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3-(2-Pyridylmethyleneamino)benzoic acid

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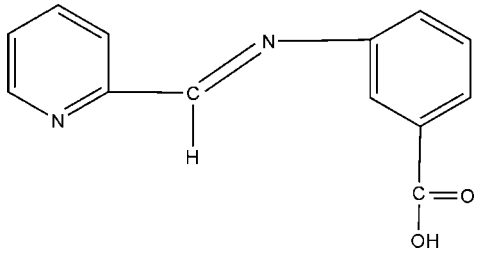
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.062; wR factor = 0.140; data-to-parameter ratio = 12.4.

In the title compound, $C_{13}H_{10}N_2O_2$, the dihedral angle between the aromatic ring planes is 1.3 (2)°. The molecules are linked into chains by intermolecular C—H···O and O—H···N hydrogen bonds.

Related literature

For general background, see: Lindoy *et al.* (1976).



Experimental

Crystal data

$C_{13}H_{10}N_2O_2$
M_r = 226.23
Monoclinic, $C2/c$
a = 27.217 (2) Å
b = 4.0536 (17) Å
c = 23.767 (2) Å
β = 123.553 (15)°
V = 2185.2 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.59 × 0.21 × 0.13 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.946, T_{max} = 0.988
5079 measured reflections
1926 independent reflections
896 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.140
S = 1.00
1926 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93	2.40	3.301 (3)	164
O2—H2···N2^{ii}	0.82	1.85	2.664 (3)	172

Symmetry codes: (i) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2632).

References

Lindoy, L. F., Lip, H. C., Power, L. F. & Rea, T. H. (1976). *Inorg. Chem.* **15**, 1724–1727.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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supplementary materials

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3-(2-Pyridylmethyleneamino)benzoic acid

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Comment

Schiff bases are important intermediates in the preparation of many substances such as dyes, liquid crystals and corrosion inhibitors (*e.g.* Lindoy *et al.*, 1976). We report here the synthesis and crystal structure of the title compound, (I), (Fig. 1), a new Schiff base.

This compound contains two aromatic rings linked through a imino group. An E configuration with respect to the C═N bond is shown by the molecule, with a C—N═C—C torsoin angle of −179.9 (3) °. The molecule of (I) is almost planr, with a dihedral angle of 1.3 (2)° between the benzene and pyridine rings.

As seen in Fig. 2, the molecules are linked into chains propagating in [100] by intermolecular C—H···O and O—H···N hydrogen bonds (Table 1). Thus, classical carboxylic acid inversion dimers do not feature in the packing.

Experimental

Pyridine-2-carboxaldehyde (5 mmol, 535.6 mg) in absolute ethanol (5 ml) was added dropwise to a absolute ethanol solution (15 ml) of *m*-aminobenzoic acid (5 mmol, 685.7 mg). The mixture was heated under reflux with stirring for 2 h and then filtered. The resulting clear pale yellow solution was diffused with diethyl ether vapor at room temperature for 12 days, after which large yellow blocks of (I) were obtained.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C, O).

Figures

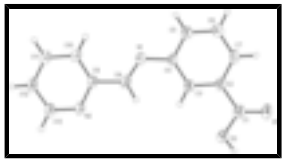

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

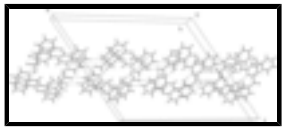

Fig. 2. The crystal packing of (I), viewed approximately along the *a* axis.

3-(2-Pyridylmethyleneamino)benzoic acid

Crystal data

$C_{13}H_{10}N_2O_2$	F_{000} = 944
M_r = 226.23	D_x = 1.375 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 781 reflections
a = 27.217 (2) Å	θ = 3.0–22.2º
b = 4.0536 (17) Å	μ = 0.10 mm^{-1}
c = 23.767 (2) Å	*T* = 298 (2) K
β = 123.553 (15)º	Block, yellow
V = 2185.2 (10) Å^3	0.59 × 0.21 × 0.13 mm
Z = 8	

Data collection

Siemens SMART CCD diffractometer	1926 independent reflections
Radiation source: fine-focus sealed tube	896 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.092
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −26→32
T_{min} = 0.946, T_{max} = 0.988	*k* = −4→4
5079 measured reflections	*l* = −28→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.062	H-atom parameters constrained
$wR(F^2)$ = 0.140	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1926 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
155 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.10556 (9)	0.7481 (7)	0.34401 (12)	0.0521 (8)
N2	0.07264 (9)	1.2019 (7)	0.44507 (12)	0.0514 (8)
O1	0.35449 (8)	0.8343 (7)	0.41129 (11)	0.0816 (9)
O2	0.32303 (8)	1.0085 (7)	0.47445 (10)	0.0703 (8)
H2	0.3564	1.0856	0.4974	0.105*
C1	0.31601 (12)	0.8605 (9)	0.42142 (16)	0.0561 (10)
C2	0.25549 (12)	0.7286 (8)	0.37490 (14)	0.0467 (9)
C3	0.21148 (11)	0.7944 (8)	0.38571 (14)	0.0466 (9)
H3	0.2201	0.9108	0.4239	0.056*
C4	0.15450 (11)	0.6866 (8)	0.33956 (14)	0.0431 (8)
C5	0.14323 (12)	0.5086 (8)	0.28483 (14)	0.0501 (9)
H5	0.1053	0.4293	0.2545	0.060*
C6	0.18674 (13)	0.4448 (10)	0.27381 (15)	0.0597 (10)
H6	0.1782	0.3248	0.2361	0.072*
C7	0.24288 (13)	0.5586 (8)	0.31864 (15)	0.0524 (9)
H7	0.2723	0.5203	0.3108	0.063*
C8	0.10902 (11)	0.9531 (9)	0.38494 (14)	0.0491 (9)
H8	0.1443	1.0656	0.4125	0.059*
C9	0.05954 (11)	1.0241 (9)	0.39133 (14)	0.0439 (8)
C10	0.00358 (11)	0.9087 (9)	0.34624 (14)	0.0538 (10)
H10	−0.0049	0.7873	0.3087	0.065*
C11	−0.03951 (12)	0.9758 (9)	0.35763 (15)	0.0568 (10)
H11	−0.0778	0.9017	0.3273	0.068*
C12	−0.02658 (13)	1.1499 (9)	0.41295 (16)	0.0581 (10)
H12	−0.0552	1.1918	0.4219	0.070*
C13	0.03026 (13)	1.2628 (9)	0.45537 (15)	0.0616 (11)
H13	0.0394	1.3871	0.4929	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0372 (14)	0.070 (2)	0.0529 (16)	0.0010 (14)	0.0276 (13)	−0.0067 (15)

N2	0.0346 (14)	0.071 (2)	0.0524 (15)	0.0037 (14)	0.0266 (13)	−0.0061 (15)
O1	0.0428 (13)	0.127 (3)	0.0893 (17)	−0.0066 (14)	0.0454 (13)	−0.0231 (16)
O2	0.0356 (12)	0.113 (2)	0.0599 (14)	−0.0092 (14)	0.0248 (12)	−0.0223 (15)
C1	0.041 (2)	0.074 (3)	0.055 (2)	0.0023 (18)	0.0277 (18)	−0.0014 (19)
C2	0.0362 (17)	0.059 (3)	0.0466 (18)	0.0035 (16)	0.0238 (16)	0.0013 (17)
C3	0.0352 (17)	0.064 (3)	0.0426 (17)	0.0080 (16)	0.0230 (16)	−0.0004 (16)
C4	0.0315 (16)	0.059 (3)	0.0424 (17)	0.0038 (16)	0.0225 (15)	0.0006 (17)
C5	0.0401 (17)	0.063 (3)	0.0478 (19)	0.0021 (17)	0.0244 (16)	0.0007 (18)
C6	0.055 (2)	0.076 (3)	0.056 (2)	−0.001 (2)	0.0359 (19)	−0.013 (2)
C7	0.0442 (19)	0.068 (3)	0.059 (2)	0.0016 (18)	0.0369 (18)	−0.0017 (19)
C8	0.0312 (16)	0.068 (3)	0.0505 (19)	−0.0021 (17)	0.0240 (16)	0.0008 (19)
C9	0.0315 (16)	0.058 (2)	0.0456 (18)	0.0012 (16)	0.0234 (15)	−0.0017 (17)
C10	0.0337 (18)	0.073 (3)	0.0525 (19)	−0.0016 (16)	0.0223 (17)	−0.0095 (18)
C11	0.0328 (17)	0.073 (3)	0.061 (2)	0.0001 (17)	0.0236 (17)	−0.004 (2)
C12	0.0362 (19)	0.080 (3)	0.065 (2)	0.0040 (18)	0.0327 (18)	−0.003 (2)
C13	0.0437 (19)	0.087 (3)	0.060 (2)	0.0037 (19)	0.0326 (18)	−0.012 (2)

Geometric parameters (Å, °)

N1—C8	1.243 (3)	C5—H5	0.9300
N1—C4	1.415 (3)	C6—C7	1.372 (4)
N2—C13	1.328 (3)	C6—H6	0.9300
N2—C9	1.332 (3)	C7—H7	0.9300
O1—C1	1.202 (3)	C8—C9	1.465 (3)
O2—C1	1.311 (3)	C8—H8	0.9300
O2—H2	0.8200	C9—C10	1.372 (4)
C1—C2	1.486 (4)	C10—C11	1.369 (3)
C2—C7	1.369 (4)	C10—H10	0.9300
C2—C3	1.383 (3)	C11—C12	1.356 (4)
C3—C4	1.385 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.377 (4)
C4—C5	1.366 (4)	C12—H12	0.9300
C5—C6	1.371 (3)	C13—H13	0.9300
C8—N1—C4	120.6 (3)	C2—C7—C6	119.9 (3)
C13—N2—C9	118.6 (3)	C2—C7—H7	120.1
C1—O2—H2	109.5	C6—C7—H7	120.1
O1—C1—O2	123.6 (3)	N1—C8—C9	122.4 (3)
O1—C1—C2	123.3 (3)	N1—C8—H8	118.8
O2—C1—C2	113.1 (2)	C9—C8—H8	118.8
C7—C2—C3	120.2 (3)	N2—C9—C10	121.8 (2)
C7—C2—C1	119.0 (3)	N2—C9—C8	115.6 (3)
C3—C2—C1	120.7 (3)	C10—C9—C8	122.6 (3)
C2—C3—C4	119.9 (3)	C11—C10—C9	118.7 (3)
C2—C3—H3	120.1	C11—C10—H10	120.6
C4—C3—H3	120.1	C9—C10—H10	120.6
C5—C4—C3	119.0 (2)	C12—C11—C10	120.2 (3)
C5—C4—N1	116.0 (3)	C12—C11—H11	119.9
C3—C4—N1	125.0 (3)	C10—C11—H11	119.9
C4—C5—C6	121.2 (3)	C11—C12—C13	117.9 (3)

C4—C5—H5	119.4	C11—C12—H12	121.1
C6—C5—H5	119.4	C13—C12—H12	121.1
C5—C6—C7	119.8 (3)	N2—C13—C12	122.8 (3)
C5—C6—H6	120.1	N2—C13—H13	118.6
C7—C6—H6	120.1	C12—C13—H13	118.6

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.93	2.40	3.301 (3)	164
O2—H2···N2^{ii}	0.82	1.85	2.664 (3)	172

Symmetry codes: (i) *x*−1/2, *y*+1/2, *z*; (ii) −*x*+1/2, −*y*+5/2, −*z*+1.

Fig. 1

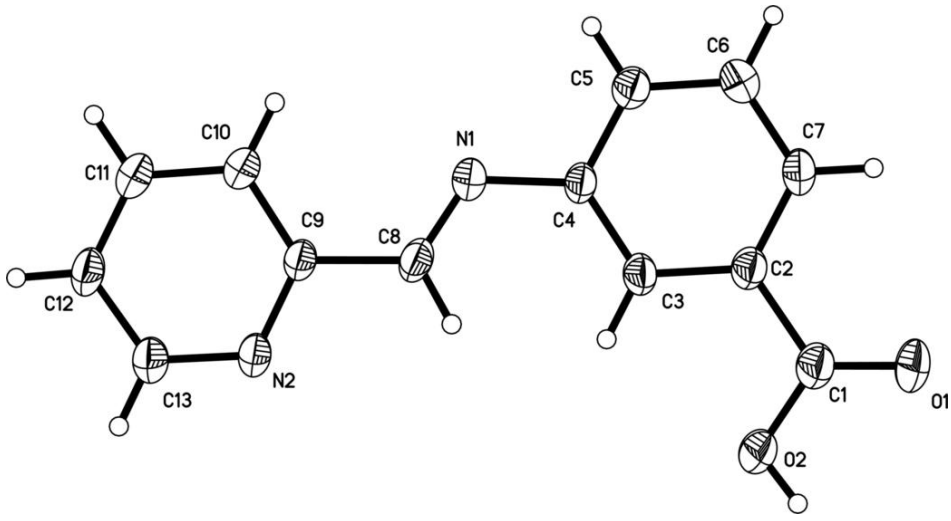

Fig. 2