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-1yl)-thiourea (PANT) has been synthesized and characterized by elemental analysis, IR spectroscopy and ^{1}H-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, *Z* = 2 with *a* = 10.284(2) Å, *b* = 10.790(2) Å, *c* = 11.305(2) Å, α= 64.92(3) °, β= 89.88(3) °, γ= 62.99(3) °, *V* = 983.7(3) Å^3 and *Dcalc* = 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, *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-chlro-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 each other. Moreover, we confirmed that these surfactant complexes had new characteristics. If an aromatic drug is a water insoluble drug, the dissolution rate is increase. If it easily takes oxygen damage, it is kept out to oxygenate. The complexes can control of the vaporization of drugs by heat treatment, too.[2, 3] We recently studied molecular complex formation between surfactant of different type in cationic surfactants, medicinal surfactants such as 1-hexadecylpyridinium bromide (abbreviated as CPB), benzyl(hexadecyl) dimethylammonium chloride (abbreviated as BCDAC), and aromatic compounds containing drugs (hydroquinone of treatment of skin pigmentation, etc). After many trials, we obtained complexes above fifteen, three of which were suitable for X-ray analysis. The three complexes, CPB/guaiacol, CPB/9-anthracenecarboxylic acid, and BCDAC/hydroquinone were obtained from alcohol or aqueous solutions. Their crystal structures were similar to that observed in the quaternary ammonium surfactant complexes. Therefore, these complexes will show the similar characteristics to those of the quaternary ammonium complexes.

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Keywords: molecular complex, surfactant, stabilization of drug

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Chiral recognition in cholamide crystals: Four-location model for hydrogen and stereogenic carbon

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A four-location model for enantioselective inclusion of secondary aliphatic and aromatic alcohols with steroidal acids and their derivatives is presented. In principle, two kinds of disordered structures of guest components may be observed in a concave cavity at least. The one is that a stereogenic carbon of the guest is disordered with a substituent, such as a hydrogen. The other is that the stereogenic carbon is almost fixed while two neighboring substituents, such as a hydrogen and a methyl group, are disordered. For example, cholamide accommodates 2-methyl-3-hexanol (**1**) and 2,2-dimethyl-3-hexanol (**2**) into its channels. (*S*)-isomer of **1** is separated in less than 20% ee, while that of **2** in more than 98% ee. Crystallographic studies brought us a profound insight for such one methyl group effect in chiral recognition. It was confirmed that the inclusion crystal of **1** exhibits a disordered structure of hydrogen around a stereogenic carbon, while that of **2** a definite structure. Such a difference requires a chirality recognition model which explains selective locations of the forth substituent, hydrogen, together with chiral carbon. Employment of a four-location model resulted in a successful interpretation for the chirality recognition. Moreover, cholamide includes various 1-phenylethanol derivatives. Among them, (*S*)-isomers of ortho-substituted 1-phenylethanols showed higher enantioselectivity than those of para-substituted ones. X-ray crystallographic analysis clarified that the former has a definite structure in the channels, while the latter has a disordered structure between hydrogen and methyl group. The four-location model enabled us to explain these experimental results for enantioresolution.

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