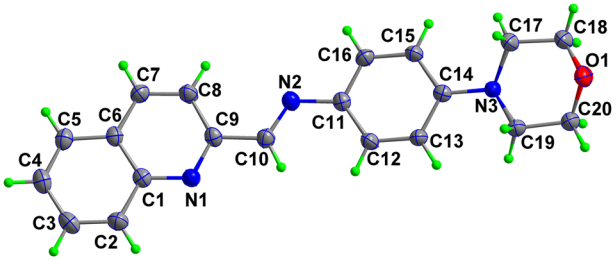
Kun-Sheng Jin and Wei-Na Wu*

Crystal structure of (*E*)-*N*-(4-morpholinophenyl)-1-(quinolin-2-yl)methanimine, $C_{20}H_{19}N_3O$



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Abstract

$C_{20}H_{19}N_3O$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.8776(10) Å, b = 7.6503(13) Å, c = 36.447(6) Å, V = 1638.8(5) Å^3, Z = 4, $R_{gt}(F)$ = 0.0374, $wR_{ref}(F^2)$ = 0.0950, T = 296 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

Quinoline-2-carbaldehyde (0.157 g, 1 mmol) and 4-morpholin-4-yl-phenylamine (0.178 g, 1 mmol) were dissolved in ethanol (10 mL). The mixture was stirred for 1 h under refluxing. The resulting solution was left in air for a few days, yielding yellow plate crystals.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [1].

***Corresponding author: Wei-Na Wu**, College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo, 454000, P. R. China, E-mail: wuwnhpu@163.com. https://orcid.org/0000-0002-0874-0703
Kun-Sheng Jin, College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo, 454000, P. R. China

Table 1: Data collection and handling.

Crystal:	Yellow plate
Size	0.20 × 0.12 × 0.04 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8371, 2872, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 2252
$N(param)_{refined}$:	218
Programs:	SHELX [1], Bruker [2]

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

Atom	*x*	*y*	*z*	U_{iso}^*/U_{eq}
O1	0.0505 (3)	0.6194 (3)	0.10134 (5)	0.0571 (6)
C1	0.3997 (5)	0.5448 (3)	0.44413 (6)	0.0427 (6)
C2	0.2859 (5)	0.4431 (4)	0.47059 (7)	0.0564 (8)
H2A	0.148077	0.390369	0.464690	0.068*
C3	0.3752 (6)	0.4212 (4)	0.50458 (7)	0.0631 (9)
H3A	0.298224	0.353727	0.521801	0.076*
C4	0.5819 (6)	0.4992 (4)	0.51390 (7)	0.0589 (8)
H4A	0.641650	0.483594	0.537305	0.071*
C5	0.6957 (5)	0.5972 (4)	0.48911 (7)	0.0529 (7)
H5A	0.833543	0.648178	0.495602	0.064*
C6	0.6082 (5)	0.6230 (3)	0.45362 (6)	0.0427 (6)
C7	0.7177 (5)	0.7241 (4)	0.42643 (7)	0.0534 (7)
H7A	0.853906	0.780604	0.431706	0.064*
C8	0.6240 (5)	0.7386 (4)	0.39276 (7)	0.0526 (7)
H8A	0.695641	0.804148	0.374651	0.063*
C9	0.4161 (5)	0.6532 (3)	0.38527 (6)	0.0437 (7)
C10	0.3145 (5)	0.6588 (3)	0.34881 (7)	0.0498 (7)
H10A	0.176410	0.602592	0.344815	0.060*
C11	0.3164 (5)	0.7359 (3)	0.28654 (6)	0.0411 (6)
C12	0.1157 (5)	0.6556 (4)	0.27595 (7)	0.0506 (7)
H12A	0.025914	0.601195	0.293578	0.061*
C13	0.0468 (5)	0.6547 (3)	0.24003 (6)	0.0481 (7)
H13A	−0.088447	0.599034	0.233779	0.058*
C14	0.1753 (4)	0.7355 (3)	0.21257 (6)	0.0373 (6)
C15	0.3730 (4)	0.8197 (3)	0.22364 (6)	0.0464 (7)
H15A	0.461289	0.877127	0.206231	0.056*
C16	0.4415 (5)	0.8201 (3)	0.25974 (7)	0.0469 (7)
H16A	0.574581	0.878118	0.266229	0.056*
C17	0.2868 (5)	0.7459 (4)	0.14848 (6)	0.0623 (8)
H17A	0.382376	0.643019	0.150501	0.075*
H17B	0.380250	0.847509	0.153652	0.075*
C18	0.1963 (5)	0.7588 (5)	0.11009 (7)	0.0658 (9)

Table 2: (continued)

Atom	*x*	*y*	*z*	U_{iso}^*/U_{eq}
H18A	0.114437	0.868111	0.107357	0.079*
H18B	0.322807	0.759903	0.092989	0.079*
C19	−0.0616 (5)	0.6034 (4)	0.16522 (7)	0.0507 (7)
H19A	−0.193016	0.612209	0.181217	0.061*
H19B	0.004355	0.488182	0.168439	0.061*
C20	−0.1365 (5)	0.6251 (4)	0.12588 (6)	0.0549 (8)
H20A	−0.242876	0.532802	0.119655	0.066*
H20B	−0.214594	0.736027	0.123193	0.066*
N1	0.3056 (4)	0.5598 (3)	0.40994 (5)	0.0484 (6)
N2	0.4092 (4)	0.7380 (3)	0.32243 (5)	0.0472 (6)
N3	0.1045 (4)	0.7354 (3)	0.17549 (5)	0.0394 (5)

The hydrogen atoms were placed at calculated positions and refined as riding atoms with constrained isotropic displacement parameters.

Comment

Schiff bases bearing quinoline units have been extensively investigated due to their excellent chelate ability [3, 4]. In this regard, several quinoline-containing Schiff bases. have been developed as probes for the fluorescent detection of metal ions [5–7]. As part of our ongoing studies on fluorescent probes, the title compound was synthesized and characterized by X-ray diffraction.

In the title structure (see the Figure), the bond length of the imine moiety C10–N2 is 1.265(3) Å, clearly indicating the Schiff base formation [8]. The quinoline ring (r.m.s. deviation 0.0092 Å) and benzene ring (r.m.s. deviation 0.0080 Å) are almost coplanar, with the dihedral angle of 9.1°. As expected, there exist no classical hydrogen bonds, while the weak C4–H4A···O1^{i} (symmetry code i: 0.5 − *x*, 1 − *y*, 0.5 + *z*) hydrogen bonds link the moledules into an one-dimensional chain along *c* axis.

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

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