metal-organic papers

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Key indicators

Single-crystal X-ray study T = 298 KMean σ (C–C) = 0.010 Å Disorder in main residue R factor = 0.050 wR factor = 0.128 Data-to-parameter ratio = 10.9

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

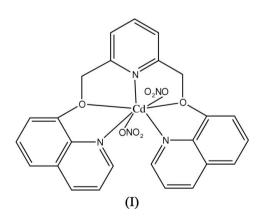
[2,6-Bis(8-quinolyloxymethyl)pyridine]dinitratocadmium(II)

In the title complex, $[Cd(NO_3)_2(C_{25}H_{19}N_3O_2)]$, the coordination environment around cadmium consists of four O and three N atoms in the form of a distorted pentagonal bipyramid.

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Comment

Recently, much interest has been shown in the investigation of open chain crown ethers, especially those containing N and O atoms, because mixed-donor open chain ligands can selectively coordinate transition and post-transition metal ions (Tummler et al., 1977; Guo & Tan, 2003; Beynek et al., 1998; Seitz et al., 2004), and have remarkable applications in extracting the lanthanide metals (Wu, 1992) and removing these metal ions from the body in cases of metal poisoning. However, there are no crystal structure reports of complexes containing the L ligand [where L is 2,6-bis(8-quinolyloxymethyl)pyridine]. In the title complex, (I), the Cd atom and the five donor atoms of L are in an approximately planar array, while the two monodentate nitrate ions occupy the axial sites to form a distorted pentagonal bipyramidal coordination geometry. The average Cd-O(L) and the Cd-N(1)(py) bond lengths are 2.442 Å and 2.360 (5) Å, respectively, which are shorter than those in [2,6-bis(2'-aminophenoxymethyl)pyridine-N, N', N'', O, O']bis(nitrato-O)cadmium(II)(2.613 and 2.398 Å, respectively; Adam et al., 1990), while the average Cd-O(nitrate) bond length (2.367 Å) is longer than the corresponding Cd-O(nitrate) length (2.361 Å) in the abovementioned compound (Adam et al., 1990).



Experimental

© 2006 International Union of Crystallography All rights reserved 2,6-Bis(8-quinolyloxymethyl)pyridine (10 ml, 1 mmol) in ethyl acetate (10 ml) was added to a solution of $Cd(NO_3)_2$ (0.1 mmol) in methanol (10 ml) with continuous stirring at room temperature for

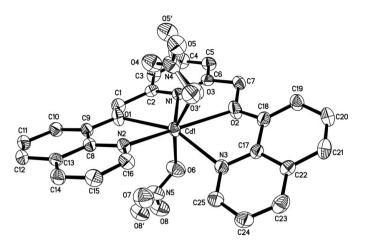


Figure 1

Drawing of the title complex, showing the atomic numbering scheme and displacement ellipsoids at the 30% probability level. H atoms have been omitted for clarity. All disordered atoms are shown.

3 h. The reaction mixture was filtered, the precipitate was dissolved in CH₃CN, and colourless single crystals were obtained by slowly evaporating the solvent (m.p. 519–521 K). Analysis calculated for $C_{25}H_{19}CdN_5O_8$: C 47.63, H 3.02, N 11.11%; found: C 47.54, H 3.06, N 11.18%.

Crystal data

 $[Cd(NO_3)_2(C_{25}H_{19}N_3O_2)]$ Z = 2 $M_r = 629.85$ $D_r = 1.734 \text{ Mg m}^{-3}$ Triclinic, $P\overline{1}$ Mo $K\alpha$ radiation a = 9.061 (2) Å Cell parameters from 6106 b = 10.523 (3) Å reflections c = 13.035 (3) Å $\theta = 2.7 - 25.0^{\circ}$ $\mu = 0.97~\mathrm{mm}^{-1}$ $\alpha = 93.573 \ (4)^{\circ}$ $\beta = 100.780 \ (3)^{\circ}$ T = 298 (2) K $\gamma = 97.351 (4)^{\circ}$ Prism, colourless V = 1206.2 (5) Å³ $0.20 \times 0.18 \times 0.10 \; \mathrm{mm}$

Data collection

Bruker SMART CCD area-detector	4145 independent reflections
diffractometer	3125 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.023$
Absorption correction: multi-scan	$\theta_{max} = 25.0^{\circ}$
(<i>SADABS</i> ; Sheldrick, 1996)	$h = -6 \rightarrow 10$
(SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 10$
$T_{min} = 0.830, T_{max} = 0.909$	$k = -12 \rightarrow 12$
6106 measured reflections	$l = -15 \rightarrow 13$

Refinement

4

F

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	+ 0.0481P]
$wR(F^2) = 0.128$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{\rm max} = 0.001$
4145 reflections	$\Delta \rho_{\rm max} = 1.10 \ {\rm e} \ {\rm \AA}^{-3}$
382 parameters	$\Delta \rho_{\rm min} = -1.42 \text{ e} \text{ Å}^{-3}$
H-atom parameters constrained	

All H atoms were placed geometrically and treated as riding on their parent atoms, with C-H = 0.93 (aromatic) or 0.97 Å (methylene). The $U_{iso}(H)$ values were set at $1.2U_{eq}(C)$. Nitrate atoms O3, O5 and O8 are disordered over two sites each. The disordered orientations were refined with site occupation factors of 0.52 (1) for O3, O5 and O8, and 0.48 (1) for O3', O5' and O8'. The highest electron density peak is 0.95 Å from Cd1 and the deepest hole 0.11 Å from O4.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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