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As the molecule adopts the syn conformation it has approximate C2 point group symmetry so that the four oxygen atoms of the two cis-fused dioxaline rings lie on the same side of the molecule. The cyclohexane rings have regular boat forms as indicated by the asymmetry parameters Δα = 3.7° and Δψ = 0.5°. One dioxaline ring has a conformation across an envelope and half chair (pseudo-rotational parameters Δ = 15.6° and Ψ = 34.6° while the other is envelope (Δ = 27.6° and Ψ = 38.2°). The six atoms of the central dicyclopropylcyclohexene moiety are coplanar and the central C=C bond length is 1.31(1) Å.

PS-06.06.09 CRYSTAL STRUCTURE STUDIES ON N-PIPERIDIN-4-ONES BY N.Sukumar and M.N.Ponnuswamy. Department of Crystallography and Biophysics, University of Madras, Guindy campus, Madras - 600 025, India and R.Jayakumar, Chemical Lab, CRI, Aruvan, Madras - 600 020, India.

Many nitrosamines are known to be carcinogenic and some N-nitroso urea are used as antilum agents or antibiotics. Their activity depends on the nature and position of the side group attached to it. The aim is to study the stereo dynamics of N-nitroso piperidines and correlate the stereochemistry with their cancer-inhibitor properties. To determine the conformational features of the piperidines the X-ray study was undertaken. The piperidine ring without N-nitroso group was found to assume chair conformation. Depending upon the electronic and steric nature of substituents, there will be a deformation from the perfect chair conformation. The introduction of the N-nitroso group at the position of nitrogen atom is known to exert a large influence on the conformation of the substituents. The following compounds have been solved.

(i) 3,5-dimethyl-2,6-dihydro-1-piperidin-4-one (DTMP) : 

ps-06.06.08 THE MOLECULAR STRUCTURE OF A CYCLO-PROPYLENE DIMER. By R.J. Greenwood and N.R. Moore. Department of Chemistry, La Trobe University, Bundoora, Victoria 3083, Australia, and M.G. Banwell, J.N. Lambert and J.M. Walter, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

An X-ray crystallographic analysis has unequivocally established that the dimerisation reaction given below yields the unexpected syn-bis[3ac,4ac,5ac,6ac,7,2-dimethyl-4-cyclopropa[f]-1,3-benzodioxal-5-ylene] with no anti-isomer detected. We believe the stereochemical outcome observed in the reaction could be quite generalizable and that the stereoelasticity associated with the initial halogen-metal exchange reaction determines whether the syn- or anti-dimer is obtained. The significance of the formation of the syn-dimer will be discussed.

Monoclinic crystals of C₂H₂O₄ belong to the space group C₂/c with a = 35.245(5), β = 6.535(1), c = 29.905(4) Å, β = 143.49° and S = 8. Refinement with 1246 observed data converged at R = 0.055 and S = 2.46 (219 parameters varied).
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PS-06.06.11 CRYSTAL STRUCTURE OF 2,2-(BENZENE SULPHONYL)-1-PARA CHLOROMETHYL CYCLOPROPA N by S. Shanmugasundara Ravikrishnan and G. Shanmugan, Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras-600 025, INDIA.

The cyclopropane ring undergoes drastic geometrical changes under influence of electron donor substituents. The interaction between a cyclopropane ring and an approximately oriented tacceptor substituent, (for eg. carbonyl group) shortens the vicinal bonds. The title compound C_{12}H_{17}O_{5}S_{2}Cl crystallizes in the monoclinic system. P2_1/a with cell constants a=10.51102, b=15.452(1), c=13.0252(2), \beta=93.70(1), V=2055.3(1)\AA^3, Z=4, D=1.489Mg\cdot m^{-3}, T=292K and CuK\alpha radiation (\lambda=1.5418\AA). The structure was solved by direct methods and refined by full-matrix least-squares procedures using 3585 observed reflections to a final R=0.066 and Rw=0.066. The cyclopropane ring is in equilateral triangle form and the benzene sulphonyl and the phenyl groups are trans to each other. The packing is stabilized by van der Waals forces.

PS-06.06.12 CRYSTAL STRUCTURE OF D- AND L- AMINO ACID SALTS OF OPTICAL RESOLVING REAGENT (-)-PHENYLETHANE SULFONIC ACID. By Tatsuya Date*, Kimio Okamura, and Ryuzo Yoshikawa, Tanabe Seiyaku Co. Ltd., Research Laboratory of organic chemistry, Kawagishi, Toda, Saitama, Japan.

The optical active (-)-Phenylethane Sulfonic acid is an excellent reagent for the optical resolution of amino acids. Generally, L-amino acid salts are observed to precipitate preferentially, but D-isomer precipitates in the case of L-Pro when dissolved in water. We have analyzed the crystal structures of D- and L-amino acid salts of (-)-PES, listed in Table 1. From the comparison of each diastereomeric crystals, we found the next characteristic features: 1) In crystals, the infinite hydrogen bonded molecular chain listed in fig. 1 are observed. In less soluble crystals, the shorter hydrogen bond between -COOH and O\cdot S- observed. In more soluble crystals, the hydrogen bond of this type are longer or cannot be observed. In the case of L-Val salt, hydrogen bond distance of -COOH and O\cdot S- is shorter than D-isomer. But this hydrogen bonds don't form infinite hydrogen bond. 2) In amino acids containing hydroxyl group or the salts having crystal water, Hydrogen bond between OH and O\cdot S- are considered to affect solubility of the salts.

Table 1

<table>
<thead>
<tr>
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<th>Fig. 1</th>
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<tbody>
<tr>
<td>D- L-Ala (-)-PES</td>
<td>O</td>
</tr>
<tr>
<td>D- L-Val (-)-PES</td>
<td>H\cdot O - H\cdot CH\cdot COOH</td>
</tr>
<tr>
<td>D- L-Leu (-)-PES</td>
<td>H\cdot R</td>
</tr>
<tr>
<td>D- L-Ser (-)-PES</td>
<td>D- L-HPG (-)-PES</td>
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</table>

WPG : Hydroxyphenylglycin

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