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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.030
 wR factor = 0.032
Data-to-parameter ratio = 10.7

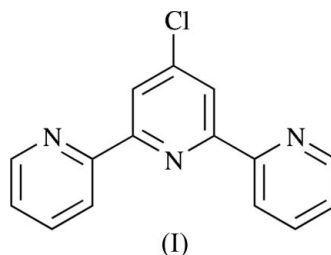
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

4'-Chloro-2,2':6',2''-terpyridine

In the title compound, $\text{C}_{15}\text{H}_{10}\text{ClN}_3$, the terpyridine unit adopts a *trans,trans* conformation. Molecules assemble into π -stacked columns along the b axis, with an interplanar distance of 3.51 Å.

Comment

Despite the widespread use of ligands based on 2,2':6',2''-terpyridine (tpy) in coordination chemistry (Andres & Schubert, 2004; Baranoff *et al.*, 2004; Constable, 1986; Hofmeier & Schubert, 2004; Thummel, 2004), few crystal structures of ligands with simple substituents have been reported. Ligands with substituents in the 4'-position (Fallahpour, 2003) are of particular significance in the design of extended assemblies with controlled stereochemistry. 4'-Chloro-2,2':6',2''-terpyridine, (I) (Constable & Ward, 1990), is commonly used as a precursor to other 4'-substituted-tpy ligands. We present here the crystal structure of (I).



Crystals of (I) were grown by slow cooling of a hot methanol solution of the ligand. Fig. 1 shows the structure of a molecule of (I). As expected, the three pyridine rings adopt a *trans,trans* conformation. Bond distances and angles are unexceptional. The molecule is close to being planar: the angles between the least-squares planes of the pyridine rings containing atoms N1 and N2, and N2 and N3 are 8.0 (1) and 5.4 (1)°, respectively. Molecules of (I) pack in π -stacked columns which run along the b axis (Fig. 2). The distance between the least-squares planes (each containing 29 atoms) of adjacent molecules is 3.51 Å. Atom Cl is not involved in any short intermolecular contacts. A search of the Cambridge Structural Database (CSD, Version 5.2.7; Allen, 2002; Bruno *et al.*, 2002) for tpy-based ligands containing single atoms (*e.g.* halogen) or short rigid-rod substituents at the 4'-position yielded no hits except for the parent 2,2':6',2''-terpyridine (Bessel *et al.*, 1992). That report describes the closest intermolecular interactions as being C—H...N contacts in the range 2.76–2.93 Å. A re-examination of the structure reveals that the packing also features π stacking (distance between least-squares planes of adjacent molecules = 3.45 Å). In

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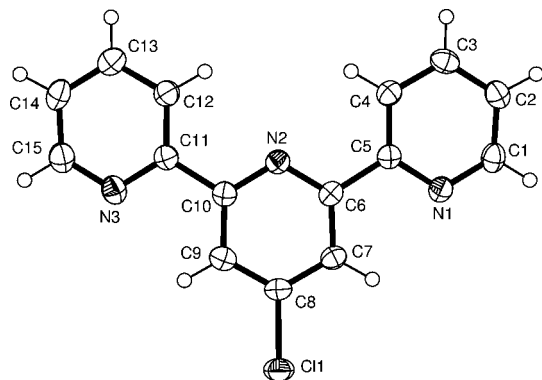


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

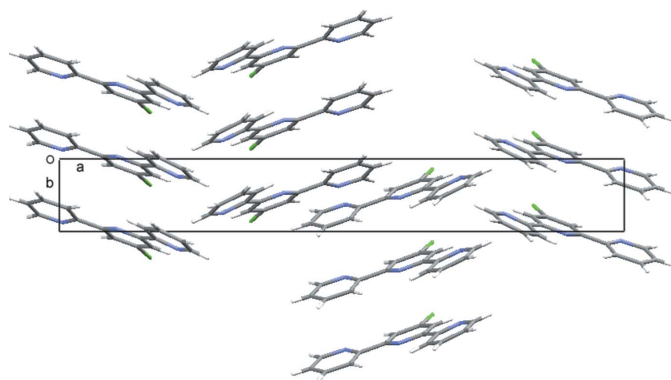


Figure 2
The packing of (I) viewed down the *c* axis, showing the π -stacked columns of molecules. Symmetry code for translation of molecules along a column (*x*, *y* + 1, *z*).

contrast to the simple stacked columns of molecules in (I), those of 2,2':6',2''-terpyridine form a more complex arrangement.

Experimental

Compound (I) was prepared as previously reported (Constable & Ward, 1990) and crystals were grown by slow cooling of a hot methanol solution.

Crystal data

$C_{15}H_{10}ClN_3$	$Z = 4$
$M_r = 267.72$	$D_x = 1.460 \text{ Mg m}^{-3}$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 29.8317 (15) \text{ \AA}$	$\mu = 0.30 \text{ mm}^{-1}$
$b = 3.8344 (2) \text{ \AA}$	$T = 173 \text{ K}$
$c = 10.6476 (5) \text{ \AA}$	Plate, colourless
$V = 1217.94 (11) \text{ \AA}^3$	$0.20 \times 0.17 \times 0.04 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer	7250 measured reflections
φ and ω scans	2554 independent reflections
Absorption correction: multi-scan (<i>DENZO/SCALEPACK</i> ; Otwinowski & Minor, 1997)	1848 reflections with $I > 3\sigma(I)$
$T_{\min} = 0.95$, $T_{\max} = 0.99$	$R_{\text{int}} = 0.098$
	$\theta_{\max} = 27.6^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F^2) + (0.02P)^2]$
$R[F > 2\sigma(F)] = 0.030$	where $P = [\max(F_o^2, 0) + 2F_c^2]/3$
$wR(F) = 0.032$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 0.94$	$\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$
1848 reflections	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$
173 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1130 Friedel pairs
	Flack parameter: $-0.04 (6)$

All H atoms were treated as riding atoms, with $C-H = 0.96 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

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