

s11.m33.p3 **Effect of High Pressure on the Crystalline Glycine: a New High-Pressure Polymorph Formation.** S.N. Ivashevskaya^{a,c}, E.V. Boldyreva^{a,b}, H. Sowa^d, H.Ahsbahs^f, H.-P. Weber^e, ^aNovosibirsk State University, Pirogova, 2, Novosibirsk, 90, 630090 Russia, ^bInstitute of Solid State Chemistry and Mechanochemistry, SB RAS, ^cInstitute of Geology, Karelian Research Center RAS, ^dPhilipps-Universität Marburg, Germany, ^eSNBL ESRF, Grenoble, France. E-mail: sveta@xray.nsu.ru

Keywords: High pressure; Powder diffraction; Polymorphism

The research of high-pressure effect on organic molecular crystals is important for prediction of behavior of drugs, materials and systems, which are based on molecular crystals in non-ambient conditions. A possibility of high-pressure polymorph formation for glycine was mentioned (Dawson A., Parsons S., Allan D., Loveday J., Guthrie M., <http://www.isis.rl.ac.uk/BCA2001/Abstract%20files/bca1>), but no data, which could confirm the hypothesis or describe the crystal structure of the new phase were published. The studies of the effect of high hydrostatic pressure on the alpha-modification of glycine did not show any phase transitions up to 4 GPa (X-ray diffraction research) [1] or up to 23 GPa (Raman scattering) [2]. There were some preliminary data that gamma-glycine may undergo a phase transition at about 3 GPa [1]. A high-resolution powder diffraction study of the effect of high hydrostatic pressure up to 8 GPa on the gamma-polymorph of glycine (P3₁) was carried out. A first-order phase transition was observed. The transition starts at about 2.73 GPa and is still not absolutely complete even at 7.85 GPa. The crystal structure of the previously unknown high-pressure polymorph of glycine could be solved and refined in the space group Pn ($a=5.379(1)\text{\AA}$, $b=5.557(1)\text{\AA}$, $c=4.780(1)\text{\AA}$, $\beta=118.25(1)^\circ$, $V=125.86(4)\text{\AA}^3$, $Z=4$). The monoclinic unit cell dimensions were determined with the indexing program TREOR90 [3] using the first 15 peak positions ($M_{15}=67$, $F_{15}=126$). The structure was solved by the grid search procedure [4] and refined with the use of bond restraints by the MRSA program [5]. H atoms were placed in geometrically calculated positions.

In this structure, glycine zwitter-ions are linked via NH...O hydrogen bonds into layers, which, in turn, form double-layered bands due to the formation of additional NH...O bonds in the direction normal to the layers. The structure of the individual layers in the high-pressure polymorph is similar to that in the previously known alpha- (P2₁/n) and beta- (P2₁) forms, but the packing of the layers is essentially different. The pressure-induced polymorphic transformation in the gamma-glycine can be compared with a change in the secondary structure of a polypeptide, when a helix is transformed into a sheet.

The study was supported by grants of SNBL (experiments 01-02-656 and 01-02-671), NO-008-X1 (BRHE), 0069 & yp.05.01.021 (Russian Ministry of Education), 02-03-33358 (RFBR), Foundation of Support of National Science (Russia).

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s11.m33.p4 **In Situ Diffraction Study of C60 Polymerization.** Leonel Marques^a, Mohamed Mezouar^b and Jean-Louis Hodeau^c, ^aDepartamento de Física, Universidade de Aveiro, 3800 Aveiro, Portugal, ^bE.S.R.F 38041 Grenoble, France, and ^cLaboratoire de Cristallographie, CNRS BP166 Cedex09, 38042 Grenoble, France. E-mail: marques@fis.ua.pt

Keywords: Fullerenes; High-pressure; Polymerization

Polymerization in pure C60 has been achieved using photochemical and high pressure-high temperature (HP-HT) methods. It has been well established that, in differently synthesized polymers, the same polymeric bond, 2+2 cycloaddition, occurs. Despite this common chemical nature of both HP-HT polymers and photopolymers, their crystal structures are very different. HP-HT polymers display ordered structures that have been elucidated by diffraction techniques [1]. Depending on pressure ($P < 8$ GPa), different polymeric phases based on 1D chains and 2D square or triangular layers are considered. In contrast, photopolymers have a disordered fcc structure, compressed with respect to the monomer, indicating a statistically random (isotropic) polymerization along all nearest neighbor directions [2]. The origin of bond order in HP-HT polymers and its absence in photopolymers, is not presently understood. Motivated by this issue, we performed an in situ HP-HT diffraction study of C60 polymerization using synchrotron radiation at the E.S.R.F. [3]. We have found that the applied anisotropic stress selects the directions of bonding inducing an anisotropic distribution of polymeric bonds. This selection is crucial to obtain ordered polymeric structures since it avoids geometrical frustration inherent to 2+2 cycloaddition interfullerene bonds in the monomer fcc lattice. The photo-induced polymerization method, having no symmetry-breaking field, leads to a frustrated disordered fcc polymer. The anisotropic polymer growth process found by us leads naturally to a highly anisotropic distribution of intermolecular bonds that should be at the origin of the observed elastic anisotropy in the C60-derived amorphous samples and the magnetic anisotropy in 2D ordered polymerized C60.

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