

resp. The crystal structures of compounds **1-4** were determined by single crystal X-ray structure analysis. Compound **5** was determined from scratch by X-ray powder diffraction.

From the crystal structures it is not evident why the compounds **1**, **3**, and **5** are fluorescent but **2** and **4** are not. Thus extensive quantum mechanical calculations have been made and the reason for the fluorescence quenching of **2** and **4** was finally found [1].

[1] Dreuw A., Wachtveitl J., Brüning J., Schmidt M. U., *in preparation*.

**Keywords:** organic pigments, crystal structures, fluorescence

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#### Structure of 19-Hydroxyneohopane

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Several fused multicyclic natural product ring systems, especially those that are saturated or nearly saturated, are poorly represented in the Cambridge Structural Database of crystallographic determinations of organic compounds.

19-hydroxyneohopane, C<sub>30</sub>H<sub>48</sub>O, is one such compound consisting of a five fused ring system (rings 1 to 4 containing six carbons and ring 5 containing five carbons) with two double bonds trans across the 2-3 ring junction. The compound was obtained from the rhizome of *Davallia solida* Sw and crystallizes in the monoclinic space group, *P*<sub>2</sub><sub>1</sub>, with two molecules in a cell of dimensions: *a* = 12.587(3), *b* = 7.558(3), *c* = 13.620(3) Å, and  $\beta$  = 102.68(3)° at *T* = 113(2) K.

Crystal Data: C<sub>30</sub>H<sub>48</sub>O, *MW* = 424.68, clear colorless plate crystal, 0.50 x 0.50 x 0.02 mm, monoclinic, *P*<sub>2</sub><sub>1</sub>, *a* = 12.587(3), *b* = 7.558(3), *c* = 13.620(3) Å,  $\beta$  = 102.68(3)°, *V* = 1264.10, *Z* = 2 *T* = 113(2) K, *d*<sub>calc</sub> = 1.116 Mg m<sup>-3</sup>,  $\mu$  = 0.48 mm<sup>-1</sup>, CuK $\alpha$  radiation, *F*(000) = 472.,  $\sin\theta/\lambda_{\max}$  = 0.545 Å<sup>-1</sup>, *R*<sub>int</sub> = 0.0688, 3876 unique data, 3404 observed *F*<sub>o</sub> > 4 $\sigma$ (*F*<sub>o</sub>), *R*<sub>i</sub> = 0.0737, *goof* = 1.126.

**Keywords:** fused ring system, natural product, hopane

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#### X-ray Investigations of Bicyclic $\alpha$ -methylene- $\delta$ -valerolactones

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The  $\alpha$ -methylene- $\delta$ -valerolactones moiety is present in various biologically active natural compounds, e.g. vernolepin, vernomenin, pentalenolactone *E*, teucrum lactone, artemisitene and crassin. However, work on isolation and synthesis of new  $\alpha$ -methylene- $\delta$ -valerolactones has not led to a significant number of crystal structure investigations. A search of the CSD (version 5.26) shows that system in which  $\delta$ -valerolactone ring is condensed with the cyclohexane moiety along the individual C $\delta$ -C $\gamma$  single bond is unique among crystal structures examined to date. Investigated compounds represent a novel group of the optically active  $\alpha$ -methylene- $\delta$ -valerolactones synthesized in a highly stereoselective Michael reaction. Recently we reported crystal structures of two compounds *i.e.* the 3-methylene-2-oxohexahydrochromene-4a-carboxylic acid ethyl ester [1] and the 4-methyl-3-methylene-octahydro-chromen-2-one [2]. The six following crystal structures will be shown in detail. In all compounds the  $\delta$ -valerolactone rings adopt a half-chair conformation. The highly polar character of the carbonyl group hinders  $\pi$  electron density delocalization within the O=C-C=C moiety. In the crystal, molecular conformation is stabilized by attractive interactions between the oppositely charged atoms. The mechanism of interactions has been investigated using *NBO* theory at the *MP2/6-31+G(d,p)* level.

[1] Krawczyk H., Śliwiński M., Wolf W.M., Bodalski R., *Synlett*, 2004, 1995.

[2] Krawczyk H., Śliwiński M., Wolf W.M., *Acta Cryst.*, 2004, C60, o897.

**Keywords:**  $\delta$ -valerolactone, crystal structure, *NBO*

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#### Conformation of Dioxaphosphopin Ring – Structures of 6-Substituted Benzo and Dibenzo [d,f] [1,3,2] Dioxaphosphopin 6-oxide (I) and Sulphide (II)

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The hetro cyclic form of organophosphorous compounds containing phosphoryl unit with suitable substitution exhibits significant physiological activity and they have unique multifaceted applications. Structural studies of organophosphorous compounds have gained considerable importance recently because of their use as insecticides, anti-cancer agents, lubricating oil additives and polymer stabilizers. As part of our continuing investigations on this molecules, we have investigated the structures of 6-substituted benzo and dibenzo [d,f] [1,3,2] dioxaphosphopin 6-oxide and sulphide to know the dependence of substituents on the conformation and geometrical parameters of dioxaphosphopin hetro ring. compound (I): C<sub>15</sub> H<sub>15</sub> O<sub>4</sub> P, colourless crystals grown from methanol are Monoclinic *P*<sub>2</sub><sub>1</sub>/*c* with *a* = 9.441(1) ; *b* = 15.202(2) and *c* = 9.746(1) Å ;  $\beta$  = 95.8(2)°; *V* = 1391.5(3) Å<sup>3</sup>; *Z* = 4; *F*(000) = 608;  $\rho_c$  = 1.385 g cm<sup>-3</sup>;  $\mu$ (M<sub>o</sub> K $\alpha$ ) = 2.08 cm<sup>-1</sup>; *R* = 4.96 and *R*<sub>w</sub> = 0.1157 for 2457 unique reflections. compound (II): C<sub>18</sub> H<sub>11</sub> O<sub>3</sub> Cl<sub>2</sub> P S, colourless crystals obtained from 2-propanol, Monoclinic *P*<sub>2</sub><sub>1</sub>/*n* with *a* = 10.816(6) ; *b* = 13.615(8) and *c* = 12.321(7) Å ;  $\beta$  = 99.6(9)°; *V* = 1789.5(2) Å<sup>3</sup>;  $\rho_c$  = 1.519 g cm<sup>-3</sup>; *Z* = 4; *F*(000) = 832;  $\lambda$ (M<sub>o</sub> K $\alpha$ ) = 0.71073 Å ; *R* = 0.048 and *R*<sub>w</sub> = 0.130 for 2410 unique reflections. based on intensity data collected on Bruker Smart Apex diffractometer using Monochromated M<sub>o</sub>K $\alpha$  radiation, structures were solved by the direct methods and refined by full-matrix least squares methods. The seven membered dioxaphosphopin ring exhibits a pseudo- chair form for the former where as a distorted boat like conformation for the later. This is evident for the structural changes with different substituents fused to the hetro ring and also attached to the phosphorous.

**Keywords:** organophosphorous compounds, conformation of dioxaphosphopin ring, seven membered hetro ring

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#### *N*-isopropylamidino-substituted Derivatives of Benzo[b]thiophene-2-carboxanilides and Benzo[b]thieno[2,3-*c*]quinolones: DNA Binding by Intercalation

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Recently, we published syntheses, characterization and antitumor evaluation of series of cyano- and *N*-isopropylamidino-substituted derivatives of benzo[b]thiophene-2-carboxanilides and benzo[b]thieno[2,3-*c*]quinolones [1]. Aromatic surface of such aromatic compounds, usually built of three or more condensed aromatic units, is more than large enough for intercalation with the DNA. On the other hand, organic cations (*i.e.* amidinium cation) are known to bind in the DNA minor groove showing various biological activities, especially anticancer properties. The X-ray crystal structure study of 4'-carbomethoxy *N*-phenyl-3-chlorobenzo[b]thiophene-2-carboxamide and *N*-[4'-(*N'*-isopropylamidino)-phenyl]-3-chlorobenzo[b]thiophene-2-carboxamide hydrochloride is undertaken in order to compare their sterical properties with some classical intercalators and to give an answer if insertion between basepairs of DNA/RNA is possible.

[1] Jarak I., Kralj M., Šuman L., Pavlović G., Dogan J., Piantanida I., Žinić M.,