

The title compound belongs to class of Coumarins. Coumarins are toxins found in many plants, notably in high concentration in the tonka bean, woodruff, and bison grass. Coumarins are important because of their extensive plant origin. They have been used in perfume industry. Coumarin and their derivatives have both clinical and medical value as the precursor for several anticoagulants, notably warfarin, used as a gain medium in some dye lasers. The compound  $C_{11}H_{10}O_2$ , crystallizes under orthorhombic system,  $P2_12_12_1$  space group, with cell parameters  $a = 5.232(2)$ ,  $b = 11.888(4)$  and  $c = 13.192(5)$  Å  $Z = 4$   $V = 820.5(5)$  Å<sup>3</sup>. The data of the compound is collected using Bruker CCD diffractometer with graphite monochromated MoK $\alpha$  radiation. The structure is solved using SHELXS-97 and refined using SHELXL-97 till R value converges to 0.0714. There are no intramolecular hydrogen bonds within the molecule. The molecular structure is stabilized by intermolecular C-H...O hydrogen bonds and C-H... $\pi$  interactions.

Keywords: single-crystal structure determination, small-molecule structures, hydrogen bonds

### P06.04.11

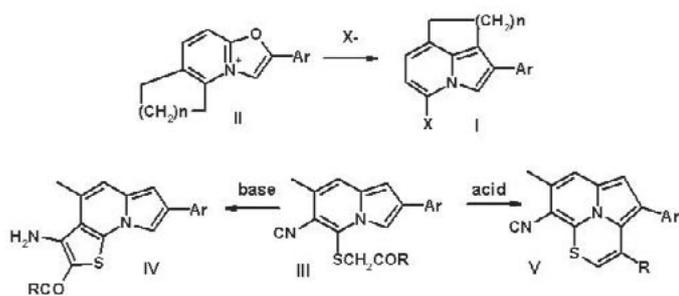
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#### X-Ray data for novel tricyclic compounds based on indolizines

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During the past decade we have investigated representative set (~50 single crystals and powders) of indolizines I and their precursors - oxazolopyridinium salts II. The structural trends in the families I, II will be overviewed, and the role of the size of third annelated cycle in the salts II on the direction of rearrangement of II to I will be discussed. Novel cyclizations have been found for indolizines III from which novel tricyclic structures IV and V can be formed under the action of bases or acids. Unusual structural features of anti-aromatic cyclazines V will be presented. This work was supported by Russian Foundation for Basic Research (grant 07-03-00921-a).



Keywords: molecular structure, heterocycle, indolizine

### P06.04.12

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#### Crystalline molecular assemblies of dehydrobenzo[12]annulenes having carboxylic groups with amines

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Dehydrobenzoannulenes (DBAs) have been of much interest from a viewpoint of their optoelectronic properties due to their rigid, planar, cyclic structures with rich pi-electrons. Moreover, DBA derivatives are adapted as building blocks of supramolecular assemblies. Recently, we reported that hexadehydrobenzo[12]annulene with carboxylic groups form face-to-face, pi-stacked one-dimensional assembly in the crystalline state. The crystal showed significantly-anisotropic charge carrier mobility along the columnar axis, indicating that molecular arrangements play an important role for such properties in the solid state, in addition to molecular structures themselves. Here we present crystal structures of organic salts of octadehydrobenzo[12]annulene having carboxylic groups (Figure) with various amines. The salts were obtained in methanol and then recrystallized from various organic solvents. The hydrogen-bonding groups construct various networks which depend on molecular structures of the amines employed. We discuss a relationship between the molecular arrangements and the optoelectronic properties.

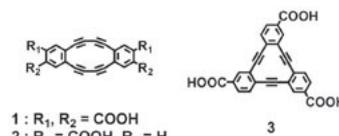


Figure. Dehydrobenzo[12]annulenes with carboxylic groups

Keywords: molecular assembly, conjugated organic compounds, organic synthesis

### P06.04.13

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#### Structures of benzo and dibenzo [d,f] [1,3,2] dioxaphosphepine 3-oxide (I, II) and 6-sulphide(III)

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Orgnophosphorus compounds are widespread in nature and they have unique multifaceted applications as anticancer agents, insecticides and lubricating oil additives and polymer stabilizers. The structures of the title compounds are determined to know the effect of substituents on the conformation of dioxaphosphepine ring. Crystal data (I):  $C_{15}H_{15}O_4P$ , Monoclinic, space group  $P2_1/n$ ,  $a = 9.441(10)$ ,  $b = 15.202(16)$ ,  $c = 9.746(10)$  Å,  $\beta = 95.782(2)^\circ$ ,  $V = 1391.5(3)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.385$  Mg m<sup>-3</sup>, 16173 reflections measured, 2457 unique [ $I > 2 \cdot (I)$ ],  $R$  value 0.0495,  $wR2 = 0.1145$ . Crystal data (II):  $C_{14}H_{12}ClO_4P$ , Monoclinic, space group  $P2_1/c$ ,  $a = 13.585(2)$ ,  $b = 8.719(1)$ ,  $c = 13.106(2)$  Å,  $\beta = 118.15(2)^\circ$ ,  $V = 1368.7(3)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.508$  Mg m<sup>-3</sup>, 6682 reflections measured, 2410 unique [ $I > 2 \cdot (I)$ ],  $R$  value 0.0512,  $wR2 = 0.1118$ . Crystal data (III):  $C_{18}H_{11}Cl_2O_3PS$ , Monoclinic, space group  $P2_1/n$ ,  $a = 10.816(6)$ ,  $b = 13.615(8)$ ,  $c = 12.321(7)$  Å,  $\beta = 99.583(9)^\circ$ ,  $V = 1789.0(18)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.519$  Mg m<sup>-3</sup>, 8553 reflections measured, 3119 unique [ $I > 2 \cdot (I)$ ],  $R$  value 0.0428,  $wR2 = 0.1086$ . The dioxaphosphepine rings exhibit twist-chair form for I & II where as distorted boat conformation for III. Fusion of the phosphepine ring to the biphenyl system causes strain, as evidenced by both widening and compression of the endocyclic

angles in the heterocyclic ring.

Keywords: organophosphorus compounds, dioxaphosphepine rings, anticancer agents

## P06.04.14

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### Crystal structure and quantum mechanical calculations of an oxime compound, $C_9H_{11}N_3O_2$

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Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine [1]. The oxime (-C=N-OH) moiety is potentially ambidentate, with possibilities of coordination through the N and/or O atoms. It is a functional group that has not been extensively explored in crystal engineering. In the solid state, oximes are usually associated via O-H...N hydrogen bonds of length 2.8 Å. Oxime groups possess stronger hydrogen-bonding capabilities than alcohols, phenols and carboxylic acids [2]. The hydrogen-bond systems in the crystals of oximes have been analysed and a correlation between a pattern of hydrogen bonding and N-O bond lengths has been suggested [3]. The configurational and/or conformational isomers of glyoxime derivatives (dioximes) have also been analysed [4]. The experimental geometry of  $C_9H_{11}N_3O_2$  obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations. It is found that the bond lengths and angles obtained from two methods are in good agreement with each other.

[1] Sevagapandian, S., Rajagopal, G., Nehru, K. & Athappan, P. (2000). *Transition Met. Chem.* 25, 388-393. [2] Marsman, A. W., Leussing, E. D., Zwikker, J. W. & Jenneskens, L. W. (1999). *Chem. Mater.* 11, 1484-1491. [3] Bertolasi, V., Gilli, G. & Veronese, A. C. (1982). *Acta Cryst.* B38, 502-511. [4] Chertanova, L., Pascard, C. & Sheremetev, A. (1994). *Acta Cryst.* B50, 708-716.

Keywords: oxime, X-ray diffraction, quantum mechanical methods

## P06.06.15

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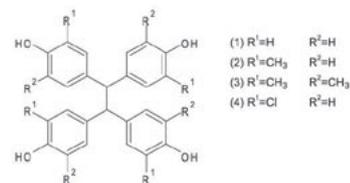
### Crystal structure analysis of inclusion crystals with tetrapodal host molecules

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Inclusion crystals have unique characteristics such as guest solubility or temperature dependent guest releasing, which is relevant to the structure of host framework enclosing guest molecules. Hence it is of great importance to investigate and develop host frameworks to design new functional materials. 1,1,2,2-tetrakis (4-hydroxyphenyl) ethane, TEP (1), has four hydroxyl phenyl groups in different directions to build different types of hydrogen bonding host frameworks corresponding to guest molecule types. In our previous study, three types of host frameworks accommodating different kind

of guest molecules via hydrogen bonds were analyzed to show TEP has well-qualified inclusion ability as an inclusion host molecule. By introducing one or two substituents next to hydroxyl group, (2)-(4), hydrogen bonding direction and pattern should be restricted and such TEP derivatives are expected to show different hydrogen bonding pattern which leads new host frameworks. In this study, inclusion crystals of TEP derivative are synthesized and their crystal structures are analyzed to compare the host framework structures.



Keywords: inclusion compounds, molecular interactions, crystal engineering

## P06.06.16

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### A detailed study of the helical conformation in 2-aminothiazole derivatives

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Aminothiazoles have many applications such as antiviral, antimicrobial, bactericidal and fungicidal agents. Aminothiazoles metal complexes display anti cancer activity.<sup>1</sup> The crystal structures of 2-Aminothiazole N-Boc protected Leucine and Valine belongs to the space group  $P 2_12_12_1$  and  $P 4_12_12$  with cell dimensions  $a=10.5247(14)\text{Å}$ ,  $b=11.2407(15)\text{Å}$ ,  $c=30.3258(3)\text{Å}$  and  $a=9.2614(4)\text{Å}$ ,  $b=9.2614(4)\text{Å}$ ,  $c=36.6412(3)\text{Å}$  respectively. The molecules are packed via intermolecular N-H...O and N-H...N hydrogen bonds giving rise to the formation of helix like structure. The helical nature and the tilt associated with the title compounds compares well with those of the B-DNA. The pitch per one complete turn of the helix is 30.30Å and 36.64Å while the pitch in B-DNA is reported to be 34Å and this aspect might have consequences related to the activity profiles of this compound. The idea is to exploit the hydrogen bonding potential in the title compound to get the supramolecular assembly into a helix and examine its features with respect to DNA.

1. Lynch, D. E. *et al*, *Acta Cryst.*, 1999, B55, 758

Keywords: supramolecular assemblies, DNA, hydrogen bonding recognition



Valine Thiazole