Crystal structure of 2[2′-cyclohexyl]ethyl benzimidazole, $C_{15}H_{20}N_2$

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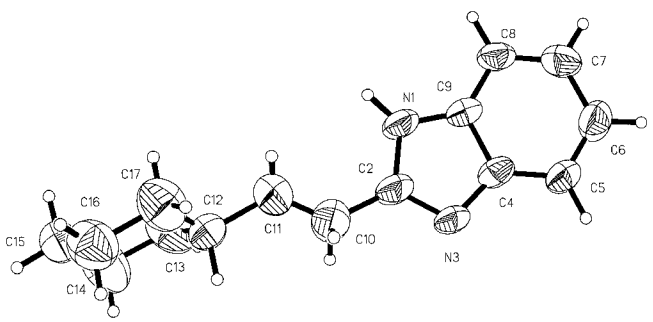

Abstract

$C_{15}H_{20}N_2$, orthorhombic, *Pbca* (No. 61), $a = 8.565(2)$ Å, $b = 9.813(2)$ Å, $c = 32.226(6)$ Å, $V = 2708.5$ Å^3, $Z = 8$, $R(F) = 0.064$, $T = 293$ K.

Discussion

Among the other, benzoxazoles and benzimidazoles possess interesting antifungal and antibacterial activity and constitute interesting objects for more effective antimicrobial agents studies [1-4]. As an extension of our studies for novel drugs the searching for correlation between structure and affinity to the receptor was postulated. Since this correlation should be based on structural and electronic parameters derived from geometrical description of the molecule, the three-dimensional structures and conformations of all investigated molecules have to be known. This prompted us to solve the structure of title compound 1 as an indispensable material for molecular modelling of the remaining molecules belonging to this group of compounds [4]. In benzimidazole moiety, C(2)–N(3) bond of 1.303(3) Å is formally treated as a double one but N(1)–C(2) equalling 1.360(2) Å is shortened comparing to the single C–N bond. The N1–C2 bond [1.360(2) Å] is longer than C2–N3 one [1.303(3) Å]. It undoubtedly indicates different hybridisation of both nitrogenous confirmed by hydrogen atom localisation at N1. All remaining bonds involving nitrogen's N1–C9 and N3–C4 also are averaging and possess bond lengths characteristic for aromatic molecules pointing at conjugation of bonds in those bicycled skeleton. The molecules are joined by H bonds of N1–H1a···N3 (0.5–x,-0.5–y, z) with distance of 2.856(2) Å forming molecules chain down y-axis.

In the molecule, mobile ethyl chain is linked with two *trans* situated cycles: planar benzimidazole and cyclohexyl in chair form. The C12–C11 bond is equatorial with respect to the ring in chair conformation. Due to ethyl chain flexibility from procedure of Random Search [5] nine variants of possible conformers for title molecule were found. It is notice worth that cyclohexyl ring possesses always chair conformation. Therefore for further structure-biological activity studies the main point will be the proper selection of the conformer being preferred in aqueous environment.

Table 1. Data collection and handling.

Crystal:	colorless cubes, size 0.2 x 0.2 x 0.2 mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ:	5.04 cm^{-1}
Diffractometer, scan mode:	KM-4, $\omega/2\theta$
$2\theta_{max}$:	163.72°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2605, 1207
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 4\,\sigma(F_{obs})$, 1207
$N(param)_{refined}$:	155
Programs:	SHELXS-86 [6], SHELXL-93 [7], XP [7]

Table 2. Atomic coordinates and displacement parameters (Å^2).

Atom	Site	x	y	z	U_{iso}
H(1A)	8*c*	0.2639	0.1952	0.3394	0.096
H(5A)	8*c*	−0.0863	−0.2070	0.3012	0.103
H(6A)	8*c*	−0.2527	−0.0670	0.2611	0.114
H(7A)	8*c*	−0.2079	0.1718	0.2579	0.114
H(8A)	8*c*	0.0058	0.2693	0.2906	0.094
H(10A)	8*c*	0.3777	−0.0748	0.4004	0.233
H(10B)	8*c*	0.4773	−0.0828	0.3604	0.233
H(11A)	8*c*	0.4328	0.1377	0.4053	0.262
H(11B)	8*c*	0.5381	0.1242	0.3662	0.262
H(12)	8*c*	0.6470	−0.0470	0.4221	0.142
H(13A)	8*c*	0.5254	0.0899	0.4718	0.173
H(13B)	8*c*	0.6074	0.2182	0.4538	0.173
H(14A)	8*c*	0.7710	0.0101	0.4924	0.204
H(14B)	8*c*	0.7470	0.1537	0.5120	0.204
H(15A)	8*c*	0.9972	0.1315	0.4820	0.163
H(15B)	8*c*	0.8995	0.2456	0.4610	0.163
H(16A)	8*c*	0.9386	−0.0159	0.4291	0.172
H(16B)	8*c*	1.0152	0.1148	0.4111	0.172
H(17A)	8*c*	0.7731	0.1964	0.3913	0.170
H(17B)	8*c*	0.7992	0.0534	0.3719	0.170

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Table 3. Atomic coordinates and displacement parameters ($Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	8*c*	0.2175(2)	0.1136(1)	0.33608(5)	0.0649(7)	0.0296(7)	0.0966(9)	−0.0031(6)	−0.0048(7)	0.0036(7)
N(3)	8*c*	0.1799(2)	−0.1098(1)	0.34001(6)	0.0810(9)	0.0244(7)	0.113(1)	0.0060(6)	−0.0264(8)	−0.0021(7)
C(2)	8*c*	0.2682(3)	−0.0080(2)	0.35112(8)	0.082(1)	0.0308(9)	0.118(2)	0.0091(8)	−0.022(1)	0.0037(9)
C(4)	8*c*	0.0621(2)	−0.0514(2)	0.31725(5)	0.0648(8)	0.0282(8)	0.0761(9)	0.0056(6)	0.0079(7)	−0.0072(7)
C(5)	8*c*	−0.0653(2)	−0.1114(2)	0.29816(7)	0.078(1)	0.0410(9)	0.087(1)	−0.0014(8)	−0.0090(9)	−0.0035(9)
C(6)	8*c*	−0.1656(3)	−0.0282(2)	0.27569(7)	0.082(1)	0.056(1)	0.090(1)	−0.004(1)	−0.012(1)	−0.016(1)
C(7)	8*c*	−0.1371(3)	0.1145(2)	0.27299(7)	0.088(1)	0.059(1)	0.081(1)	0.015(1)	−0.011(1)	0.0109(9)
C(8)	8*c*	−0.0142(3)	0.1732(2)	0.29221(5)	0.091(1)	0.0338(8)	0.0635(8)	0.0044(8)	−0.0022(9)	0.0002(7)
C(9)	8*c*	0.0852(2)	0.0893(2)	0.31444(5)	0.0622(8)	0.0304(7)	0.0658(8)	−0.0009(7)	0.0009(7)	0.0034(7)
C(10)	8*c*	0.4093(3)	−0.0232(3)	0.3762(1)	0.129(2)	0.065(1)	0.272(3)	−0.001(1)	−0.116(2)	0.007(2)
C(11)	8*c*	0.5002(4)	0.0752(3)	0.3903(1)	0.170(2)	0.091(2)	0.263(3)	−0.029(2)	−0.140(2)	0.043(2)
C(12)	8*c*	0.6371(3)	0.0512(2)	0.41718(9)	0.110(1)	0.047(1)	0.127(2)	−0.010(1)	−0.046(1)	−0.004(1)
C(13)	8*c*	0.6189(4)	0.1222(4)	0.45863(9)	0.104(2)	0.146(3)	0.097(1)	0.033(2)	0.009(1)	0.029(2)
C(14)	8*c*	0.7612(4)	0.1055(5)	0.48634(9)	0.130(2)	0.196(4)	0.082(1)	0.038(2)	−0.013(2)	−0.015(2)
C(15)	8*c*	0.9072(3)	0.1490(3)	0.4651(1)	0.111(2)	0.077(2)	0.138(2)	−0.001(2)	−0.045(2)	0.002(2)
C(16)	8*c*	0.9237(4)	0.0800(4)	0.4246(1)	0.099(2)	0.129(2)	0.117(2)	0.012(2)	0.001(2)	0.013(2)
C(17)	8*c*	0.7836(4)	0.1011(4)	0.39752(8)	0.125(2)	0.136(3)	0.078(1)	0.014(2)	−0.008(1)	−0.009(1)

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