bioactivities, antifungal bioactivities and inhibitor activities against viruses. In the past few years, we have pursued investigations on the new thiourea derivatives. As a continuation of these studies, N-(2,2-diphenylacetyl)-N'-(naphthalen-1-yl)-thiourea (PANT) has been synthesized and characterized by elemental analysis, IR spectroscopy and ¹H-NMR spectroscopy. The crystal and molecular structure of the title compound has been determined from single crystal X-ray diffraction data. It crystallizes in the triclinic space group P-1, \( a = 10.284(2) \) \( \text{Å} \), \( b = 10.790(2) \) \( \text{Å} \), \( c = 11.305(2) \) \( \text{Å} \), \( \alpha = 64.92(3) ^\circ \), \( \beta = 89.88(3) ^\circ \), \( \gamma = 62.99(3) ^\circ \), \( V = 983.7(3) \) \( \text{Å}^3 \) and \( D_{calc} = 1.339 \) Mg/m\(^3\). The molecular structure, vibrational frequencies and infrared intensities of PANT were calculated by the Hartree-Fock and Density Functional Theory methods (BLYP and B3LYP) using 6-31G(d) basis set. The calculated geometric parameters were compared to the corresponding X-ray structure of the title compound. We obtained 22 stable conformers for the title compound; however the Conformer 1 is approximately 9.53 kcal/mol more stable than the Conformer 22. The comparison of the theoretical and experimental geometry of the title compound shows that the X-ray parameters fairly well reproduce the geometry of the Conformer 17. The harmonic vibrations computed of this compound by the B3LYP/6-31G(d) method are in a good agreement with the observed IR spectral data. Theoretical vibrational spectra of the title compound were interpreted by means of PEDs using VEDA 4 program. A general better performance of the investigated methods was calculated by PAVF 1.0 program.

Keywords: crystal structure, \textit{ab-initio} calculations, thiourea derivatives

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Molecular complex formation of medicinal cationic surfactants with aromatic compounds

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Some aromatic drugs (4-chloro-m-cresol of germicide, flopropione of antispasmodic agent, etc) make molecular complexes with quaternary ammonium halides such as hexadecyltrimethylammonium bromide (abbreviated as CTAB). The structures of the complex crystals have been analyzed by X-rays.\(^1\) They were shown to be very similar to those of the title compound. The comparison of the theoretical and experimental geometry of the title compound shows that the X-ray parameters fairly well reproduce the geometry of the Conformer 17. The comparison of the theoretical and experimental geometry of the title compound shows that the X-ray parameters fairly well reproduce the geometry of the Conformer 17. The harmonic vibrations computed of this compound by the B3LYP/6-31G(d) method are in a good agreement with the observed IR spectral data. Theoretical vibrational spectra of the title compound were interpreted by means of PEDs using VEDA 4 program. A general better performance of the investigated methods was calculated by PAVF 1.0 program.

Keywords: chiral recognition, inclusion compounds, alcohols

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Protein intrinsic disorder predicted with conditional random fields

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A large fraction of eukaryotic proteins harbour significant intervals of disordered residues which allow the protein to adopt multiple, alternate conformations (Dunker, et al., 2002). Frequently, such proteins have important biological functions in the cell, such as in...