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Key indicators

Single-crystal X-ray study
 $T = 123$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.018$ Å
 Disorder in main residue
 R factor = 0.065
 wR factor = 0.244
 Data-to-parameter ratio = 14.5

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

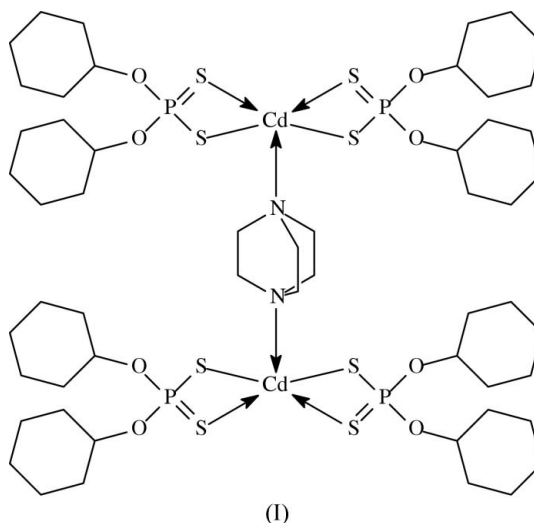
μ -1,4-Diazabicyclo[2.2.2]octane- $\kappa^2\text{N}:\text{N}'$ -bis[bis(*O,O'*-dicyclohexyl dithiophosphato- $\kappa^2\text{S},\text{S}'$)cadmium(II)]

The dinuclear title molecule, $[\text{Cd}_2(\text{C}_{12}\text{H}_{22}\text{O}_2\text{PS}_2)_4(\text{C}_6\text{H}_{12}\text{N}_2)]$, is disordered and located on a centre of inversion, and features a coordination geometry intermediate between square-pyramidal and trigonal-bipyramidal.

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Comment

Structures closely related to the title complex, (I), *viz.* $\{M_2[(i\text{-C}_3\text{H}_7\text{O})_2\text{PS}_2]_4(\text{C}_6\text{H}_{12}\text{N}_2)\}$ for $M = \text{Zn}$ (Ellis *et al.*, 2007) and Cd (Ellis & Tiekink, 2006), have been reported recently in connection with ongoing studies aimed at determining the principles of supramolecular aggregation for the zinc-triad dithiophosphates ($\text{S}_2\text{P}(\text{OR})_2$), and their adducts (Lai, Liu & Tiekink, 2004; Lai & Tiekink, 2004, 2006; Tiekink, 2003).



The structure of (I) (Fig. 1) is similar to that of the aforementioned structures, $\{M_2[(i\text{-C}_3\text{H}_7\text{O})_2\text{PS}_2]_4(\text{C}_6\text{H}_{12}\text{N}_2)\}$, in particular the Cd analogue. The complex is located on a centre of inversion and features two $\text{Cd}[\text{S}_2\text{P}(\text{OCy})_2]_2$ units bridged by a disordered 1,4-diazabicyclo[2.2.2]octane (dabco) ligand. A heavily distorted coordination geometry is found for Cd as both dithiophosphate ligands form asymmetric Cd–S bonds (Table 1). The CdNS_4 coordination geometry is intermediate between square-pyramidal (SP) and trigonal-pyramidal (TP), as seen in the value of $\tau = 0.51$; $\tau = 0.0$ and 1.0 for ideal SP and TP, respectively (Addison *et al.*, 1984).

Experimental

Compound (I) was prepared by refluxing the parent $\text{Cd}[\text{S}_2\text{P}(\text{OCy})_2]_2$ compound with 1,4-diazabicyclo[2.2.2]octane (Aldrich) according to a literature procedure (Lai & Tiekink, 2004). Colourless crystals were

isolated by the slow evaporation of a CHCl_3 /ethanol (3:1) solution of the compound (m.p. 468–470 K). IR (KBr disc): $\nu(\text{C}-\text{O})$ 1152 (w), $\nu(\text{P}-\text{O})$ 958 (s), $\nu(\text{P}-\text{S})_{\text{asym}}$ 657 (s), $\nu(\text{P}-\text{S})_{\text{sym}}$ 577 (s) cm^{-1} .

Crystal data

$[\text{Cd}_2(\text{C}_{12}\text{H}_{22}\text{O}_2\text{PS}_2)_4(\text{C}_6\text{H}_{12}\text{N}_2)]$	$V = 6824.9 (6) \text{ \AA}^3$
$M_r = 1510.52$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 23.1399 (12) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$b = 20.5858 (12) \text{ \AA}$	$T = 123 (2) \text{ K}$
$c = 16.0730 (6) \text{ \AA}$	$0.50 \times 0.10 \times 0.07 \text{ mm}$
$\beta = 116.951 (3)^\circ$	

Data collection

Bruker–Nonius KappaCCD diffractometer	30800 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	6023 independent reflections
$T_{\text{min}} = 0.730$, $T_{\text{max}} = 1$ (expected range = 0.680–0.932)	3618 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.095$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$	416 parameters
$wR(F^2) = 0.244$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{\text{max}} = 1.21 \text{ e \AA}^{-3}$
6023 reflections	$\Delta\rho_{\text{min}} = -1.25 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cd1–N1	2.318 (7)	Cd1–S3	2.521 (2)
Cd1–S1	2.530 (3)	Cd1–S4	2.818 (3)
Cd1–S2	2.760 (3)		
N1–Cd1–S1	110.83 (16)	S1–Cd1–S3	136.60 (10)
N1–Cd1–S2	94.81 (19)	S1–Cd1–S4	99.91 (9)
N1–Cd1–S3	112.54 (16)	S2–Cd1–S3	96.87 (9)
N1–Cd1–S4	97.53 (19)	S2–Cd1–S4	167.41 (9)
S1–Cd1–S2	77.89 (9)	S3–Cd1–S4	76.08 (8)

For the cyclohexyl rings, the 1,2 C–C distances were restrained to 1.54 (1) \AA and the 1,3-related distances to 2.51 (1) \AA . One of them was refined as disordered over two positions with an occupancy factor for the major component of 0.62 (1). The C atoms of the dabco ligand, which lies about an inversion centre, are disordered; the occupancy was constrained by symmetry to be 0.5. The N–C distances were restrained to 1.45 (1) \AA and the C–C distances to 1.50 (1) \AA . The C-bound H atoms were included in the riding-model approximation, with C–H = 0.99–1.00 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The final difference Fourier map had a large residual electron-density peak near C5 atom and a deep hole near Cd1. The largest peak in the final difference map was 0.4 \AA from C5 and the deepest hole was 1.0 \AA from Cd1.

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure:

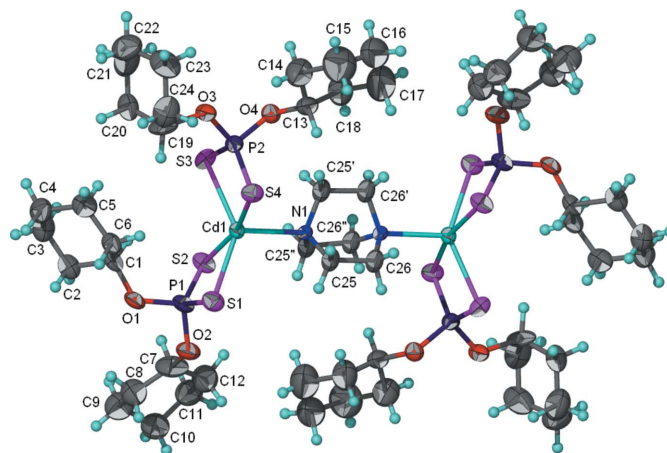


Figure 1

The molecular structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The minor disorder component of the cyclohexyl ring is not shown, and neither is one disorder component of dabco. Unlabelled atoms are generated by the symmetry operator $(1-x, 1-y, 1-z)$.

PATTY in DIRDIF92 (Beurskens *et al.*, 1992); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97.

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