

**PS06.00.12 CRYSTAL STRUCTURES OF A SOLVATED AND UNSOLVATED SULFONE CYCLIC OLIGOMER.** P. J. Cahill, L. N. Venkateshwaran, J. A. Kaduk, Amoco Corporation, P.O. Box 3011 MC F-9, Naperville IL 60566

The material causing slight cloudiness in a polysulfone was isolated, and its powder diffraction pattern could be indexed on a primitive monoclinic unit cell having  $a = 9.5703(15)$ ,  $b = 18.7582(18)$ ,  $c = 13.3945(12)$  Å, and  $\beta = 92.684(11)^\circ$ . Single crystals as large as  $80 \times 80 \times 10$  µm could be grown from boiling dimethylsulfoxide. The single crystal had a primitive monoclinic cell with  $a = 9.561(3)$ ,  $b = 18.728(5)$ ,  $c = 13.382(4)$  Å, and  $\beta = 92.66(3)^\circ$ . Both forms crystallize in  $P2_1/c$ , with  $Z = 2$ . The structure of the DMSO solvate was solved and refined using the single crystal data, and the structure of the unsolvated form was refined using powder data.

The crystal structure consists of discrete centrosymmetric cyclic oligomers, containing two of each of the diphenylsulfone and bisphenol A monomers. At the center of each macrocycle in the solvated form is a single disordered DMSO molecule. The torsion angles at the sulfone and isopropylidene linkages between the phenyl rings differ by less than  $6^\circ$  in the solvated and unsolvated forms. The torsion angles involving the ether oxygens differ by as much as  $30^\circ$ . The conformational differences are discussed in light of observed distributions of the torsion angles in diphenylsulfones, diphenylisopropylidines, and diphenyl ethers, as well as the distributions expected from conformational analyses. These structures provide valuable experimental measurements of the torsion angles in polysulfones.

**PS06.00.13 STRUCTURE OF 1-[5'-(N,N-DIETHYL)-2'-FURYL-CARBAMOYL]-2,2,2-TRICHLORO-ETHANOL.** Obel Durruthy Carbonell, Estela Margarita Roque Infante, Rolando Alba Hernandez, Oscar Au-Alvarez, Dept. of Physics and Dept. of Chemistry, University of Oriente, Santiago de Cuba 90500, Cuba, Ramon Pomes Hernandez, Angel Dago and Fabio Fajardo, National Center for Scientific Research, Havana, Cuba.

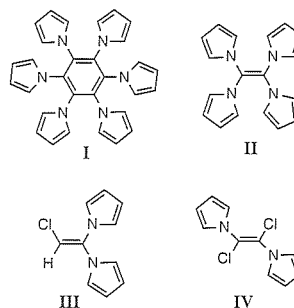
The structure consists of discrete molecules linked by van der Waals forces and presents a weak intramolecular hydrogen bond between the hydroxyl group and one chlorine atom. C-Cl distances are shorter than those expected. N atom has a  $sp^2$  planar configuration. Furl ring is planar and has bond distances and angles similar to those of furan, within experimental errors. The crystal is monoclinic,  $S.G. P2(1)/a$  with  $a=13.150(10)$ ,  $b=9.388(6)$ ,  $c=11.302(2)$  Å,  $\beta=83.4(1)$  deg and  $Z=4$ . This study tries to help in correlation of bioactivity and spectroscopic properties of this compound and its structure.

**PS06.00.14 MOLECULAR AND ELECTRONIC STRUCTURE OF 1,2,5-THIADIAZOLE 1,1-DIOXIDE DERIVATIVES.** E.E. Castellano,<sup>1</sup> O.E. Piro,<sup>2</sup> J.A. Caram,<sup>3</sup> M.V. Mirífico,<sup>3</sup> S.L. Aimone,<sup>3</sup> E.J. Vasini<sup>3</sup> and M.D. Glossman<sup>4</sup>, <sup>1</sup>Instituto de Física de São Carlos, Univ. de São Paulo, C.P. 369, 13560 São Carlos (SP), Brazil, <sup>2</sup>Dept. Física, Ftad. de C. Exactas, Univ. Nacional de La Plata, La Plata, Argentina, <sup>3</sup>INIFTA (CONICET), UNLP, La Plata, Argentina., <sup>4</sup>QUINOR (CONICET), Dept. Química, FCE, UNLP, La Plata, Argentina.

Thiadiazoles are at the basis of some polymeric organic heterocycles of interest in Material Science. Furthermore, 1,2,5-thiadiazole derivatives have pharmacological applications. As part of physical chemistry studies on several 3,4 substituted 1,1-dioxide derivatives of 1,2,5-thiadiazole, we report here a single crystal X-ray diffraction study on the molecular structure of the following derivatives: 3,4-dimethyl (I), 3-methyl-4-phenyl (II) and 3,4-diphenyl (III). We shall also report *ab initio* Molecular Orbital (MO) calculations of the electronic structure, conformation and reactivity of I and II, as well as results of semiempirical MO calculations on the electronic structure and conformation of III. The theoretical molecular conformations will be compared with the experimental X-ray diffraction results.

**PS06.00.15 HEXA-N-PYRROLEBENZENE, TETRA-N-PYRROLEETHYLENE, AND RELATED COMPOUNDS.** Frank R. Fronczek, Alfonso Dávila, Tamara R. Nauman, and Mark L. McLaughlin, Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA.

Hexa-*N*-pyrrolebenzene (I) has a propeller conformation, with pyrrole rings forming dihedral angles with the benzene plane ranging  $49.2(1)$ - $67.9(1)^\circ$ . Tetra-*N*-pyrroleethylene (II) lies on a crystallographic twofold axis, and pyrrole rings form dihedral angles of  $51.9(1)$  and  $46.5(1)^\circ$  with the plane of the double bond. In III, the pyrrole rings form dihedral angles of  $36.2(1)$  and  $56.0(1)^\circ$  with the plane of the double bond. IV lies on an inversion center, and the C=C carbon atoms are disordered into two sets of sites with relative populations *ca.* 2:1. The pyrrole plane forms a dihedral angle of  $67.7(1)^\circ$  with the plane of the double bond.



I has  $Z=4$  in  $Pna2_1$ ,  $R=0.047$ ; II has  $Z=4$  in  $C2/c$ ,  $R=0.041$ ; III has  $Z=4$  in  $P2_1/c$ ,  $R=0.055$ ; IV has  $Z=2$  in  $P2_1/n$ ,  $R=0.031$ .