A new polymorph of glycine formed at high pressure

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The crystals of amino acids can act as biomimetics, allowing one to model interactions in the biopolymers, such as peptides. Glycine is the simplest amino acid, but even at ambient conditions it is known to form three different polymorphs, well-characterized structurally and thermodynamically [1,2]. In all the three polymorphs the same structural "synthone" can be found – a "head-to-tail" chain of the zwitter-ions linked by NH…O hydrogen bonds. Via extra NH…O bonds, these chains form similar layers in the α- and the β-polymorphs (stacking of the layers in the two polymorphs being different), and triple helices linked with each other in a 3D-network – in the γ-polymorph.

When hydrostatic pressure was applied to the samples of the α-polymorph, no phase transitions were detected (unambiguously) either by X-ray diffraction at pressures up to 3.5 GPa [3], or by Raman spectroscopy at pressures below 23 GPa [4]. When pressure was applied to the γ-polymorph, a first-order not phase transition was observed that started at about 2.73 GPa and was still not absolutely complete even at 7.85 GPa. The transition was only partly reversible. The crystal structure of the previously unknown high-pressure polymorph of glycine (δ-polymorph) could be solved and refined in the space group Pn [5]. In this structure, glycine zwitter-ions are linked via NH…O hydrogen bonds into the chains and further into the layers, which form double-layered bands via additional NH…O hydrogen bonds. The structure of the individual layers in the high-pressure polymorph is similar to that in the previously known α- ($P2_1/n$) and β- ($P2_1$) forms, but the packing of the layers is essentially different. The pressure-induced polymorphic transformation in the γ -glycine can be compared with a change in the secondary structure of a peptide, when a helix is transformed into a sheet. The distortion of the chains of zwitter-ions in the γ-and in the δ-polymorphs was continuous in all the pressure range from ambient to 7.85 GPa, despite a polymorphic transformation, thus confirming that these chains can be considered as important "building blocks" preserved in all the glycine polymorphs.

The study was supported by RFBR (grant 02-03-33358), the BRHE-Program (grant NO-008-XI), Russian Ministry of Education (grants Ч0069 of the "Integration"-Program; 3H-67-01; and yp.05.01.021 of the Program "Universities of Russia"), and the National Science Support Foundation for EB (Program "Young Professors"). The diffraction experiment using synchrotron radiation was carried out at the Swiss-Norwegian Beamline at ESRF (Grenoble), experiments 01-02-656 и 01-02-671.

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