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N-Benzylpyridin-2-amine

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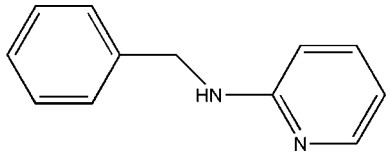
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.115; data-to-parameter ratio = 13.9.

In the crystal of the title compound, $C_{12}H_{12}N_2$, intermolecular N—H···N hydrogen bonds form rings of graph-set motif $R_2^2(8)$ and C—H···π interactions further consolidate the dimers. Neighbouring dimers are further connected into a three-dimensional network by C—H···π interactions. The benzyl and pyridyl rings form a dihedral angle of 67.2 (1)°

Related literature

For general background to the topologies and potential applications of metal coordination polymers, see: Benelli & Gatteschi (2002). For related structures, see: Davies *et al.* (2001); Wan *et al.* (2004); Zhou & Richeson (1995). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bonding graph-set motifs, see: Bernstein *et al.* (1995). For another report on the structure of *N*-benzylpyridin-2-amine, see: Wang & Zhao (2010).



Experimental

Crystal data

$C_{12}H_{12}N_2$
M_r = 184.24
Triclinic, $P\overline{1}$
a = 5.9014 (16) Å
b = 8.025 (2) Å
c = 10.561 (3) Å
α = 95.471 (4)°
β = 91.244 (4)°
γ = 94.779 (3)°
V = 495.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.23 × 0.20 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
2551 measured reflections
1762 independent reflections
1387 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.07
1762 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and N1/C8–C12 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1^{i}	0.86	2.24	3.0518 (19)	157
C12—H12···*Cg*1^{i}	0.93	2.72	3.536 (2)	147
C4—H4···*Cg*2^{ii}	0.93	3.14	3.804 (2)	130

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: RZ2510).

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supplementary materials

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Comment

The design and construction of metal-organic frameworks (MOFs) is of great research interest due to their intriguing topologies and potential applications as functional materials (Benelli & Gatteschi, 2002). The 2-benzylaminopyridine ligand possessing two nitrogen donors to coordinate to metal ions, provides unique opportunities for the construction of various coordination networks. Recently, some complexes based on this ligand have been reported (Davies *et al.*, 2001; Wan *et al.*, 2004; Zhou & Richeson, 1995). When reacted with $Ce(NO_3)_3$ under hydrothermal condition, we isolated single crystals of the 2-benzylaminopyridine ligand, whose structure is reported herein.

The structure of the title compound is depicted in Fig. 1. The benzyl and the pyridyl rings are not coplanar and form a dihedral angle of 67.2 (1)°. The C—C and C—N bond lengths show normal values (Allen *et al.*, 1987). Intermolecular N—H···N hydrogen bonds (graph set motif $R^2_2(8)$; Bernstein *et al.*, 1995) involving a centrosymmetrically related pair of molecules gives rise to a dimer, which is also stabilized by C—H···π stacking interactions (Table 1). C—H···π stacking interactions between neighbouring dimers further extend the structure to form a three-dimensional supramolecular network (Fig. 2).

Experimental

A mixture of $Ce(NO_3)_3.6H_2O$ (0.163 g, 0.5 mmol), 2-benzylaminopyridine (0.092 g, 0.5 mmol), and H_2O (10 mL) was sealed in a 15 mL Teflon-lined reactor, which was heated in an oven to 423 K for 24 h and then cooled to room temperature at a rate of 5 Kh^{-1}. Colourless crystals were obtained in a yield of 58% based on 2-benzylaminopyridine.

Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93-0.97 Å, N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Figures

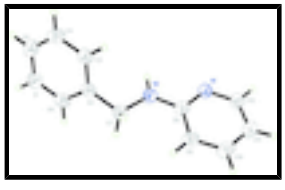

Fig. 1. The molecular structure of the title compound showing the atom numbering scheme and 50% probability displacement ellipsoids.

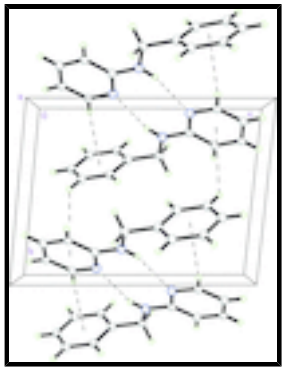

Fig. 2. View of the three-dimensional structure of the title compound. Hydrogen bonds and C—H···π interactions are shown as dased lines.

N-Benzylpyridin-2-amine

Crystal data

$C_{12}H_{12}N_2$	$Z = 2$
$M_r = 184.24$	$F(000) = 196$
Triclinic, $P\overline{1}$	$D_x = 1.234$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 5.9014$ (16) Å	Cell parameters from 3415 reflections
$b = 8.025$ (2) Å	$\theta = 1.2$–$28.0°$
$c = 10.561$ (3) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 95.471$ (4)°	$T = 296$ K
$\beta = 91.244$ (4)°	Block, colourless
$\gamma = 94.779$ (3)°	0.23 × 0.20 × 0.19 mm
$V = 495.9$ (2) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	1387 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.012$
graphite	$\theta_{max} = 25.3°$, $\theta_{min} = 1.9°$
φ and ω scans	$h = -6 \rightarrow 7$
2551 measured reflections	$k = -9 \rightarrow 9$
1762 independent reflections	$l = -9 \rightarrow 12$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.115$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.0854P]$ where $P = (F_o^2 + 2F_c^2)/3$

1762 reflections	$(\Delta/\sigma)_{max} < 0.001$
127 parameters	$\Delta\rho_{max} = 0.23$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
C1	−0.1362 (3)	0.24905 (19)	0.36541 (15)	0.0350 (4)
H1	−0.2427	0.1909	0.4122	0.042*
C2	0.0725 (3)	0.30933 (18)	0.42172 (14)	0.0308 (4)
C3	0.2280 (3)	0.39773 (19)	0.34991 (15)	0.0357 (4)
H3	0.3689	0.4396	0.3860	0.043*
C4	0.1748 (3)	0.4236 (2)	0.22596 (16)	0.0397 (4)
H4	0.2798	0.4832	0.1793	0.048*
C5	−0.0331 (3)	0.3616 (2)	0.17061 (16)	0.0408 (4)
H5	−0.0680	0.3788	0.0868	0.049*
C6	−0.1889 (3)	0.2740 (2)	0.24050 (16)	0.0403 (4)
H6	−0.3292	0.2317	0.2038	0.048*
C7	0.1283 (3)	0.2820 (2)	0.55703 (15)	0.0359 (4)
H7A	0.1617	0.3897	0.6065	0.043*
H7B	−0.0022	0.2242	0.5932	0.043*
C8	0.4265 (3)	0.15939 (18)	0.67594 (14)	0.0301 (4)
C9	0.3600 (3)	0.23242 (19)	0.79450 (14)	0.0353 (4)
H9	0.2360	0.2968	0.7998	0.042*
C10	0.4814 (3)	0.2067 (2)	0.90146 (15)	0.0412 (4)
H10	0.4406	0.2545	0.9805	0.049*
C11	0.6648 (3)	0.1099 (2)	0.89304 (15)	0.0397 (4)
H11	0.7507	0.0930	0.9649	0.048*
C12	0.7150 (3)	0.03973 (19)	0.77449 (15)	0.0359 (4)
H12	0.8367	−0.0269	0.7683	0.043*
N1	0.6010 (2)	0.06064 (16)	0.66736 (12)	0.0334 (3)
N2	0.3221 (2)	0.18353 (16)	0.56430 (12)	0.0355 (3)
H2	0.3734	0.1384	0.4947	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0330 (9)	0.0302 (8)	0.0414 (9)	0.0009 (6)	0.0061 (7)	0.0020 (7)
C2	0.0328 (8)	0.0249 (7)	0.0354 (8)	0.0081 (6)	0.0040 (6)	0.0010 (6)
C3	0.0314 (9)	0.0348 (9)	0.0405 (9)	0.0005 (7)	0.0013 (7)	0.0026 (7)
C4	0.0443 (10)	0.0352 (9)	0.0403 (9)	0.0000 (7)	0.0100 (7)	0.0075 (7)
C5	0.0503 (11)	0.0386 (9)	0.0340 (9)	0.0075 (8)	−0.0017 (7)	0.0041 (7)
C6	0.0358 (9)	0.0403 (9)	0.0431 (10)	0.0021 (7)	−0.0041 (7)	−0.0020 (7)
C7	0.0355 (9)	0.0356 (8)	0.0378 (9)	0.0096 (7)	0.0050 (7)	0.0037 (7)
C8	0.0329 (9)	0.0249 (7)	0.0326 (8)	0.0010 (6)	0.0036 (6)	0.0033 (6)
C9	0.0410 (10)	0.0312 (8)	0.0343 (9)	0.0064 (7)	0.0064 (7)	0.0015 (6)
C10	0.0544 (11)	0.0388 (9)	0.0301 (9)	0.0045 (8)	0.0067 (7)	−0.0003 (7)
C11	0.0481 (10)	0.0382 (9)	0.0323 (9)	0.0022 (8)	−0.0039 (7)	0.0043 (7)
C12	0.0355 (9)	0.0336 (8)	0.0389 (9)	0.0032 (7)	−0.0014 (7)	0.0055 (7)
N1	0.0357 (8)	0.0328 (7)	0.0322 (7)	0.0068 (6)	0.0009 (6)	0.0022 (5)
N2	0.0416 (8)	0.0377 (7)	0.0286 (7)	0.0147 (6)	0.0023 (6)	0.0012 (6)

Geometric parameters (Å, °)

C1—C2	1.385 (2)	C7—H7B	0.9700
C1—C6	1.386 (2)	C8—N1	1.3502 (19)
C1—H1	0.9300	C8—N2	1.3559 (19)
C2—C3	1.395 (2)	C8—C9	1.409 (2)
C2—C7	1.500 (2)	C9—C10	1.366 (2)
C3—C4	1.378 (2)	C9—H9	0.9300
C3—H3	0.9300	C10—C11	1.383 (2)
C4—C5	1.381 (2)	C10—H10	0.9300
C4—H4	0.9300	C11—C12	1.372 (2)
C5—C6	1.380 (2)	C11—H11	0.9300
C5—H5	0.9300	C12—N1	1.3353 (19)
C6—H6	0.9300	C12—H12	0.9300
C7—N2	1.448 (2)	N2—H2	0.8600
C7—H7A	0.9700		
C2—C1—C6	121.05 (15)	C2—C7—H7B	109.5
C2—C1—H1	119.5	H7A—C7—H7B	108.0
C6—C1—H1	119.5	N1—C8—N2	115.92 (13)
C1—C2—C3	118.30 (14)	N1—C8—C9	121.27 (14)
C1—C2—C7	120.76 (14)	N2—C8—C9	122.81 (14)
C3—C2—C7	120.94 (14)	C10—C9—C8	118.62 (15)
C4—C3—C2	120.63 (15)	C10—C9—H9	120.7
C4—C3—H3	119.7	C8—C9—H9	120.7
C2—C3—H3	119.7	C9—C10—C11	120.44 (15)
C3—C4—C5	120.50 (16)	C9—C10—H10	119.8
C3—C4—H4	119.8	C11—C10—H10	119.8
C5—C4—H4	119.8	C12—C11—C10	117.34 (15)
C6—C5—C4	119.57 (15)	C12—C11—H11	121.3

C6—C5—H5	120.2	C10—C11—H11	121.3
C4—C5—H5	120.2	N1—C12—C11	124.42 (15)
C5—C6—C1	119.96 (15)	N1—C12—H12	117.8
C5—C6—H6	120.0	C11—C12—H12	117.8
C1—C6—H6	120.0	C12—N1—C8	117.85 (13)
N2—C7—C2	110.93 (13)	C8—N2—C7	122.91 (13)
N2—C7—H7A	109.5	C8—N2—H2	118.5
C2—C7—H7A	109.5	C7—N2—H2	118.5
N2—C7—H7B	109.5		

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C1–C6 and N1/C8–C12 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1^{i}	0.86	2.24	3.0518 (19)	157
C12—H12···Cg1^{i}	0.93	2.72	3.536 (2)	147
C4—H4···Cg2^{ii}	0.93	3.14	3.804 (2)	130

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

Fig. 1

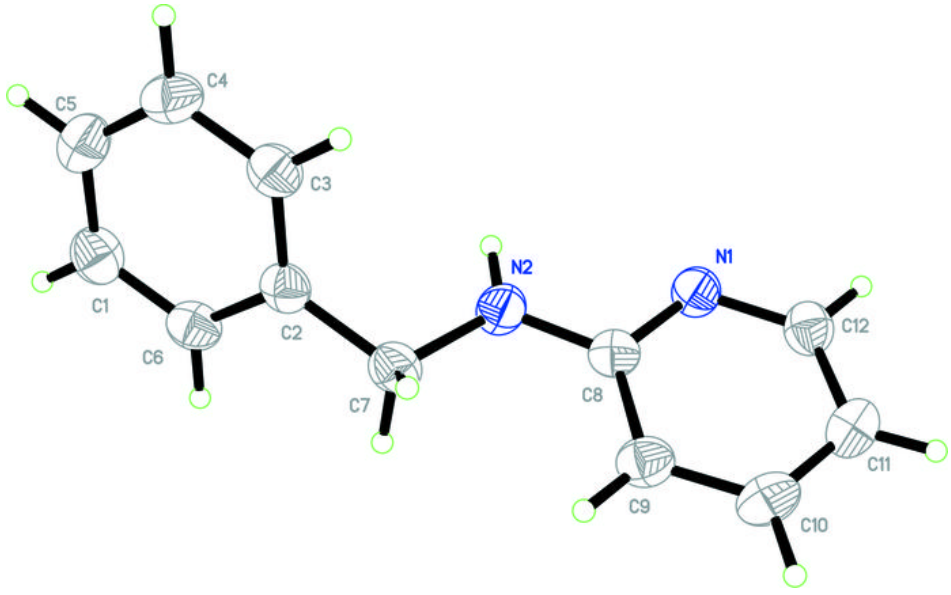

Fig. 2