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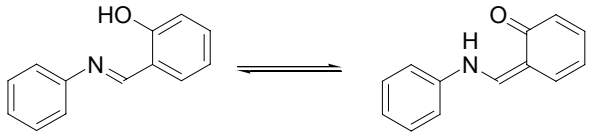
Proton tautomerism is a general phenomenon in organic molecules and plays a vital role in many fields of chemistry and biochemistry. The tautomerism of salicylideneanilines [eq(1)] has attracted a considerable attention because it is closely related to thermo- and photochromism. Salicylideneanilines greatly favor the enol form over the *cis*-keto form in the gas phase. We demonstrate here that the instability of the *cis*-keto form is substantially reduced by intermolecular hydrogen bonding and also by self-association, on the basis of our variable temperature X-ray crystallographic and UV-vis absorption spectroscopic studies.[1]-[3].



(1)

enol form *cis*-keto form

[1] Ogawa K., Kasahara Y., Ohtani Y., Harada J., *J. Am. Chem. Soc.*, 1998, **120**, 7107. [2] Ogawa K., Harada J., Fujiwara T., Yoshida S., *J. Phys. Chem. A*, 2001, **105**, 3425. [3] Fujiwara T., Harada J., Ogawa K., *J. Phys. Chem. B*, 2004, **108**, 4035.

Keywords: proton tautomerism, self-association, salicylideneanilines

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The First Observation of All Six Elastic Constants in Tetragonal Hen Egg-white Lysozyme Crystals

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It is interesting to investigate the elastic property of protein crystals. Previously, we have reported the longitudinal sound velocity of tetragonal hen egg-white (HEW) lysozyme crystals which are one of typical protein crystals using an ultrasonic pulse-echo method [1]. However, there is no measurement of all components of elastic constants, C_{ij} in tetragonal HEW lysozyme crystals since the measurements of transverse ultrasonic wave have not been carried out yet. In case of pulse-echo method, in order to generate a transverse ultrasonic wave in the crystals, a transducer must be in close contact with the crystal. However, hydrated protein crystals are fragile, and consequently, it was difficult to glue a transducer to a protein crystal. Recently, we found that the sound velocity increases with exposure to open air and approaches a constant value [2]. This suggested that the protein crystals became harder due to dehydration. Therefore, we have succeeded in the contact between a crystal and a transducer using dehydrated crystals. This led us generating a transverse ultrasonic wave through the dehydrated HEW lysozyme crystals at 42% relative humidity (RH). As a result, all components of elastic constants in dehydrated crystals were determined.

[1] a) Tachibana M., Kojima K., Ikuyama R., Kobayashi Y., Ataka M., *Chem. Phys. Lett.*, 2000, **332**, 259; b) Tachibana M., Kojima K., Ikuyama R., Kobayashi Y., Ataka M., *Chem. Phys. Lett.*, 2002, **354**, 360. [2] Tachibana M., Koizumi H., Kojima K., *Physical Review E*, 2004, **69**, 051921.

Keywords: ultrasonics, elastic properties, protein crystals

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5,5'-Disubstituted-3,3'-Methanediyl-*bis*-Indoles as Potential Antitumorals

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Certain compounds found in the diet are a potential source of new classes of chemotherapeutic and chemopreventive agents. Indole-3-carbinol, a major indole metabolite from cruciferous vegetables, and its natural condensation product 3,3'-diindolylmethane, have been found to inhibit the development of tumors in breast, uterus and liver [1-3]. However, both compounds may exhibit adverse tumor promoting activity in other organs. In search for new *anti* cancer agents we have decided to investigate 3,3'-diindolylmethane derivatives which may reduce the growth of human tumor cell lines by the inhibition of the binding of some transcription factors to the adequate sequences in DNA.

To determine structural parameters important for the biochemical activity we have performed the ^{1}H and ^{13}C NMR data and single crystal X-ray analysis of 5,5'-disubstituted-3,3'-methanediyl-*bis*-indoles. The results of these studies indicate insignificantly different molecular structures of the investigated compounds but significantly different networks of intermolecular interactions in crystals. Interesting NH$\cdots\pi$ hydrogen bonds are observed which may have a functional role in biological features.

[1] Grubbs C.J., et al., *Anticancer Res*., 1995, **15**, 709. [2] Cover C.M., et al., *J. Biol. Chem*., 1998, **273**, 3838. [3] Hong C., et al., *Bioch. Pharmacol*., 2002, **63**, 1085.

Keywords: anticancer compounds, 5,5'-disubstituted-3,3'-methanediyl-*bis*-indoles, X-ray single- crystal diffraction

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Intermolecular Interactions in 1,1'-Binaphthyl, Polymorphs and Symmetry Breaking

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A theoretical-experimental work is presented related with the chiral symmetry breaking of melting crystallization of 1,1'-binaphthyl derivatives and polymorphism. We confirm that the chiral symmetry breaking can be observed in crystallization from a melt of 1,1'-binaphthyl by a constant stirring during the crystallization. Crystallographic studies by Powder X-ray diffraction (PXRD) reveal two crystallographic forms of 1,1'-binaphthyl: one chiral form ($P42_12_1$) with either R or S enantiomers of the trans-1,1'-binaphthyl conformer and another racemic crystal (C2/c) with both enantiomers of the cis-1,1'-binaphthyl conformer. Quantum mechanical calculations of the crystal lattice for 1,1'-binaphthyl and 2,2'-dihydroxy-1,1'-binaphthyl polymorphs were performed by Density Functional Theory approximation. Our calculations reproduce the crystal lattice parameters and PXRD pattern finding the $P42_12_1$ form with lower energy than the C2/c form for 1,1'-binaphthyl. The main intermolecular interactions in 1,1'-binaphthyl crystals are weak aromatic CH/π hydrogen bonds, which are responsible for enantiomeric discrimination in the molecular recognition during crystallization. The C2/c form achieves a more efficient packing than the chiral one, but intermolecular interactions in $P42_12_1$ form are stronger than in C2/c form. In 2,2'-dihydroxy-1,1'-binaphthyl the intermolecular interactions are stronger with hydrogen bonds between the hydroxyl groups and polymorphs can be predicted by Monte Carlo simulated annealing.

Keywords: 1,1'-binaphthyl, intermolecular interactions, chiral recognition

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Experimental and Theoretical Study of Weak Interactions in Simple Molecular Solids

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