with DFT calculations [11–14]. DFT has big popularity as a cost effective general procedure for studying the physical properties

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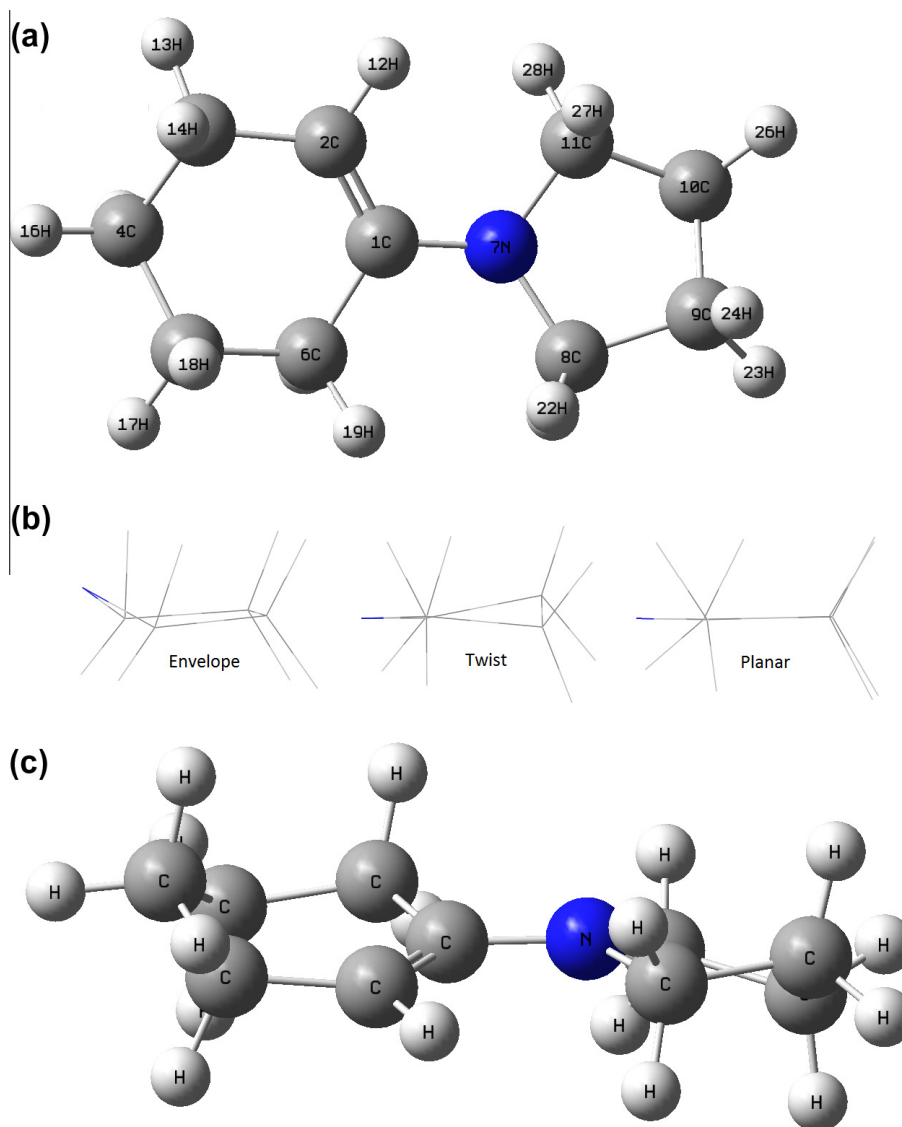


Fig. 1. Numbering of 1pych (a), possible stable conformations of pyrrolidine (b), optimized structure (conformer 8) for 1pych (c).

of molecules. Unlike Hartree Fock (HF) theory, DFT recovers electron correlation in the self-consistent Kohn–Sham procedure through the functions of electron density, so it is a cost effective and reliable method [11–14]. The DFT/B3-LYP model exhibits good performance on electron affinities, excellent performance on bond energies and reasonably good performance on vibrational frequencies and geometries of organic compounds [11–20].

Even though, 1pych has wide applications in many areas of science, to the best of our knowledge, there is no any information present in literature about its vibrational spectroscopic properties. A detailed quantum chemical study will aid in making definitive assignments to the fundamental normal modes and in clarifying the obtained experimental data of 1pych. Furthermore, all data presented may be helpful in the context of the further studies of 1pych. For the above goals, we have reported vibrational spectra of 1pych. The vibrational frequencies with PED values, HOMO and LUMO data and conformational analysis of 1pych are also investigated for its most stable conformer by means of B3-LYP/6-31+G(d,p) level. The results of the theoretical and spectroscopic studies are reported here.

Experimental

A commercial sample of 1pych in liquid phase was purchased (Sigma Aldrich, %97) and used without further purification. FT-MIR and FT-FIR spectra of 1pych in liquid phase were recorded in the region of 4000–400 cm^{-1} and 400–10 cm^{-1} with a Bruker Optics IFS66v/s FTIR spectrometer with a nominal resolution of 2 cm^{-1} . Raman spectrum was obtained using a Bruker Senterra Dispersive Raman microscope spectrometer with 532 nm excitation from a 3B diode laser having 3 cm^{-1} resolution in the spectral region of 4000–100 cm^{-1} .

Calculations

All the calculations were performed using Gaussian 09.A1 program [21] on HP DL380G7 server system and GaussView 5.0.8 [22] was used for visualization of the structure and simulated vibrational spectra. Many possible conformational isomers could be proposed for 1pych, but here, for the theoretical conformational

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