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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.053
 wR factor = 0.143
Data-to-parameter ratio = 14.7

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

(1*R*,2*R*)-Bis(4-pyridylmethyleamino)cyclohexane

The two imine moieties of the title compound, $\text{C}_{18}\text{H}_{20}\text{N}_4$, are positioned equatorially on the chair-conformation cyclohexane ring. Both also show a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond. The molecule lies on a crystallographic twofold rotation in a non-centrosymmetric space group. The dihedral angle between the two least-squares planes of the pyridine rings is 56.6 (2)°.

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Comment

The construction of transition-metal supramolecular arrays based on covalent interaction or hydrogen bonding is an area of great activity in coordination chemistry. The strategy for the preparation of these extended systems has been examined by enhancing the linking between structural units of lower dimensionality (Hernandez *et al.*, 2000). The use of spacers containing two 4-pyridyl donor units has afforded very interesting structural motifs, such as double- and triple-stranded helicates, double sheets, inter-penetrating ladders and brick-wall framework, *etc.* (Zhang *et al.*, 2001). Furthermore, in recent years, there has been renewed interest in helical chirality in inorganic and coordination chemistry (Fei *et al.*, 2000). It has been shown that silver(I) combines with a single enantiomer of a bis(pyridyl) ligand derived from *L*- or *D*-tartaric acid to give an extended single-strand helicate, whereas the corresponding racemic form of the ligand produces a disilver(I) complex incorporating both enantiomers in a *meso* arrangement (Suzuki *et al.*, 1995). A Schiff base of (1*R*,2*R*)-1,2-diaminocyclohexane reacted with a silver(I) salt to produce a homochiral single-strand polymer (Bowyer *et al.*, 1998). We have examined a new enantiomeric bis(pyridyl) ligand, (1*R*,2*R*)-bis(4-pyridylmethyleamino)cyclohexane, (I), and determined its structure. Further research on building homochiral structures is in progress.

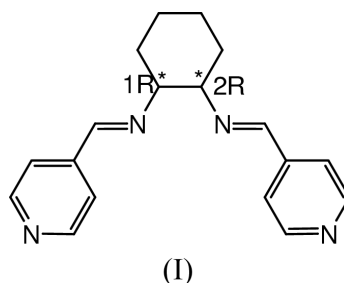


Fig. 1 shows an *ORTEP*II (Johnson, 1976) drawing of (I) with the atom-numbering scheme. The $\text{C}7-\text{N}2$ bond length of 1.456 (2) Å is within the normal range for $\text{C}-\text{N}$ single bonds, while the $\text{C}6-\text{N}2$ bond length is in the normal range expected for a $\text{C}=\text{N}$ double bond. These bond distances are compar-

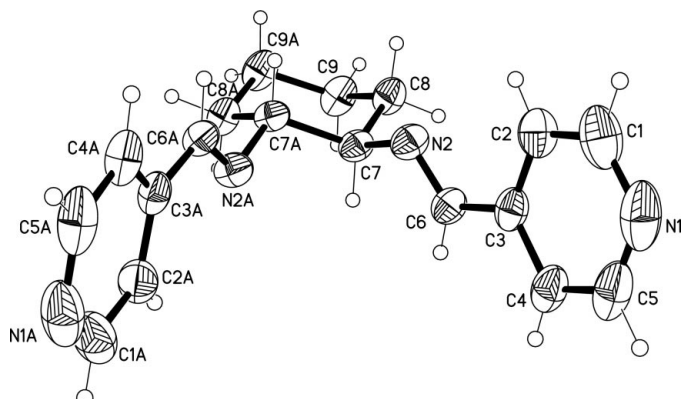


Figure 1
ORTEPII (Johnson, 1976) drawing of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.

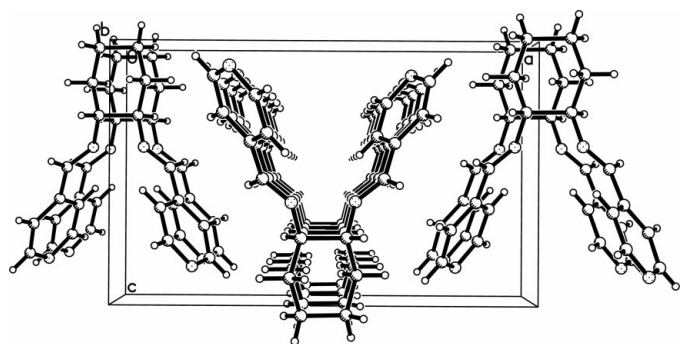


Figure 2
A packing diagram of the title compound, viewed down the *b* axis.

able with those in silver(I) complexes (Stein *et al.*, 1984, 1985; Bowyer *et al.*, 1998). Both imine moieties are equatorial with respect to the chair-conformation cyclohexane ring. The dihedral angle between the planes of the pyridine rings is $56.6(2)^\circ$. These rings are also positioned in a *trans* configuration with respect to the C=N double bond, minimizing their intramolecular interaction. The molecule has crystallographic twofold rotation symmetry. The molecular packing pattern is stabilized by steric complementarity in neighboring molecules (Fig. 2).

Experimental

The title compound, (I), was synthesized by a condensation reaction of 4-pyridylcarboxaldehyde and (1*R*,2*R*)-diaminocyclohexane, based on a modification of the procedure of Goodwin & Lions (1960). (1*R*,2*R*)-Diaminocyclohexane was mixed with 4-pyridylcarboxaldehyde in absolute ethanol in a 1:1 molar ratio. The reaction mixture was stirred at 313 K overnight, after which the solvent was evaporated under vacuum, leaving a pale-yellow solid. The residue was crystallized from a mixture of petroleum ether (333–363 K) and diethyl ether (1:1), giving colorless prismatic crystals. Colorless block crystals suitable for the crystallographic analysis were obtained by slow evaporation of a solution of (I) in a mixture of petroleum ether (333–363 K) and CHCl_3 (1:1).

Crystal data

$\text{C}_{18}\text{H}_{20}\text{N}_4$
 $M_r = 292.38$
Orthorhombic, $P2_12_12$
 $a = 15.230(4) \text{ \AA}$
 $b = 5.789(1) \text{ \AA}$
 $c = 9.415(2) \text{ \AA}$
 $V = 830.0(3) \text{ \AA}^3$
 $Z = 2$
 $D_x = 1.170 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
Cell parameters from 1006 reflections
 $\theta = 2.6\text{--}25.5^\circ$
 $\mu = 0.07 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
Block, colorless
 $0.3 \times 0.2 \times 0.2 \text{ mm}$

Data collection

Bruker CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.983$, $T_{\max} = 0.986$
1473 independent reflections
1288 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -17 \rightarrow 18$
 $k = -6 \rightarrow 6$
 $l = -11 \rightarrow 6$
4258 measured reflections

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.143$
 $S = 1.01$
1473 reflections
100 parameters
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
Absolute structure: Flack (1983);
584 Friedel pairs
Flack parameter = 0.002(1)

All H atoms were placed in geometrically calculated positions, with C–H = 0.93–0.97 Å, and were refined as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{parent atom})$.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SHELXTL (Bruker, 1997); program(s) used to solve structure: SHELXTL; program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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