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Diacetatobis[2-(2-furyl)-1*H*-imidazo[4,5-*f*]-[1,10]phenanthroline]cadmium(II)

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.070
Data-to-parameter ratio = 13.2

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

In the title complex, $[Cd(C_2H_3O_2)_2(C_{17}H_{10}N_4O)_2]$, the central Cd^{II} ion (site symmetry 2) shows an uncommon eight-coordinate CdN_4O_4 coordination geometry arising from two *N*,*N*-chelating 2-(2-furyl)-1*H*-imidazo[4,5-*f*]-1,10-phenanthroline molecules and two *O*,*O*-bidentate acetate anions.

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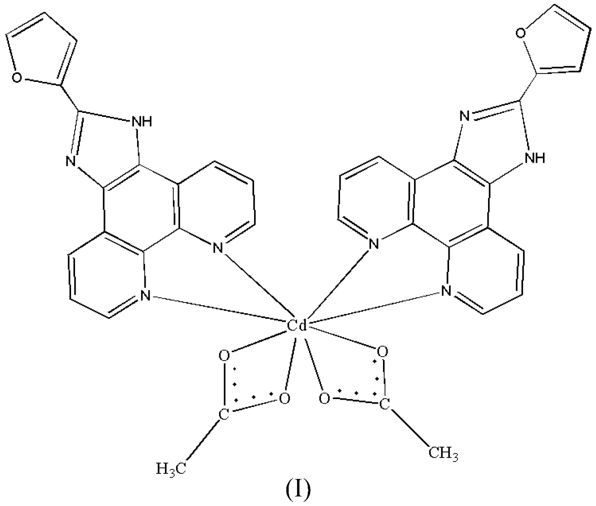
Comment

1,10-Phenanthroline (phen) is an important ligand, having often been used to build novel supramolecular architectures due to its excellent coordinating ability and extended conjugated system that can easily form π–π interactions (Chen & Liu, 2002). However, coordination polymers based on 2-(furan-2-yl)-1*H*-imidazo[4,5-*f*]-1,10-phenanthroline ($C_{17}H_{10}N_4O$; *L*) derived from phen have rarely been investigated (Li, Li, Liu & Fang, 2006). On the other hand, carboxylate ligands have already been proven to be efficient for the generation of a helical coordination polymer (Li, Li, Li & Li, 2006), so we reacted *L* with cadmium acetate, resulting in the title molecular complex, $[Cd(C_2H_3O_2)_2(L)_2]$, (I).



(I)

In complex (I), the Cd^{II} atom (site symmetry 2) adopts an unusual eight-coordinate geometry arising from four N atoms from the two bidentate *L* ligands and four O atoms from two bidentate acetate ions, resulting in a substantially distorted CdN_4O_4 dodecahedral geomtry. The average Cd—O and Cd—N distances [2.4881 (18) and 2.4462 (18) Å, respectively] are comparable with those observed for $[Cd(C_8H_4O_4)(C_{17}H_{10}N_4O)]_n$ {$C_8H_4O_4$ is benzene-1,3-dicarboxylate and $C_{17}H_{10}N_4O$ is 2-(furan-2-yl)-1*H*-imidazo[4,5-*f*]-1,10-phenanthroline; Li, Li, Liu & Fang, 2006}. The carboxylate C—O

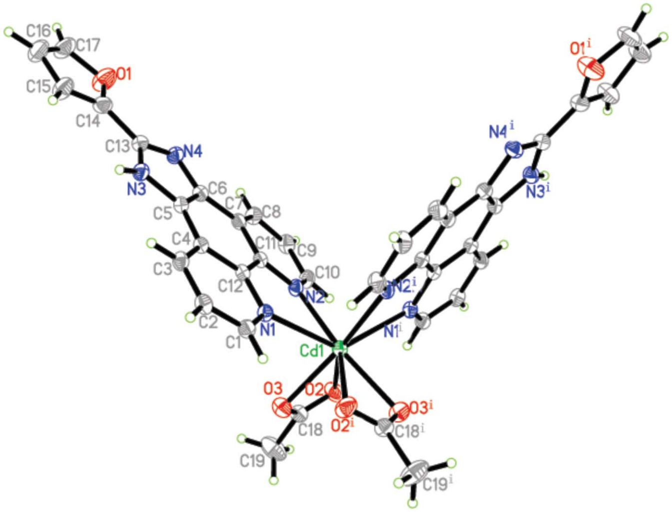


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.]

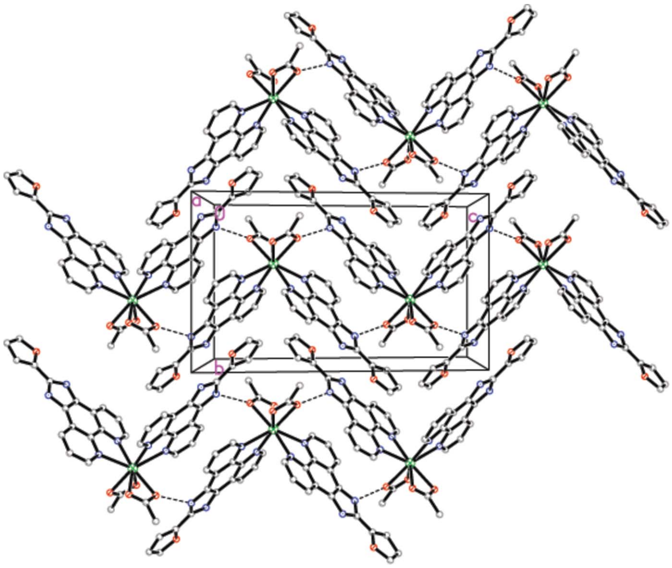


Figure 2
A view of the supramolecular structure of (I) arising from π–π interactions. H atoms have been omitted for clarity. The N$\cdots$O components of the hydrogen bonds are indicated by dashed lines.

bond lengths suggest that the bonding is largely delocalized in these groups in (I).

Neighbouring layers of molecules of (I) interact *via* π–π stacking, generating a supramolecular structure (Fig. 2). The π–π stacking distances between the mean planes of the *L* ligands in adjacent layers are 3.27 and 3.28 Å. Finally, an N—H$\cdots$O hydrogen bond (Table 2) completes the crystal structure of (I).

Experimental

2-(Furan-2-yl)-1*H*-imidazo[4,5-*f*]-1,10-phenanthroline (*L*) was synthesized according to the literature method of Steck & Day (1943). To a solution of $Cd(CH_3COO)_2$ (0.3 mmol) and the ligand *L* (0.5 mmol) in water (30 ml) was added aqueous sodium hydroxide (1 mol l^{-1}to give a pH of 7.5. The mixture was placed in a stainless steel Teflon-lined reaction vessel (40 ml) and heated to 453 K for 4 d. The vessel was then cooled slowly to room temperature at a rate of 5 K h^{-1} and yellow crystals of (I) were collected upon opening the vessel.

Crystal data

$[Cd(C_2H_3O_2)_2(C_{17}H_{10}N_4O)_2]$
$M_r = 803.08$
Monoclinic, $C2/c$
$a = 17.002$ (3) Å
$b = 10.6323$ (18) Å
$c = 17.920$ (3) Å
$\beta = 99.521$ (2)°
$V = 3194.7$ (9) Å^3
$Z = 4$
$D_x = 1.670$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.75$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.28 × 0.25 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\rm min} = 0.813$, $T_{\rm max} = 0.830$
8432 measured reflections
3181 independent reflections
2815 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\rm max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.070$
$S = 1.02$
3172 reflections
240 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.36$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O3	2.3386 (17)	Cd1—O2	2.6376 (18)
Cd1—N2	2.4070 (19)	C18—O3	1.256 (3)
Cd1—N1	2.4853 (18)	C18—O2	1.227 (3)
O3—Cd1—N2	88.87 (6)	O3—Cd1—O2	51.44 (5)
O3—Cd1—N1	83.78 (6)	N2—Cd1—O2	80.34 (6)
N2—Cd1—N1	67.48 (6)	N1—Cd1—O2	125.24 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N3—H3*A*$\cdots$O3^{i}	0.86	1.96	2.707 (2)	145

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

All H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.93 Å, and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(carrier).

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-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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