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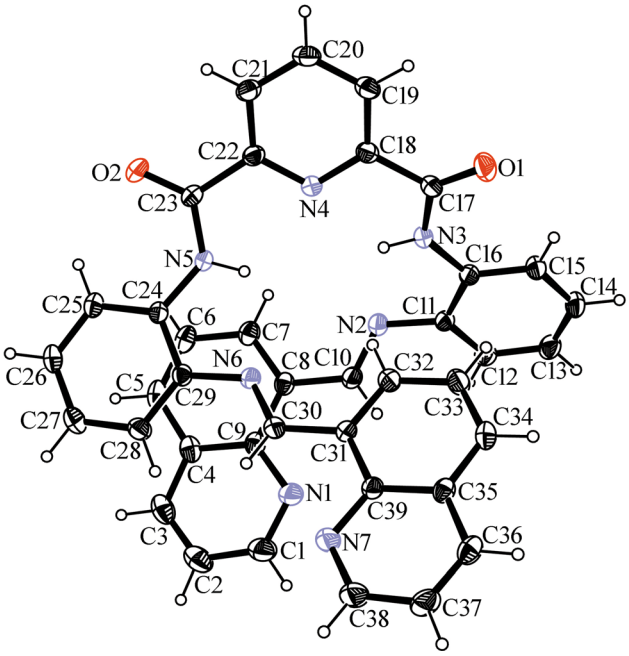
Crystal structure of N^2,N^6-bis(2-(((*E*)-quinolin-8-ylmethylene)amino)phenyl)pyridine-2,6-dicarboxamide, $C_{39}H_{27}N_7O_2$



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Abstract

$C_{39}H_{27}N_7O_2$, monoclinic, $P2_1/c$ (no. 14), a = 12.3871(18) Å, b = 19.114(3) Å, c = 13.2430(16) Å, β = 103.236(4)°, V = 3052.3(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0516, $wR_{ref}(F^2)$ = 0.1313, T = 293(2) 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.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.14 × 0.13 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker Apex-II, φ and ω
θ_{max}, completeness:	28.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	121,934, 7587, 0.078
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 5493
$N(param)_{refined}$:	433
Programs:	Olex2 [1], Bruker [2], Shelx [3], Diamond [4]

Source of material

A solution of quinoline-8-carbaldehyde (0.314 g, 2 mmol) in ethanol (30 mL) was added to a stirred ethanol solution (20 mL) of *N*,*N*′-(2-aminophenyl)-2,6-dicarboxylimide pyridine (0.347 g, 1 mmol) in a three-necked flask. The mixed solution was heated and reflowed for 9 h and cooled to room temperature. The yellow solid was separated out, filtered, and washed with ethanol for four times. 0.625 g of yellowish solid was obtained. The yield was 68%. And then, a small amount of solid was taken and dissolved in 15 mL of dichloromethane. An amount of 5 mL of ethanol was added. After slow volatilization for five days, crystals with an appropriate size were obtained.

Experimental details

Using Olex2 [1], the structure was solved using Charge Flipping and refined with the ShelXL [3] refinement. All hydrogen atoms were positioned geometrically, with the d(C–H) = 0.97–0.99 Å, U_{iso}(H) = 1.2 times U_{eq}(C) and U_{iso}(H) = 1.5 times U_{eq}(O).

Comment

Some Schiff base complexes attracted the attention of researchers because of their applications [5, 6]. Schiff base compounds containing 2,6-dicarboximide units have

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

Atom	x	y	z	U_{iso}*/U_{eq}
O1	0.44257 (12)	0.10494 (8)	0.40531 (13)	0.0651 (4)
O2	1.01718 (11)	0.11068 (7)	0.44402 (13)	0.0593 (4)
N1	0.74202 (15)	0.46819 (9)	0.25116 (15)	0.0554 (4)
N2	0.58801 (12)	0.28066 (8)	0.20201 (12)	0.0421 (3)
N3	0.52865 (12)	0.18100 (8)	0.31655 (12)	0.0418 (3)
H3	0.5939	0.1925	0.3102	0.050*
N4	0.72552 (12)	0.12622 (7)	0.40383 (11)	0.0370 (3)
N5	0.90424 (11)	0.20620 (7)	0.41424 (12)	0.0379 (3)
H5	0.8356	0.2176	0.3935	0.046*
N6	0.83046 (12)	0.32828 (7)	0.46391 (12)	0.0387 (3)
N7	0.71986 (14)	0.48220 (9)	0.62703 (14)	0.0531 (4)
C1	0.7928 (2)	0.52870 (12)	0.2730 (2)	0.0674 (6)
H1	0.7528	0.5654	0.2926	0.081*
C2	0.9032 (2)	0.54152 (14)	0.2688 (2)	0.0713 (7)
H2	0.9343	0.5856	0.2845	0.086*
C3	0.96330 (19)	0.48913 (14)	0.24175 (18)	0.0636 (6)
H3A	1.0366	0.4967	0.2386	0.076*
C4	0.91451 (16)	0.42257 (11)	0.21817 (14)	0.0480 (5)
C5	0.97201 (16)	0.36440 (13)	0.19090 (15)	0.0550 (5)
H5A	1.0459	0.3692	0.1878	0.066*
C6	0.92086 (17)	0.30162 (12)	0.16912 (15)	0.0520 (5)
H6	0.9602	0.2636	0.1523	0.062*
C7	0.80889 (16)	0.29377 (11)	0.17181 (14)	0.0459 (4)
H7	0.7747	0.2505	0.1561	0.055*
C8	0.74903 (14)	0.34865 (10)	0.19721 (13)	0.0396 (4)
C9	0.80175 (15)	0.41482 (10)	0.22214 (14)	0.0424 (4)
C10	0.63174 (15)	0.34054 (10)	0.19802 (14)	0.0424 (4)
H10	0.5879	0.3803	0.1956	0.051*
C11	0.47316 (14)	0.27547 (9)	0.19881 (14)	0.0387 (4)
C12	0.39199 (16)	0.31561 (10)	0.13565 (15)	0.0465 (4)
H12	0.4118	0.3493	0.0925	0.056*
C13	0.28122 (16)	0.30576 (11)	0.13642 (17)	0.0532 (5)
H13	0.2269	0.3330	0.0942	0.064*
C14	0.25186 (16)	0.25571 (12)	0.19952 (18)	0.0548 (5)
H14	0.1775	0.2499	0.2004	0.066*
C15	0.33098 (15)	0.21389 (10)	0.26178 (16)	0.0470 (4)
H15	0.3101	0.1803	0.3044	0.056*
C16	0.44224 (14)	0.22247 (9)	0.26011 (14)	0.0384 (4)
C17	0.52531 (15)	0.12591 (9)	0.37922 (15)	0.0423 (4)
C18	0.63571 (15)	0.09050 (9)	0.41456 (14)	0.0395 (4)
C19	0.64136 (17)	0.02350 (10)	0.45592 (16)	0.0477 (4)
H19	0.5777	0.0009	0.4648	0.057*
C20	0.74323 (18)	−0.00872 (10)	0.48353 (16)	0.0518 (5)
H20	0.7494	−0.0538	0.5106	0.062*
C21	0.83589 (17)	0.02670 (9)	0.47052 (15)	0.0466 (4)
H21	0.9053	0.0055	0.4869	0.056*
C22	0.82386 (14)	0.09442 (9)	0.43257 (13)	0.0382 (4)
C23	0.92522 (15)	0.13733 (9)	0.42909 (14)	0.0393 (4)
C24	0.98065 (13)	0.26171 (9)	0.42836 (12)	0.0344 (3)
C25	1.08887 (14)	0.25520 (11)	0.41671 (14)	0.0435 (4)
H25	1.1146	0.2122	0.3991	0.052*
C26	1.15804 (15)	0.31276 (12)	0.43130 (16)	0.0508 (5)
H26	1.2306	0.3082	0.4238	0.061*
C27	1.12113 (16)	0.37679 (11)	0.45673 (16)	0.0519 (5)
H27	1.1685	0.4152	0.4664	0.062*
C28	1.01350 (16)	0.38382 (10)	0.46782 (15)	0.0459 (4)
H28	0.9884	0.4273	0.4839	0.055*
C29	0.94217 (14)	0.32672 (9)	0.45522 (13)	0.0357 (4)
C30	0.79479 (15)	0.37666 (10)	0.51251 (15)	0.0431 (4)
H30	0.8428	0.4124	0.5419	0.052*
C31	0.68008 (14)	0.37814 (9)	0.52384 (14)	0.0376 (4)
C32	0.60569 (15)	0.32727 (10)	0.47985 (15)	0.0451 (4)
H32	0.6282	0.2922	0.4406	0.054*
C33	0.49682 (17)	0.32718 (11)	0.49295 (16)	0.0512 (5)
H33	0.4481	0.2920	0.4627	0.061*
C34	0.46179 (16)	0.37809 (11)	0.54952 (15)	0.0480 (5)
H34	0.3892	0.3775	0.5576	0.058*
C35	0.53414 (15)	0.43176 (10)	0.59598 (13)	0.0401 (4)
C36	0.50260 (18)	0.48636 (11)	0.65482 (16)	0.0529 (5)
H36	0.4308	0.4883	0.6648	0.064*
C37	0.5771 (2)	0.53564 (12)	0.69637 (18)	0.0623 (6)
H37	0.5571	0.5720	0.7350	0.075*
C38	0.6847 (2)	0.53160 (12)	0.68099 (19)	0.0631 (6)
H38	0.7350	0.5661	0.7108	0.076*
C39	0.64494 (14)	0.43182 (9)	0.58356 (13)	0.0375 (4)

multiple nitrogen atoms, and may form helical compounds and coordinate with metal ions easily. They are widely used for the recognition of metal ions [7].

Here, we report the crystal structure of the Schiff base compound N^2,N^6-bis(2-(((*E*)-quinolin-8-ylmethylene)amino) phenyl)pyridine-2,6-dicarboxamide containing structural units of quinoline ring and 2,6-dicarboximide. The crystal structure shows that the aldehyde group of quinoline-8-carbaldehyde has condensed with the amino group of *N*,*N*′-(2-aminophenyl)-2,6-dicarboxylimide pyridine, forming a helical compound. The bond lengths of imine linkage C10=N2 and C30=N6 are 1.273 and 1.263 Å, respectively. All the bond lengths and bond angles are within the normal scope [8]. The dihedral angle between two quinoline rings is 161.65° and that between two benzene rings is 124.32°. Intramolecular hydrogen bonds N3–H3···N2, N3–H3···N4, N5–H5···N4, and N5–H5···N6 exist in the molecules.

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

References

1. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution,

refinement and analysis program. *J. Appl. Crystallogr.* 2009, *42*, 339–341.
2. Bruker. *APEX2, SAINT and SADABS*; Bruker AXS Inc.: Madison, Wisconsin, USA, 2012.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Brandenburg K. *DIAMOND. Visual Crystal Structure Information System. Ver. 4.0*; Crystal Impact: Bonn, Germany, 2015.
5. Zhang X., Shen L. Y., Zhang Q. L., Yang X. J., Huang Y. L., Redshaw C., Xu H. A simple turn-off Schiff base fluorescent sensor for copper(II) ion and its application in water analysis. *Molecules* 2021, *26*, 1233.
6. Shen L. Y., Chen X. L., Yang X. J., Xu H., Huang Y. L., Zhang X., Redshaw C., Zhang Q. L. A highly selective turn-on fluorescent probe for the detection of zinc. *Molecules* 2021, *26*, 3825.
7. Yu Q., Wu S. T., Chen X. L., Zhang Q. L., Xu H., Huang Y. L., Zhu B. X., Ni X. L. Twisted Schiff-base macrocycle showing excited-state intramolecular proton-transfer (ESIPT): assembly and sensing properties. *Chem. Commun.* 2020, *56*, 2304–2307.
8. Park H., Kim J., Kwon E., Kim T. H. Crystal structure of flucetosulfuron. *Acta Crystallogr.* 2017, *E73*, 1439–1442.