The data were collected at 25 C using the Θ/2 Θscan mode, variable scan speed scan width 1.0°. Two standard reflections ($01\bar{2}$, $11\bar{1}$) monitored every 50 measurements and showed no systematic variation of intensity. Only Lorentz-Polarization corrections were applied, data ajusted to an approximately absolute scale, overall U= 0.04Å^2.

The structure was solved by direct methods, using the program MITRIL(Gilmore C.J., Journal of Appl. Cryst., 1984, 17, 42-46); Least-Squares refinement of all non-H atoms with anisotropic thermal parameters and all of the H atoms were located by a difference syntheses and refined with isotropic temperature factors.($\Delta\rho$) from -0.19 to 0.14 eÅ^{-3}, final R= 0.045, wR= 0.057.

The X-Ray study shows that in this compound there is an intermolecular approach of 3.4Å involving non-H atoms: N...O=3.018(3)Å. The molecules are held in the crystal by hydrogen bonds along [100].

PS-06.06.04 THE STRUCTURES OF THE PRODUCTS OF DIENE CONDENSATIONS WITH PARTICIPATION OF 3,3-DISUBSTITUTED CYCLOPROPENES

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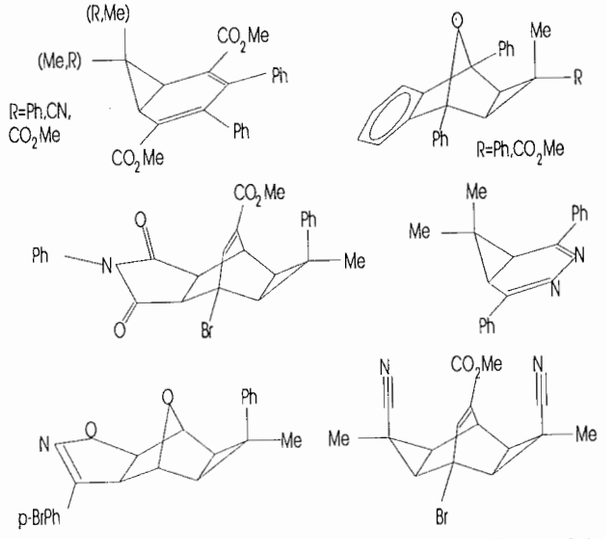
The structures of the products of Diels-Alder reaction between 3-R-3-methylcyclopropenes (R=Me, Ph, CN, COOMe) and dienes were determined by means of X-ray structure analysis (9 structures in all)



The influence of direct substituents' interactions on stabilization of the formed compounds and their spectral properties is discussed.

PS-06.06.05 CRYSTAL AND MOLECULAR STRUCTURES OF INDIRUBIN MONOOXIME (I) AND INDIRUBIN MONOOXIME ETHYL ETHER(II). By

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In order to search for a new kind of antileukemia drug, a series of derivatives of indirubin have been synthesized. Both indirubin monooxime (I) and indirubin monooxime ethyl ether (II) have been determined to possess antileukemia activity, the latter being better. In this paper we report their molecular and crystal structures.

On CAD4 diffractometer with Mokα radiation and in w/2θ mode ,in the range of 2°≤2θ≤45° for (I) and 2°≤2θ≤50° for (II), a total of 4902 and 2937 unique reflections were collected respectively. The 1846 and 1380 reflections having I>3σ(I) were used in the respective determinations. On a PDP 11/44 computer with SDP Program package, the structures of compounds (I) and (II) were solved by direct methods and fourier synthesis techniques. The crystallographic data are as follows: crystal (I) (propanone), $C_{16}H_{11}N_3O_2 \cdot CH_3COCH_3$, Mr = 335.39, monoclinic, space group C_2/C, a=2.4697(9), b=0.7243(2), c=2.4199(9)nm, β=129.98(2)°, v=3.3171(2)nm^3, z=8, Dc=1.110g/cm^3, R=0.0590, Rw=0.0590; crystal (II), $C_{18}H_{15}N_3O_2$, Mr=305.36, monoclinic, space group $P2_1/c$, a=0.9743(1), b=1.3445(1), c=1.1807(3)nm, β=101.06(1)°, v=1.5180(1)nm^3, Z=4, Dc=1.336g/cm^3, R=0.0393, Rw=0.0418. This investigation was undertaken as one part of our ongoing study in the link between the structures and antileukemia activity of derivatives of indirubin.

PS-06.06.06 CRYSTAL STRUCTURE OF AN INDOLE DERIVATIVE (A DIMER) By

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The common feature of the naturally occuring antibiotics like proflavine and ethidium is the possession of a planar chromophore with three fused rings. These planar compounds can be inserted in between adjacent base pairs of DNA molecules. The compound, Di[2-(3,4-dimethyl)]indole-3-yl methane is obtained during the synthesis of such planar chromophores. Crystals ($C_{35}H_{34}N_2O_4$; Mr = 558.68) belong to monoclinic space group A2/n. Unit cell values are a = 23.648(2), b = 8.559(3), c = 13.856(4)Å and β = 92.13(1)°; V = 2803.6 Å^3, Z = 8, Dx = 1.32 Mgm^{-3}. Structure is solved by direct methods. One half of the molecule forms the asymmetric unit. The two asymmetric units are connected through a carbon atom which lies at the centre of inversion of the dimer. One monomeric unit is refined by full-matrix least-squares methods. The indole moiety is planar and the phenyl part is perpendicular to the indole moiety. Both of the methoxy groups lie in the plane of the phenyl ring. Four dimeric molecules occupy the unit cell and packed with N - H ... O type of hydrogen bonding between the molecules.

