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

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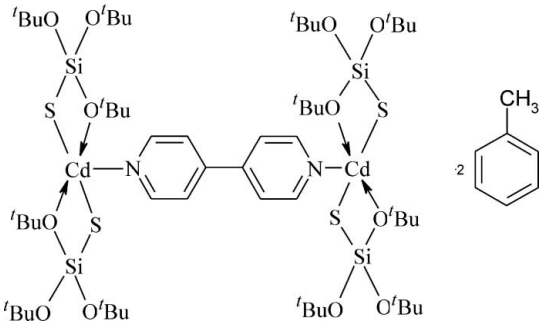
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.027; wR factor = 0.082; data-to-parameter ratio = 17.2.

The structure of the title compound, $[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_7H_8$, consists of discrete molecules, with the two halves of the complex molecule related to each other by inversion symmetry. Two (tri-*tert*-butoxysilanothiolato)-cadmium units are bridged through the 4,4′-bipyridyl ligand. The geometry of the Cd^{II} atoms is intermediate between square-pyramidal and trigonal-bipyramidal. The solvent toluene molecules pack in the voids between the mid-point of the 4,4′-bipyridine and the *tert*-butyl groups of an adjacent complex. There is disorder in the 4,4′-bipyridine molecule, with site occupancies of 0.506 (7):0.494 (7).

Related literature

For an analogous compound as the THF solvate, see: Pladzyk *et al.* (2007). For the synthetic procedure, see: Wojnowski *et al.* (1992).



Experimental

Crystal data

$[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_7H_8$
M_r = 1683.2
Monoclinic, $P2_1/c$
a = 9.8095 (2) Å
b = 19.4290 (5) Å
c = 23.1842 (6) Å
β = 94.355 (2)°
V = 4405.89 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 120 (2) K
0.14 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction KM-4 CCD diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.962, T_{max} = 1.056
27639 measured reflections
7785 independent reflections
6924 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.082
S = 1.17
7785 reflections
453 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.4 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.3097 (18)	Cd1—O1	2.5137 (13)
Cd1—S2	2.4462 (5)	Cd1—O4	2.5384 (13)
Cd1—S1	2.4560 (5)		
N1—Cd1—S2	106.15 (5)	S1—Cd1—O1	73.18 (3)
N1—Cd1—S1	104.61 (5)	N1—Cd1—O4	91.19 (5)
S2—Cd1—S1	149.156 (19)	S2—Cd1—O4	72.67 (3)
N1—Cd1—O1	90.80 (6)	S1—Cd1—O4	109.03 (3)
S2—Cd1—O1	104.03 (4)	O1—Cd1—O4	176.53 (5)

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2366).

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supplementary materials

Acta Cryst. (2007). E**63**, m3072 [**doi:10.1107/S1600536807057947**]

(μ-4,4'-Bipyridyl-κ^2N:N')bis[bis(tri-*tert*-butoxysilanethiolato-κ^2S,O)cadmium(II)] toluene disolvate

A. Dolega, K. Baranowska and A. Pladzyk

Comment

The asymmetric unit of (I) consists of one half-molecule of the complex and one toluene 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* (0,1/2,0). The 4,4'-bipy rings in compound (I) exhibit deviation from planarity, which is most probably "artificial" effect resulting from the disorder of the bipyridine moiety. The environment of the Cd can be approximated either to trigonal–bipyramidal or square pyramidal, but distortions are found for both approximations. Molecules of (I) pack in the crystal structure as discrete entities with no interactions other than van der Waals. Also position of solvating toluene is such that no pi-pi stacking can be considered.

Experimental

Compound (I) was synthesized from dimeric cadmium bis(tri-*tert*-butoxysilanethiolate) (Wojnowski *et al.* 1992). Cadmium bis(tri-*tert*-butoxysilanethiolate) (1.00 g; 0.75 mmol) was suspended in ethanol (40 ml). 4,4'-bipyridine (0.23 g, 1,5 mmol) and toluene (8 ml) were added to the suspension and the reaction mixture was heated for 1 h. The solution, kept at 269 K, yielded colourless needles suitable for X-ray analysis after approx. one month.

Refinement

All C—H hydrogen atoms were refined as riding on carbon atoms with methyl C—H = 0.98 Å, aromatic C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH and 1.5U_{eq}(C) for methyl groups. Atoms C25–C26, and C28–C29 in the 4,4'-bipyridine molecule is disordered (0.506 (7)/0.494 (7)).

Figures

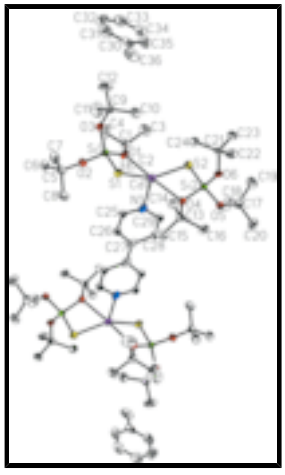


Fig. 1. A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

(μ-4,4'-Bipyridyl-κ^2*N*:*N*')bis[bis(tri-*tert*- butoxysilanethiolato-κ^2*S*,*O*)cadmium(II)] toluene disolvate

Crystal data

$[Cd_2(C_{12}H_{27}O_3SSi)_4(C_{10}H_8N_2)]\cdot 2C_7H_8$	F_{000} = 1780
M_r = 1683.2	D_x = 1.269 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 27489 reflections
a = 9.8095 (2) Å	θ = 2.1–32.5º
b = 19.4290 (5) Å	μ = 0.68 mm^{-1}
c = 23.1842 (6) Å	T = 120 (2) K
β = 94.355 (2)º	Prism, colourless
V = 4405.89 (18) Å^3	0.14 × 0.10 × 0.08 mm
Z = 2	

Data collection

Oxford Diffraction KM4 CCD diffractometer	7785 independent reflections
Monochromator: graphite	6924 reflections with $I > 2\sigma(I)$
Detector resolution: 8.1883 pixels mm^{-1}	R_{int} = 0.021
T = 120(2) K	θ_{max} = 25.1º
ω scans, 0.70 deg width	θ_{min} = 2.1º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006)	h = −11→11
T_{min} = 0.962, T_{max} = 1.056	k = −23→23
27639 measured reflections	l = −15→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.082	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 1.2954P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.17	$(\Delta/\sigma)_{max}$ = 0.002
7785 reflections	$\Delta\rho_{max}$ = 0.88 e Å^{-3}
453 parameters	$\Delta\rho_{min}$ = −0.4 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of *F*^2^ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on *F*^2^, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative *F*^2^. The threshold expression of *F*^2^ > σ(*F*^2^) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on *F*^2^ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.7392 (2)	0.39873 (11)	0.24469 (9)	0.0274 (5)	
C2	0.8606 (3)	0.43098 (18)	0.21823 (12)	0.0552 (8)	
H2A	0.9038	0.3968	0.1944	0.083*	
H2B	0.927	0.4469	0.2491	0.083*	
H2C	0.8296	0.4702	0.194	0.083*	
C3	0.7834 (3)	0.33610 (14)	0.27929 (11)	0.0495 (7)	
H3A	0.7038	0.3152	0.2955	0.074*	
H3B	0.8504	0.3495	0.3108	0.074*	
H3C	0.825	0.3028	0.2541	0.074*	
C4	0.6690 (3)	0.44959 (17)	0.28178 (13)	0.0575 (9)	
H4A	0.6457	0.4912	0.2592	0.086*	
H4B	0.7303	0.4617	0.3156	0.086*	
H4C	0.5853	0.4289	0.2946	0.086*	
C5	0.3733 (2)	0.51955 (11)	0.14177 (9)	0.0290 (5)	
C6	0.3849 (3)	0.58743 (12)	0.17434 (11)	0.0370 (6)	
H6A	0.3679	0.5797	0.215	0.056*	
H6B	0.3173	0.62	0.157	0.056*	
H6C	0.4769	0.6064	0.1721	0.056*	
C7	0.2310 (2)	0.48915 (13)	0.14482 (12)	0.0404 (6)	
H7A	0.2247	0.4457	0.1233	0.061*	
H7B	0.1627	0.5215	0.1278	0.061*	
H7C	0.214	0.4807	0.1853	0.061*	
C8	0.4073 (3)	0.52946 (13)	0.07947 (10)	0.0453 (7)	
H8A	0.501	0.5467	0.0788	0.068*	
H8B	0.3437	0.5628	0.0605	0.068*	
H8C	0.399	0.4853	0.059	0.068*	
C9	0.3271 (2)	0.31123 (11)	0.25002 (10)	0.0308 (5)	
C10	0.4065 (3)	0.24675 (12)	0.23669 (12)	0.0410 (6)	
H10A	0.4061	0.241	0.1947	0.062*	
H10B	0.3637	0.2066	0.2535	0.062*	
H10C	0.501	0.2511	0.2533	0.062*	
C11	0.1852 (3)	0.30822 (15)	0.22104 (16)	0.0566 (8)	
H11A	0.1349	0.3498	0.2305	0.085*	

H11B	0.1379	0.2676	0.2346	0.085*	
H11C	0.1901	0.3054	0.179	0.085*	
C12	0.3263 (4)	0.32048 (14)	0.31497 (12)	0.0596 (9)	
H12A	0.4206	0.324	0.332	0.089*	
H12B	0.2815	0.2808	0.3316	0.089*	
H12C	0.2764	0.3626	0.3232	0.089*	
C13	0.6504 (2)	0.19441 (11)	−0.02055 (8)	0.0220 (4)	
C14	0.5048 (2)	0.17276 (12)	−0.01138 (9)	0.0278 (5)	
H14A	0.5055	0.1269	0.0063	0.042*	
H14B	0.4509	0.1715	−0.0487	0.042*	
H14C	0.4641	0.2059	0.0142	0.042*	
C15	0.6525 (3)	0.26376 (13)	−0.05094 (10)	0.0355 (5)	
H15A	0.6078	0.2983	−0.028	0.053*	
H15B	0.6037	0.2601	−0.0893	0.053*	
H15C	0.7474	0.2775	−0.0551	0.053*	
C16	0.7220 (2)	0.13953 (12)	−0.05393 (9)	0.0312 (5)	
H16A	0.8165	0.1537	−0.0584	0.047*	
H16B	0.6737	0.1336	−0.0922	0.047*	
H16C	0.722	0.0959	−0.0327	0.047*	
C17	1.0884 (2)	0.11565 (12)	0.06581 (10)	0.0307 (5)	
C18	1.1722 (3)	0.17525 (16)	0.09261 (13)	0.0487 (7)	
H18A	1.1742	0.2129	0.0645	0.073*	
H18B	1.2657	0.1596	0.1033	0.073*	
H18C	1.1305	0.1915	0.1272	0.073*	
C19	1.0757 (3)	0.05792 (16)	0.10891 (13)	0.0529 (8)	
H19A	1.0353	0.0758	0.1433	0.079*	
H19B	1.1665	0.039	0.1201	0.079*	
H19C	1.017	0.0216	0.0913	0.079*	
C20	1.1515 (3)	0.08867 (14)	0.01263 (11)	0.0402 (6)	
H20A	1.0958	0.0507	−0.0041	0.06*	
H20B	1.2442	0.0721	0.0235	0.06*	
H20C	1.1553	0.1257	−0.0159	0.06*	
C21	0.6584 (2)	0.04645 (11)	0.12376 (9)	0.0244 (4)	
C22	0.5906 (3)	−0.01292 (12)	0.08980 (10)	0.0355 (5)	
H22A	0.5358	0.0052	0.0561	0.053*	
H22B	0.5313	−0.0382	0.1145	0.053*	
H22C	0.661	−0.0439	0.0769	0.053*	
C23	0.7478 (2)	0.02003 (12)	0.17520 (9)	0.0318 (5)	
H23A	0.8164	−0.0117	0.1618	0.048*	
H23B	0.6911	−0.0042	0.2017	0.048*	
H23C	0.7939	0.0589	0.1954	0.048*	
C24	0.5507 (2)	0.09622 (12)	0.14296 (10)	0.0333 (5)	
H24A	0.5957	0.1344	0.1644	0.05*	
H24B	0.4901	0.072	0.1679	0.05*	
H24C	0.497	0.1142	0.1089	0.05*	
C25	0.7600 (6)	0.4345 (3)	0.0605 (2)	0.0221 (14)*	0.506 (7)
H25	0.6719	0.4449	0.0724	0.046 (15)*	0.506 (7)
C26	0.8326 (6)	0.4849 (3)	0.0335 (3)	0.0240 (15)*	0.506 (7)
H26	0.7923	0.5291	0.0277	0.021 (11)*	0.506 (7)

C28	1.0182 (5)	0.4047 (2)	0.0324 (2)	0.0236 (12)*	0.506 (7)
H28	1.1098	0.3938	0.0252	0.028*	0.506 (7)
C29	0.9401 (5)	0.3570 (2)	0.0589 (2)	0.0230 (11)*	0.506 (7)
H29	0.9762	0.3131	0.0696	0.028*	0.506 (7)
C25A	0.7814 (6)	0.4448 (3)	0.0718 (3)	0.0251 (15)*	0.494 (7)
H25A	0.7082	0.459	0.0936	0.038 (14)*	0.494 (7)
C26A	0.8515 (6)	0.4949 (3)	0.0451 (3)	0.0227 (15)*	0.494 (7)
H26A	0.8267	0.542	0.0472	0.033 (13)*	0.494 (7)
C28A	0.9814 (5)	0.4081 (2)	0.0044 (2)	0.0229 (12)*	0.494 (7)
H28A	1.0457	0.394	−0.0219	0.027*	0.494 (7)
C29A	0.9070 (5)	0.3604 (2)	0.0330 (2)	0.0231 (11)*	0.494 (7)
H29A	0.9263	0.3132	0.0265	0.028*	0.494 (7)
C27	0.9606 (2)	0.47356 (11)	0.01469 (10)	0.0292 (5)	
C30	0.0194 (3)	0.20285 (15)	0.37305 (14)	0.0499 (7)	
H30	−0.0696	0.2167	0.3585	0.06*	
C31	0.0754 (3)	0.23122 (17)	0.42372 (13)	0.0514 (7)	
H31	0.025	0.2639	0.4439	0.062*	
C32	0.2049 (3)	0.21219 (13)	0.44523 (13)	0.0435 (6)	
H32	0.2446	0.232	0.48	0.052*	
C33	0.2757 (3)	0.16450 (13)	0.41587 (13)	0.0457 (7)	
H33	0.3645	0.1509	0.4307	0.055*	
C34	0.2196 (3)	0.13602 (13)	0.36497 (12)	0.0419 (6)	
H34	0.2707	0.1034	0.3451	0.05*	
C35	0.0899 (3)	0.15424 (12)	0.34249 (11)	0.0388 (6)	
C36	0.0282 (4)	0.12362 (16)	0.28714 (12)	0.0587 (8)	
H36A	0.0996	0.1172	0.2603	0.088*	
H36B	−0.0422	0.1547	0.2698	0.088*	
H36C	−0.0131	0.079	0.2952	0.088*	
Cd1	0.681416 (15)	0.293346 (7)	0.114331 (6)	0.02303 (7)	
N1	0.80907 (19)	0.37450 (9)	0.06946 (8)	0.0289 (4)	
O1	0.64763 (14)	0.37525 (8)	0.19596 (6)	0.0254 (3)	
O2	0.47662 (15)	0.47464 (7)	0.16934 (6)	0.0251 (3)	
O3	0.39076 (15)	0.37287 (7)	0.22922 (6)	0.0257 (3)	
O4	0.72132 (15)	0.20541 (6)	0.03641 (6)	0.0209 (3)	
O5	0.95533 (14)	0.14222 (7)	0.04608 (6)	0.0232 (3)	
O6	0.74521 (15)	0.07929 (7)	0.08393 (6)	0.0239 (3)	
S1	0.44513 (5)	0.33544 (3)	0.10046 (2)	0.02512 (12)	
S2	0.84466 (6)	0.20885 (3)	0.15666 (2)	0.02556 (13)	
Si1	0.48493 (5)	0.39138 (3)	0.17697 (2)	0.01919 (12)	
Si2	0.81719 (5)	0.15393 (3)	0.07939 (2)	0.01791 (12)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0249 (11)	0.0306 (11)	0.0255 (11)	0.0020 (9)	−0.0051 (9)	−0.0093 (9)
C2	0.0426 (16)	0.078 (2)	0.0428 (16)	−0.0268 (15)	−0.0084 (12)	−0.0029 (14)
C3	0.078 (2)	0.0430 (15)	0.0250 (13)	0.0088 (14)	−0.0131 (13)	−0.0032 (11)
C4	0.0446 (16)	0.070 (2)	0.0550 (18)	0.0200 (14)	−0.0185 (13)	−0.0426 (16)

C5	0.0336 (12)	0.0243 (11)	0.0287 (11)	0.0039 (9)	−0.0008 (9)	0.0041 (9)
C6	0.0467 (15)	0.0263 (12)	0.0387 (13)	0.0047 (10)	0.0072 (11)	0.0014 (10)
C7	0.0303 (13)	0.0367 (14)	0.0525 (15)	0.0050 (10)	−0.0079 (11)	0.0028 (11)
C8	0.0710 (19)	0.0338 (13)	0.0310 (13)	0.0082 (13)	0.0041 (12)	0.0064 (10)
C9	0.0374 (13)	0.0212 (10)	0.0358 (12)	−0.0076 (9)	0.0160 (10)	−0.0020 (9)
C10	0.0484 (15)	0.0264 (12)	0.0499 (15)	0.0004 (11)	0.0147 (12)	0.0062 (11)
C11	0.0326 (15)	0.0422 (15)	0.096 (2)	−0.0107 (12)	0.0097 (15)	0.0036 (16)
C12	0.107 (3)	0.0355 (15)	0.0413 (16)	−0.0214 (16)	0.0364 (16)	−0.0031 (12)
C13	0.0222 (10)	0.0257 (10)	0.0173 (10)	−0.0011 (8)	−0.0030 (8)	0.0005 (8)
C14	0.0223 (11)	0.0341 (12)	0.0264 (11)	−0.0023 (9)	−0.0023 (8)	−0.0029 (9)
C15	0.0357 (13)	0.0368 (13)	0.0330 (13)	−0.0037 (10)	−0.0045 (10)	0.0125 (10)
C16	0.0306 (12)	0.0419 (13)	0.0211 (11)	0.0032 (10)	0.0018 (9)	−0.0071 (9)
C17	0.0181 (10)	0.0386 (13)	0.0355 (12)	0.0064 (9)	0.0028 (9)	0.0029 (10)
C18	0.0224 (13)	0.0686 (19)	0.0546 (17)	−0.0019 (12)	−0.0005 (11)	−0.0181 (15)
C19	0.0419 (16)	0.0657 (19)	0.0515 (17)	0.0263 (14)	0.0066 (13)	0.0242 (14)
C20	0.0296 (13)	0.0443 (14)	0.0480 (15)	0.0058 (11)	0.0120 (11)	−0.0040 (12)
C21	0.0285 (11)	0.0243 (11)	0.0212 (10)	−0.0066 (9)	0.0072 (8)	0.0016 (8)
C22	0.0439 (14)	0.0343 (13)	0.0293 (12)	−0.0179 (11)	0.0085 (10)	−0.0021 (10)
C23	0.0388 (13)	0.0288 (12)	0.0280 (11)	−0.0030 (10)	0.0047 (10)	0.0060 (9)
C24	0.0311 (12)	0.0361 (13)	0.0342 (12)	−0.0011 (10)	0.0124 (10)	0.0045 (10)
C27	0.0262 (11)	0.0274 (11)	0.0353 (12)	−0.0081 (9)	0.0109 (9)	−0.0119 (9)
C30	0.0332 (15)	0.0565 (18)	0.0591 (18)	0.0040 (12)	−0.0027 (13)	0.0149 (14)
C31	0.0401 (16)	0.0587 (18)	0.0571 (18)	0.0004 (14)	0.0147 (13)	0.0002 (15)
C32	0.0398 (15)	0.0449 (15)	0.0459 (15)	−0.0157 (12)	0.0029 (12)	0.0059 (12)
C33	0.0316 (14)	0.0360 (14)	0.0674 (18)	−0.0092 (11)	−0.0092 (13)	0.0115 (13)
C34	0.0356 (14)	0.0314 (13)	0.0584 (17)	−0.0046 (10)	0.0024 (12)	0.0056 (12)
C35	0.0425 (14)	0.0324 (13)	0.0404 (14)	−0.0095 (11)	−0.0032 (11)	0.0179 (11)
C36	0.073 (2)	0.0538 (18)	0.0471 (17)	−0.0127 (16)	−0.0137 (15)	0.0145 (14)
Cd1	0.02256 (10)	0.02152 (10)	0.02558 (10)	−0.00129 (6)	0.00542 (6)	−0.00431 (6)
N1	0.0275 (10)	0.0277 (10)	0.0328 (10)	−0.0055 (8)	0.0099 (8)	−0.0082 (8)
O1	0.0209 (7)	0.0301 (8)	0.0250 (7)	0.0021 (6)	−0.0007 (6)	−0.0111 (6)
O2	0.0268 (8)	0.0209 (7)	0.0275 (8)	−0.0012 (6)	0.0000 (6)	0.0018 (6)
O3	0.0312 (8)	0.0197 (7)	0.0275 (8)	−0.0043 (6)	0.0112 (6)	−0.0011 (6)
O4	0.0217 (8)	0.0205 (7)	0.0200 (7)	0.0010 (5)	−0.0019 (6)	−0.0024 (5)
O5	0.0174 (7)	0.0289 (8)	0.0234 (7)	0.0009 (6)	0.0025 (6)	0.0026 (6)
O6	0.0295 (8)	0.0218 (7)	0.0214 (7)	−0.0046 (6)	0.0087 (6)	−0.0004 (6)
S1	0.0229 (3)	0.0292 (3)	0.0232 (3)	−0.0020 (2)	0.0007 (2)	−0.0060 (2)
S2	0.0284 (3)	0.0266 (3)	0.0210 (3)	−0.0005 (2)	−0.0026 (2)	−0.00446 (19)
Si1	0.0188 (3)	0.0192 (3)	0.0198 (3)	−0.0014 (2)	0.0034 (2)	−0.0011 (2)
Si2	0.0174 (3)	0.0184 (3)	0.0180 (3)	−0.0008 (2)	0.0017 (2)	0.0000 (2)

Geometric parameters (Å, °)

C1—O1	1.462 (2)	C21—O6	1.451 (2)
C1—C3	1.503 (3)	C21—C23	1.515 (3)
C1—C4	1.510 (3)	C21—C22	1.521 (3)
C1—C2	1.516 (4)	C21—C24	1.523 (3)
C2—H2A	0.98	C22—H22A	0.98
C2—H2B	0.98	C22—H22B	0.98

C2—H2C	0.98	C22—H22C	0.98
C3—H3A	0.98	C23—H23A	0.98
C3—H3B	0.98	C23—H23B	0.98
C3—H3C	0.98	C23—H23C	0.98
C4—H4A	0.98	C24—H24A	0.98
C4—H4B	0.98	C24—H24B	0.98
C4—H4C	0.98	C24—H24C	0.98
C5—O2	1.449 (3)	C25—N1	1.272 (5)
C5—C8	1.519 (3)	C25—C26	1.388 (8)
C5—C6	1.520 (3)	C25—H25	0.95
C5—C7	1.522 (3)	C26—C27	1.378 (6)
C6—H6A	0.98	C26—H26	0.95
C6—H6B	0.98	C28—C29	1.377 (6)
C6—H6C	0.98	C28—C27	1.497 (5)
C7—H7A	0.98	C28—H28	0.95
C7—H7B	0.98	C29—N1	1.369 (5)
C7—H7C	0.98	C29—H29	0.95
C8—H8A	0.98	C25A—C26A	1.365 (8)
C8—H8B	0.98	C25A—N1	1.395 (6)
C8—H8C	0.98	C25A—H25A	0.95
C9—O3	1.450 (2)	C26A—C27	1.389 (6)
C9—C11	1.501 (4)	C26A—H26A	0.95
C9—C12	1.517 (3)	C28A—C27	1.313 (5)
C9—C10	1.519 (3)	C28A—C29A	1.380 (6)
C10—H10A	0.98	C28A—H28A	0.95
C10—H10B	0.98	C29A—N1	1.355 (5)
C10—H10C	0.98	C29A—H29A	0.95
C11—H11A	0.98	C27—C27^{i}	1.482 (4)
C11—H11B	0.98	C30—C31	1.374 (4)
C11—H11C	0.98	C30—C35	1.395 (4)
C12—H12A	0.98	C30—H30	0.95
C12—H12B	0.98	C31—C32	1.379 (4)
C12—H12C	0.98	C31—H31	0.95
C13—O4	1.461 (2)	C32—C33	1.370 (4)
C13—C14	1.519 (3)	C32—H32	0.95
C13—C16	1.520 (3)	C33—C34	1.379 (4)
C13—C15	1.521 (3)	C33—H33	0.95
C14—H14A	0.98	C34—C35	1.384 (4)
C14—H14B	0.98	C34—H34	0.95
C14—H14C	0.98	C35—C36	1.500 (4)
C15—H15A	0.98	C36—H36A	0.98
C15—H15B	0.98	C36—H36B	0.98
C15—H15C	0.98	C36—H36C	0.98
C16—H16A	0.98	Cd1—N1	2.3097 (18)
C16—H16B	0.98	Cd1—S2	2.4462 (5)
C16—H16C	0.98	Cd1—S1	2.4560 (5)
C17—O5	1.445 (3)	Cd1—O1	2.5137 (13)
C17—C19	1.514 (3)	Cd1—O4	2.5384 (13)
C17—C20	1.515 (3)	Cd1—Si1	3.1428 (5)

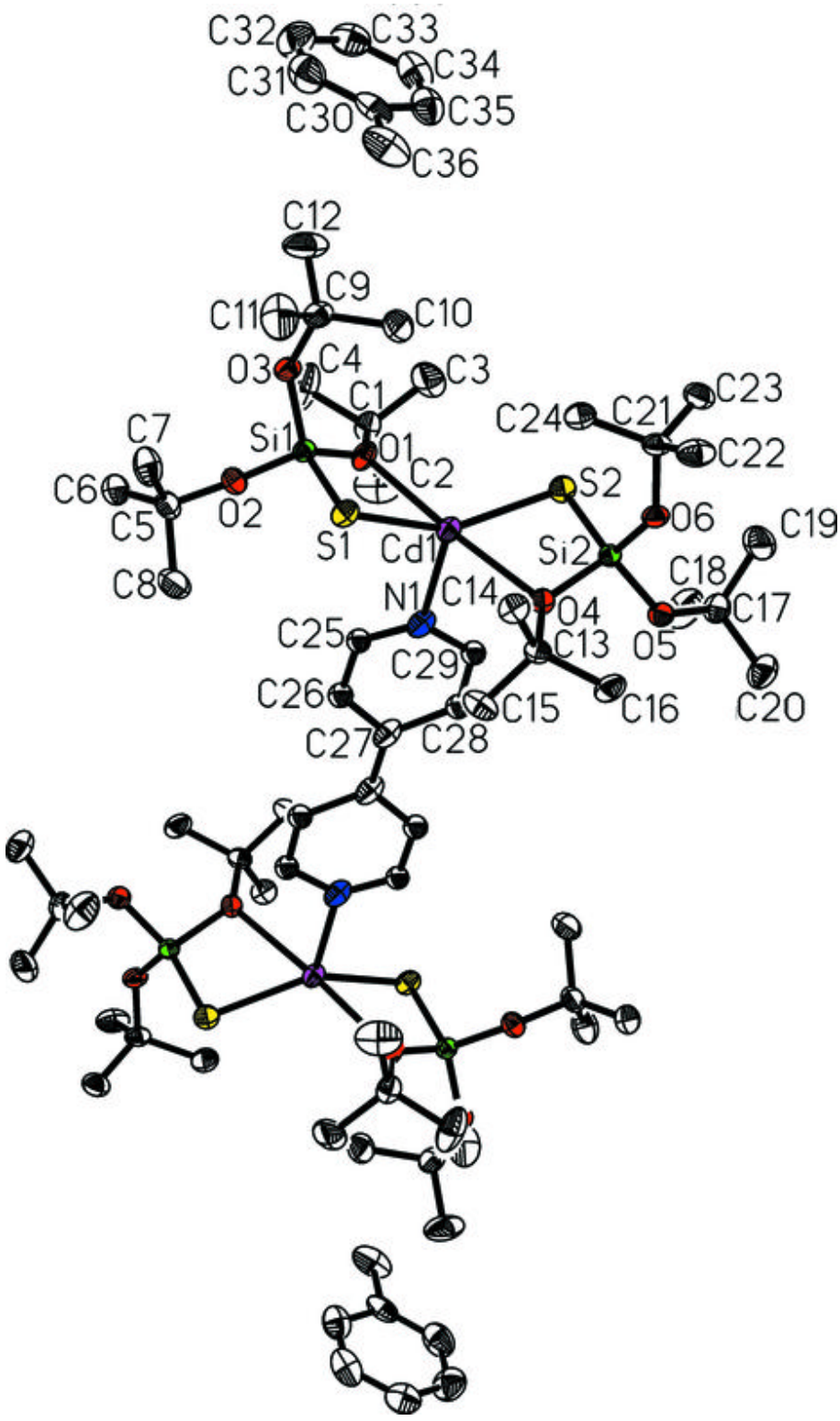
C17—C18	1.525 (4)	Cd1—Si2	3.1514 (5)
C18—H18A	0.98	O1—Si1	1.6530 (15)
C18—H18B	0.98	O2—Si1	1.6286 (15)
C18—H18C	0.98	O3—Si1	1.6187 (14)
C19—H19A	0.98	O4—Si2	1.6538 (14)
C19—H19B	0.98	O5—Si2	1.6259 (14)
C19—H19C	0.98	O6—Si2	1.6198 (14)
C20—H20A	0.98	S1—Si1	2.0916 (7)
C20—H20B	0.98	S2—Si2	2.0851 (7)
C20—H20C	0.98		
O1—C1—C3	107.18 (18)	H22B—C22—H22C	109.5
O1—C1—C4	111.37 (18)	C21—C23—H23A	109.5
C3—C1—C4	110.6 (2)	C21—C23—H23B	109.5
O1—C1—C2	105.77 (18)	H23A—C23—H23B	109.5
C3—C1—C2	110.3 (2)	C21—C23—H23C	109.5
C4—C1—C2	111.5 (2)	H23A—C23—H23C	109.5
C1—C2—H2A	109.5	H23B—C23—H23C	109.5
C1—C2—H2B	109.5	C21—C24—H24A	109.5
H2A—C2—H2B	109.5	C21—C24—H24B	109.5
C1—C2—H2C	109.5	H24A—C24—H24B	109.5
H2A—C2—H2C	109.5	C21—C24—H24C	109.5
H2B—C2—H2C	109.5	H24A—C24—H24C	109.5
C1—C3—H3A	109.5	H24B—C24—H24C	109.5
C1—C3—H3B	109.5	N1—C25—C26	121.4 (5)
H3A—C3—H3B	109.5	N1—C25—H25	119.3
C1—C3—H3C	109.5	C26—C25—H25	119.3
H3A—C3—H3C	109.5	C27—C26—C25	122.7 (5)
H3B—C3—H3C	109.5	C27—C26—H26	118.6
C1—C4—H4A	109.5	C25—C26—H26	118.6
C1—C4—H4B	109.5	C29—C28—C27	120.8 (4)
H4A—C4—H4B	109.5	C29—C28—H28	119.6
C1—C4—H4C	109.5	C27—C28—H28	119.6
H4A—C4—H4C	109.5	N1—C29—C28	118.4 (4)
H4B—C4—H4C	109.5	N1—C29—H29	120.8
O2—C5—C8	107.42 (18)	C28—C29—H29	120.8
O2—C5—C6	106.28 (18)	C26A—C25A—N1	125.0 (5)
C8—C5—C6	110.43 (19)	C26A—C25A—H25A	117.5
O2—C5—C7	111.03 (17)	N1—C25A—H25A	117.5
C8—C5—C7	111.2 (2)	C25A—C26A—C27	116.9 (5)
C6—C5—C7	110.3 (2)	C25A—C26A—H26A	121.6
C5—C6—H6A	109.5	C27—C26A—H26A	121.6
C5—C6—H6B	109.5	C27—C28A—C29A	117.9 (4)
H6A—C6—H6B	109.5	C27—C28A—H28A	121
C5—C6—H6C	109.5	C29A—C28A—H28A	121
H6A—C6—H6C	109.5	N1—C29A—C28A	126.1 (4)
H6B—C6—H6C	109.5	N1—C29A—H29A	116.9
C5—C7—H7A	109.5	C28A—C29A—H29A	116.9
C5—C7—H7B	109.5	C28A—C27—C26	111.7 (3)
H7A—C7—H7B	109.5	C28A—C27—C26A	121.1 (3)

C5—C7—H7C	109.5	C28A—C27—C27^{i}	119.6 (3)
H7A—C7—H7C	109.5	C26—C27—C27^{i}	123.6 (3)
H7B—C7—H7C	109.5	C26A—C27—C27^{i}	118.4 (3)
C5—C8—H8A	109.5	C26—C27—C28	113.0 (3)
C5—C8—H8B	109.5	C26A—C27—C28	114.6 (3)
H8A—C8—H8B	109.5	C27^{i}—C27—C28	123.1 (3)
C5—C8—H8C	109.5	C31—C30—C35	121.6 (3)
H8A—C8—H8C	109.5	C31—C30—H30	119.2
H8B—C8—H8C	109.5	C35—C30—H30	119.2
O3—C9—C11	106.9 (2)	C30—C31—C32	120.0 (3)
O3—C9—C12	105.50 (18)	C30—C31—H31	120
C11—C9—C12	112.0 (2)	C32—C31—H31	120
O3—C9—C10	111.91 (18)	C33—C32—C31	119.3 (3)
C11—C9—C10	110.4 (2)	C33—C32—H32	120.4
C12—C9—C10	109.9 (2)	C31—C32—H32	120.4
C9—C10—H10A	109.5	C32—C33—C34	120.8 (3)
C9—C10—H10B	109.5	C32—C33—H33	119.6
H10A—C10—H10B	109.5	C34—C33—H33	119.6
C9—C10—H10C	109.5	C33—C34—C35	121.0 (3)
H10A—C10—H10C	109.5	C33—C34—H34	119.5
H10B—C10—H10C	109.5	C35—C34—H34	119.5
C9—C11—H11A	109.5	C34—C35—C30	117.3 (2)
C9—C11—H11B	109.5	C34—C35—C36	121.4 (3)
H11A—C11—H11B	109.5	C30—C35—C36	121.3 (3)
C9—C11—H11C	109.5	C35—C36—H36A	109.5
H11A—C11—H11C	109.5	C35—C36—H36B	109.5
H11B—C11—H11C	109.5	H36A—C36—H36B	109.5
C9—C12—H12A	109.5	C35—C36—H36C	109.5
C9—C12—H12B	109.5	H36A—C36—H36C	109.5
H12A—C12—H12B	109.5	H36B—C36—H36C	109.5
C9—C12—H12C	109.5	N1—Cd1—S2	106.15 (5)
H12A—C12—H12C	109.5	N1—Cd1—S1	104.61 (5)
H12B—C12—H12C	109.5	S2—Cd1—S1	149.156 (19)
O4—C13—C14	107.59 (16)	N1—Cd1—O1	90.80 (6)
O4—C13—C16	110.85 (16)	S2—Cd1—O1	104.03 (4)
C14—C13—C16	110.64 (18)	S1—Cd1—O1	73.18 (3)
O4—C13—C15	105.48 (16)	N1—Cd1—O4	91.19 (5)
C14—C13—C15	110.86 (18)	S2—Cd1—O4	72.67 (3)
C16—C13—C15	111.24 (19)	S1—Cd1—O4	109.03 (3)
C13—C14—H14A	109.5	O1—Cd1—O4	176.53 (5)
C13—C14—H14B	109.5	N1—Cd1—Si1	99.61 (5)
H14A—C14—H14B	109.5	S2—Cd1—Si1	128.835 (17)
C13—C14—H14C	109.5	S1—Cd1—Si1	41.656 (15)
H14A—C14—H14C	109.5	O1—Cd1—Si1	31.56 (3)
H14B—C14—H14C	109.5	O4—Cd1—Si1	150.45 (3)
C13—C15—H15A	109.5	N1—Cd1—Si2	102.52 (5)
C13—C15—H15B	109.5	S2—Cd1—Si2	41.386 (15)
H15A—C15—H15B	109.5	S1—Cd1—Si2	131.734 (16)

C13—C15—H15C	109.5	O1—Cd1—Si2	145.10 (3)
H15A—C15—H15C	109.5	O4—Cd1—Si2	31.51 (3)
H15B—C15—H15C	109.5	Si1—Cd1—Si2	157.776 (14)
C13—C16—H16A	109.5	C25—N1—C29A	111.1 (3)
C13—C16—H16B	109.5	C25—N1—C29	123.1 (3)
H16A—C16—H16B	109.5	C29A—N1—C25A	111.8 (3)
C13—C16—H16C	109.5	C29—N1—C25A	115.9 (3)
H16A—C16—H16C	109.5	C25—N1—Cd1	119.2 (3)
H16B—C16—H16C	109.5	C29A—N1—Cd1	125.3 (2)
O5—C17—C19	110.87 (18)	C29—N1—Cd1	117.4 (2)
O5—C17—C20	106.33 (18)	C25A—N1—Cd1	122.5 (3)
C19—C17—C20	109.9 (2)	C1—O1—Si1	132.12 (12)
O5—C17—C18	107.68 (19)	C1—O1—Cd1	132.14 (11)
C19—C17—C18	111.3 (2)	Si1—O1—Cd1	95.70 (6)
C20—C17—C18	110.7 (2)	C5—O2—Si1	132.37 (13)
C17—C18—H18A	109.5	C9—O3—Si1	135.81 (13)
C17—C18—H18B	109.5	C13—O4—Si2	131.77 (12)
H18A—C18—H18B	109.5	C13—O4—Cd1	130.78 (11)
C17—C18—H18C	109.5	Si2—O4—Cd1	95.15 (6)
H18A—C18—H18C	109.5	C17—O5—Si2	131.67 (13)
H18B—C18—H18C	109.5	C21—O6—Si2	135.64 (13)
C17—C19—H19A	109.5	Si1—S1—Cd1	87.05 (2)
C17—C19—H19B	109.5	Si2—S2—Cd1	87.75 (2)
H19A—C19—H19B	109.5	O3—Si1—O2	105.98 (8)
C17—C19—H19C	109.5	O3—Si1—O1	110.67 (8)
H19A—C19—H19C	109.5	O2—Si1—O1	104.87 (8)
H19B—C19—H19C	109.5	O3—Si1—S1	116.03 (6)
C17—C20—H20A	109.5	O2—Si1—S1	114.79 (6)
C17—C20—H20B	109.5	O1—Si1—S1	103.98 (5)
H20A—C20—H20B	109.5	O3—Si1—Cd1	128.03 (6)
C17—C20—H20C	109.5	O2—Si1—Cd1	125.39 (6)
H20A—C20—H20C	109.5	O1—Si1—Cd1	52.74 (5)
H20B—C20—H20C	109.5	S1—Si1—Cd1	51.299 (18)
O6—C21—C23	108.50 (17)	O6—Si2—O5	106.78 (8)
O6—C21—C22	104.99 (16)	O6—Si2—O4	110.48 (8)
C23—C21—C22	110.78 (19)	O5—Si2—O4	104.76 (7)
O6—C21—C24	111.12 (17)	O6—Si2—S2	115.52 (6)
C23—C21—C24	110.98 (18)	O5—Si2—S2	114.94 (6)
C22—C21—C24	110.30 (19)	O4—Si2—S2	103.81 (5)
C21—C22—H22A	109.5	O6—Si2—Cd1	123.92 (5)
C21—C22—H22B	109.5	O5—Si2—Cd1	128.77 (6)
H22A—C22—H22B	109.5	O4—Si2—Cd1	53.34 (5)
C21—C22—H22C	109.5	S2—Si2—Cd1	50.863 (19)
H22A—C22—H22C	109.5		

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*.

Fig. 1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