study has also revealed some flaws in the previous model of inter-double-helix hydrogen bonding.

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## MS19 P04

**Fullerene – Fullerene Interactions in the Crystals of the Fullerene $C_{60}$ Organic Derivatives**

Aidar Gubaidullin, Alina Sayfina, Igor Litvinov, Valentina Gubskaya, Ildus Nuretdinov. *Institute of Organic and Physical Chemistry of RAS, Kazan, Russian Federation.*
E-mail: aidar@iopc.knc.ru

**Keywords: fullerenes, crystal packing, amphiphilic properties**

Functionally substituted fullerene derivatives are of interest since it is possible to obtain both biologically active substances and new materials for nanotechnology on their basis. The spherical platform of fullerene allows one to design molecules with various fragments, which are responsible for the specific properties. At the same time the crystal structure of such compounds is studied insufficiently, that is why Crystallographic Data Bases contain information about not more than 80 fullerene C60 derivatives structures. Interesting feature of these compounds (both derivatives and fullerene complexes) in solid state is their active participation in pi-electronic interactions between each other and with other compounds incorporating aromatic fragments. Owing to these interactions the compounds can form in a crystal the supramolecular structures of various type, that, apparently, finds reflection in their particular properties.
Basing on literature structural data for organic derivative of fullerene and on our original X-ray data for the bis- and mono-adducts of the methanofullerenes and pyrrolidino-fullerenes, we have analysed the intermolecular interactions, crystal packing and supramolecular structure of these compounds from the point of view of such interactions. It was found, that in spite of the presence of large substituents in the molecules and solvate molecules in the crystals, which hinder such interactions, the fullerene fragments are closely packed with different fullerene environments - honeycomb structure, zigzag-chain, dimers, columns and layers, and preferably interact face-to-face with the 5- and 6-membered aromatic rings. The majority of the compounds forms 2D-structures - layers of various topology with fullerenes coordination equal to 3 or 4. Presence of molecules-guests with aromatic fragments or aromatic fragments in the fullerene derivatives leads to their obligatory participation in such interactions and to the destruction of the fullerene-fullerene interactions.
Recently we carried out the synthesis of malonate nitroxide metanofullerene, which shows, in combination with known anticancer drug cyclophosphamide, the high antitumor activity against leukemia P-388. It was shown by X-ray single crystal analysis that methanofullerene with two nitroxide groups has a diamond-like environment in the crystal due to fullerene-fullerene interactions [1]. In the same time the first examples of the phosphorylated mono- and bis-methano-fullerenes with large substituents have lower coordination of fragments - zigzag chains and pi-dimers. The comparative analysis of the results for the organic derivatives and for the fullerene C60 inclusion compounds is presented. The topology of the crystals is analysed additionally on the base of proposed model of localization of hydrophilic and hydrophobic regions in the crystals of organic compounds.
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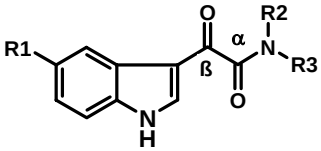
## MS19 P05

**Molecular and Supramolecular Features of Glyoxylamides**

C. H. Schwalbe[a], S. Nasima[a], S. Freeman[b], D. Mansell[b], S. D. Brandt[c], J. F. Alder[d], [a]*School of Life and Health Sciences, Aston University, Birmingham B4 7ET.* [b]*School of Pharmacy and Pharmaceutical Sciences, University of Manchester, Manchester M13 9PL.* [c]*School of Pharmacy and Chemistry, Liverpool John Moores University, Liverpool, L3 3AF.* [d]*School of Chemical Engineering and Analytical Science, University of Manchester, M60 1QD.*
E-mail: C.H.Schwalbe@aston.ac.uk

**Keywords: hydrogen bonds in organic crystals, conjugated organic compounds, conformational flexibility**

Indole-3-ylglyoxylamides are important intermediates in legal and illegal syntheses of pharmaceutically active tryptamine derivatives. We report 3 secondary glyoxylamide structures: I (R1 = R2 = H, R3 = i-Pr), II (R1 = R2 = H, R3 = t-Bu), III (R1 = OMe, R2 = H, R3 = t-Bu).




Secondary glyoxylamides in the Cambridge Structural Database (CSD) always adopt the *syn* conformation with H in the R2 position and O=C-C=O torsion angles within 40° of 180°. Tertiary glyoxylamides have O=C-C=O torsion angles within 40° of 90° or 270°, sacrificing conjugation but alleviating interference between R2 and O. When R2 ≠ R3, the usual *anti* conformation puts the bulkier substituent at R2.