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Tris(ethylxanthato-κ^2S,S')(1,10-phenanthroline)bismuth(III)

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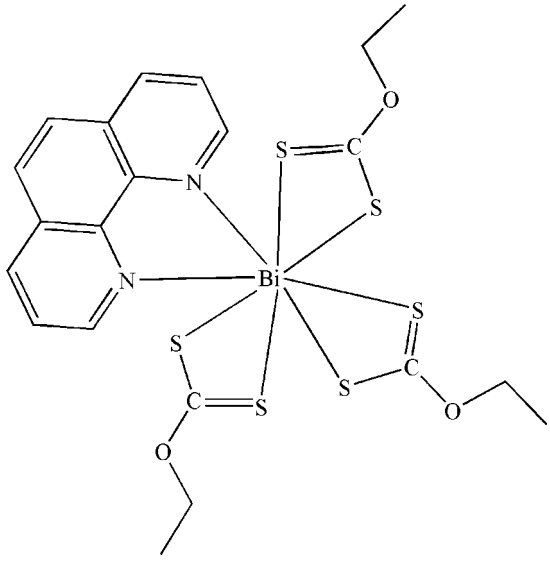
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.028 Å; R factor = 0.068; wR factor = 0.191; data-to-parameter ratio = 15.8.

The title compound, $[Bi(C_3H_5OS_2)_3(C_{12}H_8N_2)]$ [systematic name: tris(ethoxymethanedithioato-κ^2S,S')(1,10-phenanthroline)bismuth(III)], is monomeric, with the Bi atom chelated by the S atoms of three ethylxanthate ligands and the N atoms of 1,10-phenanthroline. The central Bi^{III} atom is eight-coordinate and adopts a distorted capped-pentagonal–bipyramidal geometry. In the crystal structure, weak C—H···S interactions and a close S···S contact stabilize the structure [S···S = 3.509 (3) Å].

Related literature

For uses of Bi^{III} complexes, see: Sun *et al.* (1997) and Baxter (1992). For related Bi^{III} compounds with xanthate ligands, see, for example, Snow & Tiekink (1987) and Hoskins *et al.* (1985), and with phenanthroline ligands, see, for example, Li *et al.* (2005).



Experimental

Crystal data

$[Bi(C_3H_5OS_2)_3(C_{12}H_8N_2)]$
M_r = 752.75
Triclinic, $P\overline{1}$
a = 10.7569 (16) Å
b = 11.1985 (17) Å
c = 11.2494 (17) Å
α = 96.306 (2)°
β = 91.127 (2)°
γ = 91.737 (2)°
V = 1345.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 7.04 mm^{-1}
T = 298 (2) K
0.19 × 0.18 × 0.18 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.348, T_{max} = 0.364
(expected range = 0.269–0.282)
7132 measured reflections
4698 independent reflections
3872 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.191
S = 1.04
4698 reflections
298 parameters
551 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.99 e Å^{-3}
$\Delta\rho_{min}$ = −3.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···S4^{i}	0.97	2.78	3.660 (19)	152
C5—H5B···S3^{ii}	0.97	2.90	3.851 (17)	167
C20—H20···S2^{iii}	0.93	2.99	3.73 (2)	138

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2303).

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supplementary materials

Acta Cryst. (2007). E**63**, m1544 [**doi:10.1107/S1600536807020338**]

Tris(ethylxanthato-$\kappa^2 S,S'$)(1,10-phenanthroline)bismuth(III)

F. Li, H.-D. Yin, J. Zhai and D.-Q. Wang

Comment

There has recently been increasing interest in bismuth(III) coordination chemistry, particularly in the light of the role of bismuth compounds in ^{212}Bi isotope therapy in cancer research (Sun *et al.*, 1997) and the use of bismuth complexes in the treatment of peptic ulcers (Baxter *et al.*, 1992). In particular, the interaction of bismuth(III) salts with chelating nitrogen-base ligands has been actively studied. In view of above and persuance of our interest in sulfur-containing ligands (Li *et al.*, 2005), we report here the synthesis and structure of the title compound, (I).

In this complex the bismuth atom is eight-coordinated by sulfur atoms belonging to three bidenate ethylxanthate ligands and by the nitrogen atoms of the bidentate 1,10-phenanthroline. The central Bi atom is eight-coordinate with atoms S4 and N1 in axial positions, and atoms S1, S2, S3, S5 and S6 in the equatorial plane. The remaining N atom (N2) of the 1,10-phenanthroline ligand caps the S2/S5/N1 face, giving a highly distorted capped pentagonal bipyramidal coordination geometry. Three Bi—S bonds [to S2, S3 and S5; mean = 2.897 Å] are significantly longer than the others [to S1, S4 and S6; mean = 2.805 Å], suggesting some delocalization in the system. In addition, the chelating phenanthroline ligands are bonded to the Bi atom through two N atoms. The Bi1—N1 and Bi1—N2 distances fall in the same range as in other Bi/N complexes (Li *et al.*, 2005).

The structure is stabilized by weak C—H···S interactions, Table 1, and a close S2···S2^{i} contact 3.496 Å, i = 1 − *x*, 1 − *y*, 1 − *z*.

Experimental

To a stirred solution of BiI_3 (0.2 mmol) in acetonitrile (20 ml), $C_2H_5OCS_2Na$ (0.6 mmol) was added. The reaction mixture was stirred for 2.5 h at 298 K. An orange solution was obtained and then filtered. The solvent was gradually removed by evaporation under vacuum to give a solid product which was recrystallized from ethanol yielding orange-red crystals of (I).

Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms [C—H = 0.93Å with U_{iso}(H) = 1.2U_{eq} for aromatic, C—H = 0.97Å with U_{iso}(H) = 1.2U_{eq} for CH_2, and C—H =0.96Å with U_{iso}(H) = 1.5U_{eq} for CH_3 H atoms].

Figures

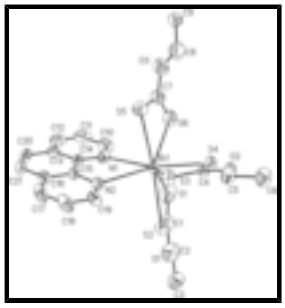

Fig. 1. The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

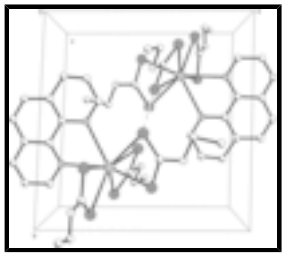

Fig. 2. Crystal packing of the title complex. The S···S interaction is shown as a dashed line.

tris(ethoxymethanedithioato-κ^2*S*,*S*')(1,10-phenanthroline)bismuth(III),

Crystal data

$[Bi(C_3H_5OS_2)_3(C_{12}H_8N_2)]$	$Z = 2$
$M_r = 752.75$	$F_{000} = 732$
Triclinic, $P\overline{1}$	$D_x = 1.857$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.7569$ (16) Å	Cell parameters from 2951 reflections
$b = 11.1985$ (17) Å	$\theta = 2.4$–24.6º
$c = 11.2494$ (17) Å	$\mu = 7.04$ mm^{-1}
$\alpha = 96.306$ (2)º	$T = 298$ (2) K
$\beta = 91.127$ (2)º	Block, orange-red
$\gamma = 91.737$ (2)º	0.19 × 0.18 × 0.18 mm
$V = 1345.9$ (4) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	4698 independent reflections
Radiation source: fine-focus sealed tube	3872 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.348$, $T_{max} = 0.364$	$k = -11 \rightarrow 13$

7132 measured reflections

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.068$

$wR(F^2) = 0.191$

$S = 1.04$

4698 reflections

298 parameters

551 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.1041P)^2 + 18.5625P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 2.99$ e Å^{-3}

$\Delta\rho_{min} = -3.36$ 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}
Bi1	0.68014 (5)	0.26489 (5)	0.68287 (5)	0.0469 (2)
N1	0.9283 (13)	0.2752 (14)	0.6203 (14)	0.065 (4)
N2	0.8064 (13)	0.4878 (13)	0.6736 (13)	0.058 (3)
O1	0.5261 (14)	0.2467 (13)	0.2990 (10)	0.0870 (17)
O2	0.3121 (9)	0.3057 (9)	0.8709 (10)	0.059 (3)
O3	0.8331 (13)	0.0829 (12)	1.0024 (12)	0.0844 (17)
S1	0.6586 (6)	0.1155 (5)	0.4631 (5)	0.0859 (10)
S2	0.5384 (5)	0.3490 (5)	0.4953 (5)	0.0749 (9)
S3	0.5113 (4)	0.4325 (4)	0.8153 (4)	0.0614 (9)
S4	0.4617 (4)	0.1707 (4)	0.7510 (4)	0.0576 (9)
S5	0.7886 (5)	0.2739 (5)	0.9215 (5)	0.0744 (10)
S6	0.7602 (5)	0.0435 (5)	0.7627 (5)	0.0768 (10)
C1	0.5798 (19)	0.226 (2)	0.4120 (14)	0.0798 (13)
C2	0.556 (2)	0.1502 (16)	0.2132 (14)	0.0860 (18)
H2A	0.5239	0.0751	0.2376	0.103*
H2B	0.6459	0.1456	0.2079	0.103*

C3	0.500 (2)	0.170 (2)	0.0914 (12)	0.091 (4)
H3A	0.5227	0.1053	0.0330	0.137*
H3B	0.5310	0.2447	0.0683	0.137*
H3C	0.4111	0.1708	0.0962	0.137*
C4	0.4271 (12)	0.3071 (15)	0.8151 (15)	0.0565 (17)
C5	0.2697 (13)	0.4150 (12)	0.9345 (16)	0.062 (2)
H5A	0.2696	0.4785	0.8824	0.075*
H5B	0.3246	0.4402	1.0027	0.075*
C6	0.1380 (13)	0.3907 (17)	0.9765 (17)	0.073 (4)
H6A	0.1078	0.4627	1.0190	0.110*
H6B	0.1392	0.3282	1.0284	0.110*
H6C	0.0844	0.3661	0.9084	0.110*
C7	0.7962 (18)	0.1240 (18)	0.8926 (15)	0.0732 (16)
C8	0.834 (2)	−0.0378 (13)	1.0278 (15)	0.084 (2)
H8A	0.8944	−0.0816	0.9786	0.101*
H8B	0.7528	−0.0762	1.0105	0.101*
C9	0.869 (2)	−0.0387 (18)	1.1604 (15)	0.085 (3)
H9A	0.8659	−0.1200	1.1803	0.127*
H9B	0.8108	0.0078	1.2084	0.127*
H9C	0.9512	−0.0046	1.1758	0.127*
C10	0.9895 (19)	0.176 (2)	0.5929 (19)	0.077 (4)
H10	0.9457	0.1026	0.5832	0.093*
C11	1.1189 (19)	0.178 (2)	0.5778 (19)	0.080 (4)
H11	1.1592	0.1066	0.5582	0.096*
C12	1.183 (2)	0.279 (2)	0.5911 (19)	0.079 (4)
H12	1.2682	0.2788	0.5803	0.095*
C13	1.1268 (18)	0.386 (2)	0.6206 (17)	0.071 (3)
C14	0.9958 (16)	0.3812 (18)	0.6365 (16)	0.065 (3)
C15	0.9313 (17)	0.4899 (18)	0.6645 (16)	0.066 (3)
C16	1.0006 (19)	0.6024 (19)	0.6805 (17)	0.071 (4)
C17	0.927 (2)	0.713 (2)	0.7052 (19)	0.082 (4)
H17	0.9666	0.7882	0.7168	0.098*
C18	0.810 (2)	0.7007 (19)	0.7100 (18)	0.078 (4)
H18	0.7633	0.7693	0.7238	0.093*
C19	0.748 (2)	0.5882 (17)	0.6955 (17)	0.070 (4)
H19	0.6617	0.5847	0.7016	0.084*
C20	1.1907 (19)	0.500 (2)	0.6358 (19)	0.079 (4)
H20	1.2761	0.5034	0.6250	0.094*
C21	1.132 (2)	0.602 (2)	0.6652 (19)	0.080 (4)
H21	1.1772	0.6744	0.6758	0.096*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0363 (3)	0.0425 (3)	0.0620 (4)	0.0043 (2)	0.0022 (2)	0.0048 (2)
N1	0.044 (8)	0.066 (9)	0.084 (10)	0.011 (7)	0.008 (7)	0.009 (8)
N2	0.050 (8)	0.054 (8)	0.073 (9)	0.000 (6)	0.005 (7)	0.011 (7)
O1	0.082 (3)	0.093 (3)	0.084 (3)	−0.004 (3)	−0.006 (3)	0.001 (3)

O2	0.044 (6)	0.062 (7)	0.070 (7)	0.000 (5)	0.009 (5)	0.003 (6)
O3	0.075 (3)	0.079 (3)	0.101 (3)	0.006 (3)	−0.003 (3)	0.022 (3)
S1	0.083 (2)	0.083 (2)	0.0848 (16)	0.0011 (17)	−0.0008 (18)	−0.0202 (15)
S2	0.0680 (19)	0.0842 (19)	0.0747 (17)	0.0015 (16)	−0.0100 (14)	0.0212 (15)
S3	0.0544 (18)	0.0551 (18)	0.0737 (19)	0.0008 (15)	0.0079 (16)	0.0006 (16)
S4	0.0477 (17)	0.0510 (17)	0.0740 (19)	0.0001 (15)	0.0071 (16)	0.0064 (16)
S5	0.073 (2)	0.077 (2)	0.0748 (14)	0.0058 (18)	−0.0127 (16)	0.0148 (16)
S6	0.068 (2)	0.0621 (19)	0.102 (2)	0.0078 (17)	−0.0019 (18)	0.0134 (18)
C1	0.073 (3)	0.095 (3)	0.0685 (17)	−0.016 (2)	−0.010 (2)	0.0006 (19)
C2	0.080 (3)	0.093 (3)	0.082 (3)	−0.004 (3)	−0.005 (3)	−0.001 (3)
C3	0.086 (6)	0.101 (7)	0.084 (6)	−0.004 (6)	−0.008 (6)	−0.001 (6)
C4	0.047 (3)	0.053 (3)	0.069 (3)	0.003 (3)	0.006 (3)	0.003 (3)
C5	0.054 (4)	0.060 (4)	0.071 (4)	0.003 (4)	0.008 (4)	−0.001 (4)
C6	0.060 (7)	0.079 (7)	0.079 (7)	0.006 (6)	0.013 (6)	−0.001 (7)
C7	0.064 (3)	0.068 (3)	0.089 (3)	0.006 (3)	−0.004 (3)	0.017 (3)
C8	0.074 (4)	0.076 (4)	0.102 (4)	0.005 (4)	−0.003 (4)	0.016 (4)
C9	0.074 (6)	0.084 (6)	0.098 (6)	0.003 (6)	−0.004 (6)	0.022 (6)
C10	0.062 (8)	0.091 (9)	0.083 (8)	0.015 (8)	0.011 (7)	0.025 (8)
C11	0.063 (8)	0.103 (9)	0.080 (8)	0.025 (8)	0.011 (7)	0.028 (8)
C12	0.060 (7)	0.106 (9)	0.076 (7)	0.005 (7)	0.005 (7)	0.028 (7)
C13	0.057 (7)	0.096 (8)	0.066 (7)	0.000 (6)	0.001 (6)	0.031 (7)
C14	0.051 (6)	0.085 (7)	0.064 (7)	−0.003 (6)	0.002 (6)	0.029 (6)
C15	0.060 (7)	0.079 (7)	0.063 (6)	−0.018 (6)	0.002 (6)	0.023 (6)
C16	0.069 (7)	0.082 (7)	0.064 (7)	−0.017 (7)	−0.002 (6)	0.022 (6)
C17	0.089 (8)	0.076 (8)	0.078 (8)	−0.024 (8)	0.001 (8)	0.011 (7)
C18	0.088 (9)	0.069 (8)	0.077 (8)	−0.007 (8)	0.005 (8)	0.011 (7)
C19	0.073 (8)	0.065 (8)	0.074 (8)	−0.005 (7)	0.006 (7)	0.021 (7)
C20	0.060 (7)	0.102 (8)	0.076 (7)	−0.016 (7)	−0.005 (6)	0.026 (7)
C21	0.070 (7)	0.093 (8)	0.078 (7)	−0.027 (7)	−0.004 (7)	0.023 (7)

Geometric parameters (Å, °)

Bi1—S4	2.706 (4)	C5—H5A	0.9700
Bi1—N1	2.776 (14)	C5—H5B	0.9700
Bi1—N2	2.819 (14)	C6—H6A	0.9600
Bi1—S1	2.830 (5)	C6—H6B	0.9600
Bi1—S2	2.839 (5)	C6—H6C	0.9600
Bi1—S6	2.878 (5)	C8—C9	1.532 (11)
Bi1—S5	2.896 (5)	C8—H8A	0.9700
Bi1—S3	2.956 (5)	C8—H8B	0.9700
N1—C10	1.32 (2)	C9—H9A	0.9600
N1—C14	1.37 (2)	C9—H9B	0.9600
N2—C19	1.31 (2)	C9—H9C	0.9600
N2—C15	1.35 (2)	C10—C11	1.41 (3)
O1—C2	1.417 (11)	C10—H10	0.9300
O1—C1	1.432 (10)	C11—C12	1.30 (3)
O2—C4	1.399 (10)	C11—H11	0.9300
O2—C5	1.440 (10)	C12—C13	1.37 (3)
O3—C8	1.412 (10)	C12—H12	0.9300

O3—C7	1.418 (10)	C13—C20	1.42 (3)
S1—C1	1.67 (2)	C13—C14	1.42 (3)
S2—C1	1.66 (2)	C14—C15	1.43 (3)
S3—C4	1.648 (16)	C15—C16	1.44 (3)
S4—C4	1.671 (17)	C16—C21	1.42 (3)
S5—C7	1.68 (2)	C16—C17	1.49 (3)
S6—C7	1.66 (2)	C17—C18	1.27 (3)
C2—C3	1.527 (11)	C17—H17	0.9300
C2—H2A	0.9700	C18—C19	1.40 (3)
C2—H2B	0.9700	C18—H18	0.9300
C3—H3A	0.9600	C19—H19	0.9300
C3—H3B	0.9600	C20—C21	1.34 (3)
C3—H3C	0.9600	C20—H20	0.9300
C5—C6	1.528 (10)	C21—H21	0.9300
S4—Bi1—N1	158.8 (3)	O2—C5—H5A	110.1
S4—Bi1—N2	141.0 (3)	C6—C5—H5A	110.1
N1—Bi1—N2	59.3 (4)	O2—C5—H5B	110.1
S4—Bi1—S1	89.76 (16)	C6—C5—H5B	110.1
N1—Bi1—S1	82.0 (4)	H5A—C5—H5B	108.4
N2—Bi1—S1	115.4 (3)	C5—C6—H6A	109.5
S4—Bi1—S2	85.59 (15)	C5—C6—H6B	109.5
N1—Bi1—S2	107.4 (3)	H6A—C6—H6B	109.5
N2—Bi1—S2	81.2 (3)	C5—C6—H6C	109.5
S1—Bi1—S2	62.52 (18)	H6A—C6—H6C	109.5
S4—Bi1—S6	79.10 (15)	H6B—C6—H6C	109.5
N1—Bi1—S6	80.3 (3)	O3—C7—S6	128.5 (15)
N2—Bi1—S6	131.5 (3)	O3—C7—S5	105.5 (13)
S1—Bi1—S6	80.86 (18)	S6—C7—S5	125.9 (9)
S2—Bi1—S6	140.30 (17)	O3—C8—C9	108.3 (10)
S4—Bi1—S5	92.46 (15)	O3—C8—H8A	110.0
N1—Bi1—S5	82.3 (4)	C9—C8—H8A	110.0
N2—Bi1—S5	85.4 (3)	O3—C8—H8B	110.0
S1—Bi1—S5	141.62 (18)	C9—C8—H8B	110.0
S2—Bi1—S5	155.84 (17)	H8A—C8—H8B	108.4
S6—Bi1—S5	62.06 (16)	C8—C9—H9A	109.5
S4—Bi1—S3	63.13 (13)	C8—C9—H9B	109.5
N1—Bi1—S3	135.0 (3)	H9A—C9—H9B	109.5
N2—Bi1—S3	78.2 (3)	C8—C9—H9C	109.5
S1—Bi1—S3	133.69 (16)	H9A—C9—H9C	109.5
S2—Bi1—S3	77.74 (15)	H9B—C9—H9C	109.5
S6—Bi1—S3	124.66 (15)	N1—C10—C11	122 (2)
S5—Bi1—S3	79.91 (15)	N1—C10—H10	119.0
C10—N1—C14	117.5 (17)	C11—C10—H10	119.0
C10—N1—Bi1	120.9 (13)	C12—C11—C10	121 (2)
C14—N1—Bi1	120.8 (12)	C12—C11—H11	119.7
C19—N2—C15	120.2 (16)	C10—C11—H11	119.7
C19—N2—Bi1	120.4 (12)	C11—C12—C13	121 (2)
C15—N2—Bi1	118.7 (12)	C11—C12—H12	119.3
C2—O1—C1	108.3 (14)	C13—C12—H12	119.3

C4—O2—C5	119.1 (11)	C12—C13—C20	124.3 (19)
C8—O3—C7	126.5 (15)	C12—C13—C14	117 (2)
C1—S1—Bi1	86.4 (7)	C20—C13—C14	119 (2)
C1—S2—Bi1	86.2 (6)	N1—C14—C13	121.8 (19)
C4—S3—Bi1	81.0 (5)	N1—C14—C15	118.4 (16)
C4—S4—Bi1	88.8 (4)	C13—C14—C15	119.7 (18)
C7—S5—Bi1	85.4 (5)	N2—C15—C14	120.7 (16)
C7—S6—Bi1	86.3 (6)	N2—C15—C16	120.1 (19)
O1—C1—S2	100.1 (13)	C14—C15—C16	119.2 (18)
O1—C1—S1	135.4 (16)	C21—C16—C15	119 (2)
S2—C1—S1	124.5 (9)	C21—C16—C17	124.7 (19)
O1—C2—C3	109.7 (10)	C15—C16—C17	116.5 (18)
O1—C2—H2A	109.7	C18—C17—C16	118 (2)
C3—C2—H2A	109.7	C18—C17—H17	120.8
O1—C2—H2B	109.7	C16—C17—H17	120.8
C3—C2—H2B	109.7	C17—C18—C19	122 (2)
H2A—C2—H2B	108.2	C17—C18—H18	118.8
C2—C3—H3A	109.5	C19—C18—H18	118.8
C2—C3—H3B	109.5	N2—C19—C18	122 (2)
H3A—C3—H3B	109.5	N2—C19—H19	118.8
C2—C3—H3C	109.5	C18—C19—H19	118.8
H3A—C3—H3C	109.5	C21—C20—C13	122 (2)
H3B—C3—H3C	109.5	C21—C20—H20	119.0
O2—C4—S3	121.3 (12)	C13—C20—H20	119.0
O2—C4—S4	111.7 (11)	C20—C21—C16	122 (2)
S3—C4—S4	127.0 (7)	C20—C21—H21	119.2
O2—C5—C6	108.0 (9)	C16—C21—H21	119.2

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···S4^{i}	0.97	2.78	3.660 (19)	152
C5—H5B···S3^{ii}	0.97	2.90	3.851 (17)	167
C20—H20···S2^{iii}	0.93	2.99	3.73 (2)	138

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

Fig. 1

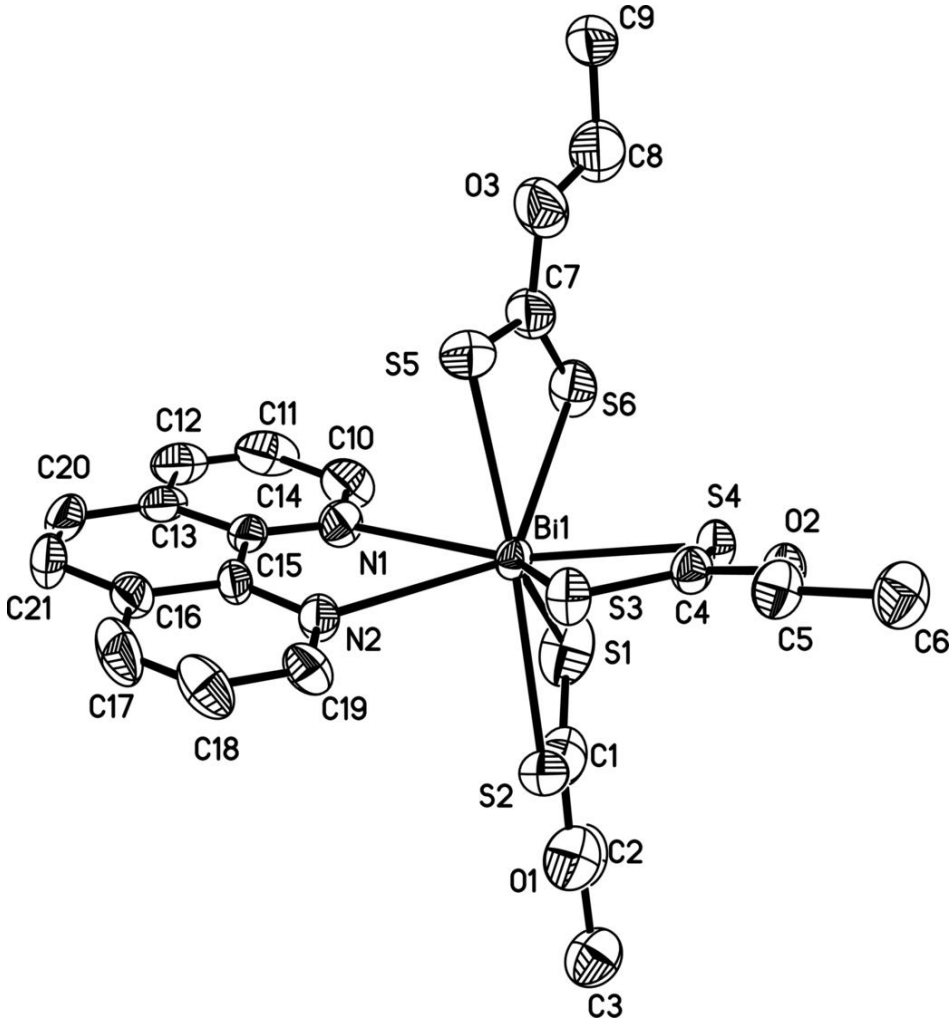
C9
C8
O3
C7
S5
S6
C12
C11
C10
C20
C14
S4
O2
C13
Bi1
C15
N1
C21
C16
S3
C4
C5
C6
N2
S1
C17
C19
C18
C1
S2
C2
O1
C3

Fig. 2