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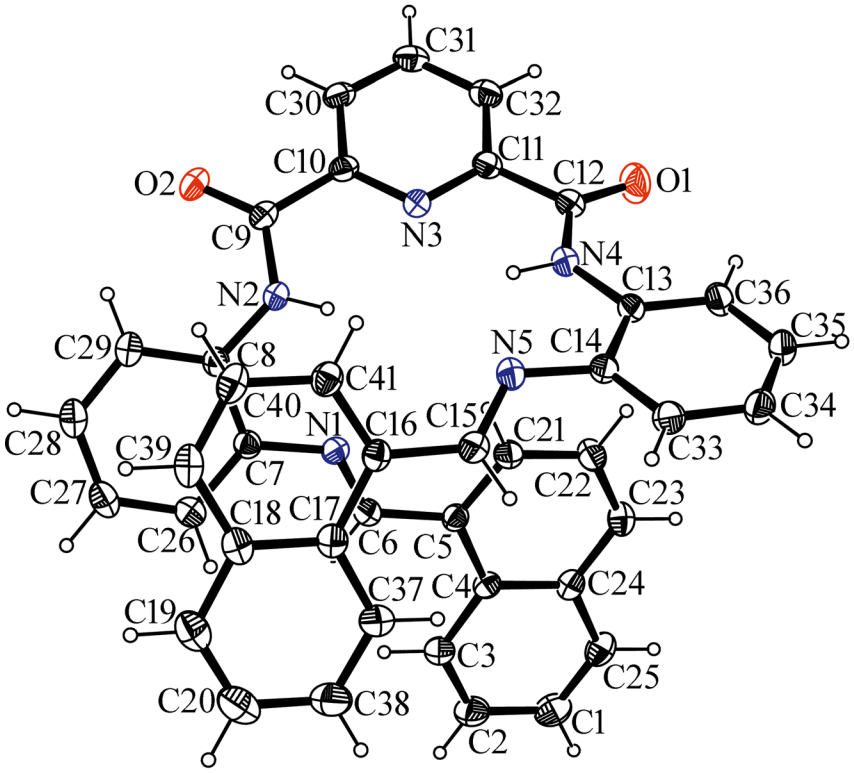
Crystal structure of N^2,N^6-bis(2-(((*E*)-naphthalen-1-ylmethylene)amino)phenyl)pyridine-2,6-dicarboxamide, $C_{41}H_{29}N_5O_2$



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Abstract

$C_{41}H_{29}N_5O_2$, monoclinic, $P2_1/c$ (no. 14), a = 12.4919(10) Å, b = 19.4010(15) Å, c = 13.2741(11) Å, β = 103.319(2)°, V = 3130.5(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0557, $wR_{ref}(F^2)$ = 0.1746, 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:	Yellow block
Size:	0.21 × 0.20 × 0.18 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	24417, 5497, 0.051
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 3415
$N(param)_{refined}$:	434
Programs:	Olex2 [1], Bruker [2], SHELX [3], Diamond [4]

Source of material

A solution of *N*,*N*′-(2-aminophenyl)-2,6-dicarboxylimide pyridine (0.69 g, 2 mmol) in methanol (60 mL) was added to a stirred methanol solution (30 mL) of 1-naphthaldehyde (0.62 g, 4 mmol) in a three-necked flask. The reaction mixture was refluxed for 12 h, then the solution was cooled

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.55558 (15)	0.89828 (11)	0.60202 (17)	0.0871 (7)
O2	−0.01580 (14)	0.89284 (9)	0.55220 (16)	0.0723 (6)
N1	0.16463 (15)	0.67733 (9)	0.53891 (15)	0.0498 (5)
N2	0.09474 (14)	0.79860 (9)	0.58806 (15)	0.0496 (5)
H2	0.1624	0.7869	0.6112	0.060*
N3	0.27386 (15)	0.87657 (9)	0.59776 (15)	0.0485 (5)
N4	0.46848 (15)	0.82222 (10)	0.68688 (16)	0.0536 (5)
H4	0.4037	0.8113	0.6934	0.064*
N5	0.40741 (15)	0.72101 (10)	0.79487 (15)	0.0526 (5)
C1	0.4327 (3)	0.47170 (16)	0.3112 (2)	0.0788 (9)
H1	0.4595	0.4373	0.2749	0.095*
C2	0.3233 (3)	0.46999 (14)	0.3190 (2)	0.0759 (8)
H2A	0.2773	0.4346	0.2876	0.091*
C3	0.2839 (2)	0.51985 (12)	0.3722 (2)	0.0627 (7)
H3	0.2106	0.5182	0.3762	0.075*
C4	0.35115 (18)	0.57420 (11)	0.42182 (17)	0.0462 (6)
C5	0.31397 (17)	0.62728 (11)	0.48055 (17)	0.0461 (6)
C6	0.20068 (19)	0.63004 (12)	0.49129 (19)	0.0534 (6)
H6	0.1528	0.5951	0.4615	0.064*
C7	0.05402 (18)	0.68051 (11)	0.54692 (18)	0.0466 (6)
C8	0.01750 (17)	0.74509 (11)	0.57391 (17)	0.0447 (5)
C9	0.07538 (19)	0.86649 (12)	0.56963 (18)	0.0497 (6)
C10	0.17666 (19)	0.90770 (11)	0.56695 (18)	0.0484 (6)
C11	0.36343 (19)	0.91161 (12)	0.58841 (19)	0.0520 (6)
C12	0.4725 (2)	0.87695 (12)	0.6258 (2)	0.0559 (6)
C13	0.55342 (18)	0.78010 (12)	0.74166 (18)	0.0476 (6)
C14	0.52119 (18)	0.72621 (12)	0.79889 (18)	0.0488 (6)
C15	0.36329 (19)	0.66305 (13)	0.80264 (19)	0.0542 (6)
H15	0.4068	0.6237	0.8085	0.065*
C16	0.24666 (18)	0.65547 (12)	0.80278 (18)	0.0478 (6)
C17	0.19164 (19)	0.59093 (12)	0.77940 (18)	0.0516 (6)
C18	0.08030 (19)	0.58558 (13)	0.78574 (18)	0.0544 (6)
C19	0.0253 (2)	0.52166 (17)	0.7650 (2)	0.0741 (8)
H19	−0.0470	0.5178	0.7713	0.089*
C20	0.0758 (3)	0.46638 (17)	0.7361 (3)	0.0872 (10)
H20	0.0382	0.4248	0.7225	0.105*
C21	0.38648 (19)	0.67793 (12)	0.52431 (19)	0.0550 (6)
H21	0.3624	0.7125	0.5623	0.066*
C22	0.4947 (2)	0.67939 (13)	0.5140 (2)	0.0613 (7)
H22	0.5417	0.7145	0.5448	0.074*
C23	0.5318 (2)	0.62953 (14)	0.4589 (2)	0.0600 (7)
H23	0.6041	0.6309	0.4518	0.072*
C24	0.46198 (19)	0.57572 (12)	0.41228 (18)	0.0516 (6)
C25	0.4997 (2)	0.52308 (15)	0.3560 (2)	0.0684 (8)
H25	0.5723	0.5238	0.3497	0.082*
C26	−0.0195 (2)	0.62547 (13)	0.5318 (2)	0.0593 (7)
H26	0.0038	0.5822	0.5154	0.071*
C27	−0.1259 (2)	0.63414 (15)	0.5409 (2)	0.0676 (8)
H27	−0.1747	0.5972	0.5290	0.081*
C28	−0.1604 (2)	0.69750 (16)	0.5675 (2)	0.0663 (7)
H28	−0.2323	0.7030	0.5744	0.080*
C29	−0.08965 (18)	0.75267 (13)	0.58379 (19)	0.0557 (6)
H29	−0.1139	0.7953	0.6016	0.067*
C30	0.1655 (2)	0.97436 (12)	0.52825 (19)	0.0564 (7)
H30	0.0966	0.9951	0.5102	0.068*
C31	0.2576 (2)	1.00928 (13)	0.5170 (2)	0.0641 (7)
H31	0.2522	1.0537	0.4901	0.077*
C32	0.3582 (2)	0.97707 (13)	0.5465 (2)	0.0612 (7)
H32	0.4217	0.9991	0.5382	0.073*
C33	0.6012 (2)	0.68441 (13)	0.8593 (2)	0.0584 (7)
H33	0.5809	0.6498	0.8996	0.070*
C34	0.7114 (2)	0.69424 (14)	0.8598 (2)	0.0653 (7)
H34	0.7647	0.6659	0.8997	0.078*
C35	0.7415 (2)	0.74577 (14)	0.8013 (2)	0.0662 (7)
H35	0.8154	0.7518	0.8014	0.079*
C36	0.66370 (19)	0.78886 (13)	0.7422 (2)	0.0590 (7)
H36	0.6852	0.8236	0.7028	0.071*
C37	0.2419 (2)	0.53151 (13)	0.7482 (2)	0.0708 (8)
H37	0.3146	0.5336	0.7423	0.085*
C38	0.1846 (3)	0.47137 (15)	0.7267 (3)	0.0857 (9)
H38	0.2185	0.4331	0.7055	0.103*
C39	0.0263 (2)	0.64432 (16)	0.8120 (2)	0.0647 (7)
H39	−0.0468	0.6410	0.8163	0.078*
C40	0.0794 (2)	0.70590 (15)	0.83114 (19)	0.0623 (7)
H40	0.0422	0.7445	0.8469	0.075*
C41	0.1900 (2)	0.71105 (13)	0.82715 (18)	0.0556 (6)
H41	0.2259	0.7532	0.8414	0.067*

to room temperature. The yellow precipitated residue was removed by filtration and then washed with methanol three times. An amount of 0.93 g of a yellow solid was obtained in 75% yield. Then, a small amount of yellow solid was dissolved in a mixed solution of 30 mL of chloroform and methanol. Single crystals were obtained from a mixture solution by slow evaporation at room temperature.

Experimental details

Crystal data, data collection and structure refinement details are summarized in Table 1. 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

Schiff base contains imine nitrogen atoms, and pair electrons are present on these imine nitrogen atoms, which easily coordinate with different metal ions, generating coordination compounds. Schiff base metal coordination compounds have some applications [5]. These special properties originate from ligand structures and metal ions. Therefore, it is of great significance to design and synthesize Schiff base ligands.

With the existence of a plurality of nitrogen atoms, Schiff base compounds containing 2,6-pyridinediimide units coordinate with metal ions more easily. Therefore, this type of compound has been widely used for the generation of Schiff base coordination compounds and for the identification and detection of metal ions [6].

As reflected by the crystal structure, condensation reaction has occurred between the amino groups of *N*,*N*′-(2-aminophenyl)-2,6-dicarboxylimide pyridine and the aldehyde groups of 1-naphthaldehyde, forming the typical "S" structured compound (see the figure). The lengths of imine bonds C6=N1 and C15=N5 are 1.255 Å and 1.267 Å respectively. All bond lengths and bond angles are within the normal range [7, 8]. There are intramolecular hydrogen bonds of N2—H2···N1, N2—H2···N3, N4—H4···N3 and N4—H4···N5.

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

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