# metal-organic compounds

# 6-Cyclohexyl-6,7-dihydrodibenzo-[c,f][1,5]azabismocin-12(5H)-yl(N→Bi) trifluoromethanesulfonate

## Nianyuan Tan[a]* and Xiaowen Zhang[b]*

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In the title compound, $[Bi(C_{20}H_{23}N)(CF_3SO_3)]$, the $Bi^{III}$ ion shows a distorted pseudo-trigonal–bipyramidal geometry, with two C atoms and a lone electron pair of the Bi atom in equatorial positions and the N and O atoms at the apical positions. The cyclohexyl group is disordered over two orientations with site-occupancy factors of 0.600 (14) and 0.400 (14).

## Related literature

For the synthesis of 12-chloro-6-cyclohexyl-5,6,7,12-tetra-hydrodibenzo[c,f][1,5]azabismocine, see: Zhang *et al.* (2009). For general background to the use of organobismuth compounds in catalysis, organic synthesis and medicine, see: Shimada *et al.* (2004); Kotani *et al.* (2005); Yin *et al.* (2008); Zhang *et al.* (2010). For related structures, see: Ohkata *et al.* (1989); Minoura *et al.* (1999).
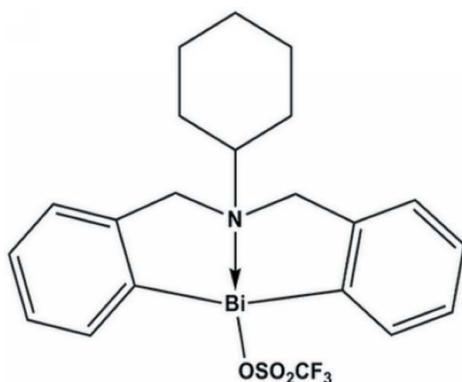


## Experimental

### Crystal data

| | |
|---|---|
| $[Bi(C_{20}H_{23}N)(CF_3O_3S)]$ | $V$ = 4375.2 (7) Å$^3$ |
| $M_r$ = 635.44 | $Z$ = 8 |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| $a$ = 12.6932 (13) Å | $\mu$ = 8.20 mm$^{-1}$ |
| $b$ = 15.0000 (14) Å | $T$ = 293 K |
| $c$ = 23.037 (2) Å | $0.31 \times 0.28 \times 0.11$ mm |
| $\beta$ = 94.040 (2)° | |

### Data collection

| | |
|---|---|
| Bruker SMART CCD diffractometer | 10954 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999) | 3860 independent reflections |
| $T_{min}$ = 0.314, $T_{max}$ = 1.000 | 2920 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.058 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.048 | 72 restraints |
| $wR(F^2)$ = 0.116 | H-atom parameters constrained |
| $S$ = 0.96 | $\Delta\rho_{max}$ = 1.81 e Å$^{-3}$ |
| 3860 reflections | $\Delta\rho_{min}$ = −1.70 e Å$^{-3}$ |
| 305 parameters | |

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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# supporting information

# 6-Cyclohexyl-6,7-dihydrodibenzo[*c,f*][1,5]azabismocin-12(5*H*)-yl(N→Bi) trifluoromethanesulfonate

**Nianyuan Tan and Xiaowen Zhang**

### S1. Comment

The utilization of organobismuth compounds in the field of catalysis, organic synthesis and medicine has been studied intensively in recent years (Shimada *et al.*, 2004; Kotani *et al.*, 2005; Yin *et al.*, 2008; Zhang, Qiu *et al.*, 2010). The 5,6,7,12-tetrahydrodibenz[c,f][1,5]azabismocine framework is highly stable as a organobismuth Fragment because the weakly coordination exists between bismuth and nitrogen atoms on 1,5-azabismocine (Ohkata *et al.*,1989; Minoura *et al.*,1999), and therefore, is suitable for the study of organobismuth compounds bearing various groups on the bismuth atom.

In the present paper, we report the crystal structure of the title compound (Fig. 1). The central bismuth-containing part of the complex exhibits a distorted pseudo trigonal-bipyramidal structure. The C (8), C (1) atoms and a lone electron pair of the Bi atom exist at the equatorial positions while the N (1) and O (1) atoms are located at the apical positions. The Bi-C (8) and Bi-C (1) distance is 2.216 (9) Å and 2.219 (9) Å, respectively. The C (8)-Bi-C (1) angle is 96.3 (3) ° while the N (1)-Bi-O (1) angle is 151.7 (2)°(rather than 180°). The Bi-N (1) distance (2.430 (6) Å) is shorter than 2.517 (4) Å of the precursor, $C_6H_{11}N(CH_2C_6H_4)_2BiCl$ (Zhang, Xia, Yan *et al.*, 2009). The cyclohexyl group is disordered over two positions with site-occupancy factors of 0.600 (14) (for atom labelled A) and 0.400 (14) (for atom labelled B) in Fig. 1.

### S2. Experimental

The following procedures are recommended for synthesis of the title compound (I):12-chloro-6-cyclohexyl-5,6,7,12-tetrahydrodibenzo[c,f][1,5]azabismocine (0.522 g, 1.0 mmol) was dissolved in 15 ml THF, then a solution of $AgOSO_2CF_3$ (0.257 g, 1.0 mmol) in 10.0 ml THF was added. After the mixture was stirred in the dark at room temperature for 3 h, it was filtered. The filtrate mixed with 1.0 ml hexane was refrigerated for 24 h, giving colorless crystals (0.610 g, 96.0%).

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C-H = 0.93 Å for aryl, 0.98 Å methine and 0.97 Å for methylene H atoms, respectively. $U_{iso}(H)= 1.2U_{eq}(C)$ for all H atoms. The cyclohexyl group was found to be disordered over two positions and modelled with site-occupancy factors, from refinement of 0.600 (14) (part A) and 0.400 (14) (part B), respectively. The displacement ellipsoids of disordered cyclohexyl group were restrained using command ISOR (0.01), both sets of C atoms were restrained using the command DELU and the distances of C–C were restrained to ±1.480 (2) Å using command DFIX.
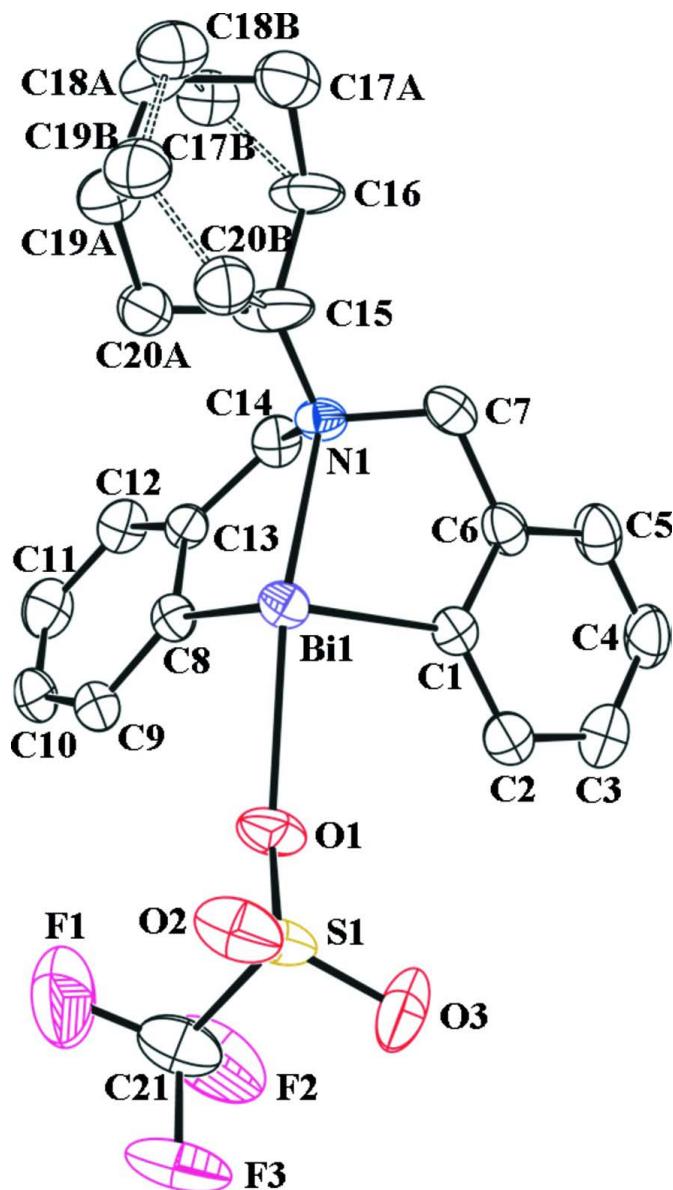
**Figure 1**

The molecular structure of the title compound with atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. All hydrogen atoms are omitted for clarity. The cyclohexyl group was found to be disordered over two positions and modelled with site-occupancy factors, from refinement of 0.600 (14)(Part A) and 0.400 (14)(Part B).

**6-Cyclohexyl-6,7-dihydrodibenzo[*c*,*f*][1,5]azabismocin- 12(5*H*)-yl(N→ Bi) trifluoromethanesulfonate**

*Crystal data*
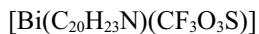
| | |
|---|---|
| [Bi(C$_{20}$H$_{23}$N)(CF$_3$O$_3$S)] | $\beta$ = 94.040 (2)° |
| $M_r$ = 635.44 | $V$ = 4375.2 (7) Å$^3$ |
| Monoclinic, *C*2/*c* | $Z$ = 8 |
| Hall symbol: -C 2yc | $F(000)$ = 2448 |
| $a$ = 12.6932 (13) Å | $D_x$ = 1.929 Mg m$^{-3}$ |
| $b$ = 15.0000 (14) Å | Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å |
| $c$ = 23.037 (2) Å | Cell parameters from 3301 reflections |

$\theta = 4.7–47.8°$
$\mu = 8.20$ mm$^{-1}$
$T = 293$ K

Prismatic, colorless
$0.31 \times 0.28 \times 0.11$ mm

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 10954 measured reflections |
| Radiation source: fine-focus sealed tube | 3860 independent reflections |
| Graphite monochromator | 2920 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.00 pixels mm$^{-1}$ | $R_{int} = 0.058$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999) | $h = -10 \rightarrow 15$ |
| | $k = -15 \rightarrow 17$ |
| $T_{min} = 0.314$, $T_{max} = 1.000$ | $l = -26 \rightarrow 27$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.116$ | H-atom parameters constrained |
| $S = 0.96$ | $w = 1/[\sigma^2(F_o^2) + (0.0687P)^2]$ |
| 3860 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 305 parameters | $(\Delta/\sigma)_{max} = 0.001$ |
| 72 restraints | $\Delta\rho_{max} = 1.81$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -1.70$ 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.

**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$^2$ > 2sigma(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) |
|---|---|---|---|---|---|
| Bi1 | 0.50647 (3) | 0.51740 (2) | 0.607770 (13) | 0.04553 (15) | |
| S1 | 0.4571 (2) | 0.75730 (17) | 0.59130 (13) | 0.0719 (8) | |
| F1 | 0.4536 (10) | 0.8079 (8) | 0.6932 (3) | 0.180 (5) | |
| F2 | 0.5912 (7) | 0.8544 (6) | 0.6476 (5) | 0.155 (4) | |
| F3 | 0.4435 (7) | 0.9161 (4) | 0.6299 (4) | 0.133 (3) | |
| O1 | 0.5181 (6) | 0.6821 (5) | 0.6099 (3) | 0.074 (2) | |
| O2 | 0.3476 (6) | 0.7462 (5) | 0.5879 (4) | 0.090 (2) | |
| O3 | 0.5008 (9) | 0.8007 (7) | 0.5390 (3) | 0.123 (3) | |
| N1 | 0.5872 (6) | 0.3705 (4) | 0.6105 (3) | 0.0472 (17) | |
| C1 | 0.6305 (7) | 0.5246 (5) | 0.5447 (3) | 0.042 (2) | |
| C2 | 0.6739 (8) | 0.6024 (7) | 0.5219 (4) | 0.058 (2) | |
| H2 | 0.6487 | 0.6582 | 0.5317 | 0.069* | |
| C3 | 0.7538 (9) | 0.5950 (8) | 0.4850 (4) | 0.075 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H3 | 0.7822 | 0.6464 | 0.4698 | 0.089* | |
| C4 | 0.7925 (11) | 0.5138 (8) | 0.4702 (5) | 0.078 (3) | |
| H4 | 0.8469 | 0.5102 | 0.4453 | 0.093* | |
| C5 | 0.7505 (9) | 0.4373 (8) | 0.4923 (4) | 0.069 (3) | |
| H5 | 0.7773 | 0.3819 | 0.4828 | 0.083* | |
| C6 | 0.6697 (8) | 0.4428 (6) | 0.5283 (4) | 0.055 (2) | |
| C7 | 0.6192 (8) | 0.3583 (6) | 0.5508 (4) | 0.056 (2) | |
| H7A | 0.5578 | 0.3428 | 0.5254 | 0.067* | |
| H7B | 0.6692 | 0.3094 | 0.5502 | 0.067* | |
| C8 | 0.6153 (7) | 0.5233 (5) | 0.6872 (4) | 0.046 (2) | |
| C9 | 0.6218 (7) | 0.5945 (6) | 0.7269 (4) | 0.056 (2) | |
| H9 | 0.5832 | 0.6464 | 0.7194 | 0.067* | |
| C10 | 0.6871 (9) | 0.5859 (8) | 0.7774 (4) | 0.066 (3) | |
| H10 | 0.6917 | 0.6326 | 0.8040 | 0.079* | |
| C11 | 0.7436 (10) | 0.5119 (8) | 0.7886 (5) | 0.075 (3) | |
| H11 | 0.7845 | 0.5069 | 0.8235 | 0.090* | |
| C12 | 0.7418 (8) | 0.4417 (7) | 0.7483 (4) | 0.060 (3) | |
| H12 | 0.7842 | 0.3918 | 0.7557 | 0.073* | |
| C13 | 0.6770 (7) | 0.4465 (6) | 0.6973 (3) | 0.047 (2) | |
| C14 | 0.6816 (7) | 0.3762 (6) | 0.6520 (3) | 0.055 (2) | |
| H14A | 0.7430 | 0.3870 | 0.6302 | 0.066* | |
| H14B | 0.6915 | 0.3190 | 0.6713 | 0.066* | |
| C15 | 0.5142 (7) | 0.2987 (5) | 0.6231 (4) | 0.097 (4) | |
| H15A | 0.4587 | 0.3044 | 0.5916 | 0.116* | 0.600 (14) |
| H15B | 0.5114 | 0.3276 | 0.6602 | 0.116* | 0.400 (14) |
| C16 | 0.5506 (7) | 0.2034 (5) | 0.6169 (4) | 0.091 (4) | |
| H16A | 0.5964 | 0.1872 | 0.6508 | 0.110* | 0.600 (14) |
| H16B | 0.5912 | 0.1985 | 0.5829 | 0.110* | 0.600 (14) |
| H16C | 0.6262 | 0.2053 | 0.6232 | 0.110* | 0.400 (14) |
| H16D | 0.5321 | 0.1815 | 0.5784 | 0.110* | 0.400 (14) |
| C17A | 0.4569 (13) | 0.1385 (12) | 0.6108 (7) | 0.080 (6) | 0.600 (14) |
| H17A | 0.4087 | 0.1546 | 0.5779 | 0.096* | 0.600 (14) |
| H17B | 0.4811 | 0.0779 | 0.6056 | 0.096* | 0.600 (14) |
| C18A | 0.4058 (17) | 0.1475 (11) | 0.6656 (8) | 0.078 (6) | 0.600 (14) |
| H18A | 0.4555 | 0.1314 | 0.6978 | 0.094* | 0.600 (14) |
| H18B | 0.3464 | 0.1067 | 0.6655 | 0.094* | 0.600 (14) |
| C19A | 0.3673 (15) | 0.2413 (10) | 0.6744 (9) | 0.078 (5) | 0.600 (14) |
| H19A | 0.3341 | 0.2448 | 0.7110 | 0.093* | 0.600 (14) |
| H19B | 0.3145 | 0.2563 | 0.6434 | 0.093* | 0.600 (14) |
| C20A | 0.4565 (12) | 0.3078 (10) | 0.6748 (6) | 0.062 (5) | 0.600 (14) |
| H20A | 0.4283 | 0.3677 | 0.6766 | 0.075* | 0.600 (14) |
| H20B | 0.5041 | 0.2983 | 0.7090 | 0.075* | 0.600 (14) |
| C17B | 0.506 (2) | 0.1385 (17) | 0.6610 (11) | 0.075 (7) | 0.400 (14) |
| H17C | 0.5259 | 0.1582 | 0.7004 | 0.090* | 0.400 (14) |
| H17D | 0.5353 | 0.0793 | 0.6560 | 0.090* | 0.400 (14) |
| C18B | 0.371 (2) | 0.136 (2) | 0.6490 (13) | 0.080 (8) | 0.400 (14) |
| H18C | 0.3509 | 0.1128 | 0.6105 | 0.096* | 0.400 (14) |
| H18D | 0.3401 | 0.0990 | 0.6777 | 0.096* | 0.400 (14) |

| | | | | | |
|------|------------|-------------|-------------|-----------|-------------|
| C19B | 0.337 (2) | 0.2284 (16) | 0.6540 (14) | 0.075 (7) | 0.400 (14) |
| H19C | 0.3388 | 0.2431 | 0.6950 | 0.090* | 0.400 (14) |
| H19D | 0.2643 | 0.2323 | 0.6385 | 0.090* | 0.400 (14) |
| C20B | 0.4007 (12) | 0.3000 (16) | 0.6236 (10) | 0.069 (7) | 0.400 (14) |
| H20C | 0.3733 | 0.3011 | 0.5832 | 0.083* | 0.400 (14) |
| H20D | 0.3823 | 0.3568 | 0.6403 | 0.083* | 0.400 (14) |
| C21 | 0.4911 (11) | 0.8380 (9) | 0.6433 (7) | 0.094 (4) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|-----------|-----------|-----------|-------------|--------------|--------------|
| Bi1 | 0.0379 (2) | 0.0445 (2) | 0.0536 (2) | 0.01047 (15) | −0.00109 (15) | −0.00054 (14) |
| S1 | 0.072 (2) | 0.0416 (14) | 0.098 (2) | 0.0118 (13) | −0.0229 (16) | −0.0123 (13) |
| F1 | 0.259 (14) | 0.205 (11) | 0.079 (5) | 0.037 (10) | 0.043 (7) | −0.006 (6) |
| F2 | 0.080 (6) | 0.144 (8) | 0.233 (10) | −0.015 (6) | −0.033 (6) | −0.093 (7) |
| F3 | 0.135 (7) | 0.045 (4) | 0.216 (9) | 0.011 (4) | −0.007 (6) | −0.032 (5) |
| O1 | 0.083 (6) | 0.046 (4) | 0.092 (5) | 0.024 (4) | −0.008 (4) | −0.004 (3) |
| O2 | 0.051 (5) | 0.070 (5) | 0.147 (7) | 0.001 (4) | 0.004 (5) | −0.024 (5) |
| O3 | 0.172 (10) | 0.140 (8) | 0.062 (5) | 0.011 (7) | 0.039 (5) | 0.035 (5) |
| N1 | 0.041 (5) | 0.038 (4) | 0.063 (4) | 0.007 (3) | 0.005 (3) | 0.001 (3) |
| C1 | 0.034 (5) | 0.050 (5) | 0.041 (4) | 0.010 (4) | −0.009 (4) | 0.000 (4) |
| C2 | 0.055 (7) | 0.062 (6) | 0.055 (5) | 0.009 (5) | −0.002 (5) | −0.002 (5) |
| C3 | 0.070 (8) | 0.096 (9) | 0.058 (6) | −0.002 (7) | 0.009 (6) | 0.011 (6) |
| C4 | 0.082 (9) | 0.096 (9) | 0.059 (6) | 0.018 (7) | 0.029 (6) | 0.002 (6) |
| C5 | 0.071 (8) | 0.082 (8) | 0.054 (6) | 0.027 (6) | 0.008 (5) | −0.003 (5) |
| C6 | 0.062 (7) | 0.058 (6) | 0.044 (5) | 0.020 (5) | −0.004 (4) | −0.006 (4) |
| C7 | 0.057 (6) | 0.049 (6) | 0.061 (5) | 0.011 (5) | 0.000 (5) | −0.012 (4) |
| C8 | 0.037 (5) | 0.053 (5) | 0.050 (5) | −0.001 (4) | 0.006 (4) | −0.003 (4) |
| C9 | 0.059 (7) | 0.058 (6) | 0.052 (5) | 0.002 (5) | 0.008 (5) | −0.005 (4) |
| C10 | 0.084 (8) | 0.074 (7) | 0.040 (5) | −0.004 (6) | 0.002 (5) | −0.014 (5) |
| C11 | 0.072 (8) | 0.099 (9) | 0.051 (6) | −0.005 (7) | −0.012 (6) | 0.007 (6) |
| C12 | 0.047 (6) | 0.074 (7) | 0.059 (6) | 0.015 (5) | −0.006 (5) | 0.014 (5) |
| C13 | 0.043 (5) | 0.047 (5) | 0.049 (5) | 0.009 (4) | 0.008 (4) | 0.006 (4) |
| C14 | 0.048 (6) | 0.062 (6) | 0.054 (5) | 0.016 (5) | −0.005 (4) | 0.007 (4) |
| C15 | 0.073 (9) | 0.037 (6) | 0.188 (13) | 0.001 (5) | 0.060 (9) | 0.002 (7) |
| C16 | 0.089 (9) | 0.033 (6) | 0.157 (12) | −0.002 (6) | 0.045 (8) | −0.009 (6) |
| C17A | 0.092 (10) | 0.063 (8) | 0.084 (8) | 0.001 (7) | 0.000 (7) | −0.004 (7) |
| C18A | 0.077 (10) | 0.063 (7) | 0.095 (9) | −0.019 (7) | 0.010 (8) | 0.012 (7) |
| C19A | 0.081 (9) | 0.067 (7) | 0.087 (10) | −0.014 (6) | 0.014 (8) | −0.001 (7) |
| C20A | 0.064 (8) | 0.057 (7) | 0.066 (8) | −0.002 (6) | 0.008 (7) | −0.006 (6) |
| C17B | 0.077 (9) | 0.067 (11) | 0.082 (11) | −0.004 (8) | 0.002 (9) | −0.001 (8) |
| C18B | 0.080 (10) | 0.069 (9) | 0.089 (12) | −0.012 (8) | −0.007 (9) | 0.001 (8) |
| C19B | 0.067 (10) | 0.070 (9) | 0.086 (12) | −0.011 (7) | 0.003 (9) | −0.002 (8) |
| C20B | 0.075 (11) | 0.063 (9) | 0.069 (10) | 0.007 (8) | 0.006 (8) | 0.006 (8) |
| C21 | 0.074 (10) | 0.068 (9) | 0.137 (13) | 0.003 (7) | −0.015 (9) | −0.028 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Bi1—C8 | 2.216 (9) | C13—C14 | 1.487 (12) |
| Bi1—C1 | 2.219 (9) | C14—H14A | 0.9700 |
| Bi1—N1 | 2.430 (6) | C14—H14B | 0.9700 |
| Bi1—O1 | 2.475 (7) | C15—C20B | 1.442 (13) |
| S1—O2 | 1.396 (8) | C15—C20A | 1.447 (11) |
| S1—O1 | 1.418 (7) | C15—C16 | 1.5127 |
| S1—O3 | 1.509 (8) | C15—H15A | 0.9800 |
| S1—C21 | 1.735 (12) | C15—H15B | 0.9600 |
| F1—C21 | 1.354 (16) | C16—C17A | 1.535 (15) |
| F2—C21 | 1.290 (14) | C16—C17B | 1.540 (17) |
| F3—C21 | 1.344 (14) | C16—H16A | 0.9700 |
| N1—C15 | 1.462 (10) | C16—H16B | 0.9700 |
| N1—C7 | 1.472 (10) | C16—H16C | 0.9600 |
| N1—C14 | 1.482 (10) | C16—H16D | 0.9600 |
| C1—C6 | 1.386 (12) | C17A—C18A | 1.465 (13) |
| C1—C2 | 1.408 (12) | C17A—H17A | 0.9700 |
| C2—C3 | 1.372 (14) | C17A—H17B | 0.9700 |
| C2—H2 | 0.9300 | C18A—C19A | 1.508 (18) |
| C3—C4 | 1.366 (14) | C18A—H18A | 0.9700 |
| C3—H3 | 0.9300 | C18A—H18B | 0.9700 |
| C4—C5 | 1.378 (16) | C19A—C20A | 1.508 (16) |
| C4—H4 | 0.9300 | C19A—H19A | 0.9700 |
| C5—C6 | 1.366 (13) | C19A—H19B | 0.9700 |
| C5—H5 | 0.9300 | C20A—H15B | 0.8483 |
| C6—C7 | 1.528 (13) | C20A—H20A | 0.9700 |
| C7—H7A | 0.9700 | C20A—H20B | 0.9700 |
| C7—H7B | 0.9700 | C17B—C18B | 1.72 (4) |
| C8—C9 | 1.403 (11) | C17B—H17C | 0.9700 |
| C8—C13 | 1.404 (12) | C17B—H17D | 0.9700 |
| C9—C10 | 1.386 (13) | C18B—C19B | 1.46 (4) |
| C9—H9 | 0.9300 | C18B—H18C | 0.9700 |
| C10—C11 | 1.337 (15) | C18B—H18D | 0.9700 |
| C10—H10 | 0.9300 | C19B—C20B | 1.54 (4) |
| C11—C12 | 1.404 (16) | C19B—H19C | 0.9700 |
| C11—H11 | 0.9300 | C19B—H19D | 0.9700 |
| C12—C13 | 1.387 (12) | C20B—H20C | 0.9700 |
| C12—H12 | 0.9300 | C20B—H20D | 0.9700 |
| | | | |
| C8—Bi1—C1 | 96.3 (3) | C15—C16—C17B | 114.1 (12) |
| C8—Bi1—N1 | 77.2 (3) | C17A—C16—C17B | 49.0 (13) |
| C1—Bi1—N1 | 75.1 (3) | C15—C16—H16A | 109.3 |
| C8—Bi1—O1 | 84.8 (3) | C17A—C16—H16A | 109.3 |
| C1—Bi1—O1 | 85.4 (3) | C17B—C16—H16A | 62.4 |
| N1—Bi1—O1 | 151.7 (2) | C15—C16—H16B | 109.3 |
| O2—S1—O1 | 116.3 (5) | C17A—C16—H16B | 109.3 |
| O2—S1—O3 | 115.3 (6) | C17B—C16—H16B | 136.3 |

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| O1—S1—O3 | 111.2 (5) | H16A—C16—H16B | 108.0 |
| O2—S1—C21 | 108.6 (6) | C15—C16—H16C | 105.4 |
| O1—S1—C21 | 104.0 (5) | C17A—C16—H16C | 142.4 |
| O3—S1—C21 | 99.3 (7) | C17B—C16—H16C | 109.0 |
| S1—O1—Bi1 | 139.2 (5) | H16A—C16—H16C | 49.6 |
| C15—N1—C7 | 108.3 (7) | H16B—C16—H16C | 62.8 |
| C15—N1—C14 | 114.1 (7) | C15—C16—H16D | 110.7 |
| C7—N1—C14 | 110.3 (7) | C17A—C16—H16D | 63.9 |
| C15—N1—Bi1 | 113.6 (5) | C17B—C16—H16D | 108.4 |
| C7—N1—Bi1 | 103.4 (5) | H16A—C16—H16D | 138.7 |
| C14—N1—Bi1 | 106.5 (5) | H16B—C16—H16D | 48.5 |
| C6—C1—C2 | 118.3 (9) | H16C—C16—H16D | 109.1 |
| C6—C1—Bi1 | 114.9 (7) | C18A—C17A—C16 | 104.5 (13) |
| C2—C1—Bi1 | 126.8 (6) | C18A—C17A—H16D | 140.6 |
| C3—C2—C1 | 119.3 (9) | C18A—C17A—H17A | 110.9 |
| C3—C2—H2 | 120.3 | C16—C17A—H17A | 110.9 |
| C1—C2—H2 | 120.3 | H16D—C17A—H17A | 83.4 |
| C4—C3—C2 | 121.4 (11) | C18A—C17A—H17B | 110.9 |
| C4—C3—H3 | 119.3 | C16—C17A—H17B | 110.9 |
| C2—C3—H3 | 119.3 | H16D—C17A—H17B | 97.6 |
| C3—C4—C5 | 119.7 (11) | H17A—C17A—H17B | 108.9 |
| C3—C4—H4 | 120.2 | C17A—C18A—C19A | 111.6 (15) |
| C5—C4—H4 | 120.2 | C17A—C18A—H18A | 109.3 |
| C6—C5—C4 | 120.0 (10) | C19A—C18A—H18A | 109.3 |
| C6—C5—H5 | 120.0 | C17A—C18A—H18B | 109.3 |
| C4—C5—H5 | 120.0 | C19A—C18A—H18B | 109.3 |
| C5—C6—C1 | 121.2 (10) | H18A—C18A—H18B | 108.0 |
| C5—C6—C7 | 120.5 (9) | C18A—C19A—C20A | 111.5 (16) |
| C1—C6—C7 | 118.3 (8) | C18A—C19A—H19A | 109.3 |
| N1—C7—C6 | 111.4 (7) | C20A—C19A—H19A | 109.3 |
| N1—C7—H7A | 109.4 | C18A—C19A—H19B | 109.3 |
| C6—C7—H7A | 109.4 | C20A—C19A—H19B | 109.3 |
| N1—C7—H7B | 109.4 | H19A—C19A—H19B | 108.0 |
| C6—C7—H7B | 109.4 | C15—C20A—C19A | 110.9 (12) |
| H7A—C7—H7B | 108.0 | C19A—C20A—H15B | 150.0 |
| C9—C8—C13 | 120.7 (8) | C15—C20A—H20A | 109.5 |
| C9—C8—Bi1 | 124.9 (7) | C19A—C20A—H20A | 109.5 |
| C13—C8—Bi1 | 114.3 (6) | H15B—C20A—H20A | 90.5 |
| C10—C9—C8 | 118.7 (9) | C15—C20A—H20B | 109.5 |
| C10—C9—H9 | 120.7 | C19A—C20A—H20B | 109.5 |
| C8—C9—H9 | 120.7 | H15B—C20A—H20B | 83.8 |
| C11—C10—C9 | 121.4 (9) | H20A—C20A—H20B | 108.0 |
| C11—C10—H10 | 119.3 | C16—C17B—C18B | 108.3 (19) |
| C9—C10—H10 | 119.3 | C16—C17B—H17C | 110.0 |
| C10—C11—C12 | 120.8 (10) | C18B—C17B—H17C | 110.0 |
| C10—C11—H11 | 119.6 | C16—C17B—H17D | 110.0 |
| C12—C11—H11 | 119.6 | C18B—C17B—H17D | 110.0 |
| C13—C12—C11 | 120.1 (10) | H17C—C17B—H17D | 108.4 |

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| C13—C12—H12 | 119.9 | C19B—C18B—C17B | 105 (2) |
| C11—C12—H12 | 119.9 | C19B—C18B—H18C | 110.7 |
| C12—C13—C8 | 118.2 (8) | C17B—C18B—H18C | 110.7 |
| C12—C13—C14 | 120.4 (8) | C19B—C18B—H18D | 110.7 |
| C8—C13—C14 | 121.0 (7) | C17B—C18B—H18D | 110.7 |
| N1—C14—C13 | 115.1 (7) | H18C—C18B—H18D | 108.8 |
| N1—C14—H14A | 108.5 | C18B—C19B—C20B | 117 (2) |
| C13—C14—H14A | 108.5 | C18B—C19B—H19C | 108.0 |
| N1—C14—H14B | 108.5 | C20B—C19B—H19C | 108.0 |
| C13—C14—H14B | 108.5 | C18B—C19B—H19D | 108.0 |
| H14A—C14—H14B | 107.5 | C20B—C19B—H19D | 108.0 |
| C20B—C15—C20A | 55.1 (11) | H19C—C19B—H19D | 107.2 |
| C20B—C15—N1 | 129.7 (11) | C15—C20B—C19B | 123.3 (16) |
| C20A—C15—N1 | 117.3 (9) | C15—C20B—H20C | 106.5 |
| C20B—C15—C16 | 109.0 (10) | C19B—C20B—H20C | 106.5 |
| C20A—C15—C16 | 110.0 (7) | C15—C20B—H20D | 106.5 |
| C20B—C15—H15A | 48.5 | C19B—C20B—H20D | 106.5 |
| C20A—C15—H15A | 102.8 | H20C—C20B—H20D | 106.5 |
| N1—C15—H15A | 102.8 | F2—C21—F3 | 106.1 (11) |
| C16—C15—H15A | 102.8 | F2—C21—F1 | 113.6 (13) |
| C20B—C15—H15B | 83.5 | F3—C21—F1 | 107.8 (12) |
| N1—C15—H15B | 84.8 | F2—C21—S1 | 112.5 (10) |
| C16—C15—H15B | 122.8 | F3—C21—S1 | 111.4 (9) |
| H15A—C15—H15B | 123.3 | F1—C21—S1 | 105.6 (10) |
| C15—C16—C17A | 111.6 (8) | | |
| | | | |
| O2—S1—O1—Bi1 | 28.9 (8) | C11—C12—C13—C8 | 0.9 (14) |
| O3—S1—O1—Bi1 | −105.8 (7) | C11—C12—C13—C14 | 174.6 (10) |
| C21—S1—O1—Bi1 | 148.2 (7) | C9—C8—C13—C12 | 2.1 (13) |
| C8—Bi1—O1—S1 | −153.4 (7) | Bi1—C8—C13—C12 | −175.4 (7) |
| C1—Bi1—O1—S1 | 109.8 (7) | C9—C8—C13—C14 | −171.7 (8) |
| N1—Bi1—O1—S1 | 156.2 (5) | Bi1—C8—C13—C14 | 10.9 (11) |
| C8—Bi1—N1—C15 | 111.1 (6) | C15—N1—C14—C13 | −100.6 (8) |
| C1—Bi1—N1—C15 | −148.8 (6) | C7—N1—C14—C13 | 137.1 (8) |
| O1—Bi1—N1—C15 | 163.0 (6) | Bi1—N1—C14—C13 | 25.6 (8) |
| C8—Bi1—N1—C7 | −131.7 (6) | C12—C13—C14—N1 | 159.8 (8) |
| C1—Bi1—N1—C7 | −31.6 (5) | C8—C13—C14—N1 | −26.6 (12) |
| O1—Bi1—N1—C7 | −79.8 (7) | C7—N1—C15—C20B | −101.8 (16) |
| C8—Bi1—N1—C14 | −15.4 (5) | C14—N1—C15—C20B | 134.9 (15) |
| C1—Bi1—N1—C14 | 84.7 (5) | Bi1—N1—C15—C20B | 12.5 (16) |
| O1—Bi1—N1—C14 | 36.5 (8) | C7—N1—C15—C20A | −167.8 (11) |
| C8—Bi1—C1—C6 | 90.0 (6) | C14—N1—C15—C20A | 69.0 (12) |
| N1—Bi1—C1—C6 | 15.1 (6) | Bi1—N1—C15—C20A | −53.4 (12) |
| O1—Bi1—C1—C6 | 174.3 (6) | C20B—C15—C16—C17A | 2.1 (11) |
| C8—Bi1—C1—C2 | −88.0 (8) | C20A—C15—C16—C17A | 60.9 (10) |
| N1—Bi1—C1—C2 | −162.9 (8) | N1—C15—C16—C17A | −160.4 (11) |
| O1—Bi1—C1—C2 | −3.7 (7) | C20B—C15—C16—C17B | −51.3 (16) |
| C6—C1—C2—C3 | −0.8 (13) | C20A—C15—C16—C17B | 7.5 (14) |

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| Bi1—C1—C2—C3 | 177.2 (7) | N1—C15—C16—C17B | 146.2 (16) |
| C1—C2—C3—C4 | −0.4 (16) | C15—C16—C17A—C18A | −62.4 (14) |
| C2—C3—C4—C5 | 0.3 (19) | C17B—C16—C17A—C18A | 41.3 (17) |
| C3—C4—C5—C6 | 0.9 (18) | C16—C17A—C18A—C19A | 61 (2) |
| C4—C5—C6—C1 | −2.0 (15) | C17A—C18A—C19A—C20A | −59 (2) |
| C4—C5—C6—C7 | 177.2 (10) | C20B—C15—C20A—C19A | 45.4 (14) |
| C2—C1—C6—C5 | 2.0 (13) | N1—C15—C20A—C19A | 166.5 (11) |
| Bi1—C1—C6—C5 | −176.2 (7) | C16—C15—C20A—C19A | −54.3 (14) |
| C2—C1—C6—C7 | −177.3 (8) | C18A—C19A—C20A—C15 | 54 (2) |
| Bi1—C1—C6—C7 | 4.6 (10) | C15—C16—C17B—C18B | 63 (2) |
| C15—N1—C7—C6 | 164.1 (7) | C17A—C16—C17B—C18B | −35.9 (16) |
| C14—N1—C7—C6 | −70.3 (9) | C16—C17B—C18B—C19B | −56 (3) |
| Bi1—N1—C7—C6 | 43.3 (8) | C17B—C18B—C19B—C20B | 44 (3) |
| C5—C6—C7—N1 | 145.0 (9) | C20A—C15—C20B—C19B | −64 (2) |
| C1—C6—C7—N1 | −35.8 (11) | N1—C15—C20B—C19B | −162.1 (19) |
| C1—Bi1—C8—C9 | 112.7 (7) | C16—C15—C20B—C19B | 38 (3) |
| N1—Bi1—C8—C9 | −174.1 (8) | C18B—C19B—C20B—C15 | −40 (4) |
| O1—Bi1—C8—C9 | 27.9 (7) | O2—S1—C21—F2 | −177.8 (11) |
| C1—Bi1—C8—C13 | −70.0 (7) | O1—S1—C21—F2 | 57.7 (13) |
| N1—Bi1—C8—C13 | 3.2 (6) | O3—S1—C21—F2 | −57.0 (12) |
| O1—Bi1—C8—C13 | −154.8 (6) | O2—S1—C21—F3 | −58.9 (12) |
| C13—C8—C9—C10 | −2.7 (13) | O1—S1—C21—F3 | 176.7 (10) |
| Bi1—C8—C9—C10 | 174.5 (7) | O3—S1—C21—F3 | 62.0 (12) |
| C8—C9—C10—C11 | 0.3 (15) | O2—S1—C21—F1 | 57.8 (11) |
| C9—C10—C11—C12 | 2.6 (18) | O1—S1—C21—F1 | −66.7 (10) |
| C10—C11—C12—C13 | −3.2 (17) | O3—S1—C21—F1 | 178.6 (10) |