## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=298 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.010 \AA$
Disorder in main residue
$R$ factor $=0.050$
$w R$ 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.

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

In the title complex, $\left[\mathrm{Cd}\left(\mathrm{NO}_{3}\right)_{2}\left(\mathrm{C}_{25} \mathrm{H}_{19} \mathrm{~N}_{3} \mathrm{O}_{2}\right)\right]$, the coordination environment around cadmium consists of four O and three N atoms in the form of a distorted pentagonal bipyramid.

## 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 ( $\mathrm{Wu}, 1992$ ) 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 $\mathrm{Cd}-\mathrm{O}(L)$ and the $\mathrm{Cd}-\mathrm{N}(1)$ (py) bond lengths are $2.442 \AA$ and 2.360 (5) $\AA$, respectively, which are shorter than those in [2,6-bis( $2^{\prime}$-aminophenoxymethyl)-pyridine- $\left.N, N^{\prime}, N^{\prime \prime}, O, O^{\prime}\right]$ bis(nitrato- $O$ )cadmium(II)(2.613 and $2.398 \AA$, respectively; Adam et al., 1990), while the average $\mathrm{Cd}-\mathrm{O}$ (nitrate) bond length $(2.367 \AA)$ is longer than the corresponding $\mathrm{Cd}-\mathrm{O}$ (nitrate) length ( $2.361 \AA$ ) in the abovementioned compound (Adam et al., 1990).

(I)

## Experimental

2,6-Bis(8-quinolyloxymethyl)pyridine $(10 \mathrm{ml}, \quad 1 \mathrm{mmol})$ in ethyl acetate $(10 \mathrm{ml})$ was added to a solution of $\mathrm{Cd}\left(\mathrm{NO}_{3}\right)_{2}(0.1 \mathrm{mmol})$ in methanol ( 10 ml ) with continuous stirring at room temperature for

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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 $\mathrm{CH}_{3} \mathrm{CN}$, and colourless single crystals were obtained by slowly evaporating the solvent (m.p. 519-521 K). Analysis calculated for $\mathrm{C}_{25} \mathrm{H}_{19} \mathrm{CdN}_{5} \mathrm{O}_{8}$ : C 47.63, H 3.02, N 11.11\%; found: C 47.54, H 3.06, N 11.18\%.

## Crystal data

| $\left[\mathrm{Cd}\left(\mathrm{NO}_{3}\right)_{2}\left(\mathrm{C}_{25} \mathrm{H}_{19} \mathrm{~N}_{3} \mathrm{O}_{2}\right)\right]$ | $Z=2$ |
| :--- | :--- |
| $M_{r}=629.85$ | $D_{x}=1.734 \mathrm{Mg} \mathrm{m}^{-3}$ |
| Triclinic, $P \overline{1}$ | Mo K radiation |
| $a=9.061(2) \AA$ | Cell parameters from 6106 |
| $b=10.523(3) \AA$ | reflections |
| $c=13.035(3) \AA$ | $\theta=2.7-25.0^{\circ}$ |
| $\alpha=93.573(4)^{\circ}$ | $\mu=0.97 \mathrm{~mm}^{-1}$ |
| $\beta=100.780(3)^{\circ}$ | $T=298(2) \mathrm{K}$ |
| $\gamma=97.351(4)^{\circ}$ | Prism, colourless |
| $V=1206.2(5) \AA^{3}$ | $0.20 \times 0.18 \times 0.10 \mathrm{~mm}$ |
|  |  |
| Data collection |  |
| Bruker SMART CCD area-detector | 4145 independent reflections |
| $\quad$ diffractometer | 3125 reflections with $I>2 \sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{\text {int }}=0.023$ |
| Absorption correction: multi-scan | $\theta_{\text {max }}=25.0^{\circ}$ |
| $\quad(S A D A B S ;$ Sheldrick, 1996$)$ | $h=-6 \rightarrow 10$ |
| $T_{\text {min }}=0.830, T_{\text {max }}=0.909$ | $k=-12 \rightarrow 12$ |
| 6106 measured reflections | $l=-15 \rightarrow 13$ |

## Refinement

Refinement on $F^{2}$

$$
\begin{aligned}
& w= 1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.0701 P)^{2}\right. \\
&+0.0481 P] \\
& \text { where } P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3 \\
&(\Delta / \sigma)_{\max }=0.001 \\
& \Delta \rho_{\max }=1.10 \mathrm{e}^{-3} \AA^{-3} \\
& \Delta \rho_{\min }=-1.42 \mathrm{e}^{-3}
\end{aligned}
$$

$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.050$
$w R\left(F^{2}\right)=0.128$
$S=1.06$
4145 reflections
382 parameters
H -atom parameters constrained

All H atoms were placed geometrically and treated as riding on their parent atoms, with $\mathrm{C}-\mathrm{H}=0.93$ (aromatic) or $0.97 \AA$ (methylene). The $U_{\text {iso }}(\mathrm{H})$ values were set at $1.2 U_{\text {eq }}(\mathrm{C})$. Nitrate atoms O3, O5 and O 8 are disordered over two sites each. The disordered orientations were refined with site occupation factors of 0.52 (1) for O 3 , O5 and O 8 , and 0.48 (1) for $\mathrm{O}^{\prime}, \mathrm{O5}^{\prime}$ and $\mathrm{O}^{\prime}$. The highest electron density peak is $0.95 \AA$ from Cd1 and the deepest hole $0.11 \AA$ 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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