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(1*R*,2*R*)-*N*,*N*′-Bis(2-pyridylmethylene)cyclohexane-1,2-diamine

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Key indicators

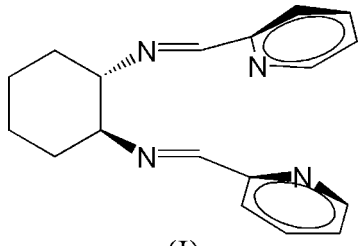
Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.097
Data-to-parameter ratio = 11.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the molecule of the title compound, $C_{18}H_{20}N_4$, the cyclohexane ring has a chair conformation. The dihedral angle between the two planar pyridine rings is 68.19 (3)°.

Comment

Schiff bases are important ligands for asymmetric catalysts. In the course of our investigation of the coordination of Schiff bases with transition metal salts, we observed that the title compound, (I), as a bidentate ligand, *N*,*N*-coordinates readily with Ni^{II} and Cu^{II} salts. We here report the crystal structure of (I).



(I)

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

Ring *A* (C1–C6) has a total puckering amplitude, Q_T, of 0.584 (3) Å and a chair conformation [φ = 7.41 (15)°, θ = 178.61 (3)°] (Cremer & Pople, 1975). Rings *B* (N3/C8–C12) and *C* (N4/C14–C18) are, of course, planar; the dihedral angle between them is 68.19 (3)°.

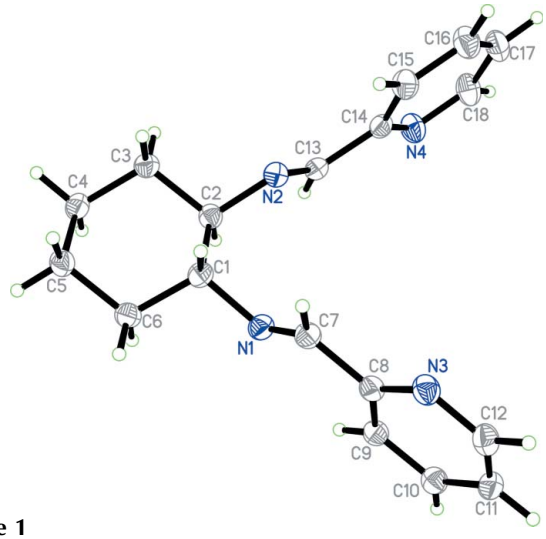


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level.

Experimental

(1*R*,2*R*)-1,2-Diaminocyclohexane (1 g, 8.77 mmol) was dissolved in methanol (5 ml) and 2-pyridinecarboxaldehyde (1.88 g, 17.55 mmol) was added. The mixture was stirred for 5 h. The resulting precipitate was filtered, recrystallized from hexane/methanol (2:1) and dried in air to afford the title compound (yield 2.2 g, 86%, m.p. 400 K). Yellow crystals suitable for X-ray analysis were obtained by slow evaporation of a hexane solution at room temperature over a period of two weeks.

Crystal data

$C_{18}H_{20}N_4$	$Z = 4$
$M_r = 292.38$	$D_x = 1.193$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.5865$ (18) Å	$\mu = 0.07$ mm^{-1}
$b = 8.7487$ (18) Å	$T = 113$ (2) K
$c = 21.661$ (5) Å	Block, yellow
$V = 1627.2$ (6) Å^3	0.24 × 0.22 × 0.16 mm

Data collection

Rigaku Saturn diffractometer	20457 measured reflections
ω scans	2239 independent reflections
Absorption correction: multi-scan (Jacobson, 1998)	2187 reflections with $I > 2\sigma(I)$
$T_{min} = 0.978$, $T_{max} = 0.988$	$R_{int} = 0.048$
	$\theta_{max} = 27.9°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.3527P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.097$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
2239 reflections	Extinction correction: *SHELXL97*
201 parameters	Extinction coefficient: 0.037 (4)
H-atom parameters constrained	

H atoms were positioned geometrically, with C—H = 0.95, 1.00 and 0.99 Å for aromatic, methine and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration was assigned on the basis of the starting material.

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2004); software used to prepare material for publication: *CrystalStructure*.

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