dian J Phys 80 (10), 1025-1027 (2006)

Note

Crystal structure of N-methyl-2-(p-octyl phenoxy)benzimidazole

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Received 24 January 2006 accepted 21 August 2006

The crystal structure of N-methyl -2(p-octyl phenoxy) benzimidazole has been determined by X-ray methods The compound monoclinic system space group $P2_1/c$ with cell parameters $a = 11.6479(2)$Å $b = 13.4292(1)$Å $c = 12.5994(9)$Å and $\beta = 98.344(8)^{\circ}$ zole ring is planar and makes a dihedral angle of 127.48(1)° with the aryloxy ring and is coplanar with N CH_3 group The two molecules ther by Van der Waals and weak inter molecular C-H N interactions

ords Crystal structure, be cyclic ring

Nos 61.10 Nz 61.66 H

midazole, a heterocyclic ring system, is present in many ally occurring cyanocobalamine Derivatives of midazoles provide a large number of biologically active ounds[1] and substitution pattern on the benzimidazole ly alters the biological activity Introduction of the long l group and additional methyl groups in the phenoxy ch enhances anti-inflammatory activity[2] 4-aminopiperidine ch attached to benzimidazole leads to potent antihistamine, mizole[3], antibacterial and antifungal activities[4], gastric ton inhibitors such as omeprazole and langprazole as pitent ulcer drugs[5] The crystal structure analysis of the title d has been undertaken to establish the solid state formation

2-hydroxy benzimidazole prepared by refluxing equimolar ities of o- phenylenedi-amine and urea in boiling amyl ol was converted to 2-chloro-1- methyl benzimidazole by method of Harrison[6] The title compound was synthesized e condensation of n-octyl phenyl in the dry DMF with 2-chloro-1- methyl benzimidazole[2] and recrystallised from ethanol The intensity data were collected using a CAD-4 diffractometer[7] The data have been corrected for Lorentz and polarization factors[8] The crystallographic data are given in Table 1 The structure has been solved by direct methods[9] and refined[10] to R (Residue factor) value 0.055 All hydrogen atoms placed in geometrically calculated positions have been kept fixed

Table 2 gives selected bond lengths and bond angles Table 3 gives hydrogen bonding geometry The chemical diagram of the molecule is shown in Figure 1 An ORTEP[11] plot of the molecule is shown in Figure 2

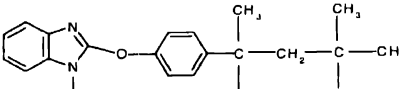

Figure 1. Chemical diagram of the molecule

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Table 1. Crystal data and refined parameters for the compound

Crystal morphology	colorless needle like
Crystal size	0.2 x 0.1 x 0.1 mm
Chemical formula	$C_{22}H_{28}N_2O$
Molecular weight	336.46
Crystal system	Monoclinic
Space group	$P2_1/c$
Cell constants	a=11.6479(2)Å
	b=13.4292(1)Å
	c=12.5994(9)Å
	β=98.344(8)°
Volume	1950.0(4)Å^3
Radiation used	Cukα
Number of formula units (Z)	4
Density(calculated) D_x	1.146 gm/cc
Unique data measured	3535
Observed data with $I>2\sigma(I)$	3158
F(000)	728
Electron density Max(ρ_{max})	0.322 e/ Å^3
Electron density Min (ρ_{min})	-0.191 e/ Å^3
R factor (R)	0.055
Weighted R (Rw)	0.161

The bond lengths and angles of the imidazole ring are in agreement with those in 2-chloro benzimidazole[12] Bond lengths N1-C1[1.362(2)Å] and N2-C1[1.293(2)Å] are in good agreement with the values reported for benzimidazole[1.364(3)Å

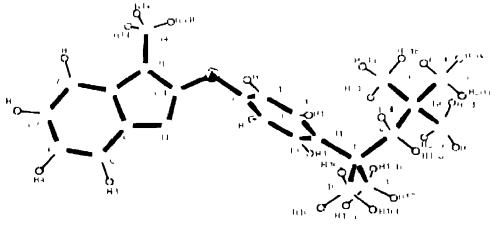

Figure 2 ORTEP PLOT of the molecule with 30% probability thermal ellipsoids

and 1.308(3)Å][13] and 2-(O-methoxy phenoxy)-1-methyl benzimidazole [1.360(2)Å and 1.295(2)Å][14] The N2-C1 bond length corresponds to a typical double bond character, while the N1-C14[1.454(2)Å] bond distance shows Csp^3-N hybridization and agrees with the literature[15] values The exocyclic angles around atom N1 show considerable asymmetry, although the sum of the valence angles around N1 [359.87(2)°] indicates no significant pyramidalization

The benzimidazole ring is coplanar with N-CH_3 group The displacement of all atoms in the ring are less than 0.01Å from the least squares planes. The dihedral angle between the phenyl

Table 2 Selected bond lengths (A) and bond angles atoms with e.s.d's are in parentheses

O1-C1	1.342(2)	O1-C8	1.416(2)
N1-C1	1.362(2)	N1-C7	1.391(2)
N1-C14	1.454(2)	N2-C1	1.293(2)
N2-C2	1.396(2)		

C1-O1-C8	116.54(1)
C1-N1-C7	105.08(1)
C1-N1-C14	127.56(2)
C7-N1-C14	127.23(2)
C1-N2-C2	103.13(1)
N2-C1-N1	116.20(2)
N2-C2-C7	110.63(1)
N1-C7-C2	104.96(1)

and imidazole ring is 1.43(5)Å The aryloxy group at angle of 127.48(1)° with the benzimidazole ring and is equatorially The observed bond length C1-O1 = 1.342 normal Csp^2-O bond showing expected residual bond of 0.09 Å due to oxygen[16] However, the C8-O1 = 1.41 comparatively larger and has been observed in the benzimidazole molecule[14]

Table 3 Hydrogen bonding geometry(A °)

D-H A		D-H	H A	D H A
C6-H6	N2$^{(i)}$	1.00(2)	2.68(2)	3.23(2
C14-H14A	N2$^{(ii)}$	0.98(4)	2.82(4)	3.71(3
C10-H10	N2$^{(iii)}$	1.01(2)	2.88(2)	1.66(2

Symmetry
(i) x, -y+1/2, z-1/2
(ii) -x+1, -y+1, -z+2

Furthermore, the conformations of the individual aryl group relative to the aromatic ring have been of vital import in the study of the hallucinogenic potency of poly meth phenyl amines The conformation of the molecule about the O1 bond is gauche The C8-O1-C1-N2 torsion angle is 3.1 which indicates the *syn* periplanar arrangement The mole are held together in crystal lattice by van der Waals forces weak intermolecular C-H .N interactions

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