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ISSN 2414-3146

Bis(4-phenyl-2-sulfanylidene-2,3-dihydro-1,3-thiazol-3-ido-κ^2S^2,N)(4-phenyl-1,3-thiazole-2-thiolato-κS^2)bismuth

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Received 22 November 2019
Accepted 20 January 2020

Edited by M. Weil, Vienna University of Technology, Austria

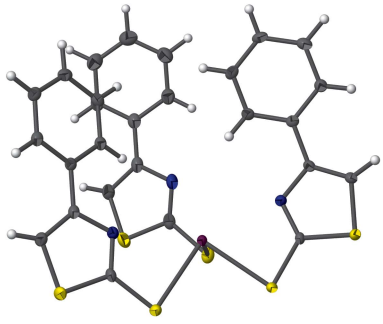
Keywords: crystal structure; bismuth; monomeric complex; N,S-donor ligand.

CCDC reference: 1979022

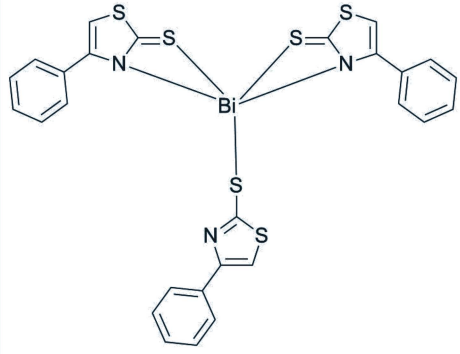
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Bi(C_9H_6NS_2)_3]$, was prepared by reacting $BiCl_3$ and 2-mercapto-4-phenylthiazole (LH) at room temperature in a stoichiometric ratio of 1:4. The molecular structure reveals a slightly distorted square-pyramidal environment around the Bi^{III} atom. Two of the three monoanionic ligands L^- coordinate in an N,S-bidentate mode, while one shows a monodentate mode through an S atom. There are no significant intermolecular interactions present in the crystal.

3D view



Chemical scheme



Structure description

For general background on this type of bismuth chemistry with S- or (N,S)-donor ligands, see: Diemer *et al.* (1995); Stavila *et al.* (2006); Briand *et al.* (2000). The coordination chemistry of bismuth with thiourea or thiosemicarbazide ligands has been studied in detail (Battaglia & Corradi, 1981,1983; Battaglia *et al.*, 1992). While thiourea ligands have been found to be S-donor ligands only, thiosemicarbazide shows an (N,S)-coordination mode. Recently, we have reported the coordination modes of three heterocyclic ligands derived from 3-mercapto-4-methyl-1,2,4-triazole (L1H), 2-mercapto-benzimidazole (L2H) and 2-mercapto-4-methylthiazole (L3H), respectively, towards bismuth(III). In the corresponding three bismuth complexes $[Bi(L1)_4(Cl)_2]Cl$, $[Bi(L2)_4Cl_2]^+[Bi(L2)_2Cl_4]^-$ and $[Bi(L3)_2Cl_2(\mu\text{-}Cl)]_2$ (Imran *et al.*, 2013, 2014), all these ligands coordinate solely *via* their S-donor atoms despite a possible (N,S) coordination.

In the title compound, the deprotonated ligand L (LH is 2-mercapto-4-phenyl thiazole) exhibits both monodentate S- and bidentate (N,S)-coordination modes (Fig. 1). Two ligands coordinate in a bidentate fashion (*via* N1, S1, and *via* N2, S3) while the third one exhibits a monodentate mode *via* the S5 donor atom, resulting in a slightly distorted

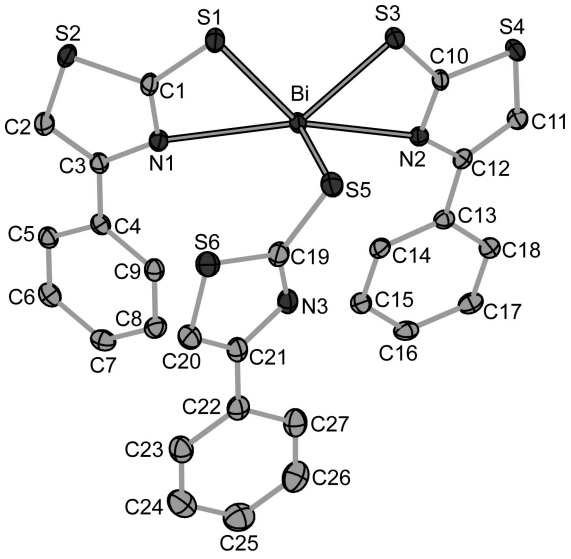


Figure 1
Molecular structure of the title compound, with anisotropic displacement ellipsoids shown at the 50% probability level. Hydrogen atoms are omitted for clarity.

square-pyramidal coordination environment. The Bi—N and Bi—S bonds differ in lengths with the Bi—S bonds shorter by $\simeq$ 0.2 Å (Table 1) but the index parameter (Addison *et al.*, 1984) of $\tau_5 = 0$ indicates an ideal value for a square-pyramidal coordination (ideal value for trigonal–bipyramidal coordination is $\tau_5 = 1$).

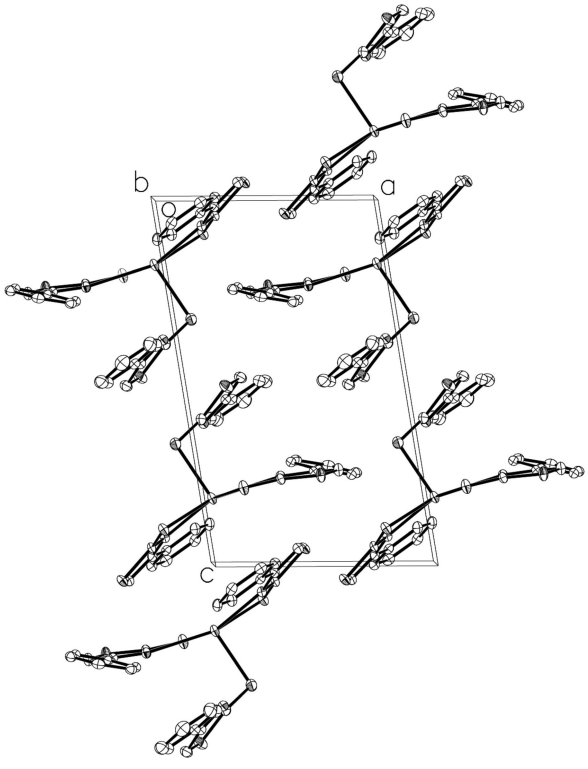


Figure 2
A packing plot of the title compound in a view along the *b* axis.

Table 1
Selected geometric parameters (Å, °).

Bi1—S1	2.6078 (5)	Bi1—N1	2.7970 (17)
Bi1—S3	2.5938 (5)	Bi1—N2	2.7342 (17)
Bi1—S5	2.5550 (6)		
S1—Bi1—N1	59.71 (4)	S5—Bi1—S1	94.838 (18)
S1—Bi1—N2	146.17 (4)	S5—Bi1—S3	87.489 (17)
S3—Bi1—S1	88.679 (16)	S5—Bi1—N1	105.90 (4)
S3—Bi1—N1	146.06 (4)	S5—Bi1—N2	96.58 (4)
S3—Bi1—N2	60.22 (4)	N2—Bi1—N1	144.35 (5)

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Bi(C_9H_6NS_2)_3]$
M_r	785.78
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	9.19758 (16), 10.8904 (2), 14.6041 (2)
α, β, γ (°)	82.0966 (15), 78.5197 (14), 70.9346 (17)
V (Å^3)	1350.77 (4)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	17.34
Crystal size (mm)	0.12 × 0.06 × 0.03
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2013)
T_{min}, T_{max}	0.085, 0.532
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25693, 5325, 5322
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.014, 0.036, 1.11
No. of reflections	5325
No. of parameters	406
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.62

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

In the crystal packing (Fig. 2), no significant intermolecular interactions are found, except a short S···S contact between S2 and S5($x + 1$, y, z) with a distance of 3.473 (1) Å.

Synthesis and crystallization

The title compound was prepared by reacting $BiCl_3$ (1 mmol, 0.315 g) and 2-mercapto-4-phenyl thiazole (LH) (4 mmol, 0.773 g) in THF at room temperature. After stirring for 4 h, the resulting yellow solution was concentrated, yielding a yellow solid that was separated by decantation and washed with small amounts of THF followed by diethyl ether. The solid was dried and recrystallized from a mixture of THF/pentane (ratio *v*:*v* = 1:3). Yellow to orange crystals suitable for X-ray diffraction were obtained by slow evaporation of the THF solution of the complex. Yield 76%; m.p. 507 K. ^{1}H NMR

($CDCl_3$): δ 7.58–7.60 (*dd*, 2H, C2H, C6H), 7.42–7.49 (*m*, 3H, C3H—C5H), 6.78, CH-thiazole ring); ^{13}C NMR ($CDCl_3$): δ 188.5 (C9), 142.5 (C8), 129.9 (C2,6), 129.4 (C3,5), 128.1 (C4), 125.9 (C1), 108.9 (C7).

Refinement

Crystal data, data collection and refinement details are summarized in Table 2.

Funding information

MI acknowledges with special thanks the Deutscher Akademischer Austausch Dienst (DAAD) for providing a PhD stipend.

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full crystallographic data

IUCrData (2020). **5**, x200067 [https://doi.org/10.1107/S241431462000067X]

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Crystal data

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M_r = 785.78
Triclinic, $P\overline{1}$
a = 9.19758 (16) Å
b = 10.8904 (2) Å
c = 14.6041 (2) Å
α = 82.0966 (15)°
β = 78.5197 (14)°
γ = 70.9346 (17)°
V = 1350.77 (4) Å^3
Z = 2
$F(000)$ = 760
D_x = 1.932 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 24519 reflections
θ = 4.3–76.1°
μ = 17.34 mm^{-1}
T = 100 K
Needle, orange
0.12 × 0.06 × 0.03 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.3114 pixels mm^{-1}
ω scans
Absorption correction: gaussian (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.085, T_{max} = 0.532
25693 measured reflections
5325 independent reflections
5322 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 72.0°, θ_{min} = 3.1°
h = −11→11
k = −12→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.036
S = 1.11
5325 reflections
406 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2 + 1.2762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Bi1	0.04854 (2)	0.79732 (2)	0.82325 (2)	0.01547 (3)
S1	0.20152 (6)	0.96640 (5)	0.79684 (4)	0.02075 (11)
S2	0.55560 (6)	0.85161 (5)	0.76213 (4)	0.02079 (11)
S3	−0.18891 (6)	0.96840 (5)	0.90975 (3)	0.01687 (10)
S4	−0.41485 (6)	0.85142 (5)	1.04776 (3)	0.01725 (10)
S5	−0.07429 (6)	0.87655 (6)	0.67505 (4)	0.02366 (11)
S6	0.19538 (7)	0.79159 (6)	0.51708 (4)	0.02644 (12)
N1	0.3712 (2)	0.71876 (17)	0.76281 (12)	0.0160 (3)
N2	−0.1935 (2)	0.72176 (17)	0.92834 (12)	0.0144 (3)
N3	0.0621 (2)	0.6322 (2)	0.61607 (12)	0.0203 (4)
C1	0.3717 (2)	0.8368 (2)	0.77210 (14)	0.0166 (4)
C2	0.6356 (3)	0.6878 (2)	0.74564 (16)	0.0199 (4)
H2	0.741 (4)	0.655 (3)	0.734 (2)	0.039 (9)*
C3	0.5213 (2)	0.6322 (2)	0.74932 (13)	0.0151 (4)
C4	0.5433 (2)	0.4935 (2)	0.74129 (13)	0.0153 (4)
C5	0.6842 (2)	0.3977 (2)	0.75534 (14)	0.0172 (4)
H5	0.765 (3)	0.424 (3)	0.7721 (18)	0.021 (6)*
C6	0.7044 (3)	0.2675 (2)	0.74796 (15)	0.0195 (4)
H6	0.801 (3)	0.202 (3)	0.759 (2)	0.025 (7)*
C7	0.5851 (3)	0.2296 (2)	0.72688 (14)	0.0198 (4)
H7	0.602 (3)	0.139 (3)	0.720 (2)	0.029 (7)*
C8	0.4447 (3)	0.3232 (2)	0.71348 (14)	0.0189 (4)
H8	0.364 (4)	0.297 (3)	0.702 (2)	0.029 (7)*
C9	0.4235 (2)	0.4543 (2)	0.72059 (14)	0.0169 (4)
H9	0.328 (3)	0.515 (3)	0.7120 (17)	0.014 (6)*
C10	−0.2588 (2)	0.8389 (2)	0.95742 (14)	0.0143 (4)
C11	−0.3889 (2)	0.6881 (2)	1.04507 (15)	0.0165 (4)
H11	−0.451 (3)	0.648 (3)	1.087 (2)	0.026 (7)*
C12	−0.2661 (2)	0.6341 (2)	0.97873 (14)	0.0145 (4)
C13	−0.2010 (2)	0.4953 (2)	0.95995 (14)	0.0149 (4)
C14	−0.0570 (2)	0.4502 (2)	0.90157 (15)	0.0179 (4)
H14	−0.004 (3)	0.506 (3)	0.8737 (18)	0.020 (6)*
C15	0.0088 (3)	0.3187 (2)	0.88689 (16)	0.0198 (4)
H15	0.103 (4)	0.290 (3)	0.850 (2)	0.029 (7)*
C16	−0.0690 (3)	0.2307 (2)	0.92946 (15)	0.0193 (4)
H16	−0.025 (3)	0.141 (3)	0.9200 (18)	0.020 (6)*
C17	−0.2140 (3)	0.2748 (2)	0.98625 (15)	0.0193 (4)
H17	−0.269 (3)	0.214 (3)	1.0171 (18)	0.016 (6)*
C18	−0.2798 (2)	0.4065 (2)	1.00132 (15)	0.0174 (4)
H18	−0.377 (3)	0.433 (3)	1.0409 (18)	0.018 (6)*
C19	0.0574 (3)	0.7542 (2)	0.60642 (15)	0.0223 (5)
C20	0.2623 (3)	0.6324 (2)	0.49126 (16)	0.0239 (5)
H20	0.344 (4)	0.605 (3)	0.440 (2)	0.032 (8)*
C21	0.1787 (3)	0.5610 (2)	0.55003 (14)	0.0201 (4)
C22	0.2029 (3)	0.4211 (2)	0.54815 (15)	0.0208 (4)

C23	0.3385 (3)	0.3415 (3)	0.49685 (16)	0.0257 (5)
H23	0.414 (3)	0.379 (3)	0.4648 (19)	0.024 (7)*
C24	0.3624 (3)	0.2088 (3)	0.49678 (18)	0.0317 (5)
H24	0.455 (4)	0.155 (3)	0.460 (2)	0.038 (8)*
C25	0.2526 (3)	0.1534 (3)	0.54776 (19)	0.0335 (6)
H25	0.272 (4)	0.058 (3)	0.548 (2)	0.040 (9)*
C26	0.1176 (3)	0.2311 (3)	0.59860 (19)	0.0314 (5)
H26	0.042 (4)	0.191 (3)	0.632 (2)	0.039 (9)*
C27	0.0928 (3)	0.3639 (3)	0.59854 (17)	0.0255 (5)
H27	0.008 (4)	0.415 (3)	0.634 (2)	0.040 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.01146 (4)	0.01291 (5)	0.02127 (5)	−0.00430 (3)	0.00139 (3)	−0.00338 (3)
S1	0.0142 (2)	0.0136 (2)	0.0332 (3)	−0.00434 (19)	−0.0004 (2)	−0.0026 (2)
S2	0.0136 (2)	0.0185 (2)	0.0324 (3)	−0.00687 (19)	−0.0033 (2)	−0.0052 (2)
S3	0.0153 (2)	0.0113 (2)	0.0222 (2)	−0.00482 (18)	0.00260 (18)	−0.00209 (18)
S4	0.0160 (2)	0.0128 (2)	0.0199 (2)	−0.00403 (18)	0.00428 (18)	−0.00268 (18)
S5	0.0182 (2)	0.0281 (3)	0.0238 (3)	−0.0052 (2)	−0.0023 (2)	−0.0057 (2)
S6	0.0263 (3)	0.0305 (3)	0.0244 (3)	−0.0150 (2)	0.0043 (2)	−0.0055 (2)
N1	0.0140 (8)	0.0163 (9)	0.0178 (8)	−0.0054 (7)	−0.0020 (6)	−0.0010 (7)
N2	0.0136 (8)	0.0131 (8)	0.0164 (8)	−0.0042 (7)	−0.0020 (6)	−0.0016 (6)
N3	0.0161 (9)	0.0288 (10)	0.0161 (8)	−0.0074 (8)	−0.0020 (7)	−0.0019 (7)
C1	0.0128 (9)	0.0198 (10)	0.0179 (9)	−0.0074 (8)	−0.0004 (7)	−0.0009 (8)
C2	0.0144 (10)	0.0188 (11)	0.0260 (11)	−0.0041 (8)	−0.0029 (8)	−0.0036 (8)
C3	0.0129 (9)	0.0185 (10)	0.0134 (9)	−0.0042 (8)	−0.0015 (7)	−0.0017 (7)
C4	0.0157 (10)	0.0169 (10)	0.0122 (9)	−0.0048 (8)	−0.0001 (7)	−0.0006 (7)
C5	0.0151 (10)	0.0210 (11)	0.0147 (9)	−0.0049 (8)	−0.0016 (7)	−0.0023 (8)
C6	0.0195 (11)	0.0187 (11)	0.0169 (10)	−0.0030 (9)	−0.0013 (8)	0.0000 (8)
C7	0.0259 (11)	0.0169 (11)	0.0158 (9)	−0.0074 (9)	−0.0003 (8)	−0.0015 (8)
C8	0.0206 (10)	0.0219 (11)	0.0165 (9)	−0.0101 (9)	−0.0020 (8)	−0.0017 (8)
C9	0.0153 (10)	0.0196 (11)	0.0151 (9)	−0.0054 (8)	−0.0019 (7)	0.0000 (8)
C10	0.0106 (9)	0.0150 (10)	0.0163 (9)	−0.0043 (7)	0.0006 (7)	−0.0016 (7)
C11	0.0171 (10)	0.0134 (10)	0.0186 (10)	−0.0060 (8)	−0.0009 (8)	0.0002 (8)
C12	0.0145 (9)	0.0142 (10)	0.0161 (9)	−0.0064 (8)	−0.0031 (7)	0.0002 (7)
C13	0.0159 (10)	0.0141 (10)	0.0155 (9)	−0.0043 (8)	−0.0052 (7)	−0.0011 (7)
C14	0.0164 (10)	0.0158 (10)	0.0235 (10)	−0.0068 (8)	−0.0035 (8)	−0.0033 (8)
C15	0.0152 (10)	0.0185 (11)	0.0254 (11)	−0.0022 (8)	−0.0048 (8)	−0.0065 (8)
C16	0.0216 (11)	0.0121 (10)	0.0249 (11)	−0.0020 (8)	−0.0092 (8)	−0.0037 (8)
C17	0.0245 (11)	0.0164 (10)	0.0201 (10)	−0.0092 (9)	−0.0072 (8)	0.0009 (8)
C18	0.0174 (10)	0.0171 (10)	0.0181 (10)	−0.0060 (8)	−0.0023 (8)	−0.0019 (8)
C19	0.0172 (10)	0.0311 (13)	0.0202 (10)	−0.0092 (9)	−0.0029 (8)	−0.0030 (9)
C20	0.0225 (11)	0.0300 (13)	0.0190 (10)	−0.0093 (10)	0.0006 (9)	−0.0049 (9)
C21	0.0159 (10)	0.0290 (12)	0.0153 (9)	−0.0060 (9)	−0.0038 (8)	−0.0018 (8)
C22	0.0184 (10)	0.0276 (12)	0.0171 (10)	−0.0065 (9)	−0.0063 (8)	−0.0006 (8)
C23	0.0227 (11)	0.0329 (13)	0.0203 (11)	−0.0077 (10)	−0.0024 (9)	−0.0024 (9)
C24	0.0314 (13)	0.0329 (14)	0.0268 (12)	−0.0037 (11)	−0.0037 (10)	−0.0058 (10)

C25	0.0375 (15)	0.0262 (13)	0.0375 (14)	−0.0082 (11)	−0.0112 (11)	−0.0014 (11)
C26	0.0286 (13)	0.0312 (14)	0.0361 (13)	−0.0128 (11)	−0.0073 (11)	0.0037 (11)
C27	0.0208 (11)	0.0295 (13)	0.0250 (11)	−0.0066 (10)	−0.0047 (9)	0.0008 (10)

Geometric parameters (Å, º)

Bi1—S1	2.6078 (5)	C8—H8	0.93 (3)
Bi1—S3	2.5938 (5)	C8—C9	1.391 (3)
Bi1—S5	2.5550 (6)	C9—H9	0.93 (3)
Bi1—N1	2.7970 (17)	C11—H11	0.92 (3)
Bi1—N2	2.7342 (17)	C11—C12	1.359 (3)
S1—C1	1.744 (2)	C12—C13	1.475 (3)
S2—C1	1.727 (2)	C13—C14	1.401 (3)
S2—C2	1.724 (2)	C13—C18	1.396 (3)
S3—C10	1.741 (2)	C14—H14	0.90 (3)
S4—C10	1.728 (2)	C14—C15	1.389 (3)
S4—C11	1.721 (2)	C15—H15	0.91 (3)
S5—C19	1.754 (2)	C15—C16	1.387 (3)
S6—C19	1.735 (2)	C16—H16	0.95 (3)
S6—C20	1.708 (3)	C16—C17	1.396 (3)
N1—C1	1.313 (3)	C17—H17	0.97 (3)
N1—C3	1.388 (3)	C17—C18	1.392 (3)
N2—C10	1.310 (3)	C18—H18	0.94 (3)
N2—C12	1.388 (3)	C20—H20	0.95 (3)
N3—C19	1.304 (3)	C20—C21	1.370 (3)
N3—C21	1.389 (3)	C21—C22	1.470 (3)
C2—H2	0.91 (3)	C22—C23	1.403 (3)
C2—C3	1.363 (3)	C22—C27	1.394 (3)
C3—C4	1.475 (3)	C23—H23	0.93 (3)
C4—C5	1.405 (3)	C23—C24	1.388 (4)
C4—C9	1.401 (3)	C24—H24	0.96 (3)
C5—H5	0.96 (3)	C24—C25	1.383 (4)
C5—C6	1.385 (3)	C25—H25	0.99 (3)
C6—H6	0.96 (3)	C25—C26	1.389 (4)
C6—C7	1.391 (3)	C26—H26	0.95 (3)
C7—H7	0.97 (3)	C26—C27	1.388 (4)
C7—C8	1.390 (3)	C27—H27	0.91 (3)
S1—Bi1—N1	59.71 (4)	N2—C10—S4	114.33 (15)
S1—Bi1—N2	146.17 (4)	S4—C11—H11	120.4 (18)
S3—Bi1—S1	88.679 (16)	C12—C11—S4	110.94 (16)
S3—Bi1—N1	146.06 (4)	C12—C11—H11	128.6 (18)
S3—Bi1—N2	60.22 (4)	N2—C12—C13	118.96 (18)
S5—Bi1—S1	94.838 (18)	C11—C12—N2	114.04 (18)
S5—Bi1—S3	87.489 (17)	C11—C12—C13	126.91 (19)
S5—Bi1—N1	105.90 (4)	C14—C13—C12	120.24 (19)
S5—Bi1—N2	96.58 (4)	C18—C13—C12	120.76 (19)
N2—Bi1—N1	144.35 (5)	C18—C13—C14	118.98 (19)

C1—S1—Bi1	87.45 (7)	C13—C14—H14	120.6 (17)
C2—S2—C1	89.48 (11)	C15—C14—C13	120.7 (2)
C10—S3—Bi1	86.69 (7)	C15—C14—H14	118.7 (17)
C11—S4—C10	89.19 (10)	C14—C15—H15	120.4 (19)
C19—S5—Bi1	95.96 (8)	C16—C15—C14	120.0 (2)
C20—S6—C19	89.33 (12)	C16—C15—H15	119.6 (19)
C1—N1—Bi1	89.15 (12)	C15—C16—H16	120.8 (17)
C1—N1—C3	111.55 (17)	C15—C16—C17	119.8 (2)
C3—N1—Bi1	156.38 (14)	C17—C16—H16	119.4 (17)
C10—N2—Bi1	90.38 (12)	C16—C17—H17	120.7 (15)
C10—N2—C12	111.48 (17)	C18—C17—C16	120.3 (2)
C12—N2—Bi1	155.75 (13)	C18—C17—H17	119.0 (16)
C19—N3—C21	110.92 (19)	C13—C18—H18	121.5 (16)
S2—C1—S1	122.72 (13)	C17—C18—C13	120.2 (2)
N1—C1—S1	123.07 (16)	C17—C18—H18	118.2 (16)
N1—C1—S2	114.17 (16)	S6—C19—S5	120.09 (14)
S2—C2—H2	117 (2)	N3—C19—S5	125.26 (17)
C3—C2—S2	110.56 (16)	N3—C19—S6	114.65 (17)
C3—C2—H2	132 (2)	S6—C20—H20	120.4 (19)
N1—C3—C4	119.18 (18)	C21—C20—S6	110.71 (18)
C2—C3—N1	114.21 (19)	C21—C20—H20	128.8 (19)
C2—C3—C4	126.61 (19)	N3—C21—C22	119.7 (2)
C5—C4—C3	120.68 (19)	C20—C21—N3	114.4 (2)
C9—C4—C3	120.76 (19)	C20—C21—C22	125.9 (2)
C9—C4—C5	118.6 (2)	C23—C22—C21	120.8 (2)
C4—C5—H5	119.0 (16)	C27—C22—C21	120.8 (2)
C6—C5—C4	120.6 (2)	C27—C22—C23	118.4 (2)
C6—C5—H5	120.4 (16)	C22—C23—H23	118.3 (18)
C5—C6—H6	120.1 (17)	C24—C23—C22	120.7 (2)
C5—C6—C7	120.4 (2)	C24—C23—H23	121.0 (18)
C7—C6—H6	119.4 (17)	C23—C24—H24	120 (2)
C6—C7—H7	119.4 (17)	C25—C24—C23	120.2 (2)
C8—C7—C6	119.6 (2)	C25—C24—H24	120 (2)
C8—C7—H7	121.0 (17)	C24—C25—H25	119.3 (19)
C7—C8—H8	119.5 (19)	C24—C25—C26	119.7 (3)
C7—C8—C9	120.3 (2)	C26—C25—H25	121.0 (19)
C9—C8—H8	120.1 (19)	C25—C26—H26	118 (2)
C4—C9—H9	120.8 (16)	C27—C26—C25	120.3 (2)
C8—C9—C4	120.5 (2)	C27—C26—H26	121 (2)
C8—C9—H9	118.7 (16)	C22—C27—H27	118 (2)
S4—C10—S3	123.72 (12)	C26—C27—C22	120.7 (2)
N2—C10—S3	121.93 (15)	C26—C27—H27	121 (2)