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

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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

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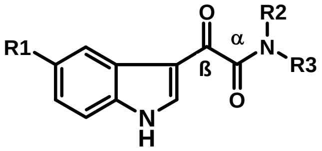
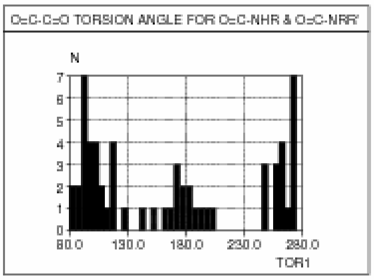
Keywords: hydrogen bonds in organic crystals, conjugated organic compounds, conformational flexibility

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.



In I-III and secondary glyoxylamides in the CSD the amide resonance makes the average α C=O longer than the β C=O, but by <0.01 Å, suggesting fairly similar abilities as hydrogen bond acceptors. From a secondary indol-2-ylglyoxylamide structure Black et al. [1] inferred that a set of 3 hydrogen-bonded rings, S(5) from amide H to β-O, $R_2^2(10)$ involving the same atoms intermolecularly, and S(6) from indole NH to α-O could be a robust supramolecular synthon. In a series of indol-3-yl analogues we find that the S(5) persists, and the S(6) replaces the indole NH with the adjacent CH as donor but remains fairly strong. However, C(4) chains linking amide H to α-O occur as often as the $R_2^2(10)$ motif.

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MS19 P06

Reaction of 1,3,5-triazacyclohexane with copper : formation of other complex

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Keywords: Triazacyclohexane , copper complexes , X-ray.

Copper complexes with three facially coordinating nitrogen atoms play an important role in the biological binding and activation of dioxygen[1]. They are used, for example, as bioinorganic model systems, reagents with high metal ion selectivity or as olefin polymerisation catalysts.

Many complexes containing triazacyclohexane and larger macrocyclic amines are known [2,3] .

The title complex 1,3,5-(4-methylphenyl)-1,3,5-triazacyclohexane **1** is prepared by reaction of formaldehyde with primary amine (4-methyl aniline)[4].

The complexantion of 1,3,5-(4-methylphenyl)-1,3,5-tricyclohexane **1** give a bimetallic complex in which the ligand is fragmented (Fig 1).

As the coordination number of these copper complexes is two short bonds between (1.879 and 1.881Å).

The Para magnetism of this complex made it difficult to get useful H-or C-NMR. The ligand and complex were characterized by X-ray crystallography.

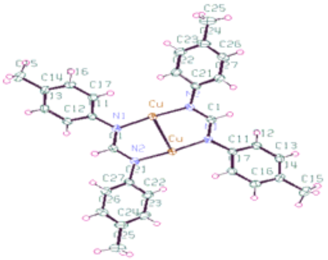

Figure 1: X- ray structure of (p-tol)NCHNH(p-tol)

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MS19 P07

The Structural Class Concept, an Extension

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Keywords: structural-class, symmetry , packing

Novacki [1] was the first to study space group frequencies at a time when the space groups were only known for about 3000 crystal structures. Since then a number of studies has appeared. An important improvement in this field was introduced by Belsky et al. [2,3] with the structural class concept, which beside the space group also includes the Z value and the distribution of molecules over equivalent positions. Implicit in this notation is also unoccupied special positions, which is of importance in discussing crystal packing, since every unoccupied position is a waste of space [4]. Therefore it is suggested that these positions should be added to the structural class notation in the following way: a semicolon shows the end of the structural class and then the unoccupied special positions are given within brackets. No unoccupied special positions are denoted ;[0]. An obvious notation would be $P2_1/c$,Z=2(-1);[(-1^3)] and $P2_1/c$,Z=4(1);[(-1^4)] etc. This notation will thus explicit give an overview of all Wyckoff positions, occupied or not, and will be helpfull in addressing questions like *i)* which molecular symmetries are retained and avoided in the solid state and *ii)* which Wyckoff postions are unoccupied. A few examples regarding complexes *cis/trans*-PtX_2L_2 and *cis/trans*-PtX_4L_2, where X=halogen and L=neutral ligand, will be discussed.

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MS19 P08

Unusual tin(II)-iron complexes $(RO)_2Sn\text{-}Fe(CO)_4$ and $\{[Li][(RO)_3Sn\text{-}Fe(CO)_4]\}_2$ (R = $CH_2CH_2NMe_2$)

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Keywords: tin(II), transition-metal complexes, X-ray diffraction analysis

Two new tin(II)-iron complexes $(RO)_2Sn\text{-}Fe(CO)_4$ (**3**) and $\{[Li][(RO)_3Sn\text{-}Fe(CO)_4]\}_2$ (**4**) (R = $CH_2CH_2NMe_2$) have been structurally characterized. Unusual types of heteronuclear bonding between heavier Group 14 elements and transition metals have been revealed. The iron atoms both in **3** and **4** have a trigonal-bipyramidal coordination typical for FeL_5-fragments. The "stannylene" ligand in **3** occupies the equatorial position, whereas the stannate ligand in **4** is axially disposed. The structures of **3** and **4** indicate that the monomeric tin(II) compound $(RO)_2Sn$ (**1**) [1] is a better π-acceptor than a σ-donor toward iron [2] and thus displays the stannylene-like properties, while the