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Crystal structure of (*E*)-(benzylidene)(pyridin-2-ylmethyl)amine

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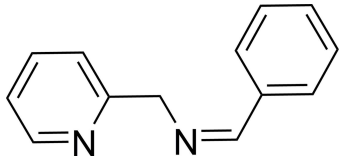
In the title molecule, $C_{13}H_{12}N_2$, all non-H atoms, except for those of the pyridine ring, are essentially coplanar, with an r.m.s. deviation of 0.025 Å. The mean plane of these atoms forms a dihedral angle of 80.98 (4)° with the pyridine ring. In the crystal, weak C—H$\cdots\pi$ interactions link the molecules, forming a three-dimensional network.

Keywords: crystal structure; 2-pyridinemethanamine; C—H$\cdots\pi$ interactions.

CCDC reference: 1440665

1. Related literature

For the synthesis of the title compound, see: Pointeau *et al.* (1986); Ménard *et al.* (1994). For the crystal structures of related Schiff base compounds, see: Pointeau *et al.* (1986); Olivo *et al.* (2015).



2. Experimental

2.1. Crystal data

$C_{13}H_{12}N_2$
M_r = 196.25
Monoclinic, $P2_1/c$
a = 9.8029 (13) Å
b = 10.4175 (13) Å
c = 11.4984 (15) Å
β = 115.138 (4)°
V = 1063.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 147 K
0.32 × 0.22 × 0.11 mm

2.2. Data collection

Bruker Kappa APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.687, T_{max} = 0.746
5375 measured reflections
2427 independent reflections
1712 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.02
2427 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of rings C8–C13 and N1/C1–C5, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2*A*$\cdots$*Cg*1^{i}	0.95	2.87	3.6655 (19)	142
C3—H3*A*$\cdots$*Cg*1^{ii}	0.95	2.71	3.4436 (19)	135
C7—H7*A*$\cdots$*Cg*2^{iii}	0.95	2.93	3.716 (2)	140
C12—H12*A*$\cdots$*Cg*2^{iv}	0.95	2.91	3.484 (2)	120

Symmetry codes: (i) $x, y-1, z$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT*; program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *PLATON* (Spek, 2009) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2014*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5247).

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supporting information

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Crystal structure of (*E*)-(benzylidene)(pyridin-2-ylmethyl)amine

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S1. Structural commentary

The synthesis of the title compound was first reported by Pointeau *et al.* (1986) who described the isolation of an oily mixture of both *E* and *Z* isomers. Ménard *et al.* (1994) provided additional synthetic and characterization details for the title compound. Schiff bases such as the title compound are ideal in the preparation of six coordinate stannanes. The bidentate ligand acts to moderate the Lewis acidity by providing additional electron density to Sn, while at the same time reducing nucleophilic attack from species such as water. The incorporation of this ligand would change the coordination number at the Sn centre from tetrahedral to a pseudo octahedral. The isolation of only a single isomer in the crystal structure of the title molecule may be a result of the dehydrating conditions of the reaction where all evolved moisture from the condensation was absorbed by activated molecular sieves.

The molecular structure of the title compound is shown in Fig. 1. In the molecule, all non-H atoms except for those of the pyridine ring are essentially coplanar with an r.m.s. deviation of 0.025 Å and the mean plane of these atoms (C8–C13/C7/N2/C6) forms a dihedral angle of 80.98 (4)° with the pyridine ring (N1/C1–C5).

In the crystal, weak C—H···π interactions link molecules forming a three-dimensional network (Fig. 2).

S2. Synthesis and crystallization

In a sealed 100 ml 3-neck round bottom flask equipped with a magnetic stir bar, 5 grams of 4Å molecular sieves were flamed dried and placed under dynamic vacuum for over 1 hr. Dried CH_2Cl_2 (25 mL), benzaldehyde (900 mg, 8.48 mmol) and 2-picolylamine (917 mg, 8.48 mmol) were placed into a flask and stirred for 12 hr under N_2. The resulting slurry was then filtered through Celite and the organic layer washed with 1N NaCl (2 x 10 ml). The solution was then filtered and the solvent removed under vacuum to yield colourless needle crystals. Analysis by NMR spectroscopy (^{1}H NMR) was similar to that previously reported by Pointeau *et al.* (1986). Yield: 92% (1.65 g, 8.41 mmol) ^{1}H NMR ($CDCl_3$): δ 4.97(s, 2H), 7.17 (ddt, ^{2}J = 5 Hz, ^{3}J = 1Hz, 1H), 7.43 (m, 4H), 7.66 (td, ^{2}J = 5 Hz, ^{3}J = 2 Hz, 1H), 7.815 (dd, ^{2}J = 5Hz, ^{3}J = 2Hz, 2H), 8.48 (s, 1H), 8.58 (d, ^{3}J = 2Hz, 1H) ppm; ^{13}C NMR 66.79, 121.98, 122.25, 128.32, 128.60, 130.87, 136.09, 136.63, 149.25, 159.31 ppm. Analysis HRMS: [M+H] Calc: 197.10787; Found 197.10804.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Hydrogen atoms bonded to C atoms were placed in calculated positions with C—H distances 0.95 and 0.99 Å and included in the refinement in a riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C).

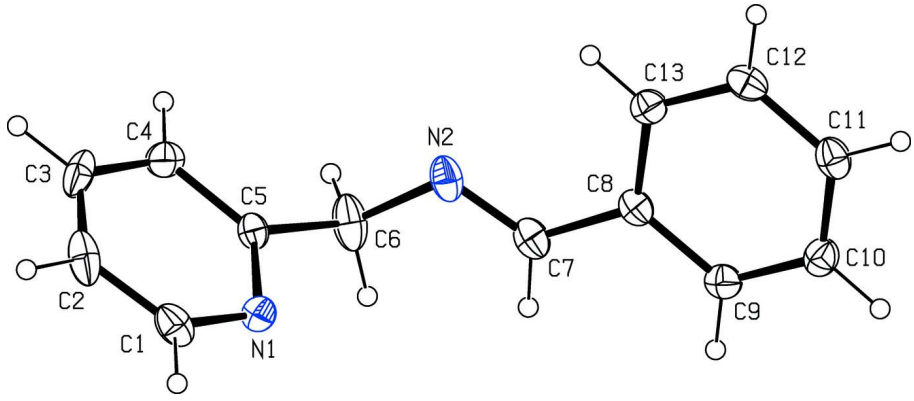

Figure 1

The molecular structure of title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

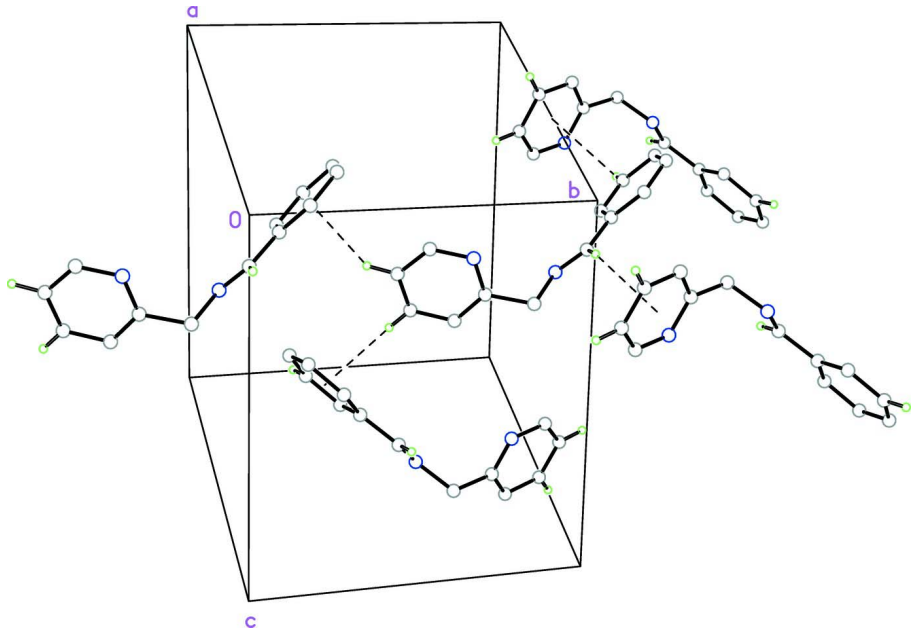

Figure 2

A partial view of the crystal packing of the title compound, with the weak C—H···π interactions shown as dashed lines (see Table 1).

(*E*)-(Benzylidene)(pyridin-2-ylmethyl)amine

Crystal data

$C_{13}H_{12}N_2$
$M_r = 196.25$
Monoclinic, $P2_1/c$
$a = 9.8029$ (13) Å
$b = 10.4175$ (13) Å
$c = 11.4984$ (15) Å
$\beta = 115.138$ (4)°
$V = 1063.0$ (2) Å^3
$Z = 4$

$F(000) = 416$
$D_x = 1.226$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2108 reflections
$\theta = 2.8$–27.4°
$\mu = 0.07$ mm^{-1}
$T = 147$ K
Needle, colourless
0.32 × 0.22 × 0.11 mm

Data collection

Bruker Kappa APEX DUO CCD diffractometer
Radiation source: sealed tube with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.687, T_{max} = 0.746
5375 measured reflections
2427 independent reflections
1712 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −12→11
k = −13→13
l = −12→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.02
2427 reflections
136 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.1728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.15560 (14)	0.68211 (12)	0.22241 (12)	0.0330 (3)
N2	0.22487 (16)	0.95797 (12)	0.30974 (14)	0.0386 (3)
C1	0.20176 (19)	0.56274 (15)	0.21743 (17)	0.0408 (4)
H1A	0.1794	0.5273	0.1352	0.049*
C2	0.27894 (19)	0.48812 (15)	0.32253 (19)	0.0452 (5)
H2A	0.3094	0.4036	0.3134	0.054*
C3	0.31131 (17)	0.53793 (16)	0.44134 (18)	0.0435 (5)
H3A	0.3647	0.4884	0.5165	0.052*
C4	0.26525 (17)	0.66143 (16)	0.45063 (15)	0.0363 (4)
H4A	0.2864	0.6982	0.5321	0.044*
C5	0.18781 (16)	0.73029 (13)	0.33913 (14)	0.0285 (3)
C6	0.1323 (2)	0.86489 (14)	0.3400 (2)	0.0484 (5)
H6A	0.0261	0.8721	0.2759	0.058*
H6B	0.1363	0.8842	0.4257	0.058*
C7	0.15547 (18)	1.02977 (13)	0.21382 (15)	0.0337 (4)
H7A	0.0496	1.0192	0.1677	0.040*
C8	0.22990 (16)	1.12861 (13)	0.16989 (14)	0.0288 (3)
C9	0.14469 (17)	1.19809 (13)	0.05954 (14)	0.0313 (3)
H9A	0.0392	1.1835	0.0161	0.038*
C10	0.21199 (18)	1.28840 (14)	0.01229 (15)	0.0346 (4)
H10A	0.1530	1.3346	−0.0639	0.042*
C11	0.36432 (19)	1.31114 (14)	0.07569 (15)	0.0357 (4)

H11A	0.4105	1.3732	0.0435	0.043*
C12	0.45054 (17)	1.24339 (15)	0.18669 (15)	0.0347 (4)
H12A	0.5556	1.2597	0.2305	0.042*
C13	0.38459 (17)	1.15228 (14)	0.23412 (14)	0.0318 (3)
H13A	0.4442	1.1060	0.3100	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0341 (7)	0.0335 (7)	0.0304 (7)	−0.0004 (6)	0.0127 (6)	0.0025 (5)
N2	0.0540 (9)	0.0231 (6)	0.0479 (8)	0.0000 (6)	0.0305 (7)	−0.0018 (6)
C1	0.0507 (10)	0.0335 (8)	0.0465 (10)	−0.0098 (8)	0.0286 (9)	−0.0102 (7)
C2	0.0496 (10)	0.0257 (7)	0.0796 (14)	0.0064 (7)	0.0459 (10)	0.0101 (8)
C3	0.0279 (8)	0.0498 (10)	0.0557 (11)	0.0094 (7)	0.0207 (8)	0.0323 (9)
C4	0.0339 (8)	0.0477 (9)	0.0289 (8)	−0.0082 (7)	0.0149 (7)	0.0028 (7)
C5	0.0302 (7)	0.0257 (7)	0.0336 (8)	−0.0020 (6)	0.0175 (6)	0.0015 (6)
C6	0.0674 (12)	0.0283 (8)	0.0715 (13)	0.0053 (8)	0.0509 (11)	0.0040 (8)
C7	0.0371 (8)	0.0256 (7)	0.0453 (9)	0.0014 (6)	0.0242 (8)	−0.0065 (7)
C8	0.0322 (8)	0.0244 (7)	0.0343 (8)	0.0012 (6)	0.0186 (7)	−0.0064 (6)
C9	0.0303 (7)	0.0293 (7)	0.0333 (8)	0.0035 (6)	0.0125 (6)	−0.0057 (6)
C10	0.0416 (9)	0.0311 (8)	0.0312 (8)	0.0049 (7)	0.0156 (7)	0.0007 (6)
C11	0.0469 (9)	0.0287 (7)	0.0397 (9)	−0.0032 (7)	0.0262 (8)	−0.0040 (7)
C12	0.0307 (8)	0.0356 (8)	0.0396 (9)	−0.0040 (7)	0.0168 (7)	−0.0094 (7)
C13	0.0343 (8)	0.0301 (7)	0.0300 (8)	0.0033 (6)	0.0127 (6)	−0.0040 (6)

Geometric parameters (Å, º)

N1—C1	1.333 (2)	C6—H6B	0.9900
N1—C5	1.3391 (18)	C7—C8	1.470 (2)
N2—C7	1.265 (2)	C7—H7A	0.9500
N2—C6	1.467 (2)	C8—C9	1.390 (2)
C1—C2	1.364 (2)	C8—C13	1.398 (2)
C1—H1A	0.9500	C9—C10	1.386 (2)
C2—C3	1.367 (3)	C9—H9A	0.9500
C2—H2A	0.9500	C10—C11	1.376 (2)
C3—C4	1.383 (2)	C10—H10A	0.9500
C3—H3A	0.9500	C11—C12	1.387 (2)
C4—C5	1.381 (2)	C11—H11A	0.9500
C4—H4A	0.9500	C12—C13	1.384 (2)
C5—C6	1.506 (2)	C12—H12A	0.9500
C6—H6A	0.9900	C13—H13A	0.9500
C1—N1—C5	116.94 (13)	H6A—C6—H6B	108.1
C7—N2—C6	116.07 (15)	N2—C7—C8	123.50 (15)
N1—C1—C2	124.36 (16)	N2—C7—H7A	118.2
N1—C1—H1A	117.8	C8—C7—H7A	118.2
C2—C1—H1A	117.8	C9—C8—C13	119.14 (13)
C1—C2—C3	118.37 (15)	C9—C8—C7	119.01 (14)

C1—C2—H2A	120.8	C13—C8—C7	121.83 (14)
C3—C2—H2A	120.8	C10—C9—C8	120.66 (14)
C2—C3—C4	119.06 (15)	C10—C9—H9A	119.7
C2—C3—H3A	120.5	C8—C9—H9A	119.7
C4—C3—H3A	120.5	C11—C10—C9	119.97 (15)
C5—C4—C3	118.71 (15)	C11—C10—H10A	120.0
C5—C4—H4A	120.6	C9—C10—H10A	120.0
C3—C4—H4A	120.6	C10—C11—C12	119.99 (14)
N1—C5—C4	122.57 (13)	C10—C11—H11A	120.0
N1—C5—C6	115.06 (13)	C12—C11—H11A	120.0
C4—C5—C6	122.37 (14)	C13—C12—C11	120.49 (14)
N2—C6—C5	110.62 (12)	C13—C12—H12A	119.8
N2—C6—H6A	109.5	C11—C12—H12A	119.8
C5—C6—H6A	109.5	C12—C13—C8	119.75 (14)
N2—C6—H6B	109.5	C12—C13—H13A	120.1
C5—C6—H6B	109.5	C8—C13—H13A	120.1

C5—N1—C1—C2	−0.2 (2)	C6—N2—C7—C8	179.81 (13)
N1—C1—C2—C3	0.2 (2)	N2—C7—C8—C9	176.78 (13)
C1—C2—C3—C4	−0.1 (2)	N2—C7—C8—C13	−1.5 (2)
C2—C3—C4—C5	0.0 (2)	C13—C8—C9—C10	1.0 (2)
C1—N1—C5—C4	0.1 (2)	C7—C8—C9—C10	−177.39 (12)
C1—N1—C5—C6	−179.47 (13)	C8—C9—C10—C11	−0.8 (2)
C3—C4—C5—N1	0.0 (2)	C9—C10—C11—C12	0.2 (2)
C3—C4—C5—C6	179.50 (14)	C10—C11—C12—C13	0.3 (2)
C7—N2—C6—C5	122.53 (16)	C11—C12—C13—C8	−0.2 (2)
N1—C5—C6—N2	−74.07 (19)	C9—C8—C13—C12	−0.5 (2)
C4—C5—C6—N2	106.40 (17)	C7—C8—C13—C12	177.85 (12)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of rings C8–C13 and N1/C1–C5, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···*Cg*1^{i}	0.95	2.87	3.6655 (19)	142
C3—H3*A*···*Cg*1^{ii}	0.95	2.71	3.4436 (19)	135
C7—H7*A*···*Cg*2^{iii}	0.95	2.93	3.716 (2)	140
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Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*, *y*+1/2, −*z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.