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catena-Poly[[tribenzyltin(IV)]- μ -4-nitrocinnamato- $\kappa^2O:O'$]

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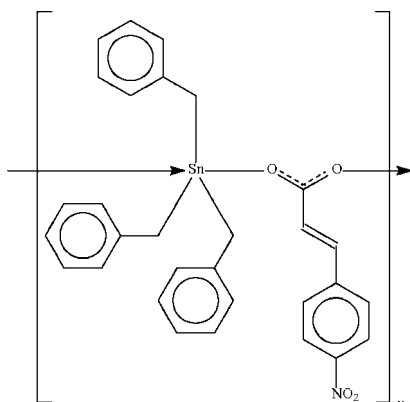
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.004$ Å; disorder in main residue; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 21.4.

The 4-nitrocinnamate anion in the title compound, $[Sn(C_7H_7)_3(C_9H_6NO_4)]_n$, bridges adjacent tribenzyltin cations into a helical chain running along the b axis. The Sn atoms in the two independent molecules adopt distorted $trans$ - C_3SnO_2 trigonal-bipyramidal geometries. The repeat distance of the polymeric chain is $b/2$.

Related literature

The trialkyltin derivatives of monocarboxylic acids generally adopt carboxylate-bridged chain structures; see: Ng *et al.* (1989). For the trialkyltin/triaryltin derivatives of cinnamic acid and other substituted cinnamic acids, see: Ng & Kumar Das (1994); Siah *et al.* (1994); Willem *et al.* (1996). For the synthesis of tribenzyltin chloride, see: Sisido *et al.* (1961). For reviews of organotin carboxylates, see: Tiekink (1991, 1994).



Experimental

Crystal data

 $[Sn(C_7H_7)_3(C_9H_6NO_4)]$
 $M_r = 584.22$ Monoclinic, $P2_1/n$ $a = 21.4850$ (3) Å $b = 10.2134$ (1) Å $c = 25.9562$ (4) Å $\beta = 112.133$ (1)° $V = 5276.0$ (1) Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 1.00$ mm⁻¹ $T = 100$ (2) K $0.36 \times 0.03 \times 0.03$ mm

Data collection

Bruker SMART APEX

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.714$, $T_{\max} = 0.971$

48779 measured reflections

12115 independent reflections

9043 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.032$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.091$ $S = 1.06$

12115 reflections

565 parameters

38 restraints

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.81$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.80$ e Å⁻³

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2314).

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supplementary materials

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catena-Poly[[tribenzyltin(IV)]- μ -4-nitrocinnamato- κ^2 O:O']

P. Y. Thong, K. M. Lo and S. W. Ng

Comment

The polymeric structure found for tribenzyl(4-nitrocinnamato)tin(IV) conforms to expectation, Fig. 1 (Ng *et al.*, 1989; Tiekink, 1991).

Experimental

Tribenzyltin chloride was synthesized from the direct reaction between tin powder and benzyl chloride in water (Sisido *et al.*, 1961). The chloride was converted to tribenzyltin hydroxide by treatment with 10% sodium hydroxide in acetone. Tribenzyltin hydroxide (1.4 g, 0.3 mmol) and 4-nitrocinnamic acid (0.5 g, 0.3 mmol) were heated in ethanol (100 ml) for 1 h. Slow evaporation of the solvent yielded yellow prisms.

Refinement

The carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.99 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. The nitro group in each independent molecule are disordered in their oxygen atoms. The nitrogen–oxygen distances for the unprimed and primed atoms were restrained to within 0.01 Å of each other. The C–NO₂ fragment was restrained to be nearly planar, and the temperature factors of the primed atoms were set to those of the unprimed ones; the anisotropic displacement parameters of the disordered atoms were restrained to be nearly isotropic. The occupancy could not be refined, and was arbitrarily set at 0.5. All phenyl and phenylene rings were refined as rigid hexagons of 1.39 Å sides.

Figures

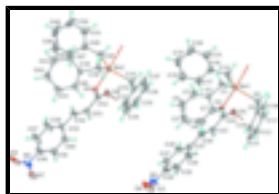


Fig. 1. 70% Probability thermal ellipsoid plot (Barbour, 2001) of $[(\text{C}_6\text{H}_5\text{CH}_2)_3\text{SnO}_2\text{CCH}=\text{CH}-\text{C}_6\text{H}_4-\text{NO}_2]_\infty$. Hydrogen atoms are drawn as spheres of arbitrary radius. Only one orientation of the disordered nitro group is shown in each case.

catena-Poly[[tribenzyltin(IV)]- μ -4-nitrocinnamato- κ^2 O:O']

Crystal data

$[\text{Sn}(\text{C}_7\text{H}_7)_3(\text{C}_9\text{H}_6\text{NO}_4)]$

$M_r = 584.22$

Monoclinic, $P2_1/n$

$F_{000} = 2368$

$D_x = 1.471 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

supplementary materials

Hall symbol: -P 2yn
 $a = 21.4850$ (3) Å
 $b = 10.2134$ (1) Å
 $c = 25.9562$ (4) Å
 $\beta = 112.133$ (1)°
 $V = 5276.0$ (1) Å³
 $Z = 8$

$\lambda = 0.71073$ Å
Cell parameters from 9977 reflections
 $\theta = 2.4$ – 28.3 °
 $\mu = 1.00$ mm⁻¹
 $T = 100$ (2) K
Prism, pale yellow
 $0.36 \times 0.03 \times 0.03$ mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 100$ (2) K
 ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.714$, $T_{\max} = 0.971$
48779 measured reflections

12115 independent reflections
9043 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 27.5$ °
 $\theta_{\text{min}} = 1.1$ °
 $h = -26 \rightarrow 27$
 $k = -13 \rightarrow 13$
 $l = -32 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.091$
 $S = 1.06$
12115 reflections
565 parameters
38 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 8.7819P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.81$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.80$ e Å⁻³
Extinction correction: none

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|---------------|---------------|--------------|----------------------------------|-----------|
| Sn1 | 0.740576 (10) | 0.624465 (18) | 0.773616 (8) | 0.01626 (6) | |
| Sn2 | 0.240598 (10) | 0.527516 (18) | 0.774258 (8) | 0.01660 (6) | |
| O1 | 0.72572 (11) | 0.46521 (19) | 0.82387 (9) | 0.0208 (4) | |
| O2 | 0.74811 (12) | 0.3133 (2) | 0.77179 (9) | 0.0285 (5) | |
| O3 | 0.5986 (4) | -0.1699 (6) | 1.0109 (5) | 0.0358 (16) | 0.50 |
| O4 | 0.6223 (5) | -0.0096 (19) | 1.0718 (4) | 0.063 (2) | 0.50 |
| O3' | 0.6225 (4) | -0.1780 (6) | 1.0239 (5) | 0.0358 (16) | 0.50 |
| O4' | 0.5957 (5) | -0.0086 (19) | 1.0602 (4) | 0.063 (2) | 0.50 |

| | | | | | |
|------|--------------|--------------|--------------|-------------|------|
| O5 | 0.22693 (12) | 0.36739 (19) | 0.82563 (9) | 0.0239 (5) | |
| O6 | 0.24714 (11) | 0.2147 (2) | 0.77260 (9) | 0.0273 (5) | |
| O7 | 0.1482 (10) | -0.2711 (10) | 1.0365 (13) | 0.039 (2) | 0.50 |
| O8 | 0.0768 (8) | -0.119 (3) | 1.0434 (7) | 0.047 (3) | 0.50 |
| O7' | 0.1347 (10) | -0.2814 (10) | 1.0294 (13) | 0.039 (2) | 0.50 |
| O8' | 0.0890 (8) | -0.125 (3) | 1.0558 (7) | 0.047 (3) | 0.50 |
| N1 | 0.61765 (12) | -0.0592 (3) | 1.02706 (11) | 0.0367 (7) | |
| N2 | 0.11891 (13) | -0.1650 (3) | 1.02647 (10) | 0.0353 (7) | |
| C1 | 0.71495 (17) | 0.7671 (3) | 0.82323 (13) | 0.0229 (6) | |
| H1A | 0.7535 | 0.8275 | 0.8394 | 0.027* | |
| H1B | 0.6765 | 0.8193 | 0.7984 | 0.027* | |
| C2 | 0.69693 (10) | 0.7136 (2) | 0.86959 (7) | 0.0190 (6) | |
| C3 | 0.63172 (9) | 0.6732 (2) | 0.85994 (8) | 0.0312 (8) | |
| H3 | 0.5977 | 0.6815 | 0.8239 | 0.037* | |
| C4 | 0.61630 (11) | 0.6204 (2) | 0.90307 (12) | 0.0484 (12) | |
| H4 | 0.5717 | 0.5928 | 0.8965 | 0.058* | |
| C5 | 0.66609 (15) | 0.6082 (2) | 0.95584 (10) | 0.0544 (14) | |
| H5 | 0.6555 | 0.5721 | 0.9853 | 0.065* | |
| C6 | 0.73130 (13) | 0.6487 (3) | 0.96549 (7) | 0.0502 (12) | |
| H6 | 0.7653 | 0.6403 | 1.0016 | 0.060* | |
| C7 | 0.74672 (8) | 0.7014 (2) | 0.92237 (8) | 0.0320 (8) | |
| H7 | 0.7913 | 0.7290 | 0.9290 | 0.038* | |
| C8 | 0.84579 (15) | 0.5814 (3) | 0.79622 (13) | 0.0225 (6) | |
| H8A | 0.8517 | 0.4871 | 0.7904 | 0.027* | |
| H8B | 0.8637 | 0.6322 | 0.7724 | 0.027* | |
| C9 | 0.88404 (10) | 0.61648 (18) | 0.85682 (6) | 0.0203 (6) | |
| C10 | 0.88920 (10) | 0.52659 (14) | 0.89844 (8) | 0.0227 (6) | |
| H10 | 0.8693 | 0.4424 | 0.8890 | 0.027* | |
| C11 | 0.92346 (10) | 0.55980 (18) | 0.95392 (7) | 0.0257 (7) | |
| H11 | 0.9270 | 0.4984 | 0.9824 | 0.031* | |
| C12 | 0.95257 (10) | 0.6829 (2) | 0.96778 (6) | 0.0278 (7) | |
| H12 | 0.9760 | 0.7056 | 1.0057 | 0.033* | |
| C13 | 0.94741 (10) | 0.77282 (15) | 0.92616 (8) | 0.0266 (7) | |
| H13 | 0.9673 | 0.8570 | 0.9356 | 0.032* | |
| C14 | 0.91314 (10) | 0.73960 (16) | 0.87068 (7) | 0.0219 (6) | |
| H14 | 0.9096 | 0.8010 | 0.8422 | 0.026* | |
| C15 | 0.66090 (15) | 0.5625 (3) | 0.69825 (13) | 0.0215 (6) | |
| H15A | 0.6636 | 0.6116 | 0.6663 | 0.026* | |
| H15B | 0.6660 | 0.4681 | 0.6920 | 0.026* | |
| C16 | 0.59325 (9) | 0.5861 (2) | 0.70202 (9) | 0.0234 (7) | |
| C17 | 0.56721 (10) | 0.49508 (17) | 0.72834 (9) | 0.0270 (7) | |
| H17 | 0.5912 | 0.4166 | 0.7428 | 0.032* | |
| C18 | 0.50613 (11) | 0.5189 (2) | 0.73352 (10) | 0.0362 (9) | |
| H18 | 0.4883 | 0.4567 | 0.7515 | 0.043* | |
| C19 | 0.47109 (9) | 0.6337 (3) | 0.71236 (11) | 0.0442 (10) | |
| H19 | 0.4293 | 0.6500 | 0.7159 | 0.053* | |
| C20 | 0.49713 (11) | 0.7247 (2) | 0.68604 (11) | 0.0467 (10) | |
| H20 | 0.4732 | 0.8032 | 0.6716 | 0.056* | |
| C21 | 0.55821 (11) | 0.70092 (19) | 0.68086 (10) | 0.0352 (8) | |

supplementary materials

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|------|--------------|---------------|--------------|-------------|
| H21 | 0.5760 | 0.7631 | 0.6629 | 0.042* |
| C22 | 0.73041 (15) | 0.3466 (3) | 0.81149 (12) | 0.0193 (6) |
| C23 | 0.71423 (15) | 0.2458 (3) | 0.84523 (12) | 0.0200 (6) |
| H23 | 0.7156 | 0.1561 | 0.8361 | 0.024* |
| C24 | 0.69782 (15) | 0.2774 (3) | 0.88809 (13) | 0.0222 (6) |
| H24 | 0.6986 | 0.3679 | 0.8967 | 0.027* |
| C25 | 0.67857 (11) | 0.18658 (16) | 0.92365 (8) | 0.0217 (6) |
| C26 | 0.66231 (12) | 0.24047 (13) | 0.96615 (9) | 0.0273 (7) |
| H26 | 0.6651 | 0.3324 | 0.9721 | 0.033* |
| C27 | 0.64194 (12) | 0.15980 (18) | 1.00000 (8) | 0.0300 (8) |
| H27 | 0.6308 | 0.1966 | 1.0290 | 0.036* |
| C28 | 0.63784 (12) | 0.02523 (17) | 0.99136 (8) | 0.0260 (7) |
| C29 | 0.65410 (13) | -0.02866 (13) | 0.94886 (9) | 0.0290 (8) |
| H29 | 0.6513 | -0.1206 | 0.9430 | 0.035* |
| C30 | 0.67447 (12) | 0.05201 (17) | 0.91501 (8) | 0.0279 (7) |
| H30 | 0.6856 | 0.0152 | 0.8860 | 0.034* |
| C31 | 0.34371 (15) | 0.4752 (3) | 0.78971 (13) | 0.0234 (7) |
| H31A | 0.3489 | 0.3789 | 0.7916 | 0.028* |
| H31B | 0.3567 | 0.5082 | 0.7593 | 0.028* |
| C32 | 0.38785 (10) | 0.5362 (2) | 0.84441 (7) | 0.0257 (7) |
| C33 | 0.39227 (11) | 0.4797 (2) | 0.89438 (9) | 0.0348 (8) |
| H33 | 0.3704 | 0.3988 | 0.8943 | 0.042* |
| C34 | 0.42867 (12) | 0.5415 (3) | 0.94443 (7) | 0.0456 (11) |
| H34 | 0.4317 | 0.5029 | 0.9786 | 0.055* |
| C35 | 0.46065 (12) | 0.6599 (3) | 0.94449 (8) | 0.0482 (11) |
| H35 | 0.4855 | 0.7021 | 0.9787 | 0.058* |
| C36 | 0.45623 (11) | 0.71638 (19) | 0.89452 (11) | 0.0425 (10) |
| H36 | 0.4781 | 0.7973 | 0.8946 | 0.051* |
| C37 | 0.41983 (11) | 0.6546 (2) | 0.84447 (8) | 0.0327 (8) |
| H37 | 0.4168 | 0.6932 | 0.8103 | 0.039* |
| C38 | 0.23174 (16) | 0.6679 (3) | 0.83283 (13) | 0.0207 (6) |
| H38A | 0.2751 | 0.6712 | 0.8650 | 0.025* |
| H38B | 0.2242 | 0.7552 | 0.8150 | 0.025* |
| C39 | 0.17661 (9) | 0.6429 (2) | 0.85455 (8) | 0.0206 (6) |
| C40 | 0.18741 (8) | 0.5606 (2) | 0.89975 (8) | 0.0258 (7) |
| H40 | 0.2299 | 0.5198 | 0.9176 | 0.031* |
| C41 | 0.13605 (11) | 0.5380 (2) | 0.91892 (8) | 0.0325 (8) |
| H41 | 0.1434 | 0.4817 | 0.9498 | 0.039* |
| C42 | 0.07389 (9) | 0.5977 (2) | 0.89288 (9) | 0.0349 (8) |
| H42 | 0.0388 | 0.5822 | 0.9060 | 0.042* |
| C43 | 0.06308 (8) | 0.6800 (2) | 0.84768 (9) | 0.0376 (9) |
| H43 | 0.0206 | 0.7208 | 0.8299 | 0.045* |
| C44 | 0.11444 (10) | 0.7026 (2) | 0.82851 (8) | 0.0293 (7) |
| H44 | 0.1071 | 0.7589 | 0.7976 | 0.035* |
| C45 | 0.15670 (16) | 0.4719 (3) | 0.70112 (14) | 0.0245 (7) |
| H45A | 0.1653 | 0.4998 | 0.6679 | 0.029* |
| H45B | 0.1527 | 0.3753 | 0.7000 | 0.029* |
| C46 | 0.09086 (9) | 0.5305 (2) | 0.69842 (10) | 0.0258 (7) |
| C47 | 0.05407 (12) | 0.4697 (2) | 0.72566 (10) | 0.0370 (9) |

| | | | | |
|-----|---------------|---------------|--------------|-------------|
| H47 | 0.0697 | 0.3901 | 0.7452 | 0.044* |
| C48 | -0.00562 (12) | 0.5252 (3) | 0.72425 (12) | 0.0517 (12) |
| H48 | -0.0308 | 0.4836 | 0.7429 | 0.062* |
| C49 | -0.02853 (10) | 0.6416 (3) | 0.69561 (12) | 0.0561 (13) |
| H49 | -0.0693 | 0.6795 | 0.6946 | 0.067* |
| C50 | 0.00826 (13) | 0.7024 (2) | 0.66837 (11) | 0.0506 (12) |
| H50 | -0.0074 | 0.7820 | 0.6488 | 0.061* |
| C51 | 0.06795 (12) | 0.6469 (2) | 0.66978 (10) | 0.0353 (8) |
| H51 | 0.0931 | 0.6885 | 0.6512 | 0.042* |
| C52 | 0.23218 (15) | 0.2495 (3) | 0.81304 (13) | 0.0198 (6) |
| C53 | 0.21856 (16) | 0.1483 (3) | 0.84854 (13) | 0.0211 (6) |
| H53 | 0.2298 | 0.0597 | 0.8450 | 0.025* |
| C54 | 0.19105 (17) | 0.1782 (3) | 0.88532 (13) | 0.0254 (7) |
| H54 | 0.1828 | 0.2683 | 0.8893 | 0.030* |
| C55 | 0.17221 (12) | 0.08569 (17) | 0.92023 (9) | 0.0255 (7) |
| C56 | 0.13401 (15) | 0.13270 (16) | 0.94915 (12) | 0.0541 (13) |
| H56 | 0.1202 | 0.2217 | 0.9454 | 0.065* |
| C57 | 0.11599 (14) | 0.0494 (2) | 0.98357 (11) | 0.0567 (14) |
| H57 | 0.0899 | 0.0816 | 1.0033 | 0.068* |
| C58 | 0.13617 (13) | -0.08082 (19) | 0.98908 (9) | 0.0283 (7) |
| C59 | 0.17438 (12) | -0.12784 (15) | 0.96017 (9) | 0.0288 (7) |
| H59 | 0.1882 | -0.2169 | 0.9639 | 0.035* |
| C60 | 0.19240 (11) | -0.04458 (19) | 0.92574 (9) | 0.0265 (7) |
| H60 | 0.2185 | -0.0767 | 0.9060 | 0.032* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|-------------|--------------|
| Sn1 | 0.02067 (11) | 0.01290 (10) | 0.01803 (10) | -0.00047 (8) | 0.01050 (8) | -0.00080 (8) |
| Sn2 | 0.01892 (10) | 0.01368 (10) | 0.02153 (11) | 0.00060 (8) | 0.01256 (8) | -0.00001 (8) |
| O1 | 0.0309 (12) | 0.0125 (10) | 0.0231 (11) | -0.0006 (9) | 0.0149 (10) | -0.0016 (8) |
| O2 | 0.0385 (14) | 0.0240 (12) | 0.0296 (12) | 0.0031 (10) | 0.0203 (11) | -0.0003 (10) |
| O3 | 0.046 (5) | 0.0261 (15) | 0.041 (4) | -0.009 (2) | 0.023 (4) | 0.0018 (18) |
| O4 | 0.120 (7) | 0.0448 (19) | 0.049 (4) | -0.019 (6) | 0.060 (4) | -0.008 (3) |
| O3' | 0.046 (5) | 0.0261 (15) | 0.041 (4) | -0.009 (2) | 0.023 (4) | 0.0018 (18) |
| O4' | 0.120 (7) | 0.0448 (19) | 0.049 (4) | -0.019 (6) | 0.060 (4) | -0.008 (3) |
| O5 | 0.0386 (13) | 0.0129 (10) | 0.0305 (12) | 0.0013 (9) | 0.0247 (11) | 0.0013 (9) |
| O6 | 0.0357 (13) | 0.0235 (12) | 0.0315 (12) | 0.0019 (10) | 0.0228 (11) | -0.0018 (10) |
| O7 | 0.035 (7) | 0.039 (2) | 0.037 (6) | -0.014 (3) | 0.008 (5) | 0.013 (2) |
| O8 | 0.084 (5) | 0.043 (3) | 0.029 (6) | -0.018 (4) | 0.040 (5) | -0.004 (6) |
| O7' | 0.035 (7) | 0.039 (2) | 0.037 (6) | -0.014 (3) | 0.008 (5) | 0.013 (2) |
| O8' | 0.084 (5) | 0.043 (3) | 0.029 (6) | -0.018 (4) | 0.040 (5) | -0.004 (6) |
| N1 | 0.063 (2) | 0.0263 (16) | 0.0308 (16) | -0.0070 (15) | 0.0295 (16) | -0.0007 (13) |
| N2 | 0.0500 (19) | 0.0320 (17) | 0.0264 (15) | -0.0184 (15) | 0.0172 (14) | -0.0017 (13) |
| C1 | 0.0378 (18) | 0.0084 (13) | 0.0267 (16) | -0.0008 (12) | 0.0169 (14) | -0.0032 (12) |
| C2 | 0.0235 (15) | 0.0129 (13) | 0.0246 (15) | 0.0027 (11) | 0.0135 (13) | -0.0024 (12) |
| C3 | 0.0278 (17) | 0.0282 (17) | 0.043 (2) | -0.0029 (14) | 0.0192 (16) | -0.0153 (16) |
| C4 | 0.057 (3) | 0.0265 (19) | 0.091 (4) | -0.0157 (18) | 0.062 (3) | -0.022 (2) |

supplementary materials

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|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C5 | 0.108 (4) | 0.0225 (19) | 0.066 (3) | 0.013 (2) | 0.070 (3) | 0.0097 (19) |
| C6 | 0.075 (3) | 0.051 (3) | 0.033 (2) | 0.032 (2) | 0.030 (2) | 0.0167 (19) |
| C7 | 0.0285 (18) | 0.042 (2) | 0.0258 (17) | 0.0099 (15) | 0.0105 (14) | -0.0001 (15) |
| C8 | 0.0256 (16) | 0.0215 (15) | 0.0253 (16) | 0.0038 (13) | 0.0152 (13) | 0.0028 (13) |
| C9 | 0.0186 (15) | 0.0209 (15) | 0.0253 (16) | 0.0035 (12) | 0.0127 (13) | 0.0033 (12) |
| C10 | 0.0217 (15) | 0.0198 (15) | 0.0293 (17) | 0.0035 (12) | 0.0127 (13) | 0.0056 (13) |
| C11 | 0.0248 (16) | 0.0286 (17) | 0.0275 (17) | 0.0080 (14) | 0.0140 (14) | 0.0099 (14) |
| C12 | 0.0263 (17) | 0.0344 (18) | 0.0230 (16) | 0.0053 (14) | 0.0098 (14) | -0.0028 (14) |
| C13 | 0.0250 (16) | 0.0219 (16) | 0.0337 (18) | 0.0021 (13) | 0.0119 (14) | -0.0034 (14) |
| C14 | 0.0222 (15) | 0.0189 (15) | 0.0291 (16) | 0.0037 (12) | 0.0146 (13) | 0.0057 (12) |
| C15 | 0.0237 (16) | 0.0210 (15) | 0.0223 (15) | -0.0019 (12) | 0.0115 (13) | -0.0034 (12) |
| C16 | 0.0212 (16) | 0.0246 (16) | 0.0233 (16) | -0.0016 (13) | 0.0071 (13) | -0.0064 (13) |
| C17 | 0.0287 (17) | 0.0275 (17) | 0.0257 (17) | -0.0075 (14) | 0.0112 (14) | -0.0077 (14) |
| C18 | 0.0291 (19) | 0.049 (2) | 0.0323 (19) | -0.0132 (17) | 0.0134 (16) | -0.0112 (17) |
| C19 | 0.0226 (18) | 0.069 (3) | 0.043 (2) | -0.0029 (18) | 0.0144 (17) | -0.010 (2) |
| C20 | 0.031 (2) | 0.054 (3) | 0.054 (3) | 0.0162 (19) | 0.0138 (19) | 0.002 (2) |
| C21 | 0.0315 (19) | 0.034 (2) | 0.040 (2) | 0.0057 (15) | 0.0131 (16) | 0.0026 (16) |
| C22 | 0.0207 (15) | 0.0162 (14) | 0.0223 (15) | 0.0007 (12) | 0.0094 (12) | -0.0022 (12) |
| C23 | 0.0235 (15) | 0.0118 (14) | 0.0251 (15) | -0.0007 (11) | 0.0097 (13) | 0.0009 (11) |
| C24 | 0.0281 (16) | 0.0139 (14) | 0.0275 (16) | -0.0021 (12) | 0.0137 (13) | -0.0006 (12) |
| C25 | 0.0275 (16) | 0.0177 (14) | 0.0230 (15) | -0.0006 (12) | 0.0130 (13) | 0.0005 (12) |
| C26 | 0.041 (2) | 0.0175 (15) | 0.0290 (17) | 0.0022 (14) | 0.0197 (15) | -0.0006 (13) |
| C27 | 0.046 (2) | 0.0271 (17) | 0.0273 (17) | 0.0006 (15) | 0.0255 (16) | -0.0036 (14) |
| C28 | 0.0375 (19) | 0.0219 (16) | 0.0228 (16) | -0.0024 (14) | 0.0162 (15) | 0.0008 (13) |
| C29 | 0.048 (2) | 0.0177 (16) | 0.0295 (18) | -0.0028 (14) | 0.0237 (17) | -0.0017 (13) |
| C30 | 0.044 (2) | 0.0207 (15) | 0.0280 (17) | -0.0046 (14) | 0.0242 (16) | -0.0037 (13) |
| C31 | 0.0234 (16) | 0.0205 (15) | 0.0306 (17) | 0.0049 (12) | 0.0152 (14) | 0.0003 (13) |
| C32 | 0.0178 (15) | 0.0264 (17) | 0.0331 (18) | 0.0069 (13) | 0.0098 (14) | 0.0017 (14) |
| C33 | 0.0247 (18) | 0.048 (2) | 0.0314 (19) | 0.0064 (16) | 0.0106 (15) | 0.0059 (17) |
| C34 | 0.028 (2) | 0.076 (3) | 0.031 (2) | 0.010 (2) | 0.0098 (16) | 0.003 (2) |
| C35 | 0.0255 (19) | 0.068 (3) | 0.043 (2) | 0.008 (2) | 0.0039 (17) | -0.020 (2) |
| C36 | 0.0274 (19) | 0.035 (2) | 0.058 (3) | 0.0038 (16) | 0.0083 (18) | -0.0115 (19) |
| C37 | 0.0241 (17) | 0.0282 (18) | 0.044 (2) | 0.0077 (14) | 0.0114 (16) | 0.0036 (16) |
| C38 | 0.0283 (16) | 0.0136 (14) | 0.0254 (16) | 0.0005 (12) | 0.0160 (13) | -0.0013 (12) |
| C39 | 0.0265 (16) | 0.0176 (15) | 0.0214 (15) | 0.0026 (12) | 0.0133 (13) | -0.0015 (12) |
| C40 | 0.0308 (17) | 0.0246 (16) | 0.0266 (17) | 0.0092 (14) | 0.0161 (14) | 0.0039 (13) |
| C41 | 0.050 (2) | 0.0233 (17) | 0.0348 (19) | 0.0058 (15) | 0.0287 (18) | 0.0055 (14) |
| C42 | 0.034 (2) | 0.042 (2) | 0.041 (2) | -0.0001 (16) | 0.0278 (17) | -0.0043 (17) |
| C43 | 0.0273 (18) | 0.056 (2) | 0.0338 (19) | 0.0129 (17) | 0.0167 (16) | 0.0014 (18) |
| C44 | 0.0311 (18) | 0.0361 (19) | 0.0250 (17) | 0.0106 (15) | 0.0155 (14) | 0.0043 (14) |
| C45 | 0.0260 (16) | 0.0216 (16) | 0.0281 (17) | -0.0034 (13) | 0.0127 (14) | -0.0052 (13) |
| C46 | 0.0207 (16) | 0.0269 (17) | 0.0284 (17) | -0.0036 (13) | 0.0076 (14) | -0.0088 (13) |
| C47 | 0.033 (2) | 0.034 (2) | 0.051 (2) | -0.0086 (16) | 0.0228 (18) | -0.0098 (17) |
| C48 | 0.029 (2) | 0.066 (3) | 0.066 (3) | -0.012 (2) | 0.024 (2) | -0.022 (2) |
| C49 | 0.024 (2) | 0.079 (3) | 0.056 (3) | 0.012 (2) | 0.0045 (19) | -0.026 (3) |
| C50 | 0.043 (2) | 0.047 (3) | 0.043 (2) | 0.019 (2) | -0.0054 (19) | -0.011 (2) |
| C51 | 0.033 (2) | 0.033 (2) | 0.0335 (19) | 0.0032 (16) | 0.0055 (16) | -0.0051 (16) |
| C52 | 0.0217 (15) | 0.0124 (14) | 0.0301 (16) | -0.0002 (11) | 0.0151 (13) | 0.0011 (12) |
| C53 | 0.0278 (16) | 0.0114 (13) | 0.0265 (16) | -0.0008 (12) | 0.0130 (13) | 0.0007 (12) |

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|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C54 | 0.0351 (18) | 0.0152 (14) | 0.0302 (17) | -0.0009 (13) | 0.0173 (15) | -0.0025 (13) |
| C55 | 0.0369 (19) | 0.0210 (15) | 0.0247 (16) | -0.0049 (14) | 0.0185 (15) | -0.0006 (13) |
| C56 | 0.106 (4) | 0.0200 (18) | 0.075 (3) | 0.008 (2) | 0.078 (3) | 0.0062 (19) |
| C57 | 0.110 (4) | 0.027 (2) | 0.073 (3) | 0.003 (2) | 0.080 (3) | 0.002 (2) |
| C58 | 0.041 (2) | 0.0245 (17) | 0.0223 (16) | -0.0130 (15) | 0.0158 (15) | -0.0032 (13) |
| C59 | 0.0326 (18) | 0.0236 (16) | 0.0310 (18) | -0.0021 (14) | 0.0129 (15) | 0.0034 (14) |
| C60 | 0.0326 (18) | 0.0217 (16) | 0.0297 (17) | -0.0009 (13) | 0.0169 (15) | 0.0009 (13) |

Geometric parameters (Å, °)

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|-----------------------|-----------|----------|-----------|
| Sn1—C1 | 2.149 (3) | C23—H23 | 0.9500 |
| Sn1—C15 | 2.153 (3) | C24—C25 | 1.473 (3) |
| Sn1—C8 | 2.156 (3) | C24—H24 | 0.9500 |
| Sn1—O1 | 2.182 (2) | C25—C26 | 1.3900 |
| Sn1—O2 ⁱ | 2.320 (2) | C25—C30 | 1.3900 |
| Sn2—C45 | 2.144 (3) | C26—C27 | 1.3900 |
| Sn2—C38 | 2.149 (3) | C26—H26 | 0.9500 |
| Sn2—C31 | 2.164 (3) | C27—C28 | 1.3900 |
| Sn2—O5 | 2.199 (2) | C27—H27 | 0.9500 |
| Sn2—O6 ⁱⁱ | 2.334 (2) | C28—C29 | 1.3900 |
| O1—C22 | 1.267 (3) | C29—C30 | 1.3900 |
| O2—C22 | 1.272 (3) | C29—H29 | 0.9500 |
| O2—Sn1 ⁱⁱⁱ | 2.320 (2) | C30—H30 | 0.9500 |
| O3—N1 | 1.222 (6) | C31—C32 | 1.513 (4) |
| O4—N1 | 1.235 (7) | C31—H31A | 0.9900 |
| O3'—N1 | 1.223 (6) | C31—H31B | 0.9900 |
| O4'—N1 | 1.238 (7) | C32—C33 | 1.3900 |
| O5—C52 | 1.264 (3) | C32—C37 | 1.3900 |
| O6—C52 | 1.259 (3) | C33—C34 | 1.3900 |
| O6—Sn2 ^{iv} | 2.334 (2) | C33—H33 | 0.9500 |
| O7—N2 | 1.231 (7) | C34—C35 | 1.3900 |
| O8—N2 | 1.240 (7) | C34—H34 | 0.9500 |
| O7'—N2 | 1.230 (7) | C35—C36 | 1.3900 |
| O8'—N2 | 1.235 (7) | C35—H35 | 0.9500 |
| N1—C28 | 1.447 (3) | C36—C37 | 1.3900 |
| N2—C58 | 1.446 (3) | C36—H36 | 0.9500 |
| C1—C2 | 1.499 (3) | C37—H37 | 0.9500 |
| C1—H1A | 0.9900 | C38—C39 | 1.513 (3) |
| C1—H1B | 0.9900 | C38—H38A | 0.9900 |
| C2—C3 | 1.3900 | C38—H38B | 0.9900 |
| C2—C7 | 1.3900 | C39—C40 | 1.3900 |
| C3—C4 | 1.3900 | C39—C44 | 1.3900 |
| C3—H3 | 0.9500 | C40—C41 | 1.3900 |
| C4—C5 | 1.3900 | C40—H40 | 0.9500 |
| C4—H4 | 0.9500 | C41—C42 | 1.3900 |
| C5—C6 | 1.3900 | C41—H41 | 0.9500 |
| C5—H5 | 0.9500 | C42—C43 | 1.3900 |
| C6—C7 | 1.3900 | C42—H42 | 0.9500 |

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|-------------------------|-------------|-------------|-------------|
| C6—H6 | 0.9500 | C43—C44 | 1.3900 |
| C7—H7 | 0.9500 | C43—H43 | 0.9500 |
| C8—C9 | 1.518 (3) | C44—H44 | 0.9500 |
| C8—H8A | 0.9900 | C45—C46 | 1.513 (3) |
| C8—H8B | 0.9900 | C45—H45A | 0.9900 |
| C9—C10 | 1.3900 | C45—H45B | 0.9900 |
| C9—C14 | 1.3900 | C46—C47 | 1.3900 |
| C10—C11 | 1.3900 | C46—C51 | 1.3900 |
| C10—H10 | 0.9500 | C47—C48 | 1.3900 |
| C11—C12 | 1.3900 | C47—H47 | 0.9500 |
| C11—H11 | 0.9500 | C48—C49 | 1.3900 |
| C12—C13 | 1.3900 | C48—H48 | 0.9500 |
| C12—H12 | 0.9500 | C49—C50 | 1.3900 |
| C13—C14 | 1.3900 | C49—H49 | 0.9500 |
| C13—H13 | 0.9500 | C50—C51 | 1.3900 |
| C14—H14 | 0.9500 | C50—H50 | 0.9500 |
| C15—C16 | 1.512 (3) | C51—H51 | 0.9500 |
| C15—H15A | 0.9900 | C52—C53 | 1.485 (4) |
| C15—H15B | 0.9900 | C53—C54 | 1.334 (4) |
| C16—C17 | 1.3900 | C53—H53 | 0.9500 |
| C16—C21 | 1.3900 | C54—C55 | 1.468 (3) |
| C17—C18 | 1.3900 | C54—H54 | 0.9500 |
| C17—H17 | 0.9500 | C55—C56 | 1.3900 |
| C18—C19 | 1.3900 | C55—C60 | 1.3900 |
| C18—H18 | 0.9500 | C56—C57 | 1.3900 |
| C19—C20 | 1.3900 | C56—H56 | 0.9500 |
| C19—H19 | 0.9500 | C57—C58 | 1.3900 |
| C20—C21 | 1.3900 | C57—H57 | 0.9500 |
| C20—H20 | 0.9500 | C58—C59 | 1.3900 |
| C21—H21 | 0.9500 | C59—C60 | 1.3900 |
| C22—C23 | 1.476 (4) | C59—H59 | 0.9500 |
| C23—C24 | 1.327 (4) | C60—H60 | 0.9500 |
| C1—Sn1—C15 | 116.64 (12) | C26—C25—C30 | 120.0 |
| C1—Sn1—C8 | 117.02 (13) | C26—C25—C24 | 117.50 (17) |
| C15—Sn1—C8 | 125.49 (12) | C30—C25—C24 | 122.48 (17) |
| C1—Sn1—O1 | 91.07 (9) | C25—C26—C27 | 120.0 |
| C15—Sn1—O1 | 94.51 (10) | C25—C26—H26 | 120.0 |
| C8—Sn1—O1 | 93.42 (10) | C27—C26—H26 | 120.0 |
| C1—Sn1—O2 ⁱ | 80.82 (10) | C26—C27—C28 | 120.0 |
| C15—Sn1—O2 ⁱ | 89.00 (10) | C26—C27—H27 | 120.0 |
| C8—Sn1—O2 ⁱ | 90.47 (10) | C28—C27—H27 | 120.0 |
| O1—Sn1—O2 ⁱ | 171.89 (8) | C29—C28—C27 | 120.0 |
| C45—Sn2—C38 | 122.28 (12) | C29—C28—N1 | 119.86 (17) |
| C45—Sn2—C31 | 123.99 (12) | C27—C28—N1 | 120.13 (17) |
| C38—Sn2—C31 | 112.99 (12) | C28—C29—C30 | 120.0 |
| C45—Sn2—O5 | 94.59 (11) | C28—C29—H29 | 120.0 |
| C38—Sn2—O5 | 89.97 (9) | C30—C29—H29 | 120.0 |
| C31—Sn2—O5 | 93.75 (10) | C29—C30—C25 | 120.0 |

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| C45—Sn2—O6 ⁱⁱ | 88.74 (10) | C29—C30—H30 | 120.0 |
| C38—Sn2—O6 ⁱⁱ | 83.09 (10) | C25—C30—H30 | 120.0 |
| C31—Sn2—O6 ⁱⁱ | 89.43 (10) | C32—C31—Sn2 | 107.96 (18) |
| O5—Sn2—O6 ⁱⁱ | 173.04 (8) | C32—C31—H31A | 110.1 |
| C22—O1—Sn1 | 121.17 (19) | Sn2—C31—H31A | 110.1 |
| C22—O2—Sn1 ⁱⁱⁱ | 139.0 (2) | C32—C31—H31B | 110.1 |
| C52—O5—Sn2 | 120.44 (19) | Sn2—C31—H31B | 110.1 |
| C52—O6—Sn2 ^{iv} | 141.3 (2) | H31A—C31—H31B | 108.4 |
| O3—N1—O4 | 126.9 (12) | C33—C32—C37 | 120.0 |
| O3'—N1—O4' | 121.7 (12) | C33—C32—C31 | 120.21 (19) |
| O3—N1—C28 | 118.3 (7) | C37—C32—C31 | 119.60 (18) |
| O3'—N1—C28 | 119.6 (7) | C32—C33—C34 | 120.0 |
| O4—N1—C28 | 114.8 (10) | C32—C33—H33 | 120.0 |
| O4'—N1—C28 | 118.7 (11) | C34—C33—H33 | 120.0 |
| O7'—N2—O8' | 118 (3) | C33—C34—C35 | 120.0 |
| O7—N2—O8 | 130 (2) | C33—C34—H34 | 120.0 |
| O7'—N2—C58 | 118.8 (18) | C35—C34—H34 | 120.0 |
| O7—N2—C58 | 115.1 (18) | C36—C35—C34 | 120.0 |
| O8'—N2—C58 | 122.7 (16) | C36—C35—H35 | 120.0 |
| O8—N2—C58 | 114.7 (15) | C34—C35—H35 | 120.0 |
| C2—C1—Sn1 | 115.87 (18) | C35—C36—C37 | 120.0 |
| C2—C1—H1A | 108.3 | C35—C36—H36 | 120.0 |
| Sn1—C1—H1A | 108.3 | C37—C36—H36 | 120.0 |
| C2—C1—H1B | 108.3 | C36—C37—C32 | 120.0 |
| Sn1—C1—H1B | 108.3 | C36—C37—H37 | 120.0 |
| H1A—C1—H1B | 107.4 | C32—C37—H37 | 120.0 |
| C3—C2—C7 | 120.0 | C39—C38—Sn2 | 116.21 (18) |
| C3—C2—C1 | 120.75 (19) | C39—C38—H38A | 108.2 |
| C7—C2—C1 | 119.23 (19) | Sn2—C38—H38A | 108.2 |
| C2—C3—C4 | 120.0 | C39—C38—H38B | 108.2 |
| C2—C3—H3 | 120.0 | Sn2—C38—H38B | 108.2 |
| C4—C3—H3 | 120.0 | H38A—C38—H38B | 107.4 |
| C5—C4—C3 | 120.0 | C40—C39—C44 | 120.0 |
| C5—C4—H4 | 120.0 | C40—C39—C38 | 120.74 (17) |
| C3—C4—H4 | 120.0 | C44—C39—C38 | 119.26 (17) |
| C4—C5—C6 | 120.0 | C39—C40—C41 | 120.0 |
| C4—C5—H5 | 120.0 | C39—C40—H40 | 120.0 |
| C6—C5—H5 | 120.0 | C41—C40—H40 | 120.0 |
| C5—C6—C7 | 120.0 | C42—C41—C40 | 120.0 |
| C5—C6—H6 | 120.0 | C42—C41—H41 | 120.0 |
| C7—C6—H6 | 120.0 | C40—C41—H41 | 120.0 |
| C6—C7—C2 | 120.0 | C41—C42—C43 | 120.0 |
| C6—C7—H7 | 120.0 | C41—C42—H42 | 120.0 |
| C2—C7—H7 | 120.0 | C43—C42—H42 | 120.0 |
| C9—C8—Sn1 | 109.68 (17) | C44—C43—C42 | 120.0 |
| C9—C8—H8A | 109.7 | C44—C43—H43 | 120.0 |
| Sn1—C8—H8A | 109.7 | C42—C43—H43 | 120.0 |
| C9—C8—H8B | 109.7 | C43—C44—C39 | 120.0 |

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| Sn1—C8—H8B | 109.7 | C43—C44—H44 | 120.0 |
| H8A—C8—H8B | 108.2 | C39—C44—H44 | 120.0 |
| C10—C9—C14 | 120.0 | C46—C45—Sn2 | 113.29 (19) |
| C10—C9—C8 | 120.19 (17) | C46—C45—H45A | 108.9 |
| C14—C9—C8 | 119.81 (17) | Sn2—C45—H45A | 108.9 |
| C9—C10—C11 | 120.0 | C46—C45—H45B | 108.9 |
| C9—C10—H10 | 120.0 | Sn2—C45—H45B | 108.9 |
| C11—C10—H10 | 120.0 | H45A—C45—H45B | 107.7 |
| C12—C11—C10 | 120.0 | C47—C46—C51 | 120.0 |
| C12—C11—H11 | 120.0 | C47—C46—C45 | 120.02 (19) |
| C10—C11—H11 | 120.0 | C51—C46—C45 | 119.97 (19) |
| C11—C12—C13 | 120.0 | C46—C47—C48 | 120.0 |
| C11—C12—H12 | 120.0 | C46—C47—H47 | 120.0 |
| C13—C12—H12 | 120.0 | C48—C47—H47 | 120.0 |
| C14—C13—C12 | 120.0 | C47—C48—C49 | 120.0 |
| C14—C13—H13 | 120.0 | C47—C48—H48 | 120.0 |
| C12—C13—H13 | 120.0 | C49—C48—H48 | 120.0 |
| C13—C14—C9 | 120.0 | C50—C49—C48 | 120.0 |
| C13—C14—H14 | 120.0 | C50—C49—H49 | 120.0 |
| C9—C14—H14 | 120.0 | C48—C49—H49 | 120.0 |
| C16—C15—Sn1 | 110.42 (18) | C49—C50—C51 | 120.0 |
| C16—C15—H15A | 109.6 | C49—C50—H50 | 120.0 |
| Sn1—C15—H15A | 109.6 | C51—C50—H50 | 120.0 |
| C16—C15—H15B | 109.6 | C50—C51—C46 | 120.0 |
| Sn1—C15—H15B | 109.6 | C50—C51—H51 | 120.0 |
| H15A—C15—H15B | 108.1 | C46—C51—H51 | 120.0 |
| C17—C16—C21 | 120.0 | O6—C52—O5 | 124.0 (3) |
| C17—C16—C15 | 119.98 (18) | O6—C52—C53 | 119.5 (3) |
| C21—C16—C15 | 119.98 (18) | O5—C52—C53 | 116.4 (3) |
| C18—C17—C16 | 120.0 | C54—C53—C52 | 121.9 (3) |
| C18—C17—H17 | 120.0 | C54—C53—H53 | 119.0 |
| C16—C17—H17 | 120.0 | C52—C53—H53 | 119.0 |
| C17—C18—C19 | 120.0 | C53—C54—C55 | 126.4 (3) |
| C17—C18—H18 | 120.0 | C53—C54—H54 | 116.8 |
| C19—C18—H18 | 120.0 | C55—C54—H54 | 116.8 |
| C20—C19—C18 | 120.0 | C56—C55—C60 | 120.0 |
| C20—C19—H19 | 120.0 | C56—C55—C54 | 117.85 (18) |
| C18—C19—H19 | 120.0 | C60—C55—C54 | 122.14 (18) |
| C19—C20—C21 | 120.0 | C57—C56—C55 | 120.0 |
| C19—C20—H20 | 120.0 | C57—C56—H56 | 120.0 |
| C21—C20—H20 | 120.0 | C55—C56—H56 | 120.0 |
| C20—C21—C16 | 120.0 | C56—C57—C58 | 120.0 |
| C20—C21—H21 | 120.0 | C56—C57—H57 | 120.0 |
| C16—C21—H21 | 120.0 | C58—C57—H57 | 120.0 |
| O1—C22—O2 | 122.5 (3) | C57—C58—C59 | 120.0 |
| O1—C22—C23 | 117.2 (3) | C57—C58—N2 | 119.3 (2) |
| O2—C22—C23 | 120.2 (3) | C59—C58—N2 | 120.7 (2) |
| C24—C23—C22 | 121.6 (3) | C60—C59—C58 | 120.0 |
| C24—C23—H23 | 119.2 | C60—C59—H59 | 120.0 |

| | | | |
|------------------------------|--------------|-------------------------------|--------------|
| C22—C23—H23 | 119.2 | C58—C59—H59 | 120.0 |
| C23—C24—C25 | 126.7 (3) | C59—C60—C55 | 120.0 |
| C23—C24—H24 | 116.6 | C59—C60—H60 | 120.0 |
| C25—C24—H24 | 116.6 | C55—C60—H60 | 120.0 |
| C1—Sn1—O1—C22 | 175.8 (2) | C28—C29—C30—C25 | 0.0 |
| C15—Sn1—O1—C22 | 58.9 (2) | C26—C25—C30—C29 | 0.0 |
| C8—Sn1—O1—C22 | -67.1 (2) | C24—C25—C30—C29 | -178.1 (2) |
| C45—Sn2—O5—C52 | 62.7 (3) | C45—Sn2—C31—C32 | 178.15 (17) |
| C38—Sn2—O5—C52 | -174.9 (3) | C38—Sn2—C31—C32 | 7.8 (2) |
| C31—Sn2—O5—C52 | -61.9 (3) | O5—Sn2—C31—C32 | -83.74 (19) |
| C15—Sn1—C1—C2 | 94.9 (2) | O6 ⁱⁱ —Sn2—C31—C32 | 90.06 (18) |
| C8—Sn1—C1—C2 | -95.0 (2) | Sn2—C31—C32—C33 | 77.7 (2) |
| O1—Sn1—C1—C2 | -0.6 (2) | Sn2—C31—C32—C37 | -97.25 (18) |
| O2 ⁱ —Sn1—C1—C2 | 179.2 (2) | C37—C32—C33—C34 | 0.0 |
| Sn1—C1—C2—C3 | -85.2 (2) | C31—C32—C33—C34 | -175.0 (2) |
| Sn1—C1—C2—C7 | 93.0 (2) | C32—C33—C34—C35 | 0.0 |
| C7—C2—C3—C4 | 0.0 | C33—C34—C35—C36 | 0.0 |
| C1—C2—C3—C4 | 178.2 (2) | C34—C35—C36—C37 | 0.0 |
| C2—C3—C4—C5 | 0.0 | C35—C36—C37—C32 | 0.0 |
| C3—C4—C5—C6 | 0.0 | C33—C32—C37—C36 | 0.0 |
| C4—C5—C6—C7 | 0.0 | C31—C32—C37—C36 | 175.0 (2) |
| C5—C6—C7—C2 | 0.0 | C45—Sn2—C38—C39 | 52.1 (2) |
| C3—C2—C7—C6 | 0.0 | C31—Sn2—C38—C39 | -137.34 (19) |
| C1—C2—C7—C6 | -178.2 (2) | O5—Sn2—C38—C39 | -43.3 (2) |
| C1—Sn1—C8—C9 | 22.8 (2) | O6 ⁱⁱ —Sn2—C38—C39 | 136.2 (2) |
| C15—Sn1—C8—C9 | -168.14 (16) | Sn2—C38—C39—C40 | 85.3 (2) |
| O1—Sn1—C8—C9 | -70.14 (18) | Sn2—C38—C39—C44 | -94.2 (2) |
| O2 ⁱ —Sn1—C8—C9 | 102.75 (18) | C44—C39—C40—C41 | 0.0 |
| Sn1—C8—C9—C10 | 86.16 (19) | C38—C39—C40—C41 | -179.5 (2) |
| Sn1—C8—C9—C14 | -92.93 (18) | C39—C40—C41—C42 | 0.0 |
| C14—C9—C10—C11 | 0.0 | C40—C41—C42—C43 | 0.0 |
| C8—C9—C10—C11 | -179.1 (2) | C41—C42—C43—C44 | 0.0 |
| C9—C10—C11—C12 | 0.0 | C42—C43—C44—C39 | 0.0 |
| C10—C11—C12—C13 | 0.0 | C40—C39—C44—C43 | 0.0 |
| C11—C12—C13—C14 | 0.0 | C38—C39—C44—C43 | 179.5 (2) |
| C12—C13—C14—C9 | 0.0 | C38—Sn2—C45—C46 | -5.7 (3) |
| C10—C9—C14—C13 | 0.0 | C31—Sn2—C45—C46 | -175.18 (18) |
| C8—C9—C14—C13 | 179.1 (2) | O5—Sn2—C45—C46 | 87.2 (2) |
| C1—Sn1—C15—C16 | -22.7 (2) | O6 ⁱⁱ —Sn2—C45—C46 | -86.7 (2) |
| C8—Sn1—C15—C16 | 168.22 (17) | Sn2—C45—C46—C47 | -84.2 (2) |
| O1—Sn1—C15—C16 | 70.77 (19) | Sn2—C45—C46—C51 | 94.3 (2) |
| O2 ⁱ —Sn1—C15—C16 | -101.91 (19) | C51—C46—C47—C48 | 0.0 |
| Sn1—C15—C16—C17 | -83.3 (2) | C45—C46—C47—C48 | 178.5 (2) |
| Sn1—C15—C16—C21 | 94.47 (19) | C46—C47—C48—C49 | 0.0 |
| C21—C16—C17—C18 | 0.0 | C47—C48—C49—C50 | 0.0 |
| C15—C16—C17—C18 | 177.8 (2) | C48—C49—C50—C51 | 0.0 |
| C16—C17—C18—C19 | 0.0 | C49—C50—C51—C46 | 0.0 |

supplementary materials

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|--------------------------------|--------------|-------------------------------|-------------|
| C17—C18—C19—C20 | 0.0 | C47—C46—C51—C50 | 0.0 |
| C18—C19—C20—C21 | 0.0 | C45—C46—C51—C50 | -178.5 (2) |
| C19—C20—C21—C16 | 0.0 | Sn2 ^{iv} —O6—C52—O5 | -176.0 (2) |
| C17—C16—C21—C20 | 0.0 | Sn2 ^{iv} —O6—C52—C53 | 3.1 (5) |
| C15—C16—C21—C20 | -177.8 (2) | Sn2—O5—C52—O6 | 2.2 (4) |
| Sn1—O1—C22—O2 | 4.7 (4) | Sn2—O5—C52—C53 | -176.9 (2) |
| Sn1—O1—C22—C23 | -175.23 (19) | O6—C52—C53—C54 | -167.7 (3) |
| Sn1 ⁱⁱⁱ —O2—C22—O1 | -175.1 (2) | O5—C52—C53—C54 | 11.4 (5) |
| Sn1 ⁱⁱⁱ —O2—C22—C23 | 4.8 (5) | C52—C53—C54—C55 | 176.5 (3) |
| O1—C22—C23—C24 | -2.4 (4) | C53—C54—C55—C56 | -169.4 (3) |
| O2—C22—C23—C24 | 177.7 (3) | C53—C54—C55—C60 | 11.8 (5) |
| C22—C23—C24—C25 | 177.8 (3) | C60—C55—C56—C57 | 0.0 |
| C23—C24—C25—C26 | -179.2 (3) | C54—C55—C56—C57 | -178.8 (2) |
| C23—C24—C25—C30 | -1.0 (4) | C55—C56—C57—C58 | 0.0 |
| C30—C25—C26—C27 | 0.0 | C56—C57—C58—C59 | 0.0 |
| C24—C25—C26—C27 | 178.2 (2) | C56—C57—C58—N2 | 178.0 (2) |
| C25—C26—C27—C28 | 0.0 | O7'—N2—C58—C57 | 177.1 (10) |
| C26—C27—C28—C29 | 0.0 | O7—N2—C58—C57 | -167.7 (10) |
| C26—C27—C28—N1 | 179.1 (2) | O8'—N2—C58—C57 | -3.0 (10) |
| O3—N1—C28—C29 | -18.7 (4) | O8—N2—C58—C57 | 12.3 (10) |
| O3'—N1—C28—C29 | 8.5 (4) | O7'—N2—C58—C59 | -4.9 (10) |
| O4—N1—C28—C29 | 160.8 (5) | O7—N2—C58—C59 | 10.2 (10) |
| O4'—N1—C28—C29 | -171.4 (4) | O8'—N2—C58—C59 | 175.0 (10) |
| O3—N1—C28—C27 | 162.2 (4) | O8—N2—C58—C59 | -169.8 (10) |
| O3'—N1—C28—C27 | -170.6 (4) | C57—C58—C59—C60 | 0.0 |
| O4—N1—C28—C27 | -18.3 (5) | N2—C58—C59—C60 | -177.9 (2) |
| O4'—N1—C28—C27 | 9.5 (4) | C58—C59—C60—C55 | 0.0 |
| C27—C28—C29—C30 | 0.0 | C56—C55—C60—C59 | 0.0 |
| N1—C28—C29—C30 | -179.1 (2) | C54—C55—C60—C59 | 178.7 (3) |

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+1/2, y+1/2, -z+3/2$; (iii) $-x+3/2, y-1/2, -z+3/2$; (iv) $-x+1/2, y-1/2, -z+3/2$.

Fig. 1

