

in their response to external actions. Crystals of amino acids are of special interest in this respect because the structure-forming units in these crystals are similar to those in the biopolymers and can be used as biomimetics. The data on response of intermolecular interactions to changes in temperature and pressure in these systems may be considered also for studying properties of complicated biomolecules such as proteins. In addition, crystalline amino acids are of interest for their ferroelectric, piezoelectrical, and nonlinear optical properties [1, 2].

In this work structural changes in DL-serine were studied in the pressure range 0.2 – 4.3 GPa. An Almax-Boehler diamond anvil cell was used to create hydrostatic pressure. Single-crystal X-ray diffraction and polarized Raman spectroscopy were selected for investigation of these crystals under high pressure. This combination of spectroscopy and diffraction made it possible to follow the changes in the individual hydrogen bonds with pressure in many details. The two techniques give complementary information: diffraction experiments provide data on the changes in atomic coordinates averaged over space and time; a detailed spectroscopy study can help in understanding the dynamic processes related to pressure changes (compression of individual intermolecular hydrogen bonds, rotation of molecules as a whole and of the individual molecular fragments).

Anisotropic structural compression of crystalline DL-serine was carefully studied in [3]; no phase transitions were detected up to 8.6 GPa. At the same time, as has been shown in the present contribution, the lengths of intermolecular hydrogen bonds linking amino-groups and serine side chains in the crystal structure depend non-linearly and non-monotonic on pressure in the range between 0.4 and 1.5 GPa. This is an interesting and unusual phenomenon. Another interesting observation is the rotation of carboxylic groups of serine with increasing pressure. The structure changes manifest themselves in the low-wavenumber range of the Raman spectra and can be detected by analyzing the redistribution of intensities and the shifts of appropriate modes.

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Pressure enhancement of CH \cdots O interactions in simple ethers

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CH \cdots O interactions attract attention of crystallographers, chemists and biochemists, although their importance was generally accepted only in the last years of 20th century [1]. Despite their weakness (typical potential energy < 4 kJ/mol), the topology of electron density redistribution accompanying the H-bond formation is similar to that of conventional hydrogen bonds [2]. Spectroscopic studies revealed that under high pressure van der Waals CH \cdots O interactions are enhanced and convert into hydrogen bonds [3]. We have recently supported this view with structural data.

Two simple ethers, tetrahydrofuran (THF) and its open-ring analogue diethyl ether (DE) have been chosen for the experiments to avoid blurring CH \cdots O interactions by stronger hydrogen bonds or Coulombic forces. For THF both isochoric crystallization at 2.25, 3.26, and 3.80 GPa and isobaric freezing at ambient pressure lead to a monoclinic phase, space group *C2/c* [4]. The CH \cdots O interactions are the strongest intermolecular forces in the THF molecular crystal, and the hierarchy of the CH \cdots O distances correlates with the electrostatic potential distribution on a molecular surface and with their alignment along the lone pair direction. In THF the exposed oxygen atom is involved in six short CH \cdots O contacts, what is not accounted for strong hydrogen bonds. In compressed THF the CH \cdots O contacts acquire the features of hydrogen bonds, and therefore the structure is stable to at least 3.80 GPa.

At low temperature DE crystallizes in the space group *P2₁2₁2₁*, *Z* = 8 [5]. The structure is fairly loosely packed, and each oxygen atom of two symmetry-independent molecules is involved in three CH \cdots O contacts shorter than 3 Å. At high pressure DE undergoes phase transitions leading to the structures with CH \cdots O contacts resembling hydrogen bonds in THF. The energetic cost of the transformation involves conformational changes facilitating the access to oxygen atom and hence the increased number of CH \cdots O contacts per molecule.

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Structure study of IPMDH from piezosensitive and piezophilic *Shewanella* species

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The organisms living in deep sea such as the Mariana Trench must be adapted to extremely high-pressure environment. For example, protein 3-isopropylmalate dehydrogenase (IPMDH) from deep-sea bacteria *Shewanella benthica* DB21MT2 (SbIPMDH) remains active under such extreme conditions, while that from land bacteria *S. oneidensis* MR-1 (SoIPMDH) becomes inactivated [1]. In order to unravel the differences existing between these two IPMDHs, we are here attempting to solve their structures by a high-pressure protein crystallography (HPPX) method using a diamond-anvil cell (DAC).

To make HPPX measurements possible at the beamline PF AR-NW12A, we have modified several equipments such as the goniometer head to accept our DAC. Using such settings, the crystal structures of SoIPMDH- and SbIPMDH-IPM complexes have been determined at about 2 Å resolution under multiple pressures and up to several hundreds MPa.

Pressure dependence of SoIPMDH- and SbIPMDH-IPM complexes is nearly uniform up to 300 MPa, and the compressibilities of the two