

**PS06.00.20 CRYSTAL STRUCTURE OF 3-[2(4-CHLOROPHENYL)SULFONYL ETHENYL]-6-METHOXY 4H-1-BENZOPYRAN 4-ONE.** K. V Narayana Raju, M. Krishnaiah, Department of Physics, Sri Venkateswara University, Tirupati-517 502, India, S. N. Rao, I. Liang Lu, Yu Sheng Chen, Department of Physics, University of Central Oklahoma, Edmond, Oklahoma, USA

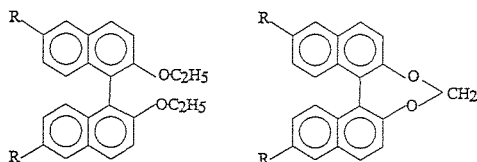
The structure of the title compound has been determined as a part of a series for studying the stereochemistry of sulfones which are well known for their clinical and commercial applications. Sulfones are used as fuel additives, plasticisers and antiicing additives. The fungicidal activity is found to vary depending upon the substance present and its stereo chemical configuration. A high degree of thermodynamical stability is associated with sulfone group and also basic properties as a proton acceptor. Sulfur with unusual and diverse properties, as constituent of a variety of inorganic, organic and biological molecules plays an important role for electron transport and associated with its exceptional versatility in bonding which is still debate with participation of 3d orbitals which more plausible when electronegative groups are involved.

Crystals obtained from methanol are colourless, monoclinic,  $C2/c$  with  $a=39.053(13)$ ,  $b=6.700(2)$ ,  $c=13.471(5)\text{\AA}$ ,  $\beta=106.62(3)^\circ$ ,  $v=3378(2)\text{\AA}^3$ ,  $z=8$ ,  $\rho_c=1.486\text{Mg/cm}^3$ ,  $\lambda=0.71073\text{\AA}$ ,  $\mu(\text{MoK}\alpha)=0.376\text{mm}^{-1}$ ,  $F(000)=1560$ . The structure has been solved by direct methods using MULTAN 80 with 2685 reflections collected on syntax P3 diffractometer. Refinement by full matrix least-square method using XRAY 80 converged at  $R=0.0687$   $R_w=0.1621$  and  $s=0.88$  for 2166 significant reflections.

The molecule contain three nearly planar segments ie benzopyranone, the chlorophenyl ring and ethylene group. The fragment C-C-C-S-C is slightly non planar and is inclined at  $60^\circ$  to the planar benzopyran ring and at  $106.17^\circ$  to the plane of the chlorophenyl group. The molecular geometry will be discussed.

**PS06.00.21 STRUCTURAL STUDIES OF SOME BINAPHTHYL DERIVATIVES.** By N.Thorup, Department of Chemistry, Technical University of Denmark, DTU-207, DK-2800 Lyngby, Denmark, H.-J. Deussen and T. Bjørnholm, CISMI, Department of Chemistry, University of Copenhagen, Denmark and K.Bechgaard, Department of Solid State Physics, Risø National Laboratory, Roskilde, Denmark and T.Geisler, Aalborg University, Aalborg, Denmark.

Crystal structures of several 1,1'-binaphthyl derivatives have been determined. In particular compounds which at the 2,2' positions have either identical ethoxy groups  $-\text{O}-\text{C}_2\text{H}_5$  or a closed bridged ether  $-\text{O}-\text{CH}_2-\text{O}-$  and furthermore have identical substitution at the 6,6' positions. The latter groups may be Br, CHO, CN or H. As would be expected, the torsional angle of the central 1-1' bond varies considerably in the open forms whereas the torsion is rather restricted in the closed forms. Optically pure crystals as well as racemic crystals have been produced in some cases. Unfortunately, good quality crystals for structural studies are difficult to grow and, therefore, rather high residuals are generally obtained. Some of the compounds are potential candidates for nonlinear optical applications and in several cases measurements of second order activity have been made.



**PS06.00.22 STRUCTURE AND CONFORMATION OF TWO NEW DIAZABICYCLO [5.3.0] DECAN-2-ONES.** D.Kumaran, M.N.Ponnuswamy and G.Shanmugam, Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras - 600 025, India, K.Sivakumar and Hoong-Kun Fun, X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia.

Several azabicyclo nonanes have been studied widely to find out various conformational possibilities and intramolecular interactions. On treating 2,4-diphenyl-3-azabicyclo [3.3.1] nonane, with sodium azide in the presence of sulfuric acid, new types of rearranged products, diazabicyclo [5.3.0] decan-2-ones compounds are obtained.

The structure of two compounds are determined. Both the crystals belong to the monoclini space group  $P21/c$  with  $Z=4$ .

Compound I :  $a = 14.462(1)$ ,  $b = 9.568(1)$   
 $c = 14.479(1)$ ,  $\beta = 118.46(1)$   
 $V = 1765.1(3)$

Compound II :  $a = 9.378(1)$ ,  $b = 8.791(1)$   
 $c = 26.306(2)$ ,  $\beta = 97.22(1)$   
 $V = 2151.5(4)$

In both the molecules the fused seven and five membered rings adopt chair-envelope conformation. The molecules are stabilized by Vander Waals forces of interaction. Further details will be discussed in detail.

**PS06.00.23 STRUCTURES OF THE SYMMETRIC CALIX[4]ARENES.** Young Ja Park, Kwanghyun No, Jung Mi Shin, Department of Chemistry, Sook Myung Women's University, Seoul, Korea 140-742

We have determined two structures of calix[4]arenes having their own two-fold rotational symmetry.

1. Tetra-butanyloxy calix[4]arene, monoclinic,  $C2/c$ ,  $a=18.435(4)$ ,  $b=13.774(2)$ ,  $c=16.941(3)\text{\AA}$ ,  $\beta=116.23(1)^\circ$ ,  $Z=4$ ,  $V=3859(1)\text{\AA}^3$ ,  $D_m=1.21\text{gcm}^{-3}$ ,  $R=0.078$  for 2605 observed reflections. The molecule is in the 1,2 alternate conformation. Twofold symmetry axis is along the line connecting between two opposite methylene carbon atoms.

2. Tetra-tert-butyl-dipropionyloxydihydroxycalix[4]arene, monoclinic,  $C2/c$ ,  $a=16.067(2)$ ,  $b=26.391(17)$ ,  $c=10.335(1)\text{\AA}$ ,  $\beta=94.26(1)^\circ$ ,  $Z=4$ ,  $V=4370(3)\text{\AA}^3$ ,  $D_m=1.16\text{gcm}^{-3}$ ,  $R=0.070$  for 2354 observed reflections. The molecule is in the 1,3 alternate conformation: two propionyloxyphenyls are up and two hydroxyphenyls are down. Two-fold symmetry axis is in the center of the molecule.

The molecular structures will be discussed with relation to NMR results and to molecular mechanics calculations.