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(μ_2-4,4′-Bipyridyl-κ^2N:N')bis[bis(tri-*tert*-butoxysilanothiolato-κ^2S,O)cadmium(II)] tetrahydrofuran disolvate

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Key indicators

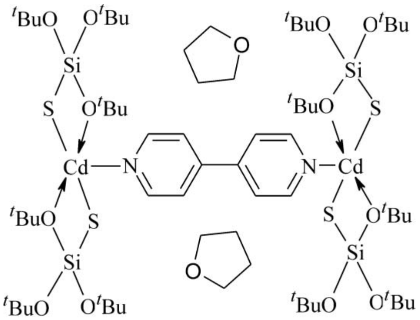
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.043
wR factor = 0.126
Data-to-parameter ratio = 17.3

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

The structure of the title compound, $[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_4H_8O$, consists of discrete molecules, with the two halves of the molecule related to each other by an inversion centre. Each Cd atom is coordinated by two S atoms, two O atoms and one N atom. The geometry of each Cd atom is intermediate between square-pyramidal and trigonal-bipyramidal. Two (tri-*tert*-butoxysilanothiolato)cadmium units are linked *via* one 4,4′-pyridyl ligand, forming an isolated molecule of the complex. Molecules of the tetrahydrofuran solvent are positioned above and below the plane of the 4,4′-bipyridyl.

Comment

The rigid bifunctional ligand 4,4′-bipyridine has been used to produce a variety of coordination polymers with interesting catalytic, electrical and optical properties. Polymeric compounds with one-, two- and three-dimensional frameworks have been synthesized (see e.g. Xiong *et al.*, 1997; Sampanthar & Vittal, 1999; Zhang *et al.*, 2001; Lai *et al.*, 2004; Zeng *et al.*, 2005). The extent of the molecular aggregation in these complexes can be controlled by the steric bulk of co-ligands, as has been demonstrated for a series of adducts of zinc dithiophosphates with bridging ligands: 4,4′-bipyridine, *trans* -1,2-bis(4-pyridyl)ethylene and 1,2-bis(4-pyridyl)ethane (Lai *et al.*, 2004).



(I)

With tri-*tert*-butoxysilanethiol as a co-ligand we anticipated formation of mono- or dinuclear complexes of 4,4′-bipyridine. The steric hindrance of tri-*tert*-butoxysilanethiol usually prevents polymerization of the resulting complexes (see *e.g.* Wojnowski *et al.*, 1985; Becker *et al.*, 2001; Dołęga *et al.*, 2004). Indeed, we obtained a dinuclear cadmium complex, (I), with the molecular structure shown in Fig. 1.

The asymmetric unit of (I) consists of one half-molecule of the complex and one tetrahydrofuran molecule. An inversion centre is located at the mid-point of the bridging C—C bond of the 4,4′-bipyridine, at Wyckoff position c (0,$\frac{1}{2}$,0). The 4,4′-bipy

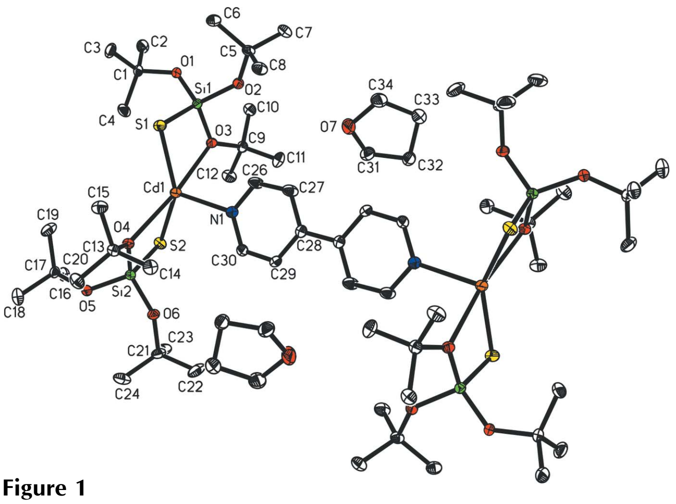


Figure 1
The molecular structure of (I) with the atomic numbering scheme given only for the independent part. Unlabelled atoms are related to labelled atoms by ($-x$, $-y + 1$, $-z + 2$). Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted.

rings in compound (I) are coplanar as a result of crystallographically imposed symmetry. This suggests, however, that the tri-*tert*-butoxysilanethiole groups on the Cd have little effect on the geometry of the ligand. The environment of the Cd can be approximated to trigonal–bipyramidal or square-pyramidal, but severe distortions are found for either geometry. The Cd—S, Cd—O and Cd—N bond lengths are within the expected ranges (Cambridge Structural Database, Version 5.28 of November 2006; Allen, 2002). The bond lengths for the 4,4′-bipyridine unit are similar to those of the free ligand (Boag *et al.*, 1999).

Molecules of (I) pack in the crystal structure as discrete entities with no interactions other than van der Waals. We checked the possibility of the formation of weak hydrogen bonds between O7 (THF) and two C—H groups, namely C11—H11 and C8—H8*C* from adjacent tri-*tert*-butoxy groups. Both distances exceed normal donor–acceptor distances [C11···O7 = 3.754 (5) and C8···O7 = 3.652 (5) Å]. Two molecules of solvent (THF) accompanying each molecule of (I) are positioned approximately parallel to the 4,4′-bipy rings, one molecule of solvent on either side of the 4,4′-bipy plane.

Experimental

Compound (I) was synthesized from dimeric cadmium bis(tri-*tert*-butoxysilanethiolate) (Wojnowski *et al.* 1992). Cadmium bis(tri-*tert*-butoxysilanethiolate) (0.675 g; 0.5 mmol) was dissolved in THF (10 ml). 4,4′-Bipyridine (0.078 g; 0.5 mmol) was added to this solution and dissolved. The reaction mixture was kept at 269 K and colourless plates suitable for X-ray analysis crystallized after 24 h.

Crystal data

$[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_4H_8O$	β = 101.882 (4)°
M_r = 1643.14	V = 4250.1 (3) Å^3
Monoclinic, $P2_1/c$	Z = 2
a = 9.8474 (4) Å	Mo $K\alpha$ radiation
b = 20.4025 (8) Å	μ = 0.71 mm^{-1}
c = 21.6171 (9) Å	T = 120 (2) K
	0.20 × 0.12 × 0.09 mm

Data collection

Oxford Diffraction KM-4-CCD diffractometer	26414 measured reflections
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)	7499 independent reflections
T_{min} = 0.803, T_{max} = 0.905	6531 reflections with $I > 2\sigma(I)$
	R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043	433 parameters
$wR(F^2)$ = 0.126	H-atom parameters constrained
S = 1.20	$\Delta\rho_{max}$ = 1.16 e Å^{-3}
7499 reflections	$\Delta\rho_{min}$ = −0.96 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—S1	2.4520 (8)	Cd1—O4	2.577 (2)
Cd1—S2	2.4335 (8)	S1—Si1	2.0868 (12)
Cd1—N1	2.332 (3)	S2—Si2	2.0813 (12)
Cd1—O3	2.552 (2)		
S1—Cd1—S2	148.43 (3)	S1—Cd1—O3	72.79 (5)
N1—Cd1—S1	102.27 (7)	S2—Cd1—O3	103.39 (5)
N1—Cd1—S2	109.30 (7)	S1—Cd1—O4	106.81 (5)
N1—Cd1—O3	95.58 (8)	S2—Cd1—O4	72.12 (5)
N1—Cd1—O4	93.20 (8)	O3—Cd1—O4	171.09 (7)

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The highest residual electron-density peak is located 0.04 Å from atom Cd1.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Becker, B., Dołęga, A., Konitz, A., Swinder, L. & Wojnowski, W. (2001). *Z. Anorg. Allg. Chem.* **627**, 280–286.
Boag, N. M., Coward, K. M., Jones, A. C., Pemble, M. E. & Thompson, J. R. (1999). *Acta Cryst.* C**55**, 672–674.
Dołęga, A., Becker, B., Chojnacki, J., Konitz, A. & Wojnowski, W. (2004). *Inorg. Chim. Acta*, **357**, 461–467.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Lai, C. S., Liu, S. & Tiekink, E. R. T. (2004). *CrystEngComm*, **6**, 221–226.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.29.9. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sampanthar, J. T. & Vittal, J. J. (1999). *J. Chem. Soc. Dalton Trans.* pp. 1993–1997.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Gottingen, Germany.
Wojnowski, W., Becker, B., Walz, L., Peters, K., Peters, E.-M. & von Schnering, H. G. (1992). *Polyhedron*, **11**, 607–612.
Wojnowski, W., Wojnowski, M., von Schnering, H. G. & Noltemeyer, M. (1985). *Z. Anorg. Allg. Chem.* **531**, 153–157.

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Xiong, R.-G., Yu, Z., Liu, C.-M. & You, X.-Z. (1997). *Polyhedron*, **16**, 2667–2671.

Zeng, Q., Wu, D., Liu, C., Ma, H., Lu, J., Xu, S., Li, Y., Wang, C. & Bai, C. (2005). *Cryst. Growth Des.* **5**, 1041–1047.

Zhang, Q.-F., Niu, Y., Xin, X., Leung, W.-H., Williams, I. D. & Song, Y. (2001). *Chem. Commun.* pp. 1126–1127.

m1436 Pladzyk *et al.* • $[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_4H_8O$ *Acta Cryst.* (2007). E**63**, m1434–m1436