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Dichlorobis(pyrazino[2,3-*f*][1,10]phenanthroline-κ^2N,N')cadmium(II)

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Key indicators

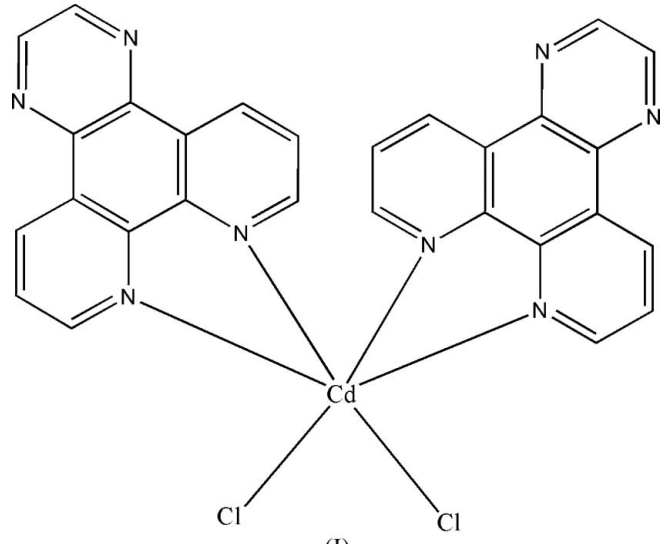
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.025
wR factor = 0.062
Data-to-parameter ratio = 13.5

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

In the title compound, $[CdCl_2(C_{14}H_8N_4)_2]$, the central Cd^{II} ion is six-coordinate in an octahedral geometry, coordinated by two Cl^- ions and four N atoms from two chelating pyrazino[2,3-*f*][1,10]phenanthroline ligands. The metal atom lies on a twofold rotation axis.

Comment

The 1,10-phenanthroline ligand has been widely used for the synthesis of coordination compounds; these are sometimes assembled into supramolecular architectures through aromatic π–π interactions (Chen & Liu, 2002). Pyrazino[2,3-*f*][1,10]phenanthroline (PyPhen) is a similarly useful ligand, and several complexes have been reported (Che *et al.*, 2006). The title compound, $[CdCl_2(PyPhen)_2]_n$ (I), has the metal lying on a twofold rotation axis in an octahedral geometry (Fig. 1). It is coordinated by two Cl^- ions and four N atoms from two PyPhen ligands.



(I)

There are π–π stacking interactions (π–π stacking distance = 3.363 Å), giving rise to a supramolecular structure (Fig. 2).

Experimental

Pyrazino[2,3-*f*][1,10]phenanthroline was synthesized according to the literature method of Dickeson & Summers (1970). To a solution of $CdCl_2$ (0.092 g, 0.5 mmol) and the ligand (0.045 g, 0.2 mmol) in 30 ml water was added aqueous sodium hydroxide to a pH of about 7.5. The mixture was placed in a stainless steel, Teflon-lined reaction vessel (40 ml) and heated to 453 K for 4 d. Dark-brown crystals were obtained (65% yield on Cd).

Crystal data

$[CdCl_2(C_{28}H_{16}N_8)]$
M_r = 647.80
Monoclinic, $C2/c$
a = 8.4987 (11) Å
b = 12.5070 (17) Å
c = 22.768 (3) Å
β = 95.267 (2)°
V = 2409.8 (6) Å^3
Z = 4
D_x = 1.786 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 292 (2) K
Block, dark brown
0.38 × 0.21 × 0.16 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.751, T_{max} = 0.828
6690 measured reflections
2382 independent reflections
2170 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.07
2382 reflections
177 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 2.0151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.3805 (18)	Cd1—Cl1	2.5382 (7)
Cd1—N2	2.425 (2)		
N1—Cd1—N2	68.85 (6)	N2—Cd1—Cl1	162.22 (5)
N1—Cd1—Cl1	94.44 (5)		

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

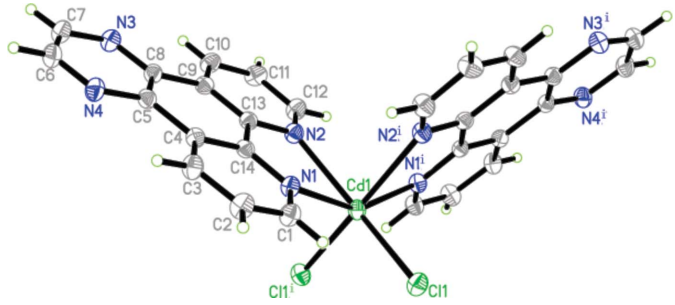


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x, y, \frac{1}{2} - z$.]

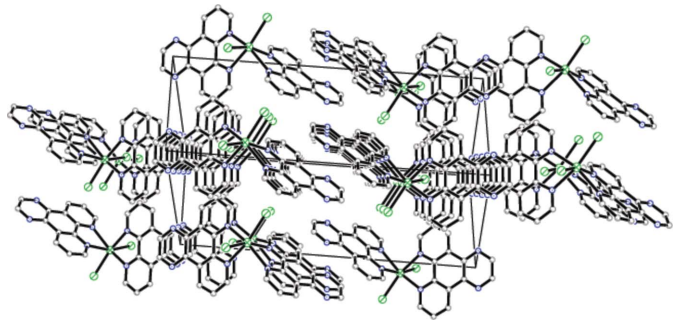


Figure 2
A view of the layer structure arising from π–π interactions.

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