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# (2,2′-Bipyridine-$\kappa^2N,N'$)(nitrato-$\kappa^2O,O'$)-bis(pyrrolidine-1-dithiocarboxylato-$\kappa^2S,S'$)bismuth(III)

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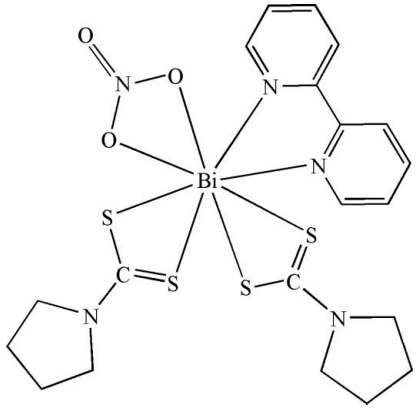
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.021 Å; $R$ factor = 0.063; $wR$ factor = 0.163; data-to-parameter ratio = 15.4.

The title compound, $[Bi(C_4H_8NS_2)_2(NO_3)(C_{10}H_8N_2)]$, is monomeric, with the Bi atom chelated by the S atoms of two pyrrolidine-1-dithiocarboxylate ligands and the N atoms of a 2,2′-bipyridine ligand. A nitrate ligand completes the coordination, with the eight-coordinated Bi atom adopting a highly distorted capped pentagonal–bipyramidal geometry.

## Related literature

For related literature, see: Baraanyi *et al.* (1977); Bardaji *et al.* (1994); Xu *et al.* (2001); Yin *et al.* (2003).




## Experimental

### Crystal data

$[Bi(C_4H_8NS_2)_2(NO_3)(C_{10}H_8N_2)]$
$M_r$ = 719.66
Triclinic, $P\overline{1}$
$a$ = 9.565 (4) Å
$b$ = 10.171 (4) Å
$c$ = 14.555 (5) Å
$\alpha$ = 73.634 (4)°
$\beta$ = 76.032 (4)°
$\gamma$ = 70.916 (4)°
$V$ = 1266.5 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 7.32 mm$^{-1}$
$T$ = 298 (2) K
0.28 × 0.24 × 0.22 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.149, $T_{max}$ = 0.212
(expected range = 0.140–0.200)
6375 measured reflections
4305 independent reflections
3408 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.163
$S$ = 0.99
4305 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −5.28 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: DN2168).

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# supplementary materials

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# (2,2'-Bipyridine-$\kappa^2N,N'$)(nitrato-$\kappa^2O,O'$)bis(pyrrolidine-1-dithiocarboxylato-$\kappa^2S,S'$)bismuth(III)

**F. Li, H.-D. Yin and D.-Q. Wang**

## Comment

Dithiocarbamates have been known as effective ligands for transition metal ions for many years. They can form chelates (Xu *et al.*, 2001) or act as bridging ligands (Bardaji *et al.*, 1994). However, the chemistry of main-group metal complexes with dithiocarbamates has been less extensively studied, and only a few reports describing bismuth(III) dithiocarbamate complexes have appeared (Yin *et al.*, 2003). As a continuation of our interest in sulfur-containing ligands, we report here the synthesis and structure of the title compound, (I).

The title compound, (I), is monomeric, with the Bi atom chelated by the S atoms of two pyrrolidine-1-dithiocarboxylate ligands and the N atoms of 2,2'-bipyridine. A nitrate ligand completes the coordination environment of the eight coordinated Bi atom (Fig. 1). The Bi atom is in a distorted pentagonal bipyramid environment, with atoms S1 and O2 in axial positions, and atoms S2, S3, S4, N3 and N4 in the equatorial plane. The remaining O atom (O1) of the nitrate ligand caps the O2/S2/N3 face of this pentagonal bipyramid, giving a highly distorted capped pentagonal bipyramid coordination geometry. One of the bidentate pyrrolidine-1-dithiocarboxylate ligands forms a significantly longer Bi—S bond [Bi1—S4 = 2.900 (4) Å] than the others in the complex. This variation in coordination strength is also signalled by the fact that the C6—S4 bond is significantly shorter than the other C—S bonds, suggesting some delocalization in the system. In addition, the chelating phenanthroline ligands are bonded to the Bi atom through two N atoms. The Bi1—N3 and Bi1—N4 distances fall in the same range as in other Bi/N complexes (Baraanyi *et al.*, 1977).

## Experimental

To an aqueous solution of $Bi(NO_3)_35H_2O$ (2.0 mmol) and mannite (2.0 mmol) was added another aqueous solution of sodium pyrrolidine-1-dithiocarboxylate (4.0 mmol) and 2,2'-bipyridine (2.0 mmol). The resulted solution was stirred for 2 h at 298 K, and then yellow solid was obtained by filtration. The solid was recrystallized from ethanol and yellow crystals of (I) were formed.

## Refinement

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

## Figures

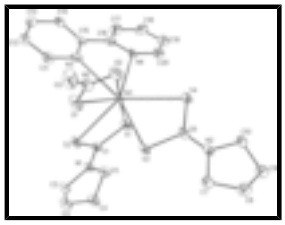


Fig. 1. The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering schemes. H atoms have been omitted for clarity.

## (2,2'-Bipyridine-κ$^2$*N*,*N*')(nitrato-κ$^2$*O*,*O*')bis(pyrrolidine-1- dithiocarboxylato-κ$^2$*S*,*S*')bismuth(III)

*Crystal data*

| | |
|---|---|
| $[Bi(C_4H_8NS_2)_2(NO_3)(C_{10}H_8N_2)]$ | $Z = 2$ |
| $M_r = 719.66$ | $F_{000} = 700$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.887$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 9.565$ (4) Å | Cell parameters from 3168 reflections |
| $b = 10.171$ (4) Å | $\theta = 2.2$–$27.3$º |
| $c = 14.555$ (5) Å | $\mu = 7.32$ mm$^{-1}$ |
| $\alpha = 73.634$ (4)º | $T = 298$ (2) K |
| $\beta = 76.032$ (4)º | Block, yellow |
| $\gamma = 70.916$ (4)º | 0.28 × 0.24 × 0.22 mm |
| $V = 1266.5$ (8) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 4305 independent reflections |
| Radiation source: fine-focus sealed tube | 3408 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.048$ |
| $T = 298$(2) K | $\theta_{max} = 25.0$º |
| φ and ω scans | $\theta_{min} = 2.2$º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -11 \rightarrow 11$ |
| $T_{min} = 0.149$, $T_{max} = 0.212$ | $k = -12 \rightarrow 11$ |
| 6375 measured reflections | $l = -17 \rightarrow 17$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | H-atom parameters constrained |
| $wR(F^2) = 0.163$ | $w = 1/[\sigma^2(F_o^2) + (0.0971P)^2]$ |

| | |
|---|---|
| | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.99$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 4305 reflections | $\Delta\rho_{max} = 2.34$ e Å$^{-3}$ |
| 280 parameters | $\Delta\rho_{min} = -5.28$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Bi1 | 0.23149 (5) | 0.12616 (4) | 0.76237 (3) | 0.03393 (19) |
| N1 | 0.1198 (11) | 0.1522 (10) | 0.4758 (7) | 0.039 (2) |
| N2 | 0.4937 (11) | 0.4557 (10) | 0.6654 (7) | 0.039 (2) |
| N3 | 0.0613 (13) | −0.0558 (13) | 0.8613 (7) | 0.051 (3) |
| N4 | −0.0642 (12) | 0.2242 (10) | 0.8629 (7) | 0.038 (2) |
| N5 | 0.4987 (12) | −0.1193 (12) | 0.8582 (8) | 0.045 (3) |
| O1 | 0.4437 (13) | −0.1199 (11) | 0.7882 (8) | 0.065 (3) |
| O2 | 0.4517 (13) | −0.0073 (12) | 0.8887 (7) | 0.065 (3) |
| O3 | 0.5935 (13) | −0.2224 (11) | 0.8937 (9) | 0.076 (3) |
| S1 | 0.0555 (4) | 0.2701 (4) | 0.6269 (2) | 0.0454 (8) |
| S2 | 0.2802 (4) | −0.0071 (3) | 0.6127 (2) | 0.0426 (8) |
| S3 | 0.4664 (4) | 0.2134 (4) | 0.6517 (3) | 0.0509 (9) |
| S4 | 0.2474 (4) | 0.3986 (4) | 0.7783 (3) | 0.0541 (9) |
| C1 | 0.1489 (12) | 0.1406 (12) | 0.5627 (8) | 0.033 (3) |
| C2 | 0.2027 (15) | 0.0460 (15) | 0.4155 (9) | 0.047 (3) |
| H2A | 0.1917 | −0.0482 | 0.4486 | 0.057* |
| H2B | 0.3085 | 0.0412 | 0.3989 | 0.057* |
| C3 | 0.126 (2) | 0.105 (2) | 0.3250 (12) | 0.074 (5) |
| H3A | 0.1995 | 0.0915 | 0.2670 | 0.088* |
| H3B | 0.0512 | 0.0575 | 0.3298 | 0.088* |
| C4 | 0.057 (2) | 0.2562 (18) | 0.3221 (11) | 0.078 (5) |
| H4A | −0.0297 | 0.2904 | 0.2896 | 0.093* |
| H4B | 0.1277 | 0.3104 | 0.2869 | 0.093* |
| C5 | 0.0100 (15) | 0.2742 (16) | 0.4259 (9) | 0.052 (4) |
| H5A | 0.0180 | 0.3642 | 0.4313 | 0.062* |
| H5B | −0.0918 | 0.2683 | 0.4514 | 0.062* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.4078 (15) | 0.3696 (13) | 0.6979 (9) | 0.042 (3) |
| C7 | 0.6380 (16) | 0.4308 (14) | 0.6002 (12) | 0.0552 (19) |
| H7A | 0.6247 | 0.4349 | 0.5354 | 0.066* |
| H7B | 0.7050 | 0.3388 | 0.6243 | 0.066* |
| C8 | 0.6979 (16) | 0.5501 (14) | 0.6004 (11) | 0.0552 (19) |
| H8A | 0.7632 | 0.5200 | 0.6486 | 0.066* |
| H8B | 0.7538 | 0.5811 | 0.5372 | 0.066* |
| C9 | 0.5667 (16) | 0.6638 (14) | 0.6241 (11) | 0.0552 (19) |
| H9A | 0.5292 | 0.7238 | 0.5654 | 0.066* |
| H9B | 0.5915 | 0.7224 | 0.6566 | 0.066* |
| C10 | 0.4503 (16) | 0.5946 (14) | 0.6899 (11) | 0.0552 (19) |
| H10A | 0.4537 | 0.5847 | 0.7576 | 0.066* |
| H10B | 0.3503 | 0.6490 | 0.6767 | 0.066* |
| C11 | 0.1268 (17) | −0.1947 (15) | 0.8675 (10) | 0.054 (4) |
| H11 | 0.2276 | −0.2237 | 0.8410 | 0.065* |
| C12 | 0.0511 (19) | −0.2988 (15) | 0.9121 (9) | 0.055 (4) |
| H12 | 0.1009 | −0.3950 | 0.9159 | 0.066* |
| C13 | −0.0973 (18) | −0.2565 (16) | 0.9498 (10) | 0.056 (4) |
| H13 | −0.1509 | −0.3234 | 0.9789 | 0.068* |
| C14 | −0.1677 (16) | −0.1112 (14) | 0.9441 (9) | 0.049 (3) |
| H14 | −0.2676 | −0.0797 | 0.9718 | 0.059* |
| C15 | −0.0852 (14) | −0.0156 (13) | 0.8964 (8) | 0.037 (3) |
| C16 | −0.1560 (14) | 0.1400 (14) | 0.8881 (8) | 0.038 (3) |
| C17 | −0.3107 (15) | 0.2003 (16) | 0.9061 (10) | 0.057 (4) |
| H17 | −0.3740 | 0.1418 | 0.9215 | 0.069* |
| C18 | −0.3706 (17) | 0.3411 (16) | 0.9016 (11) | 0.064 (5) |
| H18 | −0.4741 | 0.3797 | 0.9140 | 0.077* |
| C19 | −0.2774 (15) | 0.4260 (14) | 0.8787 (10) | 0.051 (4) |
| H19 | −0.3148 | 0.5231 | 0.8771 | 0.062* |
| C20 | −0.1275 (16) | 0.3639 (15) | 0.8580 (10) | 0.050 (3) |
| H20 | −0.0644 | 0.4229 | 0.8391 | 0.060* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Bi1 | 0.0336 (3) | 0.0278 (3) | 0.0343 (3) | 0.00256 (18) | 0.00025 (18) | −0.01551 (18) |
| N1 | 0.036 (6) | 0.039 (6) | 0.032 (6) | 0.004 (5) | −0.002 (4) | −0.012 (4) |
| N2 | 0.030 (5) | 0.029 (6) | 0.050 (6) | 0.003 (5) | 0.009 (5) | −0.023 (5) |
| N3 | 0.056 (8) | 0.061 (8) | 0.029 (6) | −0.014 (6) | 0.007 (5) | −0.015 (5) |
| N4 | 0.041 (6) | 0.028 (6) | 0.036 (6) | 0.004 (5) | 0.000 (5) | −0.017 (4) |
| N5 | 0.034 (6) | 0.043 (7) | 0.049 (7) | −0.003 (5) | 0.005 (5) | −0.017 (5) |
| O1 | 0.076 (7) | 0.060 (7) | 0.065 (7) | 0.003 (5) | −0.032 (6) | −0.034 (5) |
| O2 | 0.084 (8) | 0.062 (7) | 0.049 (6) | −0.010 (6) | −0.010 (5) | −0.025 (5) |
| O3 | 0.070 (8) | 0.047 (7) | 0.099 (9) | 0.020 (6) | −0.044 (7) | −0.016 (6) |
| S1 | 0.0452 (19) | 0.0365 (18) | 0.0375 (17) | 0.0169 (14) | −0.0010 (14) | −0.0202 (14) |
| S2 | 0.051 (2) | 0.0252 (16) | 0.0432 (18) | 0.0126 (14) | −0.0111 (15) | −0.0183 (13) |
| S3 | 0.0430 (19) | 0.043 (2) | 0.062 (2) | −0.0057 (16) | 0.0204 (16) | −0.0368 (17) |
| S4 | 0.0420 (19) | 0.050 (2) | 0.067 (2) | −0.0104 (17) | 0.0253 (17) | −0.0395 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.024 (6) | 0.034 (7) | 0.032 (6) | 0.001 (5) | 0.003 (5) | −0.009 (5) |
| C2 | 0.048 (8) | 0.050 (9) | 0.043 (8) | −0.005 (7) | 0.003 (6) | −0.029 (6) |
| C3 | 0.081 (12) | 0.091 (14) | 0.052 (10) | −0.011 (10) | −0.009 (9) | −0.037 (9) |
| C4 | 0.115 (16) | 0.064 (12) | 0.054 (10) | −0.001 (11) | −0.039 (10) | −0.021 (8) |
| C5 | 0.040 (8) | 0.062 (10) | 0.045 (8) | −0.003 (7) | −0.014 (6) | −0.005 (7) |
| C6 | 0.042 (7) | 0.028 (7) | 0.044 (7) | 0.011 (6) | 0.002 (6) | −0.019 (5) |
| C7 | 0.045 (4) | 0.036 (4) | 0.070 (5) | 0.002 (3) | 0.010 (4) | −0.019 (3) |
| C8 | 0.045 (4) | 0.036 (4) | 0.070 (5) | 0.002 (3) | 0.010 (4) | −0.019 (3) |
| C9 | 0.045 (4) | 0.036 (4) | 0.070 (5) | 0.002 (3) | 0.010 (4) | −0.019 (3) |
| C10 | 0.045 (4) | 0.036 (4) | 0.070 (5) | 0.002 (3) | 0.010 (4) | −0.019 (3) |
| C11 | 0.054 (9) | 0.046 (9) | 0.056 (9) | 0.000 (7) | −0.002 (7) | −0.021 (7) |
| C12 | 0.093 (12) | 0.039 (8) | 0.039 (8) | −0.025 (8) | −0.012 (8) | −0.008 (6) |
| C13 | 0.065 (10) | 0.058 (10) | 0.048 (9) | −0.029 (8) | 0.002 (7) | −0.010 (7) |
| C14 | 0.050 (8) | 0.046 (9) | 0.048 (8) | −0.007 (7) | 0.011 (6) | −0.028 (6) |
| C15 | 0.038 (7) | 0.045 (8) | 0.026 (6) | −0.003 (6) | 0.002 (5) | −0.022 (5) |
| C16 | 0.039 (7) | 0.046 (8) | 0.023 (6) | −0.009 (6) | −0.002 (5) | −0.004 (5) |
| C17 | 0.031 (7) | 0.061 (10) | 0.063 (10) | −0.002 (7) | −0.001 (7) | −0.005 (7) |
| C18 | 0.038 (8) | 0.048 (9) | 0.070 (11) | 0.005 (7) | 0.005 (7) | 0.011 (8) |
| C19 | 0.045 (8) | 0.030 (7) | 0.056 (9) | 0.020 (6) | −0.006 (7) | −0.013 (6) |
| C20 | 0.046 (8) | 0.049 (9) | 0.045 (8) | −0.004 (7) | 0.005 (6) | −0.016 (6) |

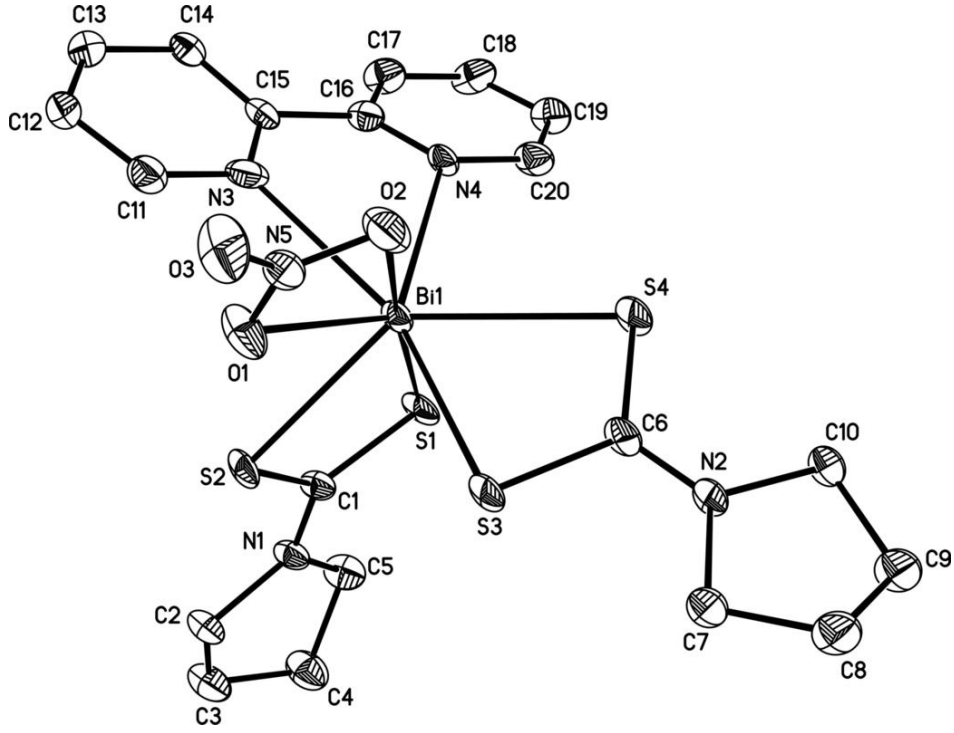
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Bi1—O1 | 2.653 (10) | C4—H4B | 0.9700 |
| Bi1—S3 | 2.680 (3) | C5—H5A | 0.9700 |
| Bi1—S1 | 2.688 (3) | C5—H5B | 0.9700 |
| Bi1—N3 | 2.736 (11) | C7—C8 | 1.503 (19) |
| Bi1—S2 | 2.749 (3) | C7—H7A | 0.9700 |
| Bi1—S4 | 2.900 (4) | C7—H7B | 0.9700 |
| N1—C1 | 1.326 (14) | C8—C9 | 1.448 (18) |
| N1—C5 | 1.475 (15) | C8—H8A | 0.9700 |
| N1—C2 | 1.484 (16) | C8—H8B | 0.9700 |
| N2—C6 | 1.309 (16) | C9—C10 | 1.507 (18) |
| N2—C10 | 1.458 (16) | C9—H9A | 0.9700 |
| N2—C7 | 1.464 (16) | C9—H9B | 0.9700 |
| N3—C11 | 1.331 (17) | C10—H10A | 0.9700 |
| N3—C15 | 1.338 (16) | C10—H10B | 0.9700 |
| N4—C20 | 1.338 (16) | C11—C12 | 1.398 (18) |
| N4—C16 | 1.341 (15) | C11—H11 | 0.9300 |
| N5—O3 | 1.220 (13) | C12—C13 | 1.36 (2) |
| N5—O2 | 1.245 (14) | C12—H12 | 0.9300 |
| N5—O1 | 1.257 (14) | C13—C14 | 1.397 (19) |
| S1—C1 | 1.711 (12) | C13—H13 | 0.9300 |
| S2—C1 | 1.719 (12) | C14—C15 | 1.381 (17) |
| S3—C6 | 1.768 (13) | C14—H14 | 0.9300 |
| S4—C6 | 1.686 (13) | C15—C16 | 1.486 (17) |
| C2—C3 | 1.54 (2) | C16—C17 | 1.395 (19) |
| C2—H2A | 0.9700 | C17—C18 | 1.35 (2) |
| C2—H2B | 0.9700 | C17—H17 | 0.9300 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.45 (2) | C18—C19 | 1.36 (2) |
| C3—H3A | 0.9700 | C18—H18 | 0.9300 |
| C3—H3B | 0.9700 | C19—C20 | 1.361 (19) |
| C4—C5 | 1.51 (2) | C19—H19 | 0.9300 |
| C4—H4A | 0.9700 | C20—H20 | 0.9300 |
| O1—Bi1—S3 | 80.9 (3) | H5A—C5—H5B | 109.3 |
| O1—Bi1—S1 | 135.0 (2) | N2—C6—S4 | 124.8 (10) |
| S3—Bi1—S1 | 92.34 (12) | N2—C6—S3 | 116.4 (9) |
| O1—Bi1—N3 | 79.5 (4) | S4—C6—S3 | 118.8 (8) |
| S3—Bi1—N3 | 158.8 (3) | N2—C7—C8 | 103.9 (11) |
| S1—Bi1—N3 | 95.9 (3) | N2—C7—H7A | 111.0 |
| O1—Bi1—S2 | 69.1 (2) | C8—C7—H7A | 111.0 |
| S3—Bi1—S2 | 80.63 (11) | N2—C7—H7B | 111.0 |
| S1—Bi1—S2 | 65.96 (10) | C8—C7—H7B | 111.0 |
| N3—Bi1—S2 | 85.0 (2) | H7A—C7—H7B | 109.0 |
| O1—Bi1—S4 | 126.4 (2) | C9—C8—C7 | 105.1 (12) |
| S3—Bi1—S4 | 64.27 (9) | C9—C8—H8A | 110.7 |
| S1—Bi1—S4 | 87.93 (12) | C7—C8—H8A | 110.7 |
| N3—Bi1—S4 | 135.3 (3) | C9—C8—H8B | 110.7 |
| S2—Bi1—S4 | 135.41 (10) | C7—C8—H8B | 110.7 |
| C1—N1—C5 | 124.5 (11) | H8A—C8—H8B | 108.8 |
| C1—N1—C2 | 122.7 (10) | C8—C9—C10 | 107.1 (11) |
| C5—N1—C2 | 112.7 (10) | C8—C9—H9A | 110.3 |
| C6—N2—C10 | 121.8 (10) | C10—C9—H9A | 110.3 |
| C6—N2—C7 | 126.6 (11) | C8—C9—H9B | 110.3 |
| C10—N2—C7 | 111.6 (10) | C10—C9—H9B | 110.3 |
| C11—N3—C15 | 117.6 (12) | H9A—C9—H9B | 108.5 |
| C11—N3—Bi1 | 117.1 (9) | N2—C10—C9 | 102.9 (10) |
| C15—N3—Bi1 | 125.0 (9) | N2—C10—H10A | 111.2 |
| C20—N4—C16 | 117.3 (11) | C9—C10—H10A | 111.2 |
| O3—N5—O2 | 122.0 (12) | N2—C10—H10B | 111.2 |
| O3—N5—O1 | 121.8 (12) | C9—C10—H10B | 111.2 |
| O2—N5—O1 | 116.3 (11) | H10A—C10—H10B | 109.1 |
| N5—O1—Bi1 | 104.5 (8) | N3—C11—C12 | 123.1 (14) |
| C1—S1—Bi1 | 88.3 (4) | N3—C11—H11 | 118.5 |
| C1—S2—Bi1 | 86.2 (4) | C12—C11—H11 | 118.5 |
| C6—S3—Bi1 | 91.2 (4) | C13—C12—C11 | 118.7 (15) |
| C6—S4—Bi1 | 85.7 (5) | C13—C12—H12 | 120.7 |
| N1—C1—S1 | 120.8 (9) | C11—C12—H12 | 120.7 |
| N1—C1—S2 | 119.9 (9) | C12—C13—C14 | 119.0 (13) |
| S1—C1—S2 | 119.3 (7) | C12—C13—H13 | 120.5 |
| N1—C2—C3 | 102.5 (11) | C14—C13—H13 | 120.5 |
| N1—C2—H2A | 111.3 | C15—C14—C13 | 118.4 (13) |
| C3—C2—H2A | 111.3 | C15—C14—H14 | 120.8 |
| N1—C2—H2B | 111.3 | C13—C14—H14 | 120.8 |
| C3—C2—H2B | 111.3 | N3—C15—C14 | 123.1 (12) |
| H2A—C2—H2B | 109.2 | N3—C15—C16 | 116.6 (11) |
| C4—C3—C2 | 105.9 (13) | C14—C15—C16 | 120.1 (11) |
| C4—C3—H3A | 110.6 | N4—C16—C17 | 119.6 (13) |

| | | | |
|---|---|---|---|
| C2—C3—H3A | 110.6 | N4—C16—C15 | 117.3 (11) |
| C4—C3—H3B | 110.6 | C17—C16—C15 | 123.2 (12) |
| C2—C3—H3B | 110.6 | C18—C17—C16 | 121.6 (14) |
| H3A—C3—H3B | 108.7 | C18—C17—H17 | 119.2 |
| C3—C4—C5 | 107.5 (12) | C16—C17—H17 | 119.2 |
| C3—C4—H4A | 110.2 | C17—C18—C19 | 118.9 (14) |
| C5—C4—H4A | 110.2 | C17—C18—H18 | 120.6 |
| C3—C4—H4B | 110.2 | C19—C18—H18 | 120.6 |
| C5—C4—H4B | 110.2 | C18—C19—C20 | 117.7 (14) |
| H4A—C4—H4B | 108.5 | C18—C19—H19 | 121.1 |
| N1—C5—C4 | 101.8 (12) | C20—C19—H19 | 121.1 |
| N1—C5—H5A | 111.4 | N4—C20—C19 | 124.9 (13) |
| C4—C5—H5A | 111.4 | N4—C20—H20 | 117.6 |
| N1—C5—H5B | 111.4 | C19—C20—H20 | 117.6 |
| C4—C5—H5B | 111.4 | | |

**Fig. 1**


C13
C14
C17
C18
C15
C16
C19
C12
C11
N3
N4
C20
O2
N5
O3
Bi1
S4
O1
S1
C6
C10
S2
C1
N2
S3
N1
C5
C9
C2
C7
C8
C3
C4