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Ammine(2-ethylpyridine-κ*N*)bis(tri-*tert*-butoxysilanethiolato-κ*S*)cobalt(II)

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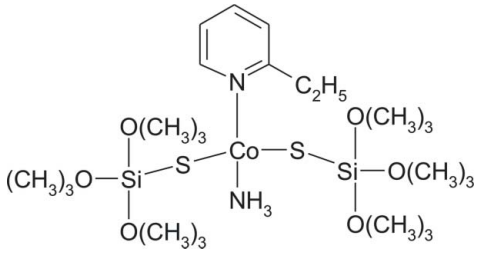
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.035; wR factor = 0.095; data-to-parameter ratio = 15.2.

The title compound, $[Co(C_{12}H_{27}O_3SSi)_2(C_7H_9N)(NH_3)]$, was obtained by the reaction of dimeric $[Co\{SSi(O^tBu)_3\}_2(NH_3)]_2$ with 2-ethylpyridine. The Co^{II} atom is coordinated by two S atoms from two silanethiolate ligands and two N atoms, one from ammonia and one from a 2-ethylpyridine molecule. The arrangement of the ligands around the Co^{II} centre facilitates the formation of an intermolecular N—H···S hydrogen bond. One of the *tert*-butyl groups and the 2-ethylpyridine ligand are disordered over two positions each, with approximate occupancy ratios of 2:1 and 3:1, respectively.

Related literature

For related literature, see: Corwin *et al.* (1987); Kimblin *et al.* (2000); Becker *et al.* (2002); Pladzyk & Baranowska (2006).



Experimental

Crystal data

$[Co(C_{12}H_{27}O_3SSi)_2(C_7H_9N)(NH_3)]$
M_r = 742.09
Triclinic, $P\overline{1}$
a = 9.6939 (4) Å
b = 13.7249 (6) Å
c = 16.1266 (6) Å
α = 78.605 (4)°
β = 88.106 (3)°
γ = 81.830 (4)°
V = 2081.94 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 120 (2) K
0.26 × 0.11 × 0.04 mm

Data collection

Kuma KM4 CCD κ-geometry diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2005)
T_{min} = 0.787, T_{max} = 0.944
13393 measured reflections
7322 independent reflections
6247 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
S = 1.08
7322 reflections
482 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···S2^{i}	0.91	2.63	3.5283 (19)	168

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); 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: GK2075).

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supplementary materials

Acta Cryst. (2007). E**63**, m1594 [**doi:10.1107/S1600536807025421**]

Ammine(2-ethylpyridine-κN)bis(tri-*tert*-butoxysilanethiolato-κS)cobalt(II)

A. Pladzyk and K. Baranowska

Comment

Complexes of transition metals with sulfur and nitrogen ligands serve as biological models of histidine-metal-cysteine centers found in zinc metalloproteins (Corwin *et al.*, 1987; Kimblin *et al.*, 2000). However, "spectroscopic silence" of zinc thiolates prevents the use of spectral experiments for simulation of enzymatic reactions in solution, *i.e.* direct measurement of the loss of substrate or product concentration increase. Since, cobalt and zinc coordination chemistry is similar and changes in coordination environment of cobalt complexes can be monitored by UV-VIS, we decided to synthesize appropriate cobalt complexes which could replace adequate complexes of zinc in spectral experiments. The objective of our research is exploration of the syntheses, geometrical structures and reactivity of model complexes. We have synthesized and characterized structurally several cobalt (II) silanethiolates with pyridine and pyridine related ligands (Becker *et al.*, 2002 and the references cited therein; Pladzyk & Baranowska, 2006).

The title complex (Fig. 1), with CoN_2S_2 core and tetrahedrally coordinated cobalt (II), is similar to [Co{SSi(*O*^{t}Bu)$_3$}$_2$(NH$_3$)(2-methylpyridine)], obtained earlier (Becker *et al.*, 2002). However, ethyl substituent on the pyridine ring forces different spatial arrangement of the ligands and, in consequence, intermolecular hydrogen bond can be formed between sulfur atom and ammonia nitrogen with the N···S distance of 3.528 (2) Å, while in [Co{SSi(*O*^{t}Bu)$_3$}$_2$(NH$_3$)(2-methylpyridine)] two N···O hydrogen bonds were present. The reorganization of ligands in the title compound involves mainly changes in the N2–Co1–N2 and S1–Co1–S2 angles, which in comparison with [Co{SSi(*O*^{t}Bu)$_3$}$_2$(NH$_3$)(2-methylpyridine)], are wider by approximately 6–7 ° in (I). The remaining N–Co–S, Si–S–Co angles are slightly smaller than those found in [Co{SSi(*O*^{t}Bu)$_3$}$_2$(NH$_3$)(2-methylpyridine)].

Experimental

[Co{SSi(O^{t}Bu)$_3$}$_2$(NH$_3$)]$_2$ was obtained as described (Becker *et al.*, 2002). All other reagents were obtained commercially. 2-Ethylpyridine was dried by standard methods, and distilled prior to use. To a solution of [Co{SSi(O^{t}Bu)$_3$}$_2$(NH$_3$)]$_2$ (0.124 g, 0.2 mmol) in 10 ml of n-hexane, freshly prepared 2-ethylpyridine (22,8µl, 0.2 mmol) was added and blue, well formed crystals of [Co{SSi(*O*^{t}Bu)$_3$}$_2$(2-ethylpyridine)(NH$_3$)] were obtained.

Refinement

All H atoms were refined in the riding mode approximation with aromatic C—H = 0.95 Å, methyl C—H = 0.98 Å, methylene C—H = 0.99 Å, and U_{iso}(H) = 1.2U_{eq}(C) for CH groups, U_{iso}(H) = 1.3U_{eq}(C) for CH_2 groups, 1.5U_{eq}(C) for CH_3 groups. The disordered ^{t}Bu group C2—C4 has site-occupancy factors of 0.660 (5) and 0.340 (5) for two orientations. Also 2-ethylpyridine was refined as disordered over two positions with occupancies of 0.736 (5) and 0.264 (5).

Figures

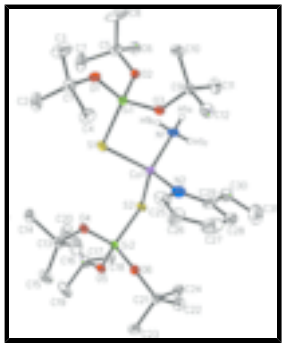

Fig. 1. The asymmetric unit of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only major orientations of the disordered groups are shown. C-bound H atoms have been omitted for clarity.

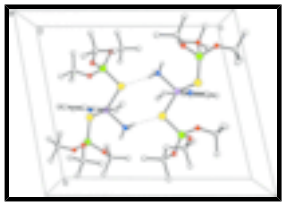

Fig. 2. The crystal packing of the title compound, viewed approximately down the *a* axis.

Ammine(2-ethylpyridine-κ*N*)bis(tri-*tert*-butoxysilanethiolato- κ*S*)cobalt(II)

Crystal data

$[Co(C_{12}H_{27}O_3SSi)_2(C_7H_9N)(NH_3)]$	$Z = 2$
$M_r = 742.09$	$F_{000} = 802$
Triclinic, $P\overline{1}$	$D_x = 1.184$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.6939$ (4) Å	Cell parameters from 12985 reflections
$b = 13.7249$ (6) Å	$\theta = 2.2$–$32.4°$
$c = 16.1266$ (6) Å	$\mu = 0.61$ mm^{-1}
$\alpha = 78.605$ (4)°	$T = 120$ (2) K
$\beta = 88.106$ (3)°	Prism, blue
$\gamma = 81.830$ (4)°	0.26 × 0.11 × 0.04 mm
$V = 2081.94$ (15) Å^3	

Data collection

Kuma KM-4-CCD κ-geometry diffractometer	7322 independent reflections
Monochromator: graphite	6247 reflections with $I > 2\sigma(I)$
Detector resolution: 8.1883 pixels mm^{-1}	$R_{int} = 0.025$
$T = 120(2)$ K	$\theta_{max} = 25.1°$
ω scans	$\theta_{min} = 2.2°$
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2005)	$h = -11 \rightarrow 11$
$T_{min} = 0.787$, $T_{max} = 0.944$	$k = -13 \rightarrow 16$

13393 measured reflections

$l = -18 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.095$

$S = 1.08$

7322 reflections

482 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.9644P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.39$ e Å^{-3}

$\Delta\rho_{min} = -0.31$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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)
Co1	0.56482 (3)	0.444200 (19)	0.684482 (17)	0.02391 (9)	
S1	0.74076 (6)	0.39705 (4)	0.78226 (3)	0.02890 (13)	
S2	0.58041 (6)	0.58892 (4)	0.58700 (3)	0.02917 (13)	
Si1	0.72768 (6)	0.24453 (4)	0.81741 (3)	0.02232 (13)	
Si2	0.56792 (6)	0.69859 (4)	0.66132 (3)	0.02210 (13)	
O1	0.82101 (15)	0.19001 (11)	0.90026 (9)	0.0288 (3)	
O2	0.78130 (14)	0.18079 (10)	0.74373 (9)	0.0251 (3)	
O3	0.56257 (15)	0.23304 (10)	0.83043 (10)	0.0288 (3)	
O4	0.67436 (16)	0.65534 (10)	0.73988 (9)	0.0292 (3)	
O5	0.60382 (15)	0.80487 (10)	0.60540 (9)	0.0270 (3)	
O6	0.41524 (15)	0.72489 (10)	0.70317 (9)	0.0267 (3)	
C1	0.8376 (2)	0.21322 (18)	0.98232 (14)	0.0361 (5)	
C2	0.9411 (5)	0.2897 (4)	0.9685 (3)	0.0587 (14)	0.660 (5)
H2A	1.0288	0.26	0.946	0.088*	0.660 (5)
H2B	0.9585	0.3082	1.0224	0.088*	0.660 (5)
H2C	0.9021	0.3496	0.9281	0.088*	0.660 (5)
C3	0.8864 (7)	0.1205 (4)	1.0388 (3)	0.0640 (17)	0.660 (5)

H3A	0.8173	0.0742	1.0419	0.096*	0.660 (5)
H3B	0.9	0.1337	1.0953	0.096*	0.660 (5)
H3C	0.975	0.0904	1.0176	0.096*	0.660 (5)
C4	0.6966 (4)	0.2650 (3)	1.0095 (2)	0.0449 (12)	0.660 (5)
H4A	0.6648	0.3241	0.9662	0.067*	0.660 (5)
H4B	0.7075	0.2857	1.0634	0.067*	0.660 (5)
H4C	0.6279	0.218	1.0162	0.067*	0.660 (5)
C2A	0.9997 (8)	0.1834 (7)	1.0065 (5)	0.051 (2)	0.340 (5)
H2D	1.0118	0.1848	1.0663	0.077*	0.340 (5)
H2E	1.0539	0.2313	0.9715	0.077*	0.340 (5)
H2F	1.0323	0.1157	0.9965	0.077*	0.340 (5)
C3A	0.7689 (12)	0.1315 (7)	1.0487 (4)	0.051 (3)	0.340 (5)
H3D	0.8001	0.0647	1.0366	0.076*	0.340 (5)
H3E	0.6672	0.1461	1.0444	0.076*	0.340 (5)
H3F	0.7973	0.1336	1.1061	0.076*	0.340 (5)
C4A	0.7904 (10)	0.3121 (6)	0.9995 (5)	0.047 (2)	0.340 (5)
H4D	0.8098	0.3129	1.0586	0.071*	0.340 (5)
H4E	0.6899	0.3289	0.9894	0.071*	0.340 (5)
H4F	0.8396	0.3615	0.9622	0.071*	0.340 (5)
C5	0.9195 (2)	0.13754 (17)	0.72242 (13)	0.0309 (5)	
C6	0.9139 (2)	0.13352 (18)	0.62931 (14)	0.0357 (5)	
H6A	0.8348	0.1003	0.6193	0.054*	
H6B	1.0006	0.0958	0.6128	0.054*	
H6C	0.9028	0.2019	0.5957	0.054*	
C7	1.0277 (3)	0.2022 (3)	0.7361 (2)	0.0624 (9)	
H7A	1.0033	0.2701	0.7027	0.094*	
H7B	1.1194	0.1731	0.7183	0.094*	
H7C	1.0303	0.2054	0.7962	0.094*	
C8	0.9478 (4)	0.0324 (2)	0.77527 (19)	0.0713 (11)	
H8A	0.9412	0.0358	0.8354	0.107*	
H8B	1.0415	0.0015	0.7626	0.107*	
H8C	0.8789	−0.0079	0.7619	0.107*	
C9	0.4871 (2)	0.14759 (16)	0.84083 (14)	0.0306 (5)	
C10	0.5736 (3)	0.05220 (17)	0.88649 (17)	0.0406 (6)	
H10A	0.6591	0.0384	0.8542	0.061*	
H10B	0.5197	−0.004	0.8918	0.061*	
H10C	0.5977	0.0607	0.9429	0.061*	
C11	0.4473 (3)	0.1358 (2)	0.75355 (17)	0.0471 (6)	
H11A	0.3952	0.1988	0.7239	0.071*	
H11B	0.3891	0.082	0.759	0.071*	
H11C	0.5318	0.1188	0.7214	0.071*	
C12	0.3577 (3)	0.1741 (2)	0.89199 (19)	0.0470 (6)	
H12A	0.3853	0.184	0.9473	0.071*	
H12B	0.3007	0.1194	0.8999	0.071*	
H12C	0.3035	0.236	0.8618	0.071*	
C13	0.6934 (2)	0.68762 (16)	0.81831 (13)	0.0315 (5)	
C14	0.8372 (3)	0.6369 (2)	0.84889 (17)	0.0460 (6)	
H14A	0.8417	0.564	0.8549	0.069*	
H14B	0.8553	0.6529	0.9038	0.069*	

H14C	0.9076	0.6608	0.8078	0.069*	
C15	0.6850 (3)	0.80104 (19)	0.80386 (17)	0.0537 (7)	
H15A	0.755	0.8232	0.7617	0.081*	
H15B	0.7027	0.821	0.8572	0.081*	
H15C	0.5919	0.8321	0.7834	0.081*	
C16	0.5838 (3)	0.6502 (2)	0.88057 (16)	0.0526 (7)	
H16A	0.491	0.678	0.8576	0.079*	
H16B	0.595	0.6716	0.9342	0.079*	
H16C	0.5943	0.5768	0.8903	0.079*	
C17	0.7164 (2)	0.82932 (17)	0.54831 (14)	0.0324 (5)	
C18	0.6719 (3)	0.82716 (18)	0.45958 (14)	0.0353 (5)	
H18A	0.6582	0.7587	0.4562	0.053*	
H18B	0.7443	0.8491	0.4192	0.053*	
H18C	0.5845	0.8723	0.446	0.053*	
C19	0.7370 (3)	0.9354 (2)	0.55490 (17)	0.0538 (8)	
H19A	0.6499	0.9807	0.5406	0.081*	
H19B	0.8106	0.9576	0.5155	0.081*	
H19C	0.7639	0.9362	0.6128	0.081*	
C20	0.8493 (3)	0.7557 (2)	0.57218 (17)	0.0497 (7)	
H20A	0.8756	0.7566	0.6302	0.075*	
H20B	0.9247	0.7754	0.5333	0.075*	
H20C	0.8327	0.6879	0.5684	0.075*	
C21	0.2913 (2)	0.79131 (16)	0.67126 (13)	0.0281 (4)	
C22	0.1732 (2)	0.75394 (18)	0.72733 (15)	0.0366 (5)	
H22A	0.1611	0.6868	0.7191	0.055*	
H22B	0.0869	0.7999	0.7124	0.055*	
H22C	0.1955	0.751	0.7867	0.055*	
C23	0.3091 (3)	0.89734 (16)	0.68011 (16)	0.0384 (5)	
H23A	0.3248	0.8984	0.7396	0.058*	
H23B	0.2247	0.9433	0.6603	0.058*	
H23C	0.3892	0.9185	0.6461	0.058*	
C24	0.2664 (2)	0.78670 (19)	0.57969 (14)	0.0376 (5)	
H24A	0.3441	0.8102	0.5446	0.056*	
H24B	0.1794	0.8296	0.5601	0.056*	
H24C	0.2596	0.7173	0.5753	0.056*	
N1	0.5957 (2)	0.33782 (13)	0.60817 (12)	0.0359 (4)	
H1A	0.5776	0.2776	0.6384	0.043*	
H1B	0.6856	0.332	0.5896	0.043*	
H1C	0.5375	0.3572	0.563	0.043*	
N2	0.3802 (2)	0.44899 (16)	0.75423 (15)	0.0262 (7)	0.736 (5)
C25	0.3889 (6)	0.4540 (3)	0.8362 (3)	0.0312 (9)	0.736 (5)
H25	0.479	0.4512	0.8588	0.037*	0.736 (5)
C26	0.2760 (6)	0.4629 (4)	0.8896 (4)	0.0490 (13)	0.736 (5)
H26	0.2875	0.4662	0.9472	0.059*	0.736 (5)
C27	0.1466 (4)	0.4668 (3)	0.8566 (3)	0.0498 (11)	0.736 (5)
H27	0.0657	0.473	0.891	0.06*	0.736 (5)
C28	0.1354 (6)	0.4615 (5)	0.7723 (4)	0.0406 (13)	0.736 (5)
H28	0.0461	0.4634	0.7491	0.049*	0.736 (5)
C29	0.2525 (4)	0.4534 (2)	0.7215 (3)	0.0328 (9)	0.736 (5)

C30	0.2485 (5)	0.4491 (4)	0.6297 (4)	0.0450 (12)	0.736 (5)
H30A	0.3227	0.4855	0.6	0.059*	0.736 (5)
H30B	0.2708	0.3781	0.6239	0.059*	0.736 (5)
C31	0.1151 (5)	0.4913 (6)	0.5867 (4)	0.0664 (15)	0.736 (5)
H31A	0.0418	0.4526	0.6124	0.1*	0.736 (5)
H31B	0.1242	0.488	0.5266	0.1*	0.736 (5)
H31C	0.0908	0.5614	0.5926	0.1*	0.736 (5)
N2A	0.3486 (7)	0.4540 (4)	0.6852 (4)	0.0206 (18)*	0.264 (5)
C25A	0.2872 (14)	0.4509 (10)	0.6126 (9)	0.031 (3)*	0.264 (5)
H25A	0.3442	0.4423	0.5648	0.037*	0.264 (5)
C26A	0.149 (2)	0.4594 (11)	0.6048 (11)	0.051 (4)*	0.264 (5)
H26A	0.1109	0.4588	0.5516	0.062*	0.264 (5)
C27A	0.0581 (10)	0.4694 (7)	0.6754 (6)	0.040 (2)*	0.264 (5)
H27A	−0.0405	0.4776	0.6706	0.048*	0.264 (5)
C28A	0.1219 (19)	0.4662 (14)	0.7485 (10)	0.029 (4)*	0.264 (5)
H28A	0.0676	0.4666	0.7986	0.035*	0.264 (5)
C29A	0.2690 (11)	0.4623 (7)	0.7529 (6)	0.020 (3)*	0.264 (5)
C30A	0.3392 (15)	0.4674 (12)	0.8331 (11)	0.042 (4)*	0.264 (5)
H30C	0.4009	0.403	0.8508	0.055*	0.264 (5)
H30D	0.4001	0.5206	0.8194	0.055*	0.264 (5)
C31A	0.2567 (19)	0.4856 (13)	0.9038 (11)	0.046 (5)*	0.264 (5)
H31D	0.1969	0.5503	0.8889	0.069*	0.264 (5)
H31E	0.3174	0.4872	0.9508	0.069*	0.264 (5)
H31F	0.1986	0.4321	0.9208	0.069*	0.264 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02190 (15)	0.01971 (15)	0.03067 (17)	−0.00157 (10)	−0.00152 (11)	−0.00691 (11)
S1	0.0379 (3)	0.0223 (3)	0.0276 (3)	−0.0090 (2)	−0.0064 (2)	−0.0031 (2)
S2	0.0435 (3)	0.0208 (2)	0.0240 (3)	−0.0019 (2)	−0.0099 (2)	−0.0064 (2)
Si1	0.0244 (3)	0.0205 (3)	0.0218 (3)	−0.0026 (2)	−0.0007 (2)	−0.0038 (2)
Si2	0.0280 (3)	0.0184 (3)	0.0206 (3)	−0.0045 (2)	−0.0045 (2)	−0.0038 (2)
O1	0.0353 (8)	0.0297 (8)	0.0192 (7)	0.0039 (6)	−0.0014 (6)	−0.0052 (6)
O2	0.0241 (7)	0.0270 (7)	0.0245 (7)	−0.0018 (6)	−0.0008 (6)	−0.0072 (6)
O3	0.0263 (8)	0.0215 (7)	0.0388 (9)	−0.0037 (6)	0.0028 (6)	−0.0062 (6)
O4	0.0370 (8)	0.0263 (7)	0.0256 (8)	−0.0024 (6)	−0.0095 (6)	−0.0077 (6)
O5	0.0337 (8)	0.0227 (7)	0.0258 (7)	−0.0078 (6)	0.0021 (6)	−0.0050 (6)
O6	0.0288 (8)	0.0256 (7)	0.0247 (7)	−0.0037 (6)	−0.0031 (6)	−0.0017 (6)
C1	0.0408 (13)	0.0453 (13)	0.0243 (11)	−0.0008 (10)	−0.0040 (10)	−0.0147 (10)
C2	0.052 (3)	0.084 (3)	0.049 (3)	−0.010 (2)	−0.019 (2)	−0.032 (2)
C3	0.097 (5)	0.060 (3)	0.025 (2)	0.029 (3)	−0.021 (2)	−0.0079 (19)
C4	0.048 (2)	0.060 (3)	0.0267 (19)	0.008 (2)	−0.0018 (17)	−0.0206 (18)
C2A	0.045 (5)	0.073 (6)	0.044 (5)	−0.013 (4)	−0.009 (4)	−0.025 (4)
C3A	0.078 (7)	0.060 (5)	0.018 (4)	−0.033 (5)	0.000 (4)	−0.004 (3)
C4A	0.070 (6)	0.046 (4)	0.023 (4)	0.002 (4)	−0.004 (4)	−0.007 (3)
C5	0.0271 (11)	0.0400 (12)	0.0243 (11)	0.0043 (9)	0.0007 (9)	−0.0094 (9)
C6	0.0371 (12)	0.0437 (13)	0.0288 (12)	−0.0053 (10)	0.0037 (10)	−0.0135 (10)

C7	0.0280 (13)	0.114 (3)	0.0615 (18)	−0.0116 (15)	0.0048 (12)	−0.0553 (19)
C8	0.077 (2)	0.0646 (19)	0.0452 (17)	0.0444 (17)	0.0192 (15)	0.0118 (14)
C9	0.0294 (11)	0.0270 (11)	0.0372 (12)	−0.0096 (9)	0.0029 (9)	−0.0070 (9)
C10	0.0467 (14)	0.0264 (11)	0.0468 (15)	−0.0097 (10)	0.0034 (11)	−0.0003 (10)
C11	0.0474 (15)	0.0544 (16)	0.0437 (15)	−0.0214 (12)	−0.0039 (12)	−0.0089 (12)
C12	0.0364 (13)	0.0441 (14)	0.0630 (18)	−0.0132 (11)	0.0158 (12)	−0.0131 (13)
C13	0.0413 (13)	0.0319 (11)	0.0241 (11)	−0.0065 (9)	−0.0114 (9)	−0.0093 (9)
C14	0.0458 (15)	0.0498 (15)	0.0453 (15)	−0.0065 (12)	−0.0207 (12)	−0.0133 (12)
C15	0.089 (2)	0.0349 (13)	0.0416 (15)	−0.0073 (13)	−0.0243 (14)	−0.0144 (11)
C16	0.0556 (17)	0.079 (2)	0.0275 (13)	−0.0196 (15)	−0.0058 (11)	−0.0134 (13)
C17	0.0364 (12)	0.0371 (12)	0.0266 (11)	−0.0181 (10)	0.0026 (9)	−0.0042 (9)
C18	0.0405 (13)	0.0389 (12)	0.0277 (12)	−0.0119 (10)	0.0010 (10)	−0.0052 (10)
C19	0.085 (2)	0.0494 (16)	0.0372 (14)	−0.0435 (15)	0.0105 (14)	−0.0105 (12)
C20	0.0303 (13)	0.0724 (19)	0.0436 (15)	−0.0147 (12)	−0.0009 (11)	0.0009 (13)
C21	0.0276 (11)	0.0297 (11)	0.0257 (11)	−0.0006 (9)	−0.0027 (8)	−0.0044 (9)
C22	0.0326 (12)	0.0446 (13)	0.0330 (12)	−0.0068 (10)	0.0025 (10)	−0.0079 (10)
C23	0.0399 (13)	0.0273 (11)	0.0465 (14)	0.0006 (10)	0.0004 (11)	−0.0076 (10)
C24	0.0344 (12)	0.0472 (14)	0.0279 (12)	0.0034 (10)	−0.0069 (9)	−0.0044 (10)
N1	0.0492 (12)	0.0247 (9)	0.0327 (10)	0.0067 (8)	−0.0174 (9)	−0.0085 (8)
N2	0.0260 (14)	0.0200 (12)	0.0311 (15)	0.0000 (9)	−0.0013 (10)	−0.0031 (10)
C25	0.036 (2)	0.0311 (19)	0.0241 (18)	0.0022 (19)	0.0007 (18)	−0.0054 (13)
C26	0.053 (3)	0.045 (3)	0.039 (3)	0.015 (2)	0.001 (2)	0.000 (2)
C27	0.042 (2)	0.043 (2)	0.054 (2)	0.0097 (16)	0.0165 (17)	0.0024 (17)
C28	0.024 (2)	0.038 (2)	0.056 (4)	0.0007 (15)	−0.002 (3)	−0.004 (3)
C29	0.0278 (19)	0.0229 (16)	0.048 (2)	0.0002 (12)	−0.0069 (17)	−0.0090 (16)
C30	0.026 (3)	0.060 (3)	0.053 (3)	0.009 (2)	−0.015 (2)	−0.028 (2)
C31	0.038 (3)	0.092 (4)	0.068 (3)	0.004 (3)	−0.017 (2)	−0.020 (3)

Geometric parameters (Å, °)

Co1—N1	2.0730 (17)	C14—H14A	0.98
Co1—N2A	2.081 (6)	C14—H14B	0.98
Co1—N2	2.082 (2)	C14—H14C	0.98
Co1—S1	2.2967 (6)	C15—H15A	0.98
Co1—S2	2.2968 (6)	C15—H15B	0.98
S1—Si1	2.0787 (7)	C15—H15C	0.98
S2—Si2	2.0899 (7)	C16—H16A	0.98
Si1—O1	1.6298 (15)	C16—H16B	0.98
Si1—O3	1.6332 (15)	C16—H16C	0.98
Si1—O2	1.6395 (14)	C17—C18	1.515 (3)
Si2—O4	1.6240 (15)	C17—C19	1.522 (3)
Si2—O6	1.6293 (15)	C17—C20	1.529 (4)
Si2—O5	1.6328 (14)	C18—H18A	0.98
O1—C1	1.440 (2)	C18—H18B	0.98
O2—C5	1.446 (2)	C18—H18C	0.98
O3—C9	1.448 (2)	C19—H19A	0.98
O4—C13	1.446 (2)	C19—H19B	0.98
O5—C17	1.438 (3)	C19—H19C	0.98
O6—C21	1.444 (2)	C20—H20A	0.98

C1—C3	1.440 (5)	C20—H20B	0.98
C1—C4A	1.447 (8)	C20—H20C	0.98
C1—C2	1.532 (5)	C21—C22	1.518 (3)
C1—C4	1.540 (4)	C21—C24	1.519 (3)
C1—C3A	1.593 (8)	C21—C23	1.524 (3)
C1—C2A	1.608 (8)	C22—H22A	0.98
C2—H2A	0.98	C22—H22B	0.98
C2—H2B	0.98	C22—H22C	0.98
C2—H2C	0.98	C23—H23A	0.98
C3—H3A	0.98	C23—H23B	0.98
C3—H3B	0.98	C23—H23C	0.98
C3—H3C	0.98	C24—H24A	0.98
C4—H4A	0.98	C24—H24B	0.98
C4—H4B	0.98	C24—H24C	0.98
C4—H4C	0.98	N1—H1A	0.91
C2A—H2D	0.98	N1—H1B	0.91
C2A—H2E	0.98	N1—H1C	0.91
C2A—H2F	0.98	N2—C25	1.343 (5)
C3A—H3D	0.98	N2—C29	1.350 (5)
C3A—H3E	0.98	C25—C26	1.377 (7)
C3A—H3F	0.98	C25—H25	0.95
C4A—H4D	0.98	C26—C27	1.369 (7)
C4A—H4E	0.98	C26—H26	0.95
C4A—H4F	0.98	C27—C28	1.384 (8)
C5—C7	1.514 (4)	C27—H27	0.95
C5—C8	1.516 (4)	C28—C29	1.382 (7)
C5—C6	1.516 (3)	C28—H28	0.95
C6—H6A	0.98	C29—C30	1.496 (7)
C6—H6B	0.98	C30—C31	1.475 (6)
C6—H6C	0.98	C30—H30A	0.99
C7—H7A	0.98	C30—H30B	0.99
C7—H7B	0.98	C31—H31A	0.98
C7—H7C	0.98	C31—H31B	0.98
C8—H8A	0.98	C31—H31C	0.98
C8—H8B	0.98	N2A—C29A	1.330 (12)
C8—H8C	0.98	N2A—C25A	1.343 (17)
C9—C11	1.517 (3)	C25A—C26A	1.33 (2)
C9—C10	1.519 (3)	C25A—H25A	0.95
C9—C12	1.519 (3)	C26A—C27A	1.434 (19)
C10—H10A	0.98	C26A—H26A	0.95
C10—H10B	0.98	C27A—C28A	1.340 (19)
C10—H10C	0.98	C27A—H27A	0.95
C11—H11A	0.98	C28A—C29A	1.42 (2)
C11—H11B	0.98	C28A—H28A	0.95
C11—H11C	0.98	C29A—C30A	1.50 (2)
C12—H12A	0.98	C30A—C31A	1.41 (2)
C12—H12B	0.98	C30A—H30C	0.99
C12—H12C	0.98	C30A—H30D	0.99
C13—C16	1.511 (4)	C31A—H31D	0.98

C13—C14	1.518 (3)	C31A—H31E	0.98
C13—C15	1.519 (3)	C31A—H31F	0.98
N1—Co1—N2A	94.65 (18)	C13—C14—H14A	109.5
N1—Co1—N2	116.09 (9)	C13—C14—H14B	109.5
N2A—Co1—N2	32.07 (18)	H14A—C14—H14B	109.5
N1—Co1—S1	104.82 (5)	C13—C14—H14C	109.5
N2A—Co1—S1	136.83 (17)	H14A—C14—H14C	109.5
N2—Co1—S1	105.70 (7)	H14B—C14—H14C	109.5
N1—Co1—S2	101.12 (6)	C13—C15—H15A	109.5
N2A—Co1—S2	97.03 (17)	C13—C15—H15B	109.5
N2—Co1—S2	113.31 (6)	H15A—C15—H15B	109.5
S1—Co1—S2	115.85 (2)	C13—C15—H15C	109.5
Si1—S1—Co1	100.10 (3)	H15A—C15—H15C	109.5
Si2—S2—Co1	103.26 (3)	H15B—C15—H15C	109.5
O1—Si1—O3	112.92 (8)	C13—C16—H16A	109.5
O1—Si1—O2	105.15 (7)	C13—C16—H16B	109.5
O3—Si1—O2	104.91 (8)	H16A—C16—H16B	109.5
O1—Si1—S1	113.09 (6)	C13—C16—H16C	109.5
O3—Si1—S1	107.06 (6)	H16A—C16—H16C	109.5
O2—Si1—S1	113.54 (6)	H16B—C16—H16C	109.5
O4—Si2—O6	106.16 (8)	O5—C17—C18	108.30 (17)
O4—Si2—O5	112.39 (8)	O5—C17—C19	105.48 (18)
O6—Si2—O5	105.35 (7)	C18—C17—C19	110.2 (2)
O4—Si2—S2	107.19 (6)	O5—C17—C20	111.37 (18)
O6—Si2—S2	114.89 (6)	C18—C17—C20	110.3 (2)
O5—Si2—S2	110.89 (6)	C19—C17—C20	111.1 (2)
C1—O1—Si1	134.13 (13)	C17—C18—H18A	109.5
C5—O2—Si1	130.97 (13)	C17—C18—H18B	109.5
C9—O3—Si1	132.79 (13)	H18A—C18—H18B	109.5
C13—O4—Si2	132.73 (13)	C17—C18—H18C	109.5
C17—O5—Si2	132.12 (13)	H18A—C18—H18C	109.5
C21—O6—Si2	132.54 (13)	H18B—C18—H18C	109.5
C3—C1—O1	107.3 (2)	C17—C19—H19A	109.5
C3—C1—C4A	130.5 (4)	C17—C19—H19B	109.5
O1—C1—C4A	121.5 (3)	H19A—C19—H19B	109.5
C3—C1—C2	114.2 (4)	C17—C19—H19C	109.5
O1—C1—C2	105.0 (2)	H19A—C19—H19C	109.5
C4A—C1—C2	62.1 (4)	H19B—C19—H19C	109.5
C3—C1—C4	113.2 (3)	C17—C20—H20A	109.5
O1—C1—C4	108.3 (2)	C17—C20—H20B	109.5
C2—C1—C4	108.3 (3)	H20A—C20—H20B	109.5
O1—C1—C3A	106.4 (3)	C17—C20—H20C	109.5
C4A—C1—C3A	109.6 (5)	H20A—C20—H20C	109.5
C2—C1—C3A	146.3 (4)	H20B—C20—H20C	109.5
O1—C1—C2A	107.3 (3)	O6—C21—C22	105.35 (17)
C4A—C1—C2A	108.7 (5)	O6—C21—C24	110.69 (17)
C4—C1—C2A	144.1 (3)	C22—C21—C24	110.61 (18)
C3A—C1—C2A	101.4 (5)	O6—C21—C23	108.24 (17)
C1—C2—H2A	109.5	C22—C21—C23	110.73 (18)

C1—C2—H2B	109.5	C24—C21—C23	111.06 (19)
C1—C2—H2C	109.5	C21—C22—H22A	109.5
C1—C3—H3A	109.5	C21—C22—H22B	109.5
C1—C3—H3B	109.5	H22A—C22—H22B	109.5
C1—C3—H3C	109.5	C21—C22—H22C	109.5
C1—C4—H4A	109.5	H22A—C22—H22C	109.5
C1—C4—H4B	109.5	H22B—C22—H22C	109.5
C1—C4—H4C	109.5	C21—C23—H23A	109.5
C1—C2A—H2D	109.5	C21—C23—H23B	109.5
C1—C2A—H2E	109.5	H23A—C23—H23B	109.5
H2D—C2A—H2E	109.5	C21—C23—H23C	109.5
C1—C2A—H2F	109.5	H23A—C23—H23C	109.5
H2D—C2A—H2F	109.5	H23B—C23—H23C	109.5
H2E—C2A—H2F	109.5	C21—C24—H24A	109.5
C1—C3A—H3D	109.5	C21—C24—H24B	109.5
C1—C3A—H3E	109.5	H24A—C24—H24B	109.5
H3D—C3A—H3E	109.5	C21—C24—H24C	109.5
C1—C3A—H3F	109.5	H24A—C24—H24C	109.5
H3D—C3A—H3F	109.5	H24B—C24—H24C	109.5
H3E—C3A—H3F	109.5	Co1—N1—H1A	109.5
C1—C4A—H4D	109.5	Co1—N1—H1B	109.5
C1—C4A—H4E	109.5	H1A—N1—H1B	109.5
H4D—C4A—H4E	109.5	Co1—N1—H1C	109.5
C1—C4A—H4F	109.5	H1A—N1—H1C	109.5
H4D—C4A—H4F	109.5	H1B—N1—H1C	109.5
H4E—C4A—H4F	109.5	C25—N2—C29	118.2 (4)
O2—C5—C7	111.27 (18)	C25—N2—Co1	117.2 (3)
O2—C5—C8	107.68 (19)	C29—N2—Co1	124.5 (2)
C7—C5—C8	112.2 (3)	N2—C25—C26	124.4 (5)
O2—C5—C6	105.45 (17)	N2—C25—H25	117.8
C7—C5—C6	109.6 (2)	C26—C25—H25	117.8
C8—C5—C6	110.4 (2)	C27—C26—C25	117.5 (5)
C5—C6—H6A	109.5	C27—C26—H26	121.3
C5—C6—H6B	109.5	C25—C26—H26	121.3
H6A—C6—H6B	109.5	C26—C27—C28	119.1 (4)
C5—C6—H6C	109.5	C26—C27—H27	120.5
H6A—C6—H6C	109.5	C28—C27—H27	120.5
H6B—C6—H6C	109.5	C29—C28—C27	120.9 (5)
C5—C7—H7A	109.5	C29—C28—H28	119.6
C5—C7—H7B	109.5	C27—C28—H28	119.6
H7A—C7—H7B	109.5	N2—C29—C28	120.1 (5)
C5—C7—H7C	109.5	N2—C29—C30	116.0 (4)
H7A—C7—H7C	109.5	C28—C29—C30	123.9 (5)
H7B—C7—H7C	109.5	C31—C30—C29	115.6 (4)
C5—C8—H8A	109.5	C31—C30—H30A	108.4
C5—C8—H8B	109.5	C29—C30—H30A	108.4
H8A—C8—H8B	109.5	C31—C30—H30B	108.4
C5—C8—H8C	109.5	C29—C30—H30B	108.4
H8A—C8—H8C	109.5	H30A—C30—H30B	107.5

H8B—C8—H8C	109.5	C29A—N2A—C25A	118.7 (9)
O3—C9—C11	107.79 (18)	C29A—N2A—Co1	124.1 (6)
O3—C9—C10	111.75 (18)	C25A—N2A—Co1	117.2 (7)
C11—C9—C10	110.4 (2)	C26A—C25A—N2A	122.5 (13)
O3—C9—C12	105.68 (17)	C26A—C25A—H25A	118.7
C11—C9—C12	110.5 (2)	N2A—C25A—H25A	118.7
C10—C9—C12	110.6 (2)	C25A—C26A—C27A	121.3 (15)
C9—C10—H10A	109.5	C25A—C26A—H26A	119.3
C9—C10—H10B	109.5	C27A—C26A—H26A	119.3
H10A—C10—H10B	109.5	C28A—C27A—C26A	115.1 (13)
C9—C10—H10C	109.5	C28A—C27A—H27A	122.4
H10A—C10—H10C	109.5	C26A—C27A—H27A	122.4
H10B—C10—H10C	109.5	C27A—C28A—C29A	121.6 (15)
C9—C11—H11A	109.5	C27A—C28A—H28A	119.2
C9—C11—H11B	109.5	C29A—C28A—H28A	119.2
H11A—C11—H11B	109.5	N2A—C29A—C28A	120.5 (11)
C9—C11—H11C	109.5	N2A—C29A—C30A	117.9 (10)
H11A—C11—H11C	109.5	C28A—C29A—C30A	121.6 (11)
H11B—C11—H11C	109.5	C31A—C30A—C29A	119.3 (13)
C9—C12—H12A	109.5	C31A—C30A—H30C	107.5
C9—C12—H12B	109.5	C29A—C30A—H30C	107.5
H12A—C12—H12B	109.5	C31A—C30A—H30D	107.5
C9—C12—H12C	109.5	C29A—C30A—H30D	107.5
H12A—C12—H12C	109.5	H30C—C30A—H30D	107
H12B—C12—H12C	109.5	C30A—C31A—H31D	109.5
O4—C13—C16	108.31 (18)	C30A—C31A—H31E	109.5
O4—C13—C14	105.12 (18)	H31D—C31A—H31E	109.5
C16—C13—C14	110.0 (2)	C30A—C31A—H31F	109.5
O4—C13—C15	110.79 (18)	H31D—C31A—H31F	109.5
C16—C13—C15	111.4 (2)	H31E—C31A—H31F	109.5
C14—C13—C15	111.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···S2^{i}	0.91	2.63	3.5283 (19)	168

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

Fig. 1

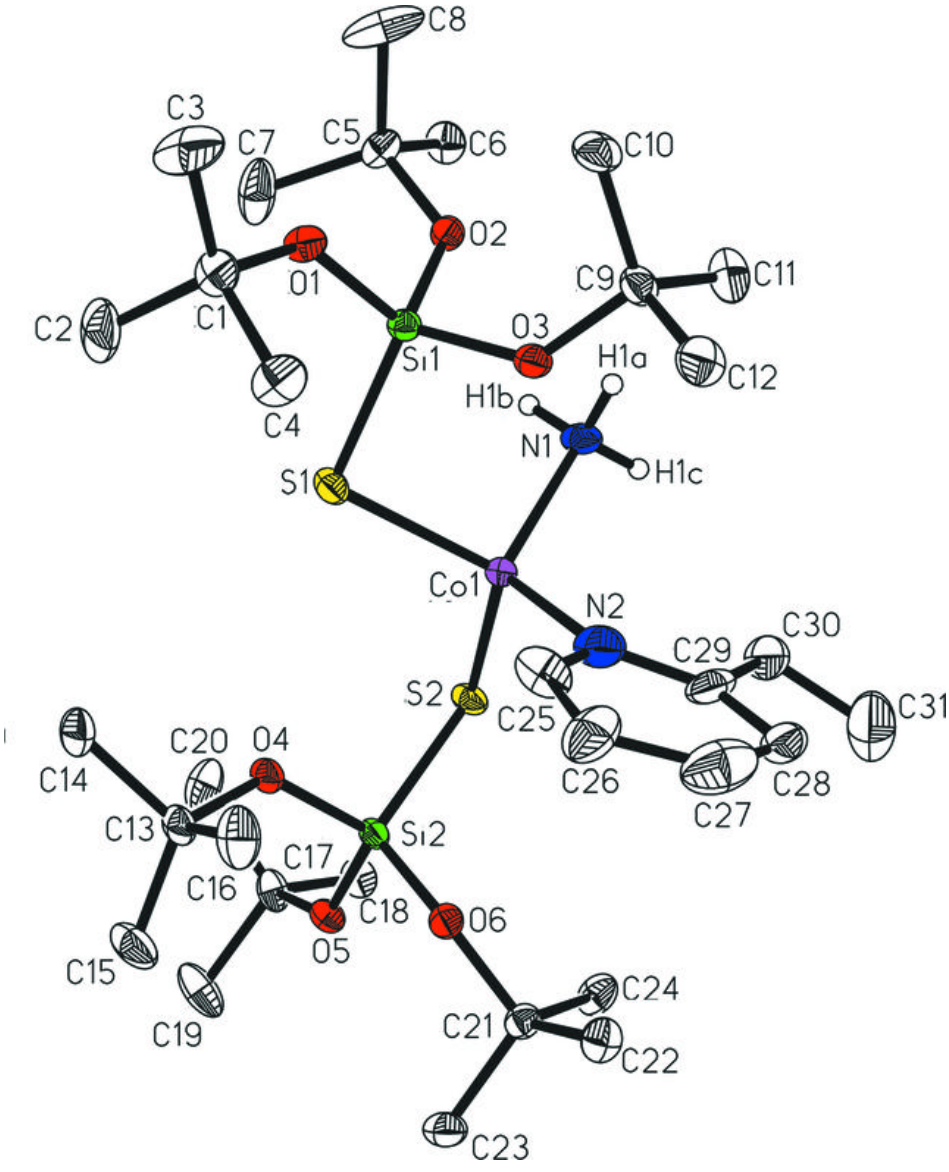
C8
C3
C7
C5
C6
C10
O2
O1
C9
C11
C2
C1
Si1
O3
H1a
C12
H1b
C4
N1
S1
H1c
Co1
N2
C30
C29
S2
C25
C31
C20
O4
C14
C26
C28
C27
C13
Si2
C17
C16
C18
O6
O5
C15
C24
C19
C21
C22
C23

Fig. 2