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# (μ-2,2′-Biquinolinyl-4,4′-dicarboxylato-κ²O:O′)bis[(dimethylformamide-κO)-triphenyltin(IV)]

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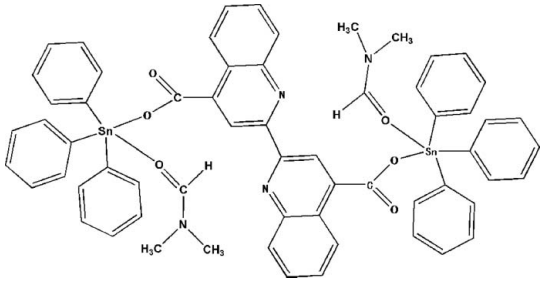
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.054; $wR$ factor = 0.170; data-to-parameter ratio = 18.6.

The molecule of the title compound, $[Sn_2(C_6H_5)_6(C_{10}H_5NO_2)_2(C_3H_7NO)_2]$, is centrosymmetric. Two triphenyltin groups are bridged by a 2,2′-biquinolinyl-4,4′-dicarboxylate dianion ($L$) through its two carboxylate groups. Each Sn atom displays a distorted trigonal–bipyramidal geometry composed of three phenyl groups, one carboxylate O atom from the $L$ dianion and one O atom of *N*,*N*-dimethylformamide. The molecules display aromatic $\pi$–$\pi$ stacking (face-to-face distance 3.406 Å).

## Related literature

For related literature, see: Basu Baul *et al.* (2004).



## Experimental

*Crystal data*

$[Sn_2(C_6H_5)_6(C_{10}H_5NO_2)_2(C_3H_7NO)_2]$
$M_r$ = 1188.47
Monoclinic, $C2/c$
$a$ = 30.4592 (17) Å
$b$ = 9.5344 (5) Å
$c$ = 22.0343 (14) Å
$\beta$ = 123.051 (2)°
$V$ = 5363.5 (5) Å³
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.99 mm$^{-1}$
$T$ = 293 (2) K
0.54 × 0.48 × 0.39 mm

*Data collection*

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.590, $T_{max}$ = 0.678
15947 measured reflections
6203 independent reflections
4618 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.170
$S$ = 1.08
6203 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.14 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Sn1—C13 | 2.125 (4) | Sn1—C1 | 2.127 (4) |
| Sn1—C7 | 2.127 (4) | Sn1—O1 | 2.187 (4) |
| C13—Sn1—C7 | 119.75 (18) | C13—Sn1—O1 | 88.78 (16) |
| C13—Sn1—C1 | 114.85 (16) | C7—Sn1—O1 | 103.41 (17) |
| C7—Sn1—C1 | 119.16 (19) | C1—Sn1—O1 | 102.48 (19) |

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The author thanks the Fok Ying Tung Education Foundation and the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2083).

## References

Basu Baul, T. S., Rynjah, W., Willem, R., Biesemans, M., Verbruggen, I., Holèapek, M., de Vos, D. & Linden, A. (2004). *J. Organomet. Chem.* **689**, 4691–4701.
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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1883 [ **doi:10.1107/S1600536807028048** ]

# (μ-2,2'-Biquinolinyl-4,4'-dicarboxylato-$\kappa^2O$:$O'$)bis[(dimethylformamide-$\kappa O$)triphenyltin(IV)]

**L.-B. Wang**

## Comment

To further widen the scope of application of organotin compounds, there is a need to prepare new series of organotin compounds. In this paper, the structure of (I) is described.

The title compound (I) contains one neutral $[Sn_2(C_6H_5)_6(C_9H_5NCOO)_2]$ molecule and two *N*,*N*-dimethyl formamide solvent molecules. As shown in Fig.1, two triphenyltin groups are bridged by the 2,2'-biquinoline-4,4'-dicarboxylate dianion, *L*, through its two carboxylate groups. The central Sn atom adopts distorted $SnC_3O_2$ trigonal bipyramid geometry composed of three phenyl groups, one carboxylate O atom from *L* and one O atom of *N*,*N*-dimethyl formamide. The *N*,*N*-dimethyl formamide, included as solvent molecule, forms no hydrogen-bonding interactions with any other atoms in the structure. In addition, the bond between Sn1 and O3 (2.605 (3) Å) is much more weaker than that of Sn1 and O1 (2.187 (4) Å) (Basu Baul *et al.*, 2004). The *L* ligand of each molecule provides two quinoline rings to form slipped π-π interaction with the face-to-face distance (*d*) being about 3.406Å (Fig. 2).

## Experimental

A mixture of $Na_2L$ (0.388 g, 1 mmol) and $Ph_3SnCl$ (0.770 g, 2 mmol) in 25 ml e thanol was refluxed for 12 h and then filtered. The resulting precipitates were washed with ethanol. Crystals suitable for X-ray diffraction were obtained by slow evaporation of a *N*,*N*-dimethyl formamide solution.

## Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, $U_{iso}$=1.2$U_{eq}$ (C) for aromatic and 0.96 Å, $U_{iso}$ = 1.5$U_{eq}$ (C) for $CH_3$ atoms. The minimum electron-density peak is located 0.96Å from atom Sn1.

## Figures

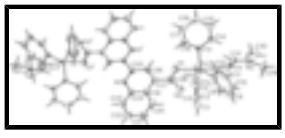

Fig. 1. View of the compound (I). Displacement ellipsoids are drawn at the 30% probability level. (symmetry code: (i) 1 − *x*, 1 − *y*, 1 − *z*)

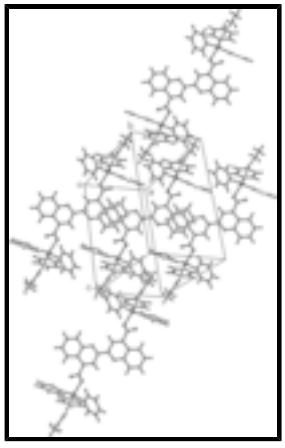

Fig. 2. A packing diagram of (I).

**(μ-2,2'-Biquinolinyl-4,4'-dicarboxylato-κ$^2$*O*:*O*')bis[(dimethylformamide- κ*O*)triphenyltin(IV)]**

*Crystal data*

| | |
|---|---|
| $[Sn_2(C_6H_5)_6(C_{10}H_5NO_2)_2(C_3H_7NO)_2]$ | $F_{000}$ = 2408 |
| $M_r$ = 1188.47 | $D_x$ = 1.472 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 6203 reflections |
| *a* = 30.4592 (17) Å | θ = 1.6–28.3º |
| *b* = 9.5344 (5) Å | μ = 0.99 mm$^{-1}$ |
| *c* = 22.0343 (14) Å | *T* = 293 (2) K |
| β = 123.051 (2)º | Block, colourless |
| *V* = 5363.5 (5) Å$^3$ | 0.54 × 0.48 × 0.39 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 6203 independent reflections |
| Radiation source: fine-focus sealed tube | 4618 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.033 |
| *T* = 293(2) K | $\theta_{max}$ = 28.3º |
| ω scans | $\theta_{min}$ = 1.6º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −40→26 |
| $T_{min}$ = 0.590, $T_{max}$ = 0.678 | *k* = −12→10 |
| 15947 measured reflections | *l* = −26→29 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.054$ | H-atom parameters constrained |
| $wR(F^2) = 0.170$ | $w = 1/[\sigma^2(F_o^2) + (0.1137P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 6203 reflections | $\Delta\rho_{max} = 2.82$ e Å$^{-3}$ |
| 334 parameters | $\Delta\rho_{min} = -1.14$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | 0.347644 (10) | 0.11246 (3) | 0.186776 (13) | 0.04892 (14) |
| C1 | 0.37845 (18) | −0.0948 (5) | 0.2087 (2) | 0.0555 (11) |
| C2 | 0.36527 (18) | −0.1935 (5) | 0.2426 (2) | 0.0593 (11) |
| H2 | 0.3448 | −0.1670 | 0.2602 | 0.071* |
| C3 | 0.3825 (2) | −0.3329 (6) | 0.2507 (3) | 0.0728 (13) |
| H3 | 0.3731 | −0.3993 | 0.2724 | 0.087* |
| C4 | 0.4137 (3) | −0.3694 (5) | 0.2257 (3) | 0.0765 (16) |
| H4 | 0.4251 | −0.4616 | 0.2304 | 0.092* |
| C5 | 0.4280 (2) | −0.2738 (7) | 0.1948 (3) | 0.0810 (15) |
| H5 | 0.4495 | −0.2999 | 0.1788 | 0.097* |
| C6 | 0.4110 (2) | −0.1384 (6) | 0.1867 (3) | 0.0693 (13) |
| H6 | 0.4216 | −0.0735 | 0.1657 | 0.083* |
| C7 | 0.27208 (17) | 0.1477 (6) | 0.1675 (2) | 0.0567 (11) |
| C8 | 0.2439 (2) | 0.0377 (8) | 0.1703 (3) | 0.0898 (17) |
| H8 | 0.2588 | −0.0513 | 0.1823 | 0.108* |
| C9 | 0.1931 (2) | 0.0564 (9) | 0.1553 (4) | 0.0997 (19) |
| H9 | 0.1751 | −0.0185 | 0.1588 | 0.120* |
| C10 | 0.1708 (2) | 0.1853 (9) | 0.1356 (3) | 0.094 (2) |
| H10 | 0.1365 | 0.1988 | 0.1225 | 0.113* |
| C11 | 0.1984 (3) | 0.2913 (9) | 0.1352 (5) | 0.121 (3) |
| H11 | 0.1839 | 0.3807 | 0.1245 | 0.145* |
| C12 | 0.2486 (3) | 0.2729 (8) | 0.1503 (4) | 0.102 (2) |
| H12 | 0.2664 | 0.3502 | 0.1485 | 0.122* |
| C13 | 0.37577 (16) | 0.2455 (4) | 0.1378 (2) | 0.0487 (9) |

| | | | | |
|---|---|---|---|---|
| C14 | 0.3425 (2) | 0.3145 (5) | 0.0722 (3) | 0.0650 (12) |
| H14 | 0.3066 | 0.2999 | 0.0481 | 0.078* |
| C15 | 0.3608 (3) | 0.4014 (6) | 0.0428 (4) | 0.0840 (18) |
| H15 | 0.3374 | 0.4478 | −0.0002 | 0.101* |
| C16 | 0.4128 (4) | 0.4219 (6) | 0.0753 (5) | 0.096 (2) |
| H16 | 0.4253 | 0.4799 | 0.0540 | 0.116* |
| C17 | 0.4480 (3) | 0.3552 (6) | 0.1413 (4) | 0.0890 (19) |
| H17 | 0.4839 | 0.3697 | 0.1645 | 0.107* |
| C18 | 0.42890 (18) | 0.2687 (5) | 0.1710 (3) | 0.0672 (12) |
| H18 | 0.4522 | 0.2243 | 0.2147 | 0.081* |
| C19 | 0.44734 (17) | 0.1592 (6) | 0.4717 (3) | 0.0637 (12) |
| C20 | 0.4307 (2) | 0.0166 (7) | 0.4709 (4) | 0.088 (2) |
| H20 | 0.4080 | −0.0268 | 0.4267 | 0.105* |
| C21 | 0.4477 (3) | −0.0562 (8) | 0.5337 (5) | 0.0917 (18) |
| H21 | 0.4369 | −0.1483 | 0.5315 | 0.110* |
| C22 | 0.4809 (2) | 0.0069 (7) | 0.6004 (4) | 0.0861 (16) |
| H22 | 0.4915 | −0.0423 | 0.6427 | 0.103* |
| C23 | 0.4981 (2) | 0.1400 (6) | 0.6043 (3) | 0.0698 (13) |
| H23 | 0.5211 | 0.1796 | 0.6495 | 0.084* |
| C24 | 0.48187 (17) | 0.2212 (5) | 0.5406 (3) | 0.0612 (11) |
| C25 | 0.48861 (15) | 0.4313 (5) | 0.4933 (2) | 0.0549 (10) |
| C26 | 0.45349 (18) | 0.3773 (5) | 0.4212 (2) | 0.0632 (13) |
| H26 | 0.4448 | 0.4320 | 0.3812 | 0.076* |
| C27 | 0.43283 (16) | 0.2450 (6) | 0.4116 (3) | 0.0658 (14) |
| C28 | 0.3947 (2) | 0.1862 (8) | 0.3373 (3) | 0.087 (2) |
| C29 | 0.2256 (3) | −0.1292 (7) | −0.0722 (4) | 0.109 (3) |
| H29A | 0.2124 | −0.1853 | −0.1149 | 0.163* |
| H29C | 0.2084 | −0.0397 | −0.0852 | 0.163* |
| H29B | 0.2190 | −0.1759 | −0.0393 | 0.163* |
| C30 | 0.3076 (4) | −0.1706 (11) | −0.0725 (6) | 0.151 (4) |
| H30B | 0.2818 | −0.2201 | −0.1154 | 0.226* |
| H30C | 0.3346 | −0.2345 | −0.0397 | 0.226* |
| H30A | 0.3226 | −0.0972 | −0.0853 | 0.226* |
| C31 | 0.3084 (2) | −0.0349 (5) | 0.0229 (3) | 0.0668 (12) |
| H31 | 0.3437 | −0.0186 | 0.0418 | 0.080* |
| N1 | 0.50173 (14) | 0.3517 (4) | 0.55044 (19) | 0.0541 (8) |
| N2 | 0.2823 (2) | −0.1090 (4) | −0.0371 (3) | 0.0769 (13) |
| O1 | 0.40005 (16) | 0.2196 (6) | 0.2896 (2) | 0.1038 (15) |
| O2 | 0.3613 (2) | 0.0932 (5) | 0.3264 (2) | 0.0980 (14) |
| O3 | 0.29056 (13) | 0.0138 (3) | 0.05551 (17) | 0.0662 (8) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn1 | 0.03819 (19) | 0.0677 (2) | 0.03760 (19) | 0.00386 (11) | 0.01859 (14) | 0.00340 (11) |
| C1 | 0.044 (2) | 0.078 (3) | 0.042 (2) | 0.0083 (19) | 0.0216 (19) | 0.0107 (19) |
| C2 | 0.056 (3) | 0.066 (3) | 0.053 (2) | 0.006 (2) | 0.029 (2) | 0.001 (2) |
| C3 | 0.062 (3) | 0.082 (3) | 0.058 (3) | −0.006 (3) | 0.023 (2) | −0.002 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.075 (4) | 0.064 (3) | 0.075 (4) | 0.010 (2) | 0.030 (3) | −0.005 (2) |
| C5 | 0.071 (3) | 0.099 (4) | 0.084 (4) | 0.021 (3) | 0.049 (3) | 0.001 (3) |
| C6 | 0.062 (3) | 0.089 (4) | 0.063 (3) | 0.016 (2) | 0.038 (3) | 0.010 (2) |
| C7 | 0.042 (2) | 0.087 (3) | 0.043 (2) | 0.004 (2) | 0.0235 (18) | −0.002 (2) |
| C8 | 0.059 (3) | 0.105 (4) | 0.110 (5) | 0.011 (3) | 0.049 (3) | 0.014 (4) |
| C9 | 0.064 (4) | 0.131 (5) | 0.112 (5) | −0.008 (4) | 0.054 (4) | 0.004 (5) |
| C10 | 0.053 (3) | 0.157 (6) | 0.078 (4) | 0.025 (4) | 0.039 (3) | 0.001 (4) |
| C11 | 0.081 (4) | 0.120 (6) | 0.174 (8) | 0.037 (4) | 0.077 (5) | 0.020 (5) |
| C12 | 0.070 (4) | 0.103 (5) | 0.141 (6) | 0.023 (3) | 0.063 (4) | 0.024 (4) |
| C13 | 0.049 (2) | 0.052 (2) | 0.048 (2) | −0.0061 (17) | 0.0279 (18) | −0.0119 (17) |
| C14 | 0.065 (3) | 0.079 (3) | 0.054 (3) | −0.006 (2) | 0.035 (2) | −0.006 (2) |
| C15 | 0.122 (6) | 0.070 (3) | 0.083 (4) | 0.006 (3) | 0.070 (4) | 0.012 (3) |
| C16 | 0.136 (7) | 0.064 (3) | 0.144 (7) | −0.009 (4) | 0.112 (6) | 0.003 (4) |
| C17 | 0.079 (4) | 0.080 (4) | 0.133 (6) | −0.027 (3) | 0.074 (4) | −0.027 (4) |
| C18 | 0.051 (3) | 0.075 (3) | 0.076 (3) | −0.006 (2) | 0.034 (2) | −0.017 (2) |
| C19 | 0.037 (2) | 0.092 (3) | 0.060 (3) | 0.001 (2) | 0.025 (2) | −0.022 (3) |
| C20 | 0.048 (3) | 0.097 (4) | 0.116 (5) | −0.016 (3) | 0.043 (3) | −0.049 (4) |
| C21 | 0.077 (4) | 0.089 (4) | 0.126 (6) | 0.007 (3) | 0.066 (4) | 0.018 (4) |
| C22 | 0.071 (4) | 0.105 (4) | 0.091 (4) | 0.007 (3) | 0.050 (3) | 0.008 (4) |
| C23 | 0.065 (3) | 0.078 (3) | 0.074 (3) | 0.004 (2) | 0.042 (3) | 0.000 (3) |
| C24 | 0.042 (2) | 0.084 (3) | 0.058 (3) | −0.002 (2) | 0.028 (2) | −0.015 (2) |
| C25 | 0.039 (2) | 0.089 (3) | 0.0334 (18) | 0.0039 (19) | 0.0180 (17) | −0.013 (2) |
| C26 | 0.042 (2) | 0.106 (4) | 0.035 (2) | 0.005 (2) | 0.0172 (19) | −0.016 (2) |
| C27 | 0.034 (2) | 0.099 (4) | 0.059 (3) | −0.009 (2) | 0.022 (2) | −0.039 (3) |
| C28 | 0.052 (3) | 0.156 (6) | 0.054 (3) | −0.018 (3) | 0.029 (2) | −0.045 (4) |
| C29 | 0.091 (5) | 0.098 (5) | 0.091 (5) | −0.041 (4) | 0.020 (4) | −0.013 (3) |
| C30 | 0.180 (9) | 0.156 (7) | 0.193 (10) | −0.066 (7) | 0.151 (9) | −0.092 (7) |
| C31 | 0.059 (3) | 0.073 (3) | 0.066 (3) | −0.020 (2) | 0.032 (2) | −0.014 (2) |
| N1 | 0.0448 (19) | 0.074 (2) | 0.0385 (17) | 0.0026 (17) | 0.0192 (15) | −0.0070 (16) |
| N2 | 0.086 (3) | 0.078 (3) | 0.072 (3) | −0.031 (2) | 0.047 (3) | −0.023 (2) |
| O1 | 0.062 (2) | 0.178 (5) | 0.048 (2) | −0.017 (3) | 0.0146 (18) | −0.008 (2) |
| O2 | 0.087 (3) | 0.118 (3) | 0.071 (3) | −0.031 (2) | 0.032 (2) | −0.003 (2) |
| O3 | 0.066 (2) | 0.072 (2) | 0.0561 (18) | −0.0086 (16) | 0.0304 (16) | −0.0120 (15) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Sn1—C13 | 2.125 (4) | C17—C18 | 1.364 (8) |
| Sn1—C7 | 2.127 (4) | C17—H17 | 0.9300 |
| Sn1—C1 | 2.127 (4) | C18—H18 | 0.9300 |
| Sn1—O1 | 2.187 (4) | C19—C27 | 1.407 (8) |
| C1—C6 | 1.384 (7) | C19—C24 | 1.422 (7) |
| C1—C2 | 1.390 (6) | C19—C20 | 1.447 (8) |
| C2—C3 | 1.404 (7) | C20—C21 | 1.371 (9) |
| C2—H2 | 0.9300 | C20—H20 | 0.9300 |
| C3—C4 | 1.377 (8) | C21—C22 | 1.387 (10) |
| C3—H3 | 0.9300 | C21—H21 | 0.9300 |
| C4—C5 | 1.344 (8) | C22—C23 | 1.358 (8) |
| C4—H4 | 0.9300 | C22—H22 | 0.9300 |
| C5—C6 | 1.366 (7) | C23—C24 | 1.433 (8) |

| | | | |
|---|---|---|---|
| C5—H5 | 0.9300 | C23—H23 | 0.9300 |
| C6—H6 | 0.9300 | C24—N1 | 1.349 (6) |
| C7—C12 | 1.337 (8) | C25—N1 | 1.331 (6) |
| C7—C8 | 1.378 (8) | C25—C25$^{i}$ | 1.436 (10) |
| C8—C9 | 1.406 (8) | C25—C26 | 1.443 (6) |
| C8—H8 | 0.9300 | C26—C27 | 1.373 (7) |
| C9—C10 | 1.356 (11) | C26—H26 | 0.9300 |
| C9—H9 | 0.9300 | C27—C28 | 1.507 (6) |
| C10—C11 | 1.318 (10) | C28—O1 | 1.190 (7) |
| C10—H10 | 0.9300 | C28—O2 | 1.270 (8) |
| C11—C12 | 1.385 (9) | C29—N2 | 1.471 (9) |
| C11—H11 | 0.9300 | C29—H29A | 0.9600 |
| C12—H12 | 0.9300 | C29—H29C | 0.9600 |
| C13—C18 | 1.383 (6) | C29—H29B | 0.9600 |
| C13—C14 | 1.397 (7) | C30—N2 | 1.482 (9) |
| C14—C15 | 1.345 (8) | C30—H30B | 0.9600 |
| C14—H14 | 0.9300 | C30—H30C | 0.9600 |
| C15—C16 | 1.351 (11) | C30—H30A | 0.9600 |
| C15—H15 | 0.9300 | C31—O3 | 1.206 (6) |
| C16—C17 | 1.403 (11) | C31—N2 | 1.316 (6) |
| C16—H16 | 0.9300 | C31—H31 | 0.9300 |
| C13—Sn1—C7 | 119.75 (18) | C18—C17—H17 | 120.4 |
| C13—Sn1—C1 | 114.85 (16) | C16—C17—H17 | 120.4 |
| C7—Sn1—C1 | 119.16 (19) | C17—C18—C13 | 121.7 (6) |
| C13—Sn1—O1 | 88.78 (16) | C17—C18—H18 | 119.2 |
| C7—Sn1—O1 | 103.41 (17) | C13—C18—H18 | 119.2 |
| C1—Sn1—O1 | 102.48 (19) | C27—C19—C24 | 115.7 (5) |
| C6—C1—C2 | 117.2 (4) | C27—C19—C20 | 127.4 (5) |
| C6—C1—Sn1 | 120.7 (4) | C24—C19—C20 | 117.0 (5) |
| C2—C1—Sn1 | 122.0 (3) | C21—C20—C19 | 121.8 (6) |
| C1—C2—C3 | 120.7 (5) | C21—C20—H20 | 119.1 |
| C1—C2—H2 | 119.7 | C19—C20—H20 | 119.1 |
| C3—C2—H2 | 119.7 | C20—C21—C22 | 120.3 (6) |
| C4—C3—C2 | 118.8 (5) | C20—C21—H21 | 119.9 |
| C4—C3—H3 | 120.6 | C22—C21—H21 | 119.9 |
| C2—C3—H3 | 120.6 | C23—C22—C21 | 120.4 (6) |
| C5—C4—C3 | 121.0 (5) | C23—C22—H22 | 119.8 |
| C5—C4—H4 | 119.5 | C21—C22—H22 | 119.8 |
| C3—C4—H4 | 119.5 | C22—C23—C24 | 121.8 (6) |
| C4—C5—C6 | 120.2 (5) | C22—C23—H23 | 119.1 |
| C4—C5—H5 | 119.9 | C24—C23—H23 | 119.1 |
| C6—C5—H5 | 119.9 | N1—C24—C19 | 124.1 (5) |
| C5—C6—C1 | 122.1 (5) | N1—C24—C23 | 117.2 (4) |
| C5—C6—H6 | 119.0 | C19—C24—C23 | 118.7 (5) |
| C1—C6—H6 | 119.0 | N1—C25—C25$^{i}$ | 117.6 (4) |
| C12—C7—C8 | 116.2 (5) | N1—C25—C26 | 119.9 (5) |
| C12—C7—Sn1 | 123.5 (4) | C25$^{i}$—C25—C26 | 122.5 (5) |
| C8—C7—Sn1 | 120.2 (4) | C27—C26—C25 | 120.0 (5) |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 121.7 (6) | C27—C26—H26 | 120.0 |
| C7—C8—H8 | 119.1 | C25—C26—H26 | 120.0 |
| C9—C8—H8 | 119.1 | C26—C27—C19 | 120.5 (4) |
| C10—C9—C8 | 119.0 (7) | C26—C27—C28 | 121.7 (6) |
| C10—C9—H9 | 120.5 | C19—C27—C28 | 117.8 (5) |
| C8—C9—H9 | 120.5 | O1—C28—O2 | 120.1 (5) |
| C11—C10—C9 | 119.2 (6) | O1—C28—C27 | 117.7 (6) |
| C11—C10—H10 | 120.4 | O2—C28—C27 | 121.8 (6) |
| C9—C10—H10 | 120.4 | N2—C29—H29A | 109.5 |
| C10—C11—C12 | 121.7 (7) | N2—C29—H29C | 109.5 |
| C10—C11—H11 | 119.2 | H29A—C29—H29C | 109.5 |
| C12—C11—H11 | 119.2 | N2—C29—H29B | 109.5 |
| C7—C12—C11 | 122.1 (7) | H29A—C29—H29B | 109.5 |
| C7—C12—H12 | 118.9 | H29C—C29—H29B | 109.5 |
| C11—C12—H12 | 118.9 | N2—C30—H30B | 109.5 |
| C18—C13—C14 | 116.8 (4) | N2—C30—H30C | 109.5 |
| C18—C13—Sn1 | 120.4 (4) | H30B—C30—H30C | 109.5 |
| C14—C13—Sn1 | 122.7 (3) | N2—C30—H30A | 109.5 |
| C15—C14—C13 | 122.1 (5) | H30B—C30—H30A | 109.5 |
| C15—C14—H14 | 119.0 | H30C—C30—H30A | 109.5 |
| C13—C14—H14 | 119.0 | O3—C31—N2 | 125.7 (5) |
| C14—C15—C16 | 120.5 (6) | O3—C31—H31 | 117.2 |
| C14—C15—H15 | 119.7 | N2—C31—H31 | 117.2 |
| C16—C15—H15 | 119.7 | C25—N1—C24 | 119.8 (4) |
| C15—C16—C17 | 119.7 (5) | C31—N2—C29 | 119.4 (5) |
| C15—C16—H16 | 120.2 | C31—N2—C30 | 122.6 (6) |
| C17—C16—H16 | 120.2 | C29—N2—C30 | 118.0 (6) |
| C18—C17—C16 | 119.1 (6) | C28—O1—Sn1 | 114.5 (4) |
| C13—Sn1—C1—C6 | −4.8 (5) | C15—C16—C17—C18 | 1.0 (10) |
| C7—Sn1—C1—C6 | 147.4 (4) | C16—C17—C18—C13 | −0.2 (8) |
| O1—Sn1—C1—C6 | −99.3 (4) | C14—C13—C18—C17 | 0.2 (7) |
| C13—Sn1—C1—C2 | 178.0 (3) | Sn1—C13—C18—C17 | −179.1 (4) |
| C7—Sn1—C1—C2 | −29.8 (4) | C27—C19—C20—C21 | −179.9 (5) |
| O1—Sn1—C1—C2 | 83.5 (4) | C24—C19—C20—C21 | −0.5 (7) |
| C6—C1—C2—C3 | −2.9 (7) | C19—C20—C21—C22 | 1.2 (8) |
| Sn1—C1—C2—C3 | 174.3 (4) | C20—C21—C22—C23 | −1.8 (9) |
| C1—C2—C3—C4 | 1.4 (7) | C21—C22—C23—C24 | 1.6 (8) |
| C2—C3—C4—C5 | 0.6 (8) | C27—C19—C24—N1 | −2.1 (6) |
| C3—C4—C5—C6 | −0.9 (9) | C20—C19—C24—N1 | 178.5 (4) |
| C4—C5—C6—C1 | −0.8 (9) | C27—C19—C24—C23 | 179.8 (4) |
| C2—C1—C6—C5 | 2.7 (8) | C20—C19—C24—C23 | 0.3 (6) |
| Sn1—C1—C6—C5 | −174.6 (4) | C22—C23—C24—N1 | −179.2 (5) |
| C13—Sn1—C7—C12 | −26.3 (6) | C22—C23—C24—C19 | −0.9 (7) |
| C1—Sn1—C7—C12 | −177.2 (5) | N1—C25—C26—C27 | 1.3 (6) |
| O1—Sn1—C7—C12 | 70.0 (5) | $C25^{i}$—C25—C26—C27 | −180.0 (5) |
| C13—Sn1—C7—C8 | 151.7 (4) | C25—C26—C27—C19 | −2.6 (6) |
| C1—Sn1—C7—C8 | 0.9 (5) | C25—C26—C27—C28 | 178.1 (4) |
| O1—Sn1—C7—C8 | −111.9 (4) | C24—C19—C27—C26 | 2.9 (6) |

| | | | |
|---|---|---|---|
| C12—C7—C8—C9 | 0.5 (9) | C20—C19—C27—C26 | −177.7 (4) |
| Sn1—C7—C8—C9 | −177.7 (5) | C24—C19—C27—C28 | −177.8 (4) |
| C7—C8—C9—C10 | 2.0 (10) | C20—C19—C27—C28 | 1.6 (7) |
| C8—C9—C10—C11 | −4.1 (11) | C26—C27—C28—O1 | 33.8 (9) |
| C9—C10—C11—C12 | 3.8 (13) | C19—C27—C28—O1 | −145.5 (6) |
| C8—C7—C12—C11 | −0.8 (11) | C26—C27—C28—O2 | −153.2 (6) |
| Sn1—C7—C12—C11 | 177.3 (7) | C19—C27—C28—O2 | 27.5 (8) |
| C10—C11—C12—C7 | −1.3 (14) | $C25^{i}$—C25—N1—C24 | −179.2 (4) |
| C7—Sn1—C13—C18 | 151.2 (3) | C26—C25—N1—C24 | −0.4 (6) |
| C1—Sn1—C13—C18 | −56.8 (4) | C19—C24—N1—C25 | 0.9 (6) |
| O1—Sn1—C13—C18 | 46.4 (4) | C23—C24—N1—C25 | 179.0 (4) |
| C7—Sn1—C13—C14 | −28.0 (4) | O3—C31—N2—C29 | 4.4 (8) |
| C1—Sn1—C13—C14 | 124.0 (4) | O3—C31—N2—C30 | −177.3 (7) |
| O1—Sn1—C13—C14 | −132.8 (4) | O2—C28—O1—Sn1 | 1.2 (9) |
| C18—C13—C14—C15 | −1.0 (7) | C27—C28—O1—Sn1 | 174.3 (4) |
| Sn1—C13—C14—C15 | 178.2 (4) | C13—Sn1—O1—C28 | 173.5 (5) |
| C13—C14—C15—C16 | 1.9 (9) | C7—Sn1—O1—C28 | 53.1 (6) |
| C14—C15—C16—C17 | −1.9 (10) | C1—Sn1—O1—C28 | −71.3 (5) |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

**Fig. 1**

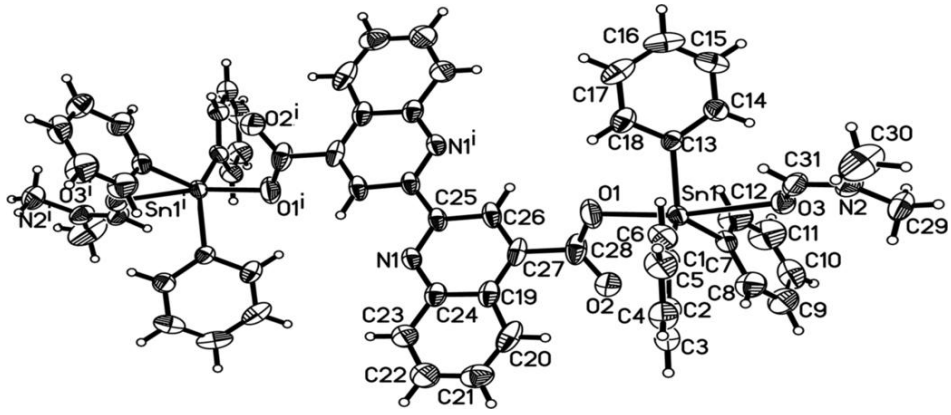
C16
C15
C17
C14
C18
C13
C30
C31
O2i
N1i
O3i
Sn1i
O1i
N2i
C25
C26
O1
Sn1
C12
O3
N2
C29
C6
C11
C28
N1
C27
C1
C7
C10
C5
C8
C19
O2
C4
C2
C9
C23
C24
C3
C20
C22
C21

**Fig. 2**