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. Coumarines are important because of their extensive plant origin. They have been using 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^3. The data of the compound is collected using Bruker CCD diffractometer with graphite monochromated MoKα 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...π interactions.

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

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X-Ray data for novel tricyclic compounds based on indolizines

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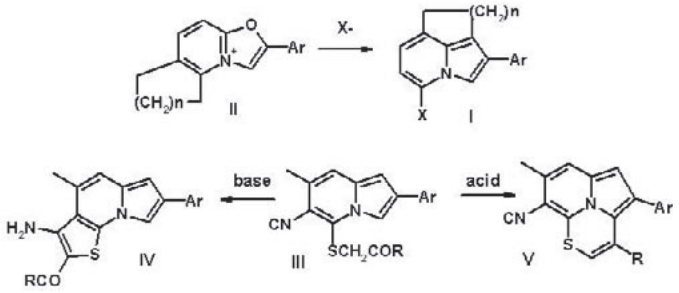
During the past decade we have investigated representative set (~50 single crystals and powders) of indolizines I and their precursors - oxazolopyridinium salts II. The structural trends in the families I, II will be overviewed, and the role of the size of third annelated cycle in the salts II on the 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

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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.

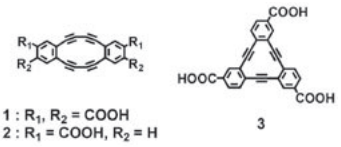

Figure. Dehydrobenzo[12]annulenes with carboxylic groups

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_4 P, Monoclinic, space group $P2_1/n$, a = 9.441(10), b = 15.202(16), c =9.746(10) Å, β = 95.782(2)°, V = 1391.5(3) Å^3, Z = 4, Dc = 1.385 Mgm^{-3}, 16173 reflections measured, 2457 unique [I>2・(I)], R value 0.0495, w$R2$ =0.1145. Crystal data (II): C_{14} H_{12} Cl O_4 P, Monoclinic, space group $P2_1/c$, a = 13.585(2), b= 8.719(1), c =13.106(2) Å, β = 118.15(2)°, V = 1368.7(3) Å^3, Z = 4, Dc = 1.508 Mg m^{-3}, 6682 reflections measured, 2410 unique [I>2・(I)], R value 0.0512, w$R2$ =0.1118. Crystal data (III): C_{18} H_{11} Cl_2 O_3 P S, Monoclinic, space group $P2_1/n$, a = 10.816(6), b = 13.615(8), c =12.321(7) Å, β = 99.583(9)°, V = 1789.0(18) Å^3, Z = 4, Dc = 1.519 Mg m^{-3}, 8553 reflections measured, 3119 unique [I>2・(I)], R value 0.0428, w$R2$ =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