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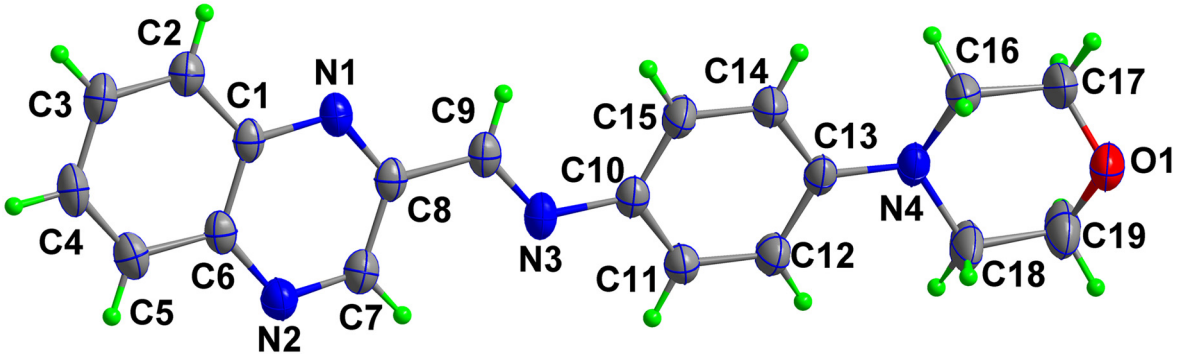
Crystal structure of (*E*)-*N*-(4-morpholinophenyl)-1-(quinoxalin-2-yl)methanimine, $C_{19}H_{18}N_4O$



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Abstract

$C_{19}H_{18}N_4O$, monoclinic, $P2_1/c$ (no. 14), a = 9.7995(9) Å, b = 10.0627(10) Å, c = 32.490(3) Å, β = 96.180(2)°, V = 3185.2(5) Å^3, Z = 8, $R_{gt}(F)$ = 0.0502, $wR_{ref}(F^2)$ = 0.1597, T = 296 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

Quinoxaline-2-carbaldehyde (0.158 g, 1 mmol) and 4-morpholin-4-yl-phenylamine (0.178 g, 1 mmol) was dissolved in an ethanol solution (10 ml). The mixture was stirred for 1 h under refluxing. The resulting solution was left in air for a few days, yielding red rod-shaped crystals.

Table 1: Data collection and handling.

Crystal:	Rod, red
Size:	0.20 × 0.08 × 0.06 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15,810, 5603, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3478
$N(param)_{refined}$:	433
Programs:	Bruker programs [1], SHELX [2]

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Quinoxaline derivatives are widely distributed in nature and have various biological applications [3]. Particularly, quinoxaline-based Schiff base complexes have attracted more and more attention because of their interesting chemical and biological properties [4]. Moreover, some quinoline-containing Schiff bases have been developed as probes for the fluorescent detection of metal ions [5]. As

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.55805 (19)	0.1428 (2)	0.34400 (5)	0.0876 (6)
O2	0.40323 (19)	0.16572 (19)	0.57136 (5)	0.0803 (5)
N1	−0.01266 (17)	0.16713 (18)	0.01612 (5)	0.0519 (4)
N2	−0.26081 (18)	0.0363 (2)	0.02704 (5)	0.0621 (5)
N3	0.06024 (18)	0.06130 (18)	0.11954 (5)	0.0572 (5)
N4	0.43326 (18)	0.0754 (2)	0.26381 (5)	0.0603 (5)
N5	−0.10473 (18)	0.15735 (19)	0.23576 (5)	0.0577 (5)
N6	−0.2164 (2)	−0.0997 (2)	0.22278 (6)	0.0747 (6)
N7	0.00561 (18)	0.01724 (19)	0.33272 (5)	0.0606 (5)
N8	0.30538 (17)	0.09231 (17)	0.48890 (5)	0.0516 (5)
C1	−0.1186 (2)	0.1617 (2)	−0.01509 (6)	0.0477 (5)
C2	−0.1038 (2)	0.2233 (2)	−0.05319 (6)	0.0580 (6)
H2B	−0.021952	0.265850	−0.057162	0.070*
C3	−0.2083 (3)	0.2211 (2)	−0.08421 (7)	0.0647 (6)
H3B	−0.197987	0.262200	−0.109318	0.078*
C4	−0.3315 (3)	0.1569 (3)	−0.07845 (7)	0.0685 (7)
H4A	−0.402528	0.155997	−0.099868	0.082*
C5	−0.3489 (2)	0.0962 (2)	−0.04215 (7)	0.0623 (6)
H5B	−0.431250	0.053566	−0.038863	0.075*
C6	−0.2428 (2)	0.0976 (2)	−0.00954 (6)	0.0507 (5)
C7	−0.1569 (2)	0.0412 (2)	0.05583 (6)	0.0578 (6)
H7B	−0.165234	−0.001131	0.080876	0.069*
C8	−0.0326 (2)	0.1076 (2)	0.05087 (6)	0.0487 (5)
C9	0.0773 (2)	0.1138 (2)	0.08499 (6)	0.0540 (6)
H9A	0.159542	0.156065	0.081369	0.065*
C10	0.1596 (2)	0.0686 (2)	0.15389 (6)	0.0530 (5)
C11	0.1426 (2)	−0.0128 (2)	0.18675 (6)	0.0600 (6)
H11A	0.068253	−0.070700	0.184705	0.072*
C12	0.2307 (2)	−0.0124 (2)	0.22253 (7)	0.0623 (6)
H12A	0.215557	−0.070427	0.243845	0.075*
C13	0.3425 (2)	0.0736 (2)	0.22740 (6)	0.0526 (6)
C14	0.3602 (3)	0.1557 (3)	0.19380 (7)	0.0767 (8)
H14A	0.434069	0.214166	0.195751	0.092*
C15	0.2728 (3)	0.1532 (3)	0.15821 (7)	0.0759 (8)
H15A	0.289026	0.208934	0.136434	0.091*
C16	0.5219 (3)	0.1893 (3)	0.27102 (7)	0.0933 (10)
H16A	0.466441	0.268025	0.273665	0.112*
H16B	0.573374	0.201751	0.247429	0.112*
C17	0.6201 (3)	0.1729 (5)	0.30948 (8)	0.1347 (17)
H17A	0.684802	0.102960	0.304868	0.162*
H17B	0.671712	0.254671	0.314453	0.162*
C18	0.3799 (3)	0.0340 (4)	0.30091 (7)	0.1097 (12)
H18A	0.336908	−0.052348	0.296259	0.132*
H18B	0.309453	0.096204	0.307194	0.132*
C19	0.4862 (3)	0.0249 (3)	0.33744 (8)	0.1015 (10)
H19A	0.441972	0.003336	0.361913	0.122*
H19B	0.549774	−0.046177	0.332982	0.122*
C20	−0.1880 (2)	0.1267 (2)	0.20050 (6)	0.0530 (6)
C21	−0.2168 (2)	0.2240 (3)	0.16995 (6)	0.0656 (6)
H21A	−0.173838	0.306375	0.172757	0.079*
C22	−0.3074 (3)	0.1982 (3)	0.13623 (7)	0.0730 (7)
H22A	−0.328085	0.263772	0.116354	0.088*
C23	−0.3697 (3)	0.0734 (3)	0.13137 (7)	0.0758 (8)
H23A	−0.432884	0.057422	0.108441	0.091*
C24	−0.3399 (2)	−0.0245 (3)	0.15933 (7)	0.0715 (7)
H24A	−0.380293	−0.107774	0.155197	0.086*
C25	−0.2476 (2)	−0.0002 (2)	0.19463 (6)	0.0592 (6)
C26	−0.1368 (3)	−0.0681 (3)	0.25601 (7)	0.0705 (7)
H26A	−0.114097	−0.133559	0.275769	0.085*
C27	−0.0832 (2)	0.0616 (2)	0.26345 (6)	0.0548 (6)
C28	−0.0017 (2)	0.0957 (2)	0.30225 (6)	0.0596 (6)
H28A	0.045316	0.176123	0.304569	0.072*
C29	0.0825 (2)	0.0461 (2)	0.37102 (6)	0.0513 (5)
C30	0.0723 (2)	−0.0441 (2)	0.40243 (6)	0.0630 (6)
H30A	0.015398	−0.117547	0.397397	0.076*
C31	0.1432 (2)	−0.0290 (2)	0.44088 (6)	0.0605 (6)
H31A	0.132830	−0.091945	0.461270	0.073*
C32	0.2305 (2)	0.0786 (2)	0.45002 (6)	0.0460 (5)
C33	0.2402 (2)	0.1697 (2)	0.41811 (6)	0.0599 (6)
H33A	0.297232	0.243239	0.422931	0.072*
C34	0.1684 (2)	0.1542 (2)	0.37996 (6)	0.0623 (6)
H34A	0.177347	0.217485	0.359561	0.075*
C35	0.3748 (3)	0.2168 (3)	0.49852 (7)	0.0729 (7)
H35A	0.307387	0.285719	0.501534	0.088*
H35B	0.426391	0.241711	0.475836	0.088*
C36	0.4703 (3)	0.2073 (3)	0.53752 (7)	0.0824 (8)
H36A	0.543061	0.144912	0.533426	0.099*
H36B	0.511951	0.293441	0.543649	0.099*
C37	0.2457 (3)	0.0389 (3)	0.52440 (7)	0.0857 (9)
H37A	0.214751	−0.051273	0.518438	0.103*
H37B	0.166477	0.091816	0.529513	0.103*
C38	0.3473 (3)	0.0392 (3)	0.56231 (7)	0.0936 (10)
H38A	0.302476	0.008185	0.585719	0.112*
H38B	0.420960	−0.022282	0.558304	0.112*

part of our ongoing studies on fluorescent probes, the title compound was synthesized and characterized by X-ray diffraction.

In the title structure, there are two independent molecules in the asymmetric unit (one of them is shown in the Figure). The bond lengths of C9–N3 and C28–N7 are found to be 1.268(3) and 1.262(3) Å, respectively, clearly indicating the Schiff base formation. The quinoxaline ring (C1–C8/N1, N2 and C20–C27/N5, N6, r.m.s. deviations of 0.0054 and 0.0333 Å, respectively) and the aryl ring (C10–C15 and C29–C34, r.m.s. deviations of 0.0047 and 0.0021 Å, respectively) in each molecule are almost coplanar, with the dihedral angles of 14.7 and 16.5°, respectively. Bond lengths and angles are all in the expected ranges for molecules containing a (quinoxalin-2-yl)methanimine moiety [6].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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