(2,2′-Bipyridine)bis(tri-*tert*-butoxysilanethiolato-$\kappa^2 O,S$)cadmium(II)

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In the title compound, [Cd($C_{12}H_{27}O_3SiS$)$_2$($C_{10}H_8N_2$)], the Cd^{II} atom has a distorted octahedral coordination formed by two N atoms of the bipyridine ligand and two pairs of S and O atoms from two *S,O*-chelating tri-*tert*-butoxysilanethiolate ligands. The O atoms occupy axial positions and the two halves of the molecule are related by a twofold axis which passes through the Cd atom.

Comment

Previously we described the preparation of a dimeric cadmium silanethiolate [Cd{SSi(OBu^t)$_3$}$_2$]$_2$ and its reactions with 2,2′-bipyridine or 1,10-phenanthroline giving complexes of a formal [Cd(*L*){SSi(OBu^t)$_3$}$_2$] stoichiometry, where *L* = bipy (I) or phen (Wojnowski *et al.*, 1992); however, structural work was not carried out. Subsequently, we obtained a related Zn complex, [Zn(bipy){SSi(OBu^t)$_3$}$_2$], (II), and found that Zn is in a distorted tetrahedral environment within a ZnN_2S_2 core (Becker *et al.*, 1996). Recently a related manganese(II)-based complex, [Mn(bipy){SSi(OBu^t)$_3$}$_2$], (III), was structurally characterized, showing Mn in a distorted octahedral environment with an $MnN_2O_2S_2$ core (Kropidłowska *et al.*, 2006). A search of the Cambridge Structural Database (CSD; Version of 2006 with updates; Allen, 2002) revealed no Mn complexes with the same core and bipyridine (or phenanthroline) as a ligand. A similar search for cadmium produced only one example of a compound where the use of a potentially *O,S*-chelating thiobenzoate ligand leads to the complex [Cd(bipy)(SOCPh)$_2$], (IV), with a $CdN_2O_2S_2$ core (CSD refcode SAMDEQ; Zhang *et al.*, 2004).

(I)
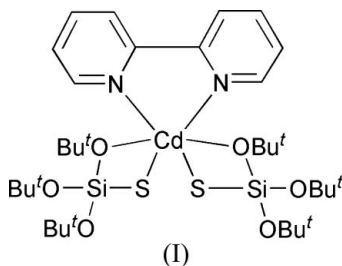
The structure of (I) is shown in Fig. 1, while selected geometric parameters are given in Table 1. The two halves of the molecule are related by a twofold axis which passes through atom Cd1. Compound (I) is isomorphous with the manganese(II) compound (III). In both complexes the six-coordination results from the *O,S*-chelating ability of the tri-*tert*-butoxysilanethiolate ligand. This property manifests itself only in certain cases – for the stoichiometrically related zinc
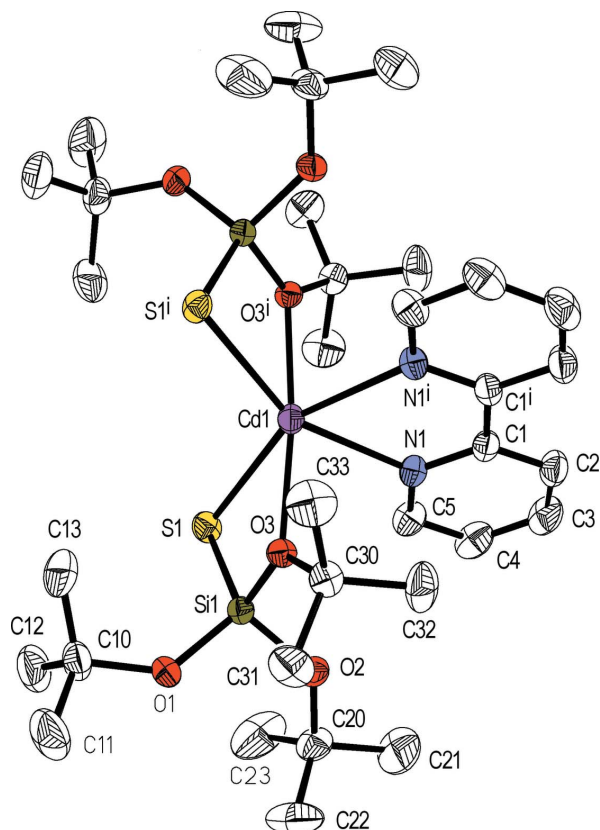
Figure 1
The molecular structure and atom-numbering scheme for (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.]

complex (II) the metal is four-coordinate. In the absence of any significant electronic effects, it is the difference in covalent radii, Cd > Mn > Zn, which may serve as a plausible explanation, especially if one takes into account the large steric hindrance imposed by the bulky tri-*tert*-butoxysilanethiolate ligand.

The chelation by the silanethiolate ligand in (I) results in distortions of the geometric parameters related to atoms O1, O2 and O3 since the Si1—O3 bond is longer and the O3—Si1—S1 angle smaller than others. The octahedral coordination in (I) is distorted (Fig. 1) because of the three bite angles imposed by the three chelating ligands (Table 1). Nevertheless, the O3—Cd1—O3^i angle closely approaches 180°. The Si1—S1 bond length is typical and close to that found in the manganese complex (III) [2.070 (1) Å]. A comparison of (I) with the thiobenzoate derivative (IV) shows the latter to be more distorted, particularly with respect to the O—Cd—O angle of 132.7°. The Cd—S, Cd—N, and Cd—O distances are also significantly different.

Experimental

Crystals of (I) suitable for X-ray measurements were obtained according to a previously described procedure (Wojnowski *et al.*, 1992). The compound is very stable and may be stored for years without decomposition.

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.410 (3)	Si1—O2	1.620 (3)
Cd1—S1	2.5224 (11)	Si1—O1	1.622 (3)
Cd1—O3	2.680 (2)	Si1—O3	1.653 (3)
S1—Si1	2.0778 (15)		
N1—Cd1—N1^i	67.32 (17)	O2—Si1—O1	104.68 (16)
N1—Cd1—S1	93.38 (9)	O2—Si1—O3	104.89 (14)
N1^i—Cd1—S1	154.88 (9)	O1—Si1—O3	112.24 (16)
S1—Cd1—S1^i	109.20 (5)	O2—Si1—S1	115.23 (13)
S1—Cd1—O3	69.38 (6)	O1—Si1—S1	114.91 (12)
O3^i—Cd1—O3	176.03 (11)	O3—Si1—S1	104.63 (10)
Si1—S1—Cd1	89.28 (5)		

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

All H atoms were treated as riding, with C—H = 0.96 Å (methyl groups) or 0.93 Å (all others) and with U_{iso}(H) values of $1.5U_{eq}$(parent) for methyl H atoms or $1.2U_{eq}$(parent) for all other H atoms.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); 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) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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