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(1,2-Dimethoxyethane-κO)bis(tri-*tert*-butoxysilanethiolato-$\kappa^2 O,S$)chromium(II)

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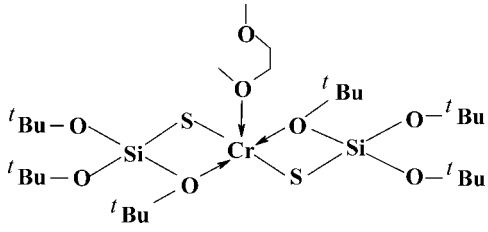
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.035; wR factor = 0.097; data-to-parameter ratio = 17.2.

The title compound, $[Cr(C_4H_{10}O_2)(C_{12}H_{27}O_3SSi)_2]$, is a molecular chromium(II) thiolate that has the 1,2-dimethoxyethane ligand coordinating through one of its two O atoms. The metal is *O*,*S*-chelated by the thiolate anion, and the O atom from the 1,2-dimethoxyethane ligand occupies the apical position of the square-pyramidal coodination geometry. The asymmetric unit contains two molecules. Three C atoms of one ^{t}Bu group are disordered approximately equally over two positions. One C atom of another ^{t}Bu group is disordered over two positions, with site occupancies of *ca.* 0.6 and 0.4.

Related literature

For the THF-coordinated analogue, see: Ciborska *et al.* (2007). For other *O*,*S*-chelated compounds, see: Becker *et al.* (1996); Dołęga *et al.* (2006); Wojnowski *et al.* (1985). For synthetic procedures, see: Piękoś & Wojnowski (1962); Wojnowska & Wojnowski (1974). For comparison Cr—S bond lengths, see: Okura *et al.* (1985); Nguyen *et al.* (2005); Ciborska *et al.* (2007).



Experimental

Crystal data

$[Cr(C_4H_{10}O_2)(C_{12}H_{27}O_3SSi)_2]$
M_r = 701.09
Triclinic, $P\overline{1}$
a = 8.6809 (3) Å
b = 21.3180 (9) Å
c = 21.7316 (10) Å
α = 87.828 (4)°
β = 84.745 (4)°
γ = 88.372 (3)°
V = 4000.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 150 (2) K
0.38 × 0.38 × 0.21 mm

Data collection

Oxford Diffraction KM4 CCD diffractometer
Absorption correction: none
27543 measured reflections
14104 independent reflections
12702 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.14
14104 reflections
821 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—Cr1	2.1248 (12)	O15—Cr2	2.3463 (13)
O4—Cr1	2.1201 (11)	S1—Cr1	2.4323 (5)
O7—Cr1	2.3273 (13)	S2—Cr1	2.4332 (5)
O9—Cr2	2.1234 (12)	S3—Cr2	2.4308 (5)
O12—Cr2	2.1283 (11)	S4—Cr2	2.4365 (5)

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: NG2360).

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supplementary materials

Acta Cryst. (2007). E**63**, m2972 [**doi:10.1107/S1600536807055614**]

(1,2-Dimethoxyethane-κO)bis(tri-*tert*-butoxysilanethiolato-$\kappa^2 O,S$)chromium(II)

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Comment

Here we report the structure of the title complex (I), which results from the reaction of $CrCl_2$ with $(O^tBu)_3SiSNa$ in dimethoxyethane solution. In this complex, tri-*tert*-butoxysilanethiol serves both as an *S*-only and as an *O,S* ligand. The property has also been observed for other silanethiolates, for example (Wojnowski *et al.*, 1985; Becker *et al.*, 1996; Dołęga *et al.*, 2006). Complex (I) is centrosymmetric about the chromium atom (Fig. 1). This coordination geometry is further reflected in the O—Cr—O angles, which are very close to 90°. The Cr—S distances are very similar to average values of *ca* 2.4 Å observed in the silanethiolates complexes (Ciborska *et al.*, 2007) and thiolate complexes (Okura *et al.*, 1985; Nguyen *et al.*, 2005). The Cr—$O_{(DME)}$ bond length is longer than the Cr—$O_{(THF)}$ distance in $Cr(C_{12}H_{27}O_3SSi)_2(C_4H_8O)$. The others important bond lengths and angles are collected in Table 1. Molecules pack in the crystal structure as discrete entities, with no intermolecular contacts (Fig. 2). Compound (I) is a analogue of the recently published THF compound (Ciborska *et al.*, 2007).

Experimental

All manipulations were performer under an atmosphere of nitrogen using standard Schlenk techniques. The $(^tBuO)_3SiSNa$ was prepared by literature methods (Piękoś & Wojnowski, 1962; Wojnowska &Wojnowski, 1974). A dimethoxyethane solution (15 ml) of $CrCl_2$ (0,196 g, 1,6 mmol) was added to a dimethoxyethane solution (10 ml) of $(^tBuO)_3SiSNa$ (1 g, 3,3 mmol) at room temperature. The resulting pale green solution was refluxed for 24 h and filtered. Concentration and cooling (−23°C) of this solution gave colourless crystals of (I), suitable for X-ray diffraction analysis.

Refinement

All H atoms were refined as riding on C atoms with methyl C—H = 0.98 Å, methylene C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2 groups and 1.5U_{eq}(C) for methyl groups. One *tert*-butyl group in (I) was found disordered in two positions; C10–C12 with probabilities of 0.513 (5) and 0.487 (5), and atom C38 with site occupation factors of 0.42 (5) and 0.58 (5).

Figures

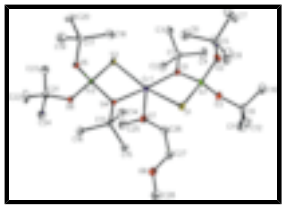

Fig. 1. A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms of *tert*-butyl groups and of 1,2-dimethoxyethan have been omitted.

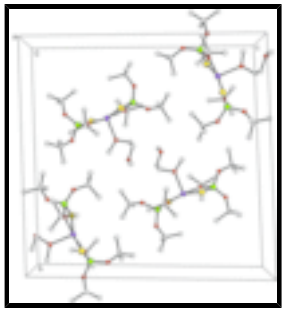

Fig. 2. A packing diagram of (I), viewed along the *a*-axis. Cr atoms are purple, S atoms are yellow, Si atoms are green, O atoms are red, C atoms are white. H atoms of *tert*-butyl groups and of 1,2- dimethoxyethan have been omitted.

(1,2-Dimethoxyethane-κ*O*)bis(tri-*tert*-butoxysilanethiolato- κ^2*O*,*S*)chromium(II)

Crystal data

$[Cr(C_4H_{10}O_2)(C_{12}H_{27}O_3SSi)_2]$	$Z = 4$
$M_r = 701.09$	$F_{000} = 1520$
Triclinic, $P\overline{1}$	$D_x = 1.164$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.6809$ (3) Å	Cell parameters from 32370 reflections
$b = 21.3180$ (9) Å	$\theta = 2.1$–32.5º
$c = 21.7316$ (10) Å	$\mu = 0.49$ mm^{-1}
$\alpha = 87.828$ (4)º	$T = 150$ (2) K
$\beta = 84.745$ (4)º	Prism, colourless
$\gamma = 88.372$ (3)º	0.38 × 0.38 × 0.21 mm
$V = 4000.6$ (3) Å^3	

Data collection

Oxford Diffraction KM4 CCD diffractometer	12702 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
Detector resolution: 8.1883 pixels mm^{-1}	$\theta_{max} = 25.1$º
$T = 150(2)$ K	$\theta_{min} = 2.1$º
ω scans, 0.75 deg width	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -22 \rightarrow 25$
27543 measured reflections	$l = -25 \rightarrow 25$
14104 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 1.4202P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.14	$(\Delta/\sigma)_{max}$ = 0.003
14104 reflections	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
821 parameters	$\Delta\rho_{min}$ = −0.42 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 $F^2 > \sigma(F^2)$ 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)
C1	0.70845 (19)	0.28522 (10)	0.42446 (8)	0.0270 (4)	
C2	0.6467 (2)	0.35164 (10)	0.41363 (9)	0.0329 (4)	
H2A	0.689	0.3796	0.4423	0.049*	
H2B	0.5335	0.3524	0.4206	0.049*	
H2C	0.6776	0.3658	0.371	0.049*	
C3	0.6515 (2)	0.23944 (10)	0.38053 (10)	0.0320 (4)	
H3A	0.6896	0.2515	0.338	0.048*	
H3B	0.5381	0.2402	0.3844	0.048*	
H3C	0.69	0.197	0.3907	0.048*	
C4	0.6634 (2)	0.26328 (13)	0.49108 (10)	0.0433 (6)	
H4A	0.7127	0.2222	0.4991	0.065*	
H4B	0.5507	0.2598	0.4977	0.065*	
H4C	0.6978	0.2937	0.5193	0.065*	
C5	1.0449 (3)	0.12730 (9)	0.42336 (10)	0.0405 (5)	
C6	1.0281 (3)	0.14287 (10)	0.35535 (10)	0.0400 (5)	
H6A	0.9203	0.155	0.35	0.06*	
H6B	1.0578	0.1059	0.331	0.06*	
H6C	1.0953	0.1777	0.3412	0.06*	
C7	0.9382 (5)	0.07414 (12)	0.44652 (16)	0.0830 (11)	
H7A	0.949	0.0649	0.4905	0.125*	
H7B	0.9663	0.0366	0.4229	0.125*	
H7C	0.8308	0.0868	0.4411	0.125*	
C8	1.2114 (4)	0.11179 (13)	0.43290 (12)	0.0617 (8)	
H8A	1.2743	0.1486	0.4213	0.093*	
H8B	1.2482	0.0767	0.4071	0.093*	
H8C	1.2202	0.1	0.4765	0.093*	
C9	1.0542 (2)	0.27704 (10)	0.57819 (8)	0.0295 (4)	

C10	0.9863 (8)	0.2200 (3)	0.6106 (2)	0.070 (2)	0.513 (5)
H10A	0.874	0.2261	0.6181	0.105*	0.513 (5)
H10B	1.0311	0.2128	0.6501	0.105*	0.513 (5)
H10C	1.0093	0.1836	0.5848	0.105*	0.513 (5)
C11	1.0150 (8)	0.3355 (3)	0.6132 (2)	0.0616 (19)	0.513 (5)
H11A	1.0585	0.3719	0.5894	0.092*	0.513 (5)
H11B	1.0584	0.3319	0.6533	0.092*	0.513 (5)
H11C	0.9023	0.341	0.6197	0.092*	0.513 (5)
C12	1.2301 (5)	0.2685 (3)	0.5664 (2)	0.0559 (17)	0.513 (5)
H12A	1.2546	0.2315	0.5416	0.084*	0.513 (5)
H12B	1.2753	0.2628	0.606	0.084*	0.513 (5)
H12C	1.2731	0.3058	0.5441	0.084*	0.513 (5)
C10A	1.1352 (8)	0.2145 (3)	0.5844 (2)	0.064 (2)	0.487 (5)
H10D	1.0599	0.1811	0.5845	0.095*	0.487 (5)
H10E	1.1845	0.2118	0.6233	0.095*	0.487 (5)
H10F	1.2142	0.2095	0.5496	0.095*	0.487 (5)
C11A	0.9224 (6)	0.2830 (3)	0.6298 (2)	0.0548 (18)	0.487 (5)
H11D	0.8661	0.323	0.6243	0.082*	0.487 (5)
H11E	0.9655	0.2815	0.67	0.082*	0.487 (5)
H11F	0.8515	0.2482	0.6282	0.082*	0.487 (5)
C12A	1.1620 (8)	0.3311 (3)	0.5788 (3)	0.073 (2)	0.487 (5)
H12D	1.2439	0.3274	0.5449	0.11*	0.487 (5)
H12E	1.2084	0.3303	0.6183	0.11*	0.487 (5)
H12F	1.1039	0.3707	0.5736	0.11*	0.487 (5)
C13	1.33304 (18)	0.36231 (9)	0.24341 (8)	0.0213 (4)	
C14	1.4062 (2)	0.29707 (9)	0.24427 (9)	0.0291 (4)	
H14A	1.3699	0.2744	0.2827	0.044*	
H14B	1.519	0.3001	0.2418	0.044*	
H14C	1.377	0.2744	0.2089	0.044*	
C15	1.3798 (2)	0.40187 (9)	0.29508 (8)	0.0252 (4)	
H15A	1.3228	0.4422	0.2947	0.038*	
H15B	1.4912	0.4092	0.2889	0.038*	
H15C	1.3556	0.3797	0.335	0.038*	
C16	1.3752 (2)	0.39646 (11)	0.18157 (9)	0.0333 (5)	
H16A	1.3381	0.3729	0.1483	0.05*	
H16B	1.4879	0.3999	0.1748	0.05*	
H16C	1.3268	0.4386	0.1819	0.05*	
C17	1.0489 (2)	0.24676 (8)	0.13400 (9)	0.0261 (4)	
C18	1.0608 (2)	0.20439 (9)	0.19140 (10)	0.0331 (4)	
H18A	1.1629	0.2084	0.2065	0.05*	
H18B	1.0467	0.1607	0.1811	0.05*	
H18C	0.9804	0.2168	0.2236	0.05*	
C19	1.1709 (3)	0.22733 (10)	0.08315 (10)	0.0392 (5)	
H19A	1.1678	0.2569	0.0476	0.059*	
H19B	1.15	0.185	0.0704	0.059*	
H19C	1.2734	0.2275	0.0986	0.059*	
C20	0.8874 (3)	0.24609 (11)	0.11278 (11)	0.0417 (5)	
H20A	0.8128	0.2625	0.1452	0.063*	
H20B	0.8616	0.2029	0.1045	0.063*	

H20C	0.8834	0.2724	0.075	0.063*
C21	0.9853 (2)	0.45813 (8)	0.11767 (8)	0.0252 (4)
C22	1.1029 (3)	0.44335 (12)	0.06350 (10)	0.0443 (6)
H22A	1.2036	0.4597	0.071	0.066*
H22B	1.0685	0.463	0.0255	0.066*
H22C	1.1123	0.3978	0.0592	0.066*
C23	0.8264 (3)	0.43494 (10)	0.10801 (11)	0.0413 (5)
H23A	0.8332	0.3898	0.1007	0.062*
H23B	0.7875	0.4574	0.0722	0.062*
H23C	0.7557	0.4426	0.1449	0.062*
C24	0.9775 (3)	0.52780 (9)	0.12900 (10)	0.0380 (5)
H24A	0.9036	0.536	0.1648	0.057*
H24B	0.9437	0.5507	0.0924	0.057*
H24C	1.0801	0.5418	0.1371	0.057*
C25	0.9560 (3)	0.48230 (10)	0.33693 (11)	0.0428 (5)
H25A	0.8537	0.4977	0.3535	0.064*
H25B	0.9525	0.4717	0.2936	0.064*
H25C	1.032	0.515	0.3397	0.064*
C26	1.0141 (2)	0.43783 (10)	0.43569 (9)	0.0342 (4)
H26A	0.9861	0.399	0.4602	0.041*
H26B	0.9402	0.4716	0.4499	0.041*
C27	1.1742 (3)	0.45543 (10)	0.44773 (9)	0.0362 (5)
H27A	1.186	0.4508	0.4926	0.043*
H27B	1.2508	0.4268	0.4259	0.043*
C28	1.3538 (4)	0.53529 (15)	0.43686 (13)	0.0652 (8)
H28A	1.3693	0.5298	0.4809	0.098*
H28B	1.3683	0.5794	0.4237	0.098*
H28C	1.4289	0.5087	0.4127	0.098*
C29	0.80317 (19)	0.06784 (9)	0.77367 (10)	0.0276 (4)
C30	0.8774 (2)	0.11637 (10)	0.72867 (10)	0.0333 (4)
H30A	0.8453	0.1102	0.6873	0.05*
H30B	0.9903	0.1118	0.7276	0.05*
H30C	0.8449	0.1585	0.7419	0.05*
C31	0.8533 (2)	0.07277 (10)	0.83835 (10)	0.0327 (4)
H31A	0.8298	0.1153	0.8528	0.049*
H31B	0.9648	0.064	0.8377	0.049*
H31C	0.7975	0.0423	0.8663	0.049*
C32	0.8401 (2)	0.00221 (10)	0.75049 (13)	0.0460 (6)
H32A	0.7955	−0.0289	0.7808	0.069*
H32B	0.9526	−0.0045	0.7447	0.069*
H32C	0.7961	−0.0022	0.711	0.069*
C33	0.4360 (2)	−0.08711 (8)	0.77133 (9)	0.0297 (4)
C34	0.4596 (3)	−0.12696 (11)	0.82988 (12)	0.0496 (6)
H34A	0.5705	−0.1319	0.8346	0.074*
H34B	0.4153	−0.1683	0.8267	0.074*
H34C	0.4081	−0.1061	0.8659	0.074*
C35	0.5228 (3)	−0.11776 (11)	0.71600 (12)	0.0478 (6)
H35A	0.5123	−0.0912	0.6788	0.072*
H35B	0.4797	−0.159	0.7106	0.072*

H35C	0.6325	−0.1229	0.7229	0.072*	
C36	0.2675 (3)	−0.07706 (12)	0.76294 (15)	0.0553 (7)	
H36A	0.2157	−0.057	0.7993	0.083*	
H36B	0.2206	−0.1176	0.7579	0.083*	
H36C	0.256	−0.05	0.7261	0.083*	
C37	0.4894 (3)	0.07508 (11)	0.62279 (10)	0.0473 (6)	
C38	0.631 (3)	0.0626 (8)	0.5691 (7)	0.058 (4)	0.42 (5)
H38A	0.7305	0.0687	0.586	0.087*	0.42 (5)
H38B	0.6208	0.0921	0.534	0.087*	0.42 (5)
H38C	0.6275	0.0195	0.5552	0.087*	0.42 (5)
C38A	0.572 (3)	0.0454 (12)	0.5682 (5)	0.071 (4)	0.58 (5)
H38D	0.6834	0.0451	0.5717	0.107*	0.58 (5)
H38E	0.5484	0.0692	0.5305	0.107*	0.58 (5)
H38F	0.5376	0.0021	0.5661	0.107*	0.58 (5)
C39	0.3213 (4)	0.06326 (14)	0.61343 (13)	0.0683 (9)	
H39A	0.3078	0.0182	0.609	0.102*	
H39B	0.2931	0.0863	0.5761	0.102*	
H39C	0.2547	0.0776	0.6493	0.102*	
C40	0.5144 (3)	0.14403 (11)	0.63386 (12)	0.0513 (6)	
H40A	0.4426	0.1577	0.6685	0.077*	
H40B	0.4954	0.1693	0.5966	0.077*	
H40C	0.6211	0.1494	0.6436	0.077*	
C41	0.19308 (18)	0.24842 (8)	0.85513 (8)	0.0214 (4)	
C42	0.1260 (2)	0.19445 (9)	0.89539 (9)	0.0252 (4)	
H42A	0.1526	0.1548	0.8752	0.038*	
H42B	0.0132	0.1998	0.9014	0.038*	
H42C	0.1688	0.1939	0.9356	0.038*	
C43	0.1372 (2)	0.25078 (9)	0.79080 (9)	0.0282 (4)	
H43A	0.1795	0.2876	0.7674	0.042*	
H43B	0.0239	0.2537	0.7941	0.042*	
H43C	0.1722	0.2126	0.7694	0.042*	
C44	0.1533 (2)	0.31001 (9)	0.88668 (10)	0.0324 (4)	
H44A	0.1898	0.3079	0.9281	0.049*	
H44B	0.0409	0.3173	0.8901	0.049*	
H44C	0.2035	0.3445	0.8622	0.049*	
C45	0.5522 (2)	0.35694 (9)	0.95746 (9)	0.0280 (4)	
C46	0.5132 (2)	0.34058 (11)	1.02538 (9)	0.0392 (5)	
H46A	0.4005	0.3406	1.0346	0.059*	
H46B	0.5573	0.3717	1.0503	0.059*	
H46C	0.5565	0.2988	1.0352	0.059*	
C47	0.7269 (2)	0.35374 (12)	0.94174 (10)	0.0429 (6)	
H47A	0.7667	0.3117	0.9527	0.064*	
H47B	0.7756	0.385	0.9651	0.064*	
H47C	0.7507	0.3625	0.8973	0.064*	
C48	0.4835 (3)	0.42099 (10)	0.94066 (12)	0.0496 (6)	
H48A	0.5034	0.4295	0.896	0.074*	
H48B	0.5313	0.4533	0.963	0.074*	
H48C	0.3717	0.4215	0.9521	0.074*	
C49	0.5261 (2)	0.37284 (9)	0.74822 (9)	0.0291 (4)	

C50	0.6892 (3)	0.39694 (10)	0.74655 (10)	0.0393 (5)
H50A	0.6917	0.4302	0.7764	0.059*
H50B	0.7214	0.4138	0.7049	0.059*
H50C	0.7599	0.3624	0.7573	0.059*
C51	0.5195 (3)	0.31975 (10)	0.70355 (9)	0.0373 (5)
H51A	0.5943	0.2864	0.7134	0.056*
H51B	0.5449	0.3359	0.6611	0.056*
H51C	0.4152	0.3028	0.7074	0.056*
C52	0.4118 (3)	0.42558 (11)	0.73404 (12)	0.0481 (6)
H52A	0.3076	0.4088	0.7353	0.072*
H52B	0.4409	0.4441	0.6928	0.072*
H52C	0.4131	0.4579	0.7649	0.072*
C53	0.4401 (3)	0.04834 (9)	0.93200 (10)	0.0370 (5)
H53A	0.5296	0.0252	0.9466	0.055*
H53B	0.4123	0.0302	0.8939	0.055*
H53C	0.3524	0.0455	0.9637	0.055*
C54	0.5027 (2)	0.14608 (9)	0.97425 (9)	0.0298 (4)
H54A	0.4359	0.1284	1.0097	0.036*
H54B	0.4709	0.1907	0.968	0.036*
C55	0.6677 (2)	0.14282 (9)	0.98987 (9)	0.0306 (4)
H55A	0.7371	0.1549	0.9529	0.037*
H55B	0.6817	0.1726	1.0226	0.037*
C56	0.8646 (3)	0.07441 (11)	1.02153 (13)	0.0474 (6)
H56A	0.9294	0.084	0.9832	0.071*
H56B	0.8864	0.0312	1.0358	0.071*
H56C	0.8872	0.1034	1.0533	0.071*
O1	0.88055 (13)	0.28833 (6)	0.41183 (5)	0.0214 (3)
O2	0.99325 (16)	0.18001 (6)	0.46173 (6)	0.0299 (3)
O3	0.98450 (14)	0.28511 (6)	0.52045 (6)	0.0260 (3)
O4	1.16195 (12)	0.35507 (5)	0.25458 (5)	0.0185 (2)
O5	1.08382 (14)	0.31099 (5)	0.14615 (5)	0.0215 (3)
O6	1.03991 (14)	0.42900 (6)	0.17293 (5)	0.0216 (3)
O7	0.99953 (16)	0.42779 (6)	0.37185 (6)	0.0304 (3)
O8	1.2029 (2)	0.51804 (7)	0.42723 (7)	0.0471 (4)
O9	0.63219 (13)	0.08135 (5)	0.77873 (6)	0.0234 (3)
O10	0.50831 (14)	−0.02842 (5)	0.78013 (6)	0.0230 (3)
O11	0.53121 (16)	0.03569 (6)	0.67500 (6)	0.0294 (3)
O12	0.36414 (12)	0.23727 (5)	0.84763 (5)	0.0183 (2)
O13	0.48026 (13)	0.30947 (5)	0.92475 (5)	0.0213 (3)
O14	0.47807 (14)	0.35165 (6)	0.81096 (6)	0.0244 (3)
O15	0.47810 (15)	0.11296 (6)	0.92004 (6)	0.0272 (3)
O16	0.70647 (16)	0.08111 (6)	1.01049 (7)	0.0341 (3)
Si1	1.01765 (5)	0.25499 (2)	0.45317 (2)	0.01928 (11)
Si2	1.03128 (5)	0.35793 (2)	0.20198 (2)	0.01669 (10)
Si3	0.49386 (5)	0.04145 (2)	0.74897 (2)	0.01813 (10)
Si4	0.50487 (5)	0.28879 (2)	0.85326 (2)	0.01674 (10)
S1	1.21321 (5)	0.28461 (2)	0.40067 (2)	0.02403 (10)
S2	0.83362 (5)	0.33759 (2)	0.257828 (19)	0.02265 (10)
S3	0.30171 (5)	0.09422 (2)	0.77934 (2)	0.02244 (10)

S4	0.69667 (5)	0.233062 (19)	0.82966 (2)	0.02145 (10)
Cr1	1.02010 (3)	0.326594 (12)	0.334825 (12)	0.01619 (7)
Cr2	0.49821 (3)	0.156658 (12)	0.818976 (12)	0.01619 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0125 (8)	0.0450 (11)	0.0223 (9)	0.0009 (7)	0.0012 (7)	0.0060 (8)
C2	0.0218 (9)	0.0451 (12)	0.0305 (10)	0.0097 (8)	0.0011 (8)	−0.0030 (9)
C3	0.0188 (9)	0.0402 (11)	0.0369 (11)	−0.0068 (8)	−0.0025 (8)	0.0043 (9)
C4	0.0215 (10)	0.0783 (17)	0.0277 (11)	−0.0015 (10)	0.0033 (8)	0.0155 (11)
C5	0.0626 (15)	0.0214 (10)	0.0354 (12)	0.0067 (9)	0.0042 (10)	0.0000 (8)
C6	0.0509 (13)	0.0349 (11)	0.0349 (12)	0.0085 (10)	−0.0058 (10)	−0.0119 (9)
C7	0.140 (3)	0.0244 (13)	0.078 (2)	−0.0131 (16)	0.030 (2)	−0.0018 (13)
C8	0.087 (2)	0.0579 (16)	0.0391 (14)	0.0454 (15)	−0.0119 (13)	−0.0023 (12)
C9	0.0329 (10)	0.0413 (11)	0.0146 (9)	0.0028 (8)	−0.0058 (7)	0.0027 (8)
C10	0.102 (5)	0.080 (4)	0.030 (3)	−0.041 (4)	−0.022 (3)	0.026 (3)
C11	0.090 (5)	0.068 (4)	0.029 (2)	0.032 (3)	−0.021 (3)	−0.019 (2)
C12	0.038 (3)	0.101 (5)	0.030 (2)	0.011 (3)	−0.0137 (19)	−0.004 (3)
C10A	0.076 (4)	0.085 (4)	0.030 (3)	0.045 (4)	−0.024 (3)	−0.003 (3)
C11A	0.052 (3)	0.092 (5)	0.017 (2)	0.019 (3)	0.001 (2)	0.002 (2)
C12A	0.088 (5)	0.096 (5)	0.042 (3)	−0.038 (4)	−0.036 (3)	0.004 (3)
C13	0.0110 (8)	0.0328 (10)	0.0203 (9)	−0.0041 (7)	−0.0016 (6)	−0.0017 (7)
C14	0.0159 (8)	0.0375 (11)	0.0343 (10)	0.0020 (7)	−0.0011 (7)	−0.0101 (8)
C15	0.0221 (9)	0.0309 (10)	0.0232 (9)	−0.0077 (7)	−0.0036 (7)	−0.0019 (7)
C16	0.0210 (9)	0.0569 (13)	0.0220 (10)	−0.0117 (9)	−0.0003 (7)	0.0033 (9)
C17	0.0322 (10)	0.0198 (9)	0.0272 (10)	−0.0063 (7)	−0.0044 (8)	−0.0051 (7)
C18	0.0373 (11)	0.0239 (10)	0.0374 (11)	−0.0039 (8)	0.0003 (9)	0.0034 (8)
C19	0.0539 (13)	0.0293 (11)	0.0333 (11)	−0.0049 (9)	0.0073 (10)	−0.0116 (9)
C20	0.0429 (12)	0.0384 (12)	0.0479 (13)	−0.0085 (10)	−0.0198 (10)	−0.0124 (10)
C21	0.0294 (9)	0.0238 (9)	0.0219 (9)	0.0032 (7)	−0.0045 (7)	0.0053 (7)
C22	0.0558 (14)	0.0486 (13)	0.0249 (11)	0.0208 (11)	0.0037 (10)	0.0104 (9)
C23	0.0420 (12)	0.0380 (12)	0.0467 (13)	−0.0044 (9)	−0.0235 (10)	0.0115 (10)
C24	0.0496 (13)	0.0259 (10)	0.0384 (12)	0.0018 (9)	−0.0068 (10)	0.0042 (9)
C25	0.0599 (15)	0.0271 (11)	0.0425 (13)	0.0091 (10)	−0.0138 (11)	−0.0014 (9)
C26	0.0456 (12)	0.0309 (10)	0.0253 (10)	0.0034 (9)	0.0026 (9)	−0.0088 (8)
C27	0.0518 (13)	0.0317 (11)	0.0254 (10)	0.0045 (9)	−0.0036 (9)	−0.0088 (8)
C28	0.080 (2)	0.076 (2)	0.0418 (15)	−0.0345 (16)	−0.0110 (13)	−0.0041 (13)
C29	0.0114 (8)	0.0266 (9)	0.0457 (12)	0.0034 (7)	−0.0033 (7)	−0.0132 (8)
C30	0.0174 (9)	0.0423 (12)	0.0400 (11)	0.0005 (8)	0.0026 (8)	−0.0123 (9)
C31	0.0201 (9)	0.0324 (10)	0.0464 (12)	0.0046 (8)	−0.0099 (8)	−0.0016 (9)
C32	0.0194 (10)	0.0354 (12)	0.0851 (18)	0.0078 (8)	−0.0079 (10)	−0.0271 (12)
C33	0.0334 (10)	0.0185 (9)	0.0368 (11)	−0.0073 (7)	0.0022 (8)	−0.0043 (8)
C34	0.0620 (16)	0.0309 (12)	0.0532 (15)	−0.0014 (11)	0.0054 (12)	0.0081 (10)
C35	0.0631 (16)	0.0307 (11)	0.0495 (14)	−0.0046 (10)	0.0020 (12)	−0.0135 (10)
C36	0.0370 (13)	0.0374 (13)	0.093 (2)	−0.0127 (10)	−0.0111 (13)	−0.0021 (13)
C37	0.0700 (16)	0.0472 (13)	0.0224 (10)	0.0285 (12)	−0.0029 (10)	0.0050 (9)
C38	0.091 (10)	0.046 (6)	0.028 (4)	0.024 (6)	0.028 (6)	0.005 (4)

C38A	0.083 (9)	0.094 (8)	0.028 (3)	0.045 (6)	0.015 (4)	0.027 (4)
C39	0.098 (2)	0.0595 (17)	0.0553 (17)	0.0180 (16)	−0.0532 (17)	−0.0090 (13)
C40	0.0541 (15)	0.0444 (14)	0.0511 (15)	0.0132 (11)	0.0041 (11)	0.0219 (11)
C41	0.0107 (8)	0.0222 (9)	0.0313 (10)	0.0006 (6)	0.0003 (7)	−0.0044 (7)
C42	0.0180 (8)	0.0286 (9)	0.0284 (10)	−0.0025 (7)	0.0037 (7)	−0.0048 (8)
C43	0.0179 (9)	0.0302 (10)	0.0367 (11)	0.0015 (7)	−0.0056 (7)	0.0029 (8)
C44	0.0185 (9)	0.0252 (10)	0.0528 (13)	0.0016 (7)	0.0032 (8)	−0.0110 (9)
C45	0.0272 (9)	0.0302 (10)	0.0275 (10)	−0.0094 (8)	0.0015 (7)	−0.0139 (8)
C46	0.0341 (11)	0.0573 (14)	0.0271 (11)	−0.0136 (10)	0.0022 (8)	−0.0164 (10)
C47	0.0307 (11)	0.0610 (15)	0.0379 (12)	−0.0209 (10)	0.0060 (9)	−0.0223 (11)
C48	0.0702 (17)	0.0276 (11)	0.0519 (15)	−0.0037 (11)	−0.0034 (12)	−0.0173 (10)
C49	0.0349 (10)	0.0264 (10)	0.0242 (10)	−0.0029 (8)	0.0038 (8)	0.0072 (8)
C50	0.0428 (12)	0.0351 (11)	0.0382 (12)	−0.0128 (9)	0.0082 (9)	0.0014 (9)
C51	0.0447 (12)	0.0409 (12)	0.0261 (10)	−0.0085 (9)	0.0006 (9)	−0.0004 (9)
C52	0.0536 (14)	0.0441 (13)	0.0429 (13)	0.0095 (11)	0.0035 (11)	0.0192 (10)
C53	0.0533 (13)	0.0257 (10)	0.0332 (11)	−0.0123 (9)	−0.0101 (9)	0.0057 (8)
C54	0.0393 (11)	0.0264 (10)	0.0238 (10)	0.0003 (8)	−0.0039 (8)	−0.0014 (8)
C55	0.0409 (11)	0.0256 (10)	0.0266 (10)	−0.0053 (8)	−0.0088 (8)	−0.0018 (8)
C56	0.0401 (12)	0.0421 (13)	0.0629 (16)	0.0045 (10)	−0.0190 (11)	−0.0080 (11)
O1	0.0136 (6)	0.0318 (7)	0.0181 (6)	0.0003 (5)	−0.0008 (4)	0.0050 (5)
O2	0.0395 (8)	0.0250 (7)	0.0234 (7)	0.0021 (6)	0.0039 (6)	0.0031 (5)
O3	0.0261 (6)	0.0348 (7)	0.0171 (6)	0.0080 (5)	−0.0043 (5)	−0.0010 (5)
O4	0.0129 (5)	0.0273 (6)	0.0151 (6)	−0.0023 (4)	−0.0007 (4)	0.0008 (5)
O5	0.0265 (6)	0.0201 (6)	0.0181 (6)	−0.0059 (5)	−0.0013 (5)	−0.0017 (5)
O6	0.0243 (6)	0.0228 (6)	0.0180 (6)	−0.0007 (5)	−0.0036 (5)	0.0011 (5)
O7	0.0410 (8)	0.0251 (7)	0.0252 (7)	0.0049 (6)	−0.0037 (6)	−0.0041 (5)
O8	0.0686 (11)	0.0389 (9)	0.0363 (9)	−0.0143 (8)	−0.0139 (8)	−0.0025 (7)
O9	0.0126 (6)	0.0205 (6)	0.0381 (7)	0.0016 (5)	−0.0030 (5)	−0.0109 (5)
O10	0.0230 (6)	0.0176 (6)	0.0290 (7)	−0.0011 (5)	−0.0046 (5)	−0.0023 (5)
O11	0.0388 (8)	0.0280 (7)	0.0209 (7)	0.0130 (6)	−0.0034 (5)	−0.0018 (5)
O12	0.0121 (5)	0.0172 (6)	0.0256 (6)	0.0003 (4)	−0.0008 (4)	−0.0040 (5)
O13	0.0213 (6)	0.0211 (6)	0.0217 (6)	−0.0046 (5)	0.0003 (5)	−0.0057 (5)
O14	0.0278 (7)	0.0197 (6)	0.0242 (7)	0.0004 (5)	0.0041 (5)	0.0011 (5)
O15	0.0363 (7)	0.0231 (6)	0.0231 (7)	−0.0059 (5)	−0.0076 (5)	0.0021 (5)
O16	0.0352 (8)	0.0284 (7)	0.0396 (8)	−0.0003 (6)	−0.0098 (6)	0.0005 (6)
Si1	0.0178 (2)	0.0244 (2)	0.0153 (2)	0.00282 (18)	−0.00170 (17)	0.00259 (18)
Si2	0.0157 (2)	0.0206 (2)	0.0140 (2)	−0.00209 (17)	−0.00261 (17)	0.00074 (17)
Si3	0.0157 (2)	0.0168 (2)	0.0225 (2)	0.00117 (17)	−0.00403 (17)	−0.00487 (18)
Si4	0.0150 (2)	0.0148 (2)	0.0202 (2)	−0.00163 (16)	0.00031 (17)	−0.00285 (17)
S1	0.0148 (2)	0.0348 (2)	0.0221 (2)	0.00182 (17)	−0.00275 (16)	0.00556 (18)
S2	0.0143 (2)	0.0361 (2)	0.0176 (2)	−0.00300 (17)	−0.00285 (15)	0.00343 (17)
S3	0.0140 (2)	0.0221 (2)	0.0323 (2)	0.00120 (16)	−0.00492 (17)	−0.01009 (18)
S4	0.01327 (19)	0.0193 (2)	0.0319 (2)	−0.00123 (15)	0.00013 (16)	−0.00643 (17)
Cr1	0.01336 (13)	0.02138 (14)	0.01365 (14)	0.00070 (10)	−0.00128 (10)	0.00082 (10)
Cr2	0.01234 (13)	0.01478 (13)	0.02179 (15)	−0.00002 (10)	−0.00202 (10)	−0.00415 (10)

Geometric parameters (Å, °)

C1—O1	1.497 (2)	C31—H31C	0.98

C1—C3	1.514 (3)	C32—H32A	0.98
C1—C2	1.517 (3)	C32—H32B	0.98
C1—C4	1.524 (3)	C32—H32C	0.98
C2—H2A	0.98	C33—O10	1.443 (2)
C2—H2B	0.98	C33—C36	1.499 (3)
C2—H2C	0.98	C33—C35	1.519 (3)
C3—H3A	0.98	C33—C34	1.529 (3)
C3—H3B	0.98	C34—H34A	0.98
C3—H3C	0.98	C34—H34B	0.98
C4—H4A	0.98	C34—H34C	0.98
C4—H4B	0.98	C35—H35A	0.98
C4—H4C	0.98	C35—H35B	0.98
C5—O2	1.460 (2)	C35—H35C	0.98
C5—C8	1.505 (4)	C36—H36A	0.98
C5—C6	1.522 (3)	C36—H36B	0.98
C5—C7	1.525 (4)	C36—H36C	0.98
C6—H6A	0.98	C37—O11	1.453 (2)
C6—H6B	0.98	C37—C38A	1.482 (12)
C6—H6C	0.98	C37—C39	1.521 (4)
C7—H7A	0.98	C37—C40	1.523 (4)
C7—H7B	0.98	C37—C38	1.64 (2)
C7—H7C	0.98	C38—H38A	0.98
C8—H8A	0.98	C38—H38B	0.98
C8—H8B	0.98	C38—H38C	0.98
C8—H8C	0.98	C38A—H38D	0.98
C9—O3	1.445 (2)	C38A—H38E	0.98
C9—C10	1.490 (5)	C38A—H38F	0.98
C9—C10A	1.497 (6)	C39—H39A	0.98
C9—C11	1.500 (5)	C39—H39B	0.98
C9—C12A	1.506 (6)	C39—H39C	0.98
C9—C12	1.532 (5)	C40—H40A	0.98
C9—C11A	1.534 (5)	C40—H40B	0.98
C10—H10A	0.98	C40—H40C	0.98
C10—H10B	0.98	C41—O12	1.4923 (19)
C10—H10C	0.98	C41—C42	1.515 (3)
C11—H11A	0.98	C41—C43	1.520 (3)
C11—H11B	0.98	C41—C44	1.521 (2)
C11—H11C	0.98	C42—H42A	0.98
C12—H12A	0.98	C42—H42B	0.98
C12—H12B	0.98	C42—H42C	0.98
C12—H12C	0.98	C43—H43A	0.98
C10A—H10D	0.98	C43—H43B	0.98
C10A—H10E	0.98	C43—H43C	0.98
C10A—H10F	0.98	C44—H44A	0.98
C11A—H11D	0.98	C44—H44B	0.98
C11A—H11E	0.98	C44—H44C	0.98
C11A—H11F	0.98	C45—O13	1.446 (2)
C12A—H12D	0.98	C45—C46	1.514 (3)
C12A—H12E	0.98	C45—C48	1.519 (3)

C12A—H12F	0.98	C45—C47	1.524 (3)
C13—O4	1.4942 (19)	C46—H46A	0.98
C13—C14	1.513 (3)	C46—H46B	0.98
C13—C15	1.521 (2)	C46—H46C	0.98
C13—C16	1.524 (3)	C47—H47A	0.98
C14—H14A	0.98	C47—H47B	0.98
C14—H14B	0.98	C47—H47C	0.98
C14—H14C	0.98	C48—H48A	0.98
C15—H15A	0.98	C48—H48B	0.98
C15—H15B	0.98	C48—H48C	0.98
C15—H15C	0.98	C49—O14	1.448 (2)
C16—H16A	0.98	C49—C50	1.517 (3)
C16—H16B	0.98	C49—C52	1.520 (3)
C16—H16C	0.98	C49—C51	1.524 (3)
C17—O5	1.450 (2)	C50—H50A	0.98
C17—C20	1.517 (3)	C50—H50B	0.98
C17—C19	1.519 (3)	C50—H50C	0.98
C17—C18	1.522 (3)	C51—H51A	0.98
C18—H18A	0.98	C51—H51B	0.98
C18—H18B	0.98	C51—H51C	0.98
C18—H18C	0.98	C52—H52A	0.98
C19—H19A	0.98	C52—H52B	0.98
C19—H19B	0.98	C52—H52C	0.98
C19—H19C	0.98	C53—O15	1.434 (2)
C20—H20A	0.98	C53—H53A	0.98
C20—H20B	0.98	C53—H53B	0.98
C20—H20C	0.98	C53—H53C	0.98
C21—O6	1.443 (2)	C54—O15	1.432 (2)
C21—C24	1.513 (3)	C54—C55	1.501 (3)
C21—C23	1.514 (3)	C54—H54A	0.99
C21—C22	1.522 (3)	C54—H54B	0.99
C22—H22A	0.98	C55—O16	1.415 (2)
C22—H22B	0.98	C55—H55A	0.99
C22—H22C	0.98	C55—H55B	0.99
C23—H23A	0.98	C56—O16	1.417 (3)
C23—H23B	0.98	C56—H56A	0.98
C23—H23C	0.98	C56—H56B	0.98
C24—H24A	0.98	C56—H56C	0.98
C24—H24B	0.98	O1—Si1	1.6817 (12)
C24—H24C	0.98	O1—Cr1	2.1248 (12)
C25—O7	1.425 (2)	O2—Si1	1.6198 (14)
C25—H25A	0.98	O3—Si1	1.6174 (13)
C25—H25B	0.98	O4—Si2	1.6809 (11)
C25—H25C	0.98	O4—Cr1	2.1201 (11)
C26—O7	1.429 (2)	O5—Si2	1.6267 (12)
C26—C27	1.498 (3)	O6—Si2	1.6201 (12)
C26—H26A	0.99	O7—Cr1	2.3273 (13)
C26—H26B	0.99	O9—Si3	1.6810 (12)
C27—O8	1.413 (3)	O9—Cr2	2.1234 (12)

C27—H27A	0.99	O10—Si3	1.6191 (13)
C27—H27B	0.99	O11—Si3	1.6190 (13)
C28—O8	1.406 (3)	O12—Si4	1.6816 (11)
C28—H28A	0.98	O12—Cr2	2.1283 (11)
C28—H28B	0.98	O13—Si4	1.6246 (12)
C28—H28C	0.98	O14—Si4	1.6195 (13)
C29—O9	1.4988 (19)	O15—Cr2	2.3463 (13)
C29—C30	1.513 (3)	Si1—S1	2.0577 (6)
C29—C31	1.517 (3)	Si2—S2	2.0558 (6)
C29—C32	1.521 (3)	Si3—S3	2.0570 (6)
C30—H30A	0.98	Si4—S4	2.0553 (6)
C30—H30B	0.98	S1—Cr1	2.4323 (5)
C30—H30C	0.98	S2—Cr1	2.4332 (5)
C31—H31A	0.98	S3—Cr2	2.4308 (5)
C31—H31B	0.98	S4—Cr2	2.4365 (5)
O1—C1—C3	107.83 (14)	C35—C33—C34	109.37 (19)
O1—C1—C2	105.77 (15)	C33—C34—H34A	109.5
C3—C1—C2	112.57 (16)	C33—C34—H34B	109.5
O1—C1—C4	110.98 (14)	H34A—C34—H34B	109.5
C3—C1—C4	109.83 (17)	C33—C34—H34C	109.5
C2—C1—C4	109.79 (17)	H34A—C34—H34C	109.5
C1—C2—H2A	109.5	H34B—C34—H34C	109.5
C1—C2—H2B	109.5	C33—C35—H35A	109.5
H2A—C2—H2B	109.5	C33—C35—H35B	109.5
C1—C2—H2C	109.5	H35A—C35—H35B	109.5
H2A—C2—H2C	109.5	C33—C35—H35C	109.5
H2B—C2—H2C	109.5	H35A—C35—H35C	109.5
C1—C3—H3A	109.5	H35B—C35—H35C	109.5
C1—C3—H3B	109.5	C33—C36—H36A	109.5
H3A—C3—H3B	109.5	C33—C36—H36B	109.5
C1—C3—H3C	109.5	H36A—C36—H36B	109.5
H3A—C3—H3C	109.5	C33—C36—H36C	109.5
H3B—C3—H3C	109.5	H36A—C36—H36C	109.5
C1—C4—H4A	109.5	H36B—C36—H36C	109.5
C1—C4—H4B	109.5	O11—C37—C38A	104.4 (5)
H4A—C4—H4B	109.5	O11—C37—C39	107.9 (2)
C1—C4—H4C	109.5	C38A—C37—C39	101.7 (12)
H4A—C4—H4C	109.5	O11—C37—C40	110.83 (19)
H4B—C4—H4C	109.5	C38A—C37—C40	119.6 (12)
O2—C5—C8	108.47 (19)	C39—C37—C40	111.5 (2)
O2—C5—C6	111.25 (16)	O11—C37—C38	103.9 (6)
C8—C5—C6	110.2 (2)	C39—C37—C38	122.6 (10)
O2—C5—C7	104.55 (19)	C40—C37—C38	99.7 (9)
C8—C5—C7	112.1 (2)	C37—C38—H38A	109.5
C6—C5—C7	110.2 (2)	C37—C38—H38B	109.5
C5—C6—H6A	109.5	C37—C38—H38C	109.5
C5—C6—H6B	109.5	C37—C38A—H38D	109.5
H6A—C6—H6B	109.5	C37—C38A—H38E	109.5
C5—C6—H6C	109.5	H38D—C38A—H38E	109.5

H6A—C6—H6C	109.5	C37—C38A—H38F	109.5
H6B—C6—H6C	109.5	H38D—C38A—H38F	109.5
C5—C7—H7A	109.5	H38E—C38A—H38F	109.5
C5—C7—H7B	109.5	C37—C39—H39A	109.5
H7A—C7—H7B	109.5	C37—C39—H39B	109.5
C5—C7—H7C	109.5	H39A—C39—H39B	109.5
H7A—C7—H7C	109.5	C37—C39—H39C	109.5
H7B—C7—H7C	109.5	H39A—C39—H39C	109.5
C5—C8—H8A	109.5	H39B—C39—H39C	109.5
C5—C8—H8B	109.5	C37—C40—H40A	109.5
H8A—C8—H8B	109.5	C37—C40—H40B	109.5
C5—C8—H8C	109.5	H40A—C40—H40B	109.5
H8A—C8—H8C	109.5	C37—C40—H40C	109.5
H8B—C8—H8C	109.5	H40A—C40—H40C	109.5
O3—C9—C10	106.9 (2)	H40B—C40—H40C	109.5
O3—C9—C10A	112.4 (2)	O12—C41—C42	106.75 (13)
C10—C9—C10A	54.4 (4)	O12—C41—C43	107.17 (13)
O3—C9—C11	106.4 (2)	C42—C41—C43	112.61 (15)
C10—C9—C11	112.5 (4)	O12—C41—C44	110.51 (13)
C10A—C9—C11	141.2 (3)	C42—C41—C44	109.54 (15)
O3—C9—C12A	105.0 (3)	C43—C41—C44	110.19 (16)
C10—C9—C12A	148.1 (3)	C41—C42—H42A	109.5
C10A—C9—C12A	112.8 (4)	C41—C42—H42B	109.5
C11—C9—C12A	56.4 (4)	H42A—C42—H42B	109.5
O3—C9—C12	110.6 (2)	C41—C42—H42C	109.5
C10—C9—C12	110.2 (4)	H42A—C42—H42C	109.5
C10A—C9—C12	57.5 (4)	H42B—C42—H42C	109.5
C11—C9—C12	110.1 (4)	C41—C43—H43A	109.5
C12A—C9—C12	57.8 (4)	C41—C43—H43B	109.5
O3—C9—C11A	106.6 (2)	H43A—C43—H43B	109.5
C10—C9—C11A	59.3 (4)	C41—C43—H43C	109.5
C10A—C9—C11A	109.7 (4)	H43A—C43—H43C	109.5
C11—C9—C11A	55.6 (4)	H43B—C43—H43C	109.5
C12A—C9—C11A	110.3 (4)	C41—C44—H44A	109.5
C12—C9—C11A	142.8 (3)	C41—C44—H44B	109.5
C9—C10—H10A	109.5	H44A—C44—H44B	109.5
C9—C10—H10B	109.5	C41—C44—H44C	109.5
C9—C10—H10C	109.5	H44A—C44—H44C	109.5
C9—C11—H11A	109.5	H44B—C44—H44C	109.5
C9—C11—H11B	109.5	O13—C45—C46	105.33 (15)
C9—C11—H11C	109.5	O13—C45—C48	109.15 (16)
C9—C12—H12A	109.5	C46—C45—C48	110.58 (18)
C9—C12—H12B	109.5	O13—C45—C47	109.67 (15)
C9—C12—H12C	109.5	C46—C45—C47	110.07 (18)
C9—C10A—H10D	109.5	C48—C45—C47	111.82 (19)
C9—C10A—H10E	109.5	C45—C46—H46A	109.5
H10D—C10A—H10E	109.5	C45—C46—H46B	109.5
C9—C10A—H10F	109.5	H46A—C46—H46B	109.5
H10D—C10A—H10F	109.5	C45—C46—H46C	109.5

H10E—C10A—H10F	109.5	H46A—C46—H46C	109.5
C9—C11A—H11D	109.5	H46B—C46—H46C	109.5
C9—C11A—H11E	109.5	C45—C47—H47A	109.5
H11D—C11A—H11E	109.5	C45—C47—H47B	109.5
C9—C11A—H11F	109.5	H47A—C47—H47B	109.5
H11D—C11A—H11F	109.5	C45—C47—H47C	109.5
H11E—C11A—H11F	109.5	H47A—C47—H47C	109.5
C9—C12A—H12D	109.5	H47B—C47—H47C	109.5
C9—C12A—H12E	109.5	C45—C48—H48A	109.5
H12D—C12A—H12E	109.5	C45—C48—H48B	109.5
C9—C12A—H12F	109.5	H48A—C48—H48B	109.5
H12D—C12A—H12F	109.5	C45—C48—H48C	109.5
H12E—C12A—H12F	109.5	H48A—C48—H48C	109.5
O4—C13—C14	107.23 (13)	H48B—C48—H48C	109.5
O4—C13—C15	106.37 (13)	O14—C49—C50	108.34 (16)
C14—C13—C15	112.70 (15)	O14—C49—C52	104.82 (16)
O4—C13—C16	110.83 (13)	C50—C49—C52	111.11 (18)
C14—C13—C16	110.65 (16)	O14—C49—C51	110.86 (15)
C15—C13—C16	108.98 (15)	C50—C49—C51	110.69 (17)
C13—C14—H14A	109.5	C52—C49—C51	110.85 (19)
C13—C14—H14B	109.5	C49—C50—H50A	109.5
H14A—C14—H14B	109.5	C49—C50—H50B	109.5
C13—C14—H14C	109.5	H50A—C50—H50B	109.5
H14A—C14—H14C	109.5	C49—C50—H50C	109.5
H14B—C14—H14C	109.5	H50A—C50—H50C	109.5
C13—C15—H15A	109.5	H50B—C50—H50C	109.5
C13—C15—H15B	109.5	C49—C51—H51A	109.5
H15A—C15—H15B	109.5	C49—C51—H51B	109.5
C13—C15—H15C	109.5	H51A—C51—H51B	109.5
H15A—C15—H15C	109.5	C49—C51—H51C	109.5
H15B—C15—H15C	109.5	H51A—C51—H51C	109.5
C13—C16—H16A	109.5	H51B—C51—H51C	109.5
C13—C16—H16B	109.5	C49—C52—H52A	109.5
H16A—C16—H16B	109.5	C49—C52—H52B	109.5
C13—C16—H16C	109.5	H52A—C52—H52B	109.5
H16A—C16—H16C	109.5	C49—C52—H52C	109.5
H16B—C16—H16C	109.5	H52A—C52—H52C	109.5
O5—C17—C20	108.33 (15)	H52B—C52—H52C	109.5
O5—C17—C19	104.93 (15)	O15—C53—H53A	109.5
C20—C17—C19	111.59 (17)	O15—C53—H53B	109.5
O5—C17—C18	110.92 (14)	H53A—C53—H53B	109.5
C20—C17—C18	110.82 (17)	O15—C53—H53C	109.5
C19—C17—C18	110.11 (17)	H53A—C53—H53C	109.5
C17—C18—H18A	109.5	H53B—C53—H53C	109.5
C17—C18—H18B	109.5	O15—C54—C55	113.36 (16)
H18A—C18—H18B	109.5	O15—C54—H54A	108.9
C17—C18—H18C	109.5	C55—C54—H54A	108.9
H18A—C18—H18C	109.5	O15—C54—H54B	108.9
H18B—C18—H18C	109.5	C55—C54—H54B	108.9

C17—C19—H19A	109.5	H54A—C54—H54B	107.7
C17—C19—H19B	109.5	O16—C55—C54	109.88 (15)
H19A—C19—H19B	109.5	O16—C55—H55A	109.7
C17—C19—H19C	109.5	C54—C55—H55A	109.7
H19A—C19—H19C	109.5	O16—C55—H55B	109.7
H19B—C19—H19C	109.5	C54—C55—H55B	109.7
C17—C20—H20A	109.5	H55A—C55—H55B	108.2
C17—C20—H20B	109.5	O16—C56—H56A	109.5
H20A—C20—H20B	109.5	O16—C56—H56B	109.5
C17—C20—H20C	109.5	H56A—C56—H56B	109.5
H20A—C20—H20C	109.5	O16—C56—H56C	109.5
H20B—C20—H20C	109.5	H56A—C56—H56C	109.5
O6—C21—C24	105.20 (15)	H56B—C56—H56C	109.5
O6—C21—C23	110.35 (15)	C1—O1—Si1	128.26 (10)
C24—C21—C23	110.33 (17)	C1—O1—Cr1	131.03 (10)
O6—C21—C22	108.07 (15)	Si1—O1—Cr1	100.45 (6)
C24—C21—C22	110.91 (18)	C5—O2—Si1	132.53 (12)
C23—C21—C22	111.75 (18)	C9—O3—Si1	134.27 (12)
C21—C22—H22A	109.5	C13—O4—Si2	127.75 (10)
C21—C22—H22B	109.5	C13—O4—Cr1	131.44 (9)
H22A—C22—H22B	109.5	Si2—O4—Cr1	100.32 (5)
C21—C22—H22C	109.5	C17—O5—Si2	134.02 (11)
H22A—C22—H22C	109.5	C21—O6—Si2	132.50 (11)
H22B—C22—H22C	109.5	C25—O7—C26	114.72 (15)
C21—C23—H23A	109.5	C25—O7—Cr1	124.82 (12)
C21—C23—H23B	109.5	C26—O7—Cr1	120.11 (11)
H23A—C23—H23B	109.5	C28—O8—C27	111.6 (2)
C21—C23—H23C	109.5	C29—O9—Si3	128.18 (10)
H23A—C23—H23C	109.5	C29—O9—Cr2	131.13 (10)
H23B—C23—H23C	109.5	Si3—O9—Cr2	100.59 (5)
C21—C24—H24A	109.5	C33—O10—Si3	133.75 (12)
C21—C24—H24B	109.5	C37—O11—Si3	132.40 (12)
H24A—C24—H24B	109.5	C41—O12—Si4	128.49 (10)
C21—C24—H24C	109.5	C41—O12—Cr2	130.72 (9)
H24A—C24—H24C	109.5	Si4—O12—Cr2	100.56 (5)
H24B—C24—H24C	109.5	C45—O13—Si4	131.78 (11)
O7—C25—H25A	109.5	C49—O14—Si4	135.87 (11)
O7—C25—H25B	109.5	C54—O15—C53	114.05 (14)
H25A—C25—H25B	109.5	C54—O15—Cr2	124.96 (11)
O7—C25—H25C	109.5	C53—O15—Cr2	120.99 (11)
H25A—C25—H25C	109.5	C55—O16—C56	112.09 (16)
H25B—C25—H25C	109.5	O3—Si1—O2	107.82 (7)
O7—C26—C27	112.82 (17)	O3—Si1—O1	104.05 (6)
O7—C26—H26A	109	O2—Si1—O1	110.29 (7)
C27—C26—H26A	109	O3—Si1—S1	116.03 (5)
O7—C26—H26B	109	O2—Si1—S1	117.46 (5)
C27—C26—H26B	109	O1—Si1—S1	100.01 (5)
H26A—C26—H26B	107.8	O6—Si2—O5	107.19 (6)
O8—C27—C26	110.52 (18)	O6—Si2—O4	104.26 (6)

O8—C27—H27A	109.5	O5—Si2—O4	110.56 (6)
C26—C27—H27A	109.5	O6—Si2—S2	115.59 (5)
O8—C27—H27B	109.5	O5—Si2—S2	117.87 (5)
C26—C27—H27B	109.5	O4—Si2—S2	100.31 (4)
H27A—C27—H27B	108.1	O11—Si3—O10	107.53 (7)
O8—C28—H28A	109.5	O11—Si3—O9	110.74 (7)
O8—C28—H28B	109.5	O10—Si3—O9	104.01 (6)
H28A—C28—H28B	109.5	O11—Si3—S3	117.35 (5)
O8—C28—H28C	109.5	O10—Si3—S3	116.14 (5)
H28A—C28—H28C	109.5	O9—Si3—S3	99.97 (5)
H28B—C28—H28C	109.5	O14—Si4—O13	106.57 (6)
O9—C29—C30	107.24 (15)	O14—Si4—O12	111.02 (6)
O9—C29—C31	106.15 (14)	O13—Si4—O12	103.98 (6)
C30—C29—C31	112.43 (16)	O14—Si4—S4	117.77 (5)
O9—C29—C32	110.89 (14)	O13—Si4—S4	116.30 (5)
C30—C29—C32	110.10 (18)	O12—Si4—S4	100.19 (4)
C31—C29—C32	109.95 (18)	Si1—S1—Cr1	81.32 (2)
C29—C30—H30A	109.5	Si2—S2—Cr1	81.086 (19)
C29—C30—H30B	109.5	Si3—S3—Cr2	81.412 (19)
H30A—C30—H30B	109.5	Si4—S4—Cr2	81.438 (19)
C29—C30—H30C	109.5	O4—Cr1—O1	173.99 (5)
H30A—C30—H30C	109.5	O4—Cr1—O7	92.86 (5)
H30B—C30—H30C	109.5	O1—Cr1—O7	93.15 (5)
C29—C31—H31A	109.5	O4—Cr1—S1	101.08 (3)
C29—C31—H31B	109.5	O1—Cr1—S1	77.90 (3)
H31A—C31—H31B	109.5	O7—Cr1—S1	97.94 (4)
C29—C31—H31C	109.5	O4—Cr1—S2	78.11 (3)
H31A—C31—H31C	109.5	O1—Cr1—S2	101.12 (3)
H31B—C31—H31C	109.5	O7—Cr1—S2	98.87 (4)
C29—C32—H32A	109.5	S1—Cr1—S2	163.19 (2)
C29—C32—H32B	109.5	O9—Cr2—O12	172.66 (5)
H32A—C32—H32B	109.5	O9—Cr2—O15	95.83 (5)
C29—C32—H32C	109.5	O12—Cr2—O15	91.50 (5)
H32A—C32—H32C	109.5	O9—Cr2—S3	77.90 (3)
H32B—C32—H32C	109.5	O12—Cr2—S3	100.81 (3)
O10—C33—C36	111.03 (16)	O15—Cr2—S3	97.17 (3)
O10—C33—C35	108.01 (16)	O9—Cr2—S4	101.37 (3)
C36—C33—C35	111.9 (2)	O12—Cr2—S4	77.80 (3)
O10—C33—C34	104.92 (16)	O15—Cr2—S4	98.97 (3)
C36—C33—C34	111.35 (19)	S3—Cr2—S4	163.82 (2)

Fig. 1

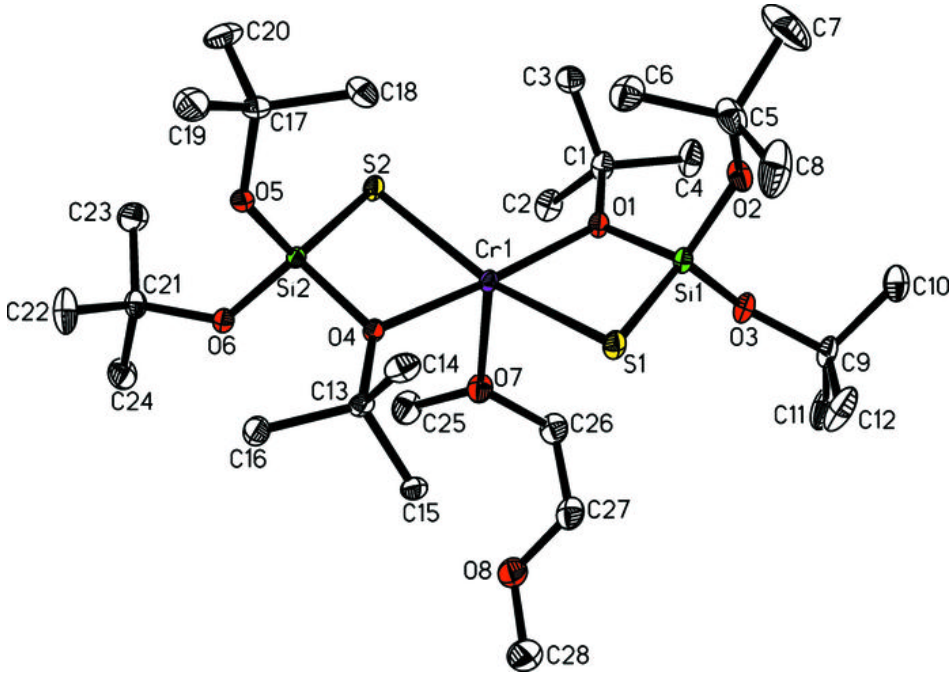
C20
C18
C19
C17
S2
O5
C23
C21
C22
O6
Si2
O4
C24
C14
C13
C16
C15
C25
O7
Cr1
C26
C27
O8
C28
C3
C6
C7
C5
C1
C8
C4
C2
O1
O2
Si1
C10
O3
S1
C9
C11
C12

Fig. 2