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# Dimethyl(4′-pyridyl-2,2′:6′,2″-terpyridine-$\kappa^3N^1,N^{1'},N^{1''}$)bis(thiocyanato-$\kappa N$)-tin(IV)

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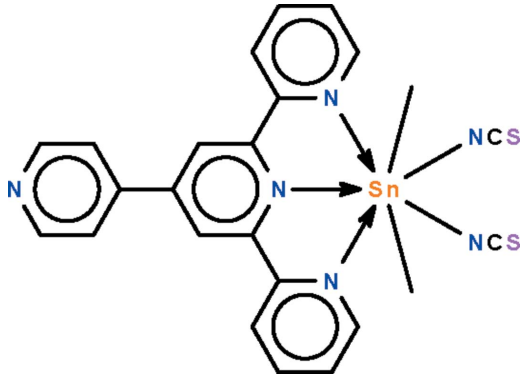
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.024; $wR$ factor = 0.060; data-to-parameter ratio = 17.2.

The Sn atom in the title compound, $[Sn(CH_3)_2(NCS)_2(C_{20}H_{14}N_4)]$, is $N,N',N''$-chelated by the terpyridine part of the $N$-heterocycle. The Sn atom exists in a *trans*-$C_2SnN_5$ pentagonal–bipyramidal geometry [C—Sn—C = 173.66 (8)°] with the methyl groups in axial and the N atoms in equatorial positions.

## Related literature

For the dimethyltin dichloride–terpyridine adduct, see: Naik & Scheidt (1973).




## Experimental

### Crystal data

$[Sn(CH_3)_2(NCS)_2(C_{20}H_{14}N_4)]$
$M_r$ = 575.27
Triclinic, $P\overline{1}$
$a$ = 9.3269 (3) Å
$b$ = 10.5017 (3) Å
$c$ = 13.1503 (4) Å
$\alpha$ = 66.814 (3)°
$\beta$ = 87.665 (3)°
$\gamma$ = 83.552 (2)°
$V$ = 1176.52 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.29 mm$^{-1}$
$T$ = 100 K
0.20 × 0.20 × 0.10 mm

### Data collection

Agilent Technologies SuperNova diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
$T_{min}$ = 0.783, $T_{max}$ = 0.882
15704 measured reflections
5168 independent reflections
4728 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.060
$S$ = 1.04
5168 reflections
300 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$

Data collection: *CrysAlis PRO* (Agilent Technologies, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5461).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m211 [ **doi:10.1107/S1600536811001309** ]

# Dimethyl(4'-pyridyl-2,2':6',2''-terpyridine-$\kappa^3N^1,N^{1'},N^{1''}$)bis(thiocyanato-$\kappa N$)tin(IV)

**E. Najafi, M. M. Amini and S. W. Ng**

## Comment

Diorganotin dihalides/pseudohalides form a number of adducts with terpyridine and its derivatives. The dimethyltin diisocyanate forms an adduct with terpyridine itself (Naik & Scheidt, 1973); the ligand chelates to the tin atom through its three N atoms. The 4'-pyridylterpyridine has a similar seven-coordinate structure (Scheme I, Fig. 1). It also features the chelated tin atom in a seven-coordinate geometry.

## Experimental

Dimethyltin diisothiocyanate and 4'-pyridyl-2,2':6',2''-terpyridine (1 mmol) were loaded into a convection tube. The tube was filled with dry methanol and kept at 333 K. Colorless crystals were collected from the side arm after several days.

## Refinement

H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, $U_{iso}$(H) 1.2 to 1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

## Figures

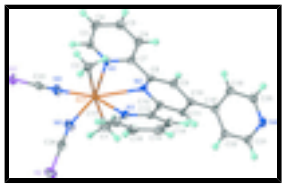


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of diisothiocyanatodimethyl(4'-pyridylterpyridine)tin at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## Dimethyl(4'-pyridyl-2,2':6',2''-terpyridine- $\kappa^3N^1,N^{1'},N^{1''}$)bis(thiocyanato-$\kappa N$)tin(IV)

*Crystal data*

| | |
|---|---|
| $[Sn(CH_3)_2(NCS)_2(C_{20}H_{14}N_4)]$ | $Z = 2$ |
| $M_r = 575.27$ | $F(000) = 576$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.624$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.3269$ (3) Å | Cell parameters from 10240 reflections |
| $b = 10.5017$ (3) Å | $\theta = 2.2$–$29.4°$ |
| $c = 13.1503$ (4) Å | $\mu = 1.29$ mm$^{-1}$ |
| $\alpha = 66.814$ (3)° | $T = 100$ K |
| $\beta = 87.665$ (3)° | Prism, colorless |

| | |
|---|---|
| γ = 83.552 (2)° | 0.20 × 0.20 × 0.10 mm |
| $V$ = 1176.52 (6) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Agilent Technologies SuperNova (Dual, Cu at zero) diffractometer with an Atlas detector | 5168 independent reflections |
| Radiation source: SuperNova (Mo) X-ray Source | 4728 reflections with $I > 2\sigma(I)$ |
| Mirror | $R_{int}$ = 0.028 |
| Detector resolution: 10.4041 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.2° |
| ω scans | $h$ = −12→11 |
| Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010) | $k$ = −13→13 |
| $T_{min}$ = 0.783, $T_{max}$ = 0.882 | $l$ = −17→16 |
| 15704 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.024 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.060 | H-atom parameters constrained |
| $S$ = 1.04 | $w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 0.2766P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 5168 reflections | $(\Delta/\sigma)_{max}$ = 0.001 |
| 300 parameters | $\Delta\rho_{max}$ = 0.51 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.49 e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | 0.670329 (15) | 0.378196 (13) | 0.343774 (11) | 0.01570 (6) |
| S1 | 0.14249 (6) | 0.55757 (6) | 0.27483 (5) | 0.02139 (12) |
| S2 | 0.54381 (7) | 0.07411 (6) | 0.72375 (5) | 0.02716 (14) |
| N1 | 0.65080 (18) | 0.52567 (17) | 0.13746 (14) | 0.0154 (4) |
| N2 | 0.88281 (18) | 0.34503 (16) | 0.22361 (14) | 0.0137 (4) |
| N3 | 0.90522 (19) | 0.26172 (17) | 0.44304 (14) | 0.0166 (4) |
| N4 | 1.26459 (19) | −0.03774 (18) | −0.05850 (15) | 0.0184 (4) |
| N5 | 0.4323 (2) | 0.45490 (19) | 0.32114 (15) | 0.0241 (4) |
| N6 | 0.5991 (2) | 0.2807 (2) | 0.51867 (15) | 0.0256 (4) |
| C1 | 0.6332 (2) | 0.1957 (2) | 0.3225 (2) | 0.0232 (5) |
| H1A | 0.6343 | 0.2139 | 0.2434 | 0.035* |
| H1B | 0.5391 | 0.1673 | 0.3536 | 0.035* |
| H1C | 0.7091 | 0.1210 | 0.3606 | 0.035* |
| C2 | 0.7301 (2) | 0.5579 (2) | 0.35758 (18) | 0.0201 (5) |
| H2A | 0.7350 | 0.5426 | 0.4359 | 0.030* |

| | | | | |
|---|---|---|---|---|
| H2B | 0.6583 | 0.6369 | 0.3198 | 0.030* |
| H2C | 0.8247 | 0.5779 | 0.3235 | 0.030* |
| C3 | 0.5515 (2) | 0.6360 (2) | 0.09447 (18) | 0.0183 (4) |
| H3 | 0.4899 | 0.6621 | 0.1439 | 0.022* |
| C4 | 0.5342 (2) | 0.7135 (2) | −0.01779 (18) | 0.0200 (5) |
| H4 | 0.4632 | 0.7915 | −0.0447 | 0.024* |
| C5 | 0.6229 (2) | 0.6748 (2) | −0.08986 (17) | 0.0185 (4) |
| H5 | 0.6121 | 0.7244 | −0.1675 | 0.022* |
| C6 | 0.7274 (2) | 0.5631 (2) | −0.04746 (17) | 0.0166 (4) |
| H6 | 0.7900 | 0.5355 | −0.0956 | 0.020* |
| C7 | 0.7396 (2) | 0.4917 (2) | 0.06618 (17) | 0.0142 (4) |
| C8 | 0.8551 (2) | 0.3767 (2) | 0.11653 (17) | 0.0138 (4) |
| C9 | 0.9287 (2) | 0.3065 (2) | 0.05728 (17) | 0.0152 (4) |
| H9 | 0.9077 | 0.3327 | −0.0188 | 0.018* |
| C10 | 1.0339 (2) | 0.1968 (2) | 0.11041 (17) | 0.0146 (4) |
| C11 | 1.0643 (2) | 0.1662 (2) | 0.22092 (17) | 0.0155 (4) |
| H11 | 1.1366 | 0.0935 | 0.2594 | 0.019* |
| C12 | 0.9879 (2) | 0.2429 (2) | 0.27423 (17) | 0.0142 (4) |
| C13 | 1.0163 (2) | 0.2199 (2) | 0.39065 (17) | 0.0158 (4) |
| C14 | 1.1508 (2) | 0.1658 (2) | 0.43977 (18) | 0.0186 (5) |
| H14 | 1.2260 | 0.1346 | 0.4015 | 0.022* |
| C15 | 1.1733 (2) | 0.1583 (2) | 0.54597 (18) | 0.0206 (5) |
| H15 | 1.2647 | 0.1238 | 0.5811 | 0.025* |
| C16 | 1.0606 (2) | 0.2018 (2) | 0.59894 (18) | 0.0214 (5) |
| H16 | 1.0731 | 0.1974 | 0.6716 | 0.026* |
| C17 | 0.9282 (2) | 0.2523 (2) | 0.54579 (18) | 0.0202 (5) |
| H17 | 0.8509 | 0.2813 | 0.5837 | 0.024* |
| C18 | 1.1117 (2) | 0.1161 (2) | 0.05122 (17) | 0.0148 (4) |
| C19 | 1.1493 (2) | 0.1789 (2) | −0.05975 (17) | 0.0165 (4) |
| H19 | 1.1225 | 0.2753 | −0.1005 | 0.020* |
| C20 | 1.2262 (2) | 0.0990 (2) | −0.11010 (17) | 0.0172 (4) |
| H20 | 1.2531 | 0.1439 | −0.1853 | 0.021* |
| C21 | 1.2265 (2) | −0.0968 (2) | 0.04727 (18) | 0.0176 (4) |
| H21 | 1.2523 | −0.1940 | 0.0853 | 0.021* |
| C22 | 1.1520 (2) | −0.0258 (2) | 0.10523 (17) | 0.0156 (4) |
| H22 | 1.1286 | −0.0733 | 0.1809 | 0.019* |
| C23 | 0.3116 (2) | 0.4974 (2) | 0.30293 (17) | 0.0173 (4) |
| C24 | 0.5756 (2) | 0.1937 (2) | 0.60383 (18) | 0.0198 (5) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn1 | 0.01512 (9) | 0.01554 (8) | 0.01612 (9) | −0.00096 (6) | 0.00146 (6) | −0.00616 (6) |
| S1 | 0.0158 (3) | 0.0253 (3) | 0.0245 (3) | 0.0018 (2) | 0.0006 (2) | −0.0123 (2) |
| S2 | 0.0260 (3) | 0.0268 (3) | 0.0212 (3) | −0.0053 (2) | 0.0007 (3) | −0.0008 (2) |
| N1 | 0.0135 (9) | 0.0140 (8) | 0.0186 (9) | −0.0003 (7) | 0.0013 (7) | −0.0068 (7) |
| N2 | 0.0137 (8) | 0.0124 (8) | 0.0152 (9) | 0.0003 (7) | −0.0017 (7) | −0.0059 (7) |
| N3 | 0.0198 (9) | 0.0161 (9) | 0.0148 (9) | −0.0019 (7) | 0.0007 (8) | −0.0069 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N4 | 0.0171 (9) | 0.0202 (9) | 0.0200 (10) | 0.0007 (7) | 0.0010 (8) | −0.0107 (8) |
| N5 | 0.0177 (10) | 0.0272 (10) | 0.0232 (10) | 0.0003 (8) | 0.0035 (8) | −0.0065 (8) |
| N6 | 0.0252 (11) | 0.0283 (10) | 0.0178 (10) | −0.0040 (8) | 0.0061 (9) | −0.0034 (8) |
| C1 | 0.0242 (12) | 0.0159 (10) | 0.0304 (13) | −0.0034 (9) | −0.0040 (10) | −0.0091 (10) |
| C2 | 0.0256 (12) | 0.0136 (10) | 0.0220 (12) | −0.0013 (9) | 0.0013 (10) | −0.0082 (9) |
| C3 | 0.0154 (11) | 0.0178 (10) | 0.0224 (12) | 0.0005 (8) | 0.0033 (9) | −0.0096 (9) |
| C4 | 0.0172 (11) | 0.0154 (10) | 0.0244 (12) | 0.0043 (9) | −0.0036 (10) | −0.0057 (9) |
| C5 | 0.0198 (11) | 0.0189 (10) | 0.0141 (11) | 0.0002 (9) | −0.0040 (9) | −0.0040 (9) |
| C6 | 0.0170 (11) | 0.0184 (10) | 0.0166 (11) | −0.0009 (8) | −0.0001 (9) | −0.0094 (9) |
| C7 | 0.0133 (10) | 0.0127 (9) | 0.0185 (11) | −0.0009 (8) | −0.0019 (9) | −0.0081 (8) |
| C8 | 0.0125 (10) | 0.0120 (9) | 0.0164 (10) | −0.0012 (8) | −0.0001 (8) | −0.0049 (8) |
| C9 | 0.0155 (10) | 0.0155 (10) | 0.0148 (10) | −0.0016 (8) | 0.0002 (9) | −0.0064 (8) |
| C10 | 0.0133 (10) | 0.0142 (9) | 0.0177 (11) | −0.0030 (8) | 0.0028 (9) | −0.0076 (8) |
| C11 | 0.0141 (10) | 0.0130 (9) | 0.0174 (11) | 0.0004 (8) | 0.0003 (9) | −0.0041 (8) |
| C12 | 0.0124 (10) | 0.0153 (10) | 0.0151 (10) | −0.0014 (8) | 0.0003 (8) | −0.0062 (8) |
| C13 | 0.0182 (11) | 0.0111 (9) | 0.0171 (11) | −0.0009 (8) | 0.0005 (9) | −0.0046 (8) |
| C14 | 0.0173 (11) | 0.0178 (10) | 0.0199 (11) | 0.0039 (9) | −0.0038 (9) | −0.0078 (9) |
| C15 | 0.0208 (11) | 0.0162 (10) | 0.0226 (12) | 0.0007 (9) | −0.0102 (10) | −0.0049 (9) |
| C16 | 0.0287 (12) | 0.0208 (11) | 0.0155 (11) | −0.0032 (10) | −0.0044 (10) | −0.0075 (9) |
| C17 | 0.0230 (12) | 0.0212 (11) | 0.0181 (11) | −0.0026 (9) | 0.0011 (10) | −0.0095 (9) |
| C18 | 0.0120 (10) | 0.0163 (10) | 0.0186 (11) | −0.0013 (8) | 0.0001 (9) | −0.0097 (9) |
| C19 | 0.0156 (10) | 0.0154 (10) | 0.0179 (11) | 0.0001 (8) | −0.0007 (9) | −0.0063 (8) |
| C20 | 0.0160 (11) | 0.0203 (10) | 0.0147 (11) | −0.0020 (9) | 0.0011 (9) | −0.0063 (9) |
| C21 | 0.0153 (10) | 0.0146 (10) | 0.0224 (12) | 0.0014 (8) | −0.0006 (9) | −0.0075 (9) |
| C22 | 0.0133 (10) | 0.0172 (10) | 0.0154 (10) | −0.0006 (8) | 0.0007 (9) | −0.0057 (8) |
| C23 | 0.0216 (12) | 0.0164 (10) | 0.0131 (10) | −0.0041 (9) | 0.0058 (9) | −0.0050 (8) |
| C24 | 0.0131 (10) | 0.0261 (11) | 0.0228 (12) | 0.0001 (9) | −0.0008 (9) | −0.0129 (10) |

*Geometric parameters (Å, °)*

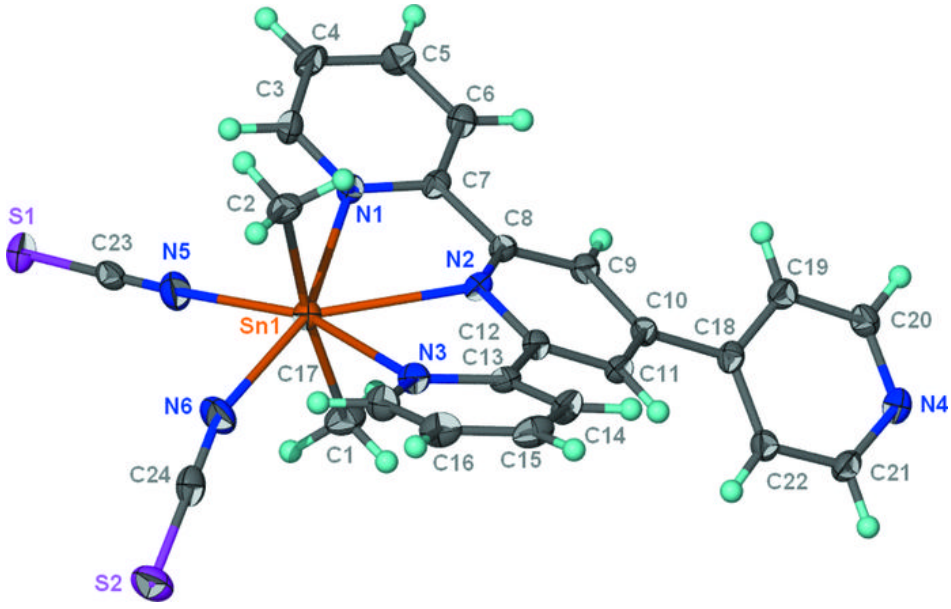
| | | | |
|---|---|---|---|
| Sn1—C2 | 2.102 (2) | C5—C6 | 1.382 (3) |
| Sn1—C1 | 2.110 (2) | C5—H5 | 0.9500 |
| Sn1—N6 | 2.2258 (18) | C6—C7 | 1.386 (3) |
| Sn1—N5 | 2.2645 (19) | C6—H6 | 0.9500 |
| Sn1—N3 | 2.5246 (17) | C7—C8 | 1.481 (3) |
| Sn1—N1 | 2.5418 (17) | C8—C9 | 1.385 (3) |
| Sn1—N2 | 2.5630 (17) | C9—C10 | 1.395 (3) |
| S1—C23 | 1.632 (2) | C9—H9 | 0.9500 |
| S2—C24 | 1.624 (2) | C10—C11 | 1.393 (3) |
| N1—C3 | 1.343 (3) | C10—C18 | 1.478 (3) |
| N1—C7 | 1.351 (3) | C11—C12 | 1.387 (3) |
| N2—C8 | 1.342 (3) | C11—H11 | 0.9500 |
| N2—C12 | 1.345 (3) | C12—C13 | 1.483 (3) |
| N3—C17 | 1.340 (3) | C13—C14 | 1.389 (3) |
| N3—C13 | 1.349 (3) | C14—C15 | 1.391 (3) |
| N4—C21 | 1.332 (3) | C14—H14 | 0.9500 |
| N4—C20 | 1.337 (3) | C15—C16 | 1.372 (3) |
| N5—C23 | 1.161 (3) | C15—H15 | 0.9500 |
| N6—C24 | 1.164 (3) | C16—C17 | 1.388 (3) |

| | | | |
|---|---|---|---|
| C1—H1A | 0.9800 | C16—H16 | 0.9500 |
| C1—H1B | 0.9800 | C17—H17 | 0.9500 |
| C1—H1C | 0.9800 | C18—C22 | 1.389 (3) |
| C2—H2A | 0.9800 | C18—C19 | 1.393 (3) |
| C2—H2B | 0.9800 | C19—C20 | 1.385 (3) |
| C2—H2C | 0.9800 | C19—H19 | 0.9500 |
| C3—C4 | 1.383 (3) | C20—H20 | 0.9500 |
| C3—H3 | 0.9500 | C21—C22 | 1.382 (3) |
| C4—C5 | 1.383 (3) | C21—H21 | 0.9500 |
| C4—H4 | 0.9500 | C22—H22 | 0.9500 |
| C2—Sn1—C1 | 173.66 (8) | C7—C6—C5 | 119.20 (19) |
| C2—Sn1—N6 | 95.00 (8) | C7—C6—H6 | 120.4 |
| C1—Sn1—N6 | 88.97 (8) | C5—C6—H6 | 120.4 |
| C2—Sn1—N5 | 94.55 (8) | N1—C7—C6 | 122.26 (18) |
| C1—Sn1—N5 | 90.97 (8) | N1—C7—C8 | 116.12 (18) |
| N6—Sn1—N5 | 80.75 (7) | C6—C7—C8 | 121.57 (18) |
| C2—Sn1—N3 | 84.97 (7) | N2—C8—C9 | 122.46 (18) |
| C1—Sn1—N3 | 91.04 (7) | N2—C8—C7 | 115.30 (17) |
| N6—Sn1—N3 | 77.94 (6) | C9—C8—C7 | 122.25 (18) |
| N5—Sn1—N3 | 158.55 (6) | C8—C9—C10 | 119.37 (19) |
| C2—Sn1—N1 | 85.50 (7) | C8—C9—H9 | 120.3 |
| C1—Sn1—N1 | 92.67 (7) | C10—C9—H9 | 120.3 |
| N6—Sn1—N1 | 158.04 (6) | C11—C10—C9 | 117.91 (18) |
| N5—Sn1—N1 | 77.33 (6) | C11—C10—C18 | 120.97 (18) |
| N3—Sn1—N1 | 123.89 (5) | C9—C10—C18 | 121.12 (19) |
| C2—Sn1—N2 | 97.06 (7) | C12—C11—C10 | 119.39 (19) |
| C1—Sn1—N2 | 76.72 (7) | C12—C11—H11 | 120.3 |
| N6—Sn1—N2 | 138.11 (6) | C10—C11—H11 | 120.3 |
| N5—Sn1—N2 | 137.58 (6) | N2—C12—C11 | 122.32 (19) |
| N3—Sn1—N2 | 63.44 (5) | N2—C12—C13 | 114.86 (17) |
| N1—Sn1—N2 | 63.18 (5) | C11—C12—C13 | 122.81 (18) |
| C3—N1—C7 | 117.48 (17) | N3—C13—C14 | 122.62 (19) |
| C3—N1—Sn1 | 122.53 (13) | N3—C13—C12 | 115.37 (18) |
| C7—N1—Sn1 | 119.96 (12) | C14—C13—C12 | 121.93 (19) |
| C8—N2—C12 | 118.48 (17) | C15—C14—C13 | 118.8 (2) |
| C8—N2—Sn1 | 117.17 (13) | C15—C14—H14 | 120.6 |
| C12—N2—Sn1 | 116.78 (13) | C13—C14—H14 | 120.6 |
| C17—N3—C13 | 117.84 (18) | C16—C15—C14 | 118.5 (2) |
| C17—N3—Sn1 | 120.77 (14) | C16—C15—H15 | 120.7 |
| C13—N3—Sn1 | 121.07 (13) | C14—C15—H15 | 120.7 |
| C21—N4—C20 | 116.62 (17) | C15—C16—C17 | 119.7 (2) |
| C23—N5—Sn1 | 176.01 (17) | C15—C16—H16 | 120.2 |
| C24—N6—Sn1 | 159.06 (18) | C17—C16—H16 | 120.2 |
| Sn1—C1—H1A | 109.5 | N3—C17—C16 | 122.5 (2) |
| Sn1—C1—H1B | 109.5 | N3—C17—H17 | 118.7 |
| H1A—C1—H1B | 109.5 | C16—C17—H17 | 118.7 |
| Sn1—C1—H1C | 109.5 | C22—C18—C19 | 117.38 (18) |
| H1A—C1—H1C | 109.5 | C22—C18—C10 | 120.88 (18) |
| H1B—C1—H1C | 109.5 | C19—C18—C10 | 121.73 (18) |

| | | | |
|---|---|---|---|
| Sn1—C2—H2A | 109.5 | C20—C19—C18 | 119.26 (19) |
| Sn1—C2—H2B | 109.5 | C20—C19—H19 | 120.4 |
| H2A—C2—H2B | 109.5 | C18—C19—H19 | 120.4 |
| Sn1—C2—H2C | 109.5 | N4—C20—C19 | 123.52 (19) |
| H2A—C2—H2C | 109.5 | N4—C20—H20 | 118.2 |
| H2B—C2—H2C | 109.5 | C19—C20—H20 | 118.2 |
| N1—C3—C4 | 123.57 (19) | N4—C21—C22 | 124.19 (19) |
| N1—C3—H3 | 118.2 | N4—C21—H21 | 117.9 |
| C4—C3—H3 | 118.2 | C22—C21—H21 | 117.9 |
| C3—C4—C5 | 118.28 (19) | C21—C22—C18 | 119.01 (19) |
| C3—C4—H4 | 120.9 | C21—C22—H22 | 120.5 |
| C5—C4—H4 | 120.9 | C18—C22—H22 | 120.5 |
| C6—C5—C4 | 119.17 (19) | N5—C23—S1 | 178.9 (2) |
| C6—C5—H5 | 120.4 | N6—C24—S2 | 178.9 (2) |
| C4—C5—H5 | 120.4 | | |
| C2—Sn1—N1—C3 | −65.95 (16) | Sn1—N1—C7—C8 | −6.5 (2) |
| C1—Sn1—N1—C3 | 120.14 (17) | C5—C6—C7—N1 | 1.4 (3) |
| N6—Sn1—N1—C3 | 26.3 (3) | C5—C6—C7—C8 | −176.24 (19) |
| N5—Sn1—N1—C3 | 29.74 (16) | C12—N2—C8—C9 | 1.2 (3) |
| N3—Sn1—N1—C3 | −146.81 (15) | Sn1—N2—C8—C9 | −147.48 (16) |
| N2—Sn1—N1—C3 | −166.20 (17) | C12—N2—C8—C7 | −179.06 (17) |
| C2—Sn1—N1—C7 | 116.06 (16) | Sn1—N2—C8—C7 | 32.2 (2) |
| C1—Sn1—N1—C7 | −57.86 (16) | N1—C7—C8—N2 | −17.1 (3) |
| N6—Sn1—N1—C7 | −151.74 (18) | C6—C7—C8—N2 | 160.63 (18) |
| N5—Sn1—N1—C7 | −148.25 (16) | N1—C7—C8—C9 | 162.59 (18) |
| N3—Sn1—N1—C7 | 35.19 (16) | C6—C7—C8—C9 | −19.7 (3) |
| N2—Sn1—N1—C7 | 15.81 (13) | N2—C8—C9—C10 | 1.2 (3) |
| C2—Sn1—N2—C8 | −106.42 (14) | C7—C8—C9—C10 | −178.43 (18) |
| C1—Sn1—N2—C8 | 74.85 (14) | C8—C9—C10—C11 | −2.5 (3) |
| N6—Sn1—N2—C8 | 147.95 (14) | C8—C9—C10—C18 | 177.98 (18) |
| N5—Sn1—N2—C8 | −1.71 (18) | C9—C10—C11—C12 | 1.3 (3) |
| N3—Sn1—N2—C8 | 172.83 (15) | C18—C10—C11—C12 | −179.16 (18) |
| N1—Sn1—N2—C8 | −25.11 (13) | C8—N2—C12—C11 | −2.5 (3) |
| C2—Sn1—N2—C12 | 104.32 (15) | Sn1—N2—C12—C11 | 146.34 (16) |
| C1—Sn1—N2—C12 | −74.41 (15) | C8—N2—C12—C13 | 176.96 (17) |
| N6—Sn1—N2—C12 | −1.31 (19) | Sn1—N2—C12—C13 | −34.2 (2) |
| N5—Sn1—N2—C12 | −150.97 (14) | C10—C11—C12—N2 | 1.2 (3) |
| N3—Sn1—N2—C12 | 23.57 (13) | C10—C11—C12—C13 | −178.18 (18) |
| N1—Sn1—N2—C12 | −174.37 (16) | C17—N3—C13—C14 | 1.2 (3) |
| C2—Sn1—N3—C17 | 62.31 (16) | Sn1—N3—C13—C14 | 174.64 (15) |
| C1—Sn1—N3—C17 | −122.63 (16) | C17—N3—C13—C12 | −175.43 (18) |
| N6—Sn1—N3—C17 | −33.91 (16) | Sn1—N3—C13—C12 | −2.0 (2) |
| N5—Sn1—N3—C17 | −27.3 (3) | N2—C12—C13—N3 | 24.1 (3) |
| N1—Sn1—N3—C17 | 143.45 (14) | C11—C12—C13—N3 | −156.48 (19) |
| N2—Sn1—N3—C17 | 162.79 (17) | N2—C12—C13—C14 | −152.59 (19) |
| C2—Sn1—N3—C13 | −110.95 (16) | C11—C12—C13—C14 | 26.9 (3) |
| C1—Sn1—N3—C13 | 64.12 (16) | N3—C13—C14—C15 | −2.0 (3) |
| N6—Sn1—N3—C13 | 152.84 (16) | C12—C13—C14—C15 | 174.45 (19) |
| N5—Sn1—N3—C13 | 159.42 (17) | C13—C14—C15—C16 | 1.4 (3) |

| | | | |
|---|---|---|---|
| N1—Sn1—N3—C13 | −29.80 (17) | C14—C15—C16—C17 | −0.2 (3) |
| N2—Sn1—N3—C13 | −10.47 (14) | C13—N3—C17—C16 | 0.1 (3) |
| C2—Sn1—N6—C24 | −150.2 (5) | Sn1—N3—C17—C16 | −173.39 (15) |
| C1—Sn1—N6—C24 | 24.8 (5) | C15—C16—C17—N3 | −0.5 (3) |
| N5—Sn1—N6—C24 | 116.0 (5) | C11—C10—C18—C22 | 35.8 (3) |
| N3—Sn1—N6—C24 | −66.5 (5) | C9—C10—C18—C22 | −144.7 (2) |
| N1—Sn1—N6—C24 | 119.4 (5) | C11—C10—C18—C19 | −143.3 (2) |
| N2—Sn1—N6—C24 | −43.8 (5) | C9—C10—C18—C19 | 36.3 (3) |
| C7—N1—C3—C4 | 1.3 (3) | C22—C18—C19—C20 | −1.2 (3) |
| Sn1—N1—C3—C4 | −176.70 (15) | C10—C18—C19—C20 | 177.93 (19) |
| N1—C3—C4—C5 | 0.7 (3) | C21—N4—C20—C19 | −0.7 (3) |
| C3—C4—C5—C6 | −1.7 (3) | C18—C19—C20—N4 | 1.5 (3) |
| C4—C5—C6—C7 | 0.7 (3) | C20—N4—C21—C22 | −0.4 (3) |
| C3—N1—C7—C6 | −2.4 (3) | N4—C21—C22—C18 | 0.7 (3) |
| Sn1—N1—C7—C6 | 175.74 (15) | C19—C18—C22—C21 | 0.1 (3) |
| C3—N1—C7—C8 | 175.36 (18) | C10—C18—C22—C21 | −178.98 (19) |

**Fig. 1**


C4
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C16
C15
C24
C22
C21
S2