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Bis(benzyl phenyl sulfoxide-κO)-dichloridodiphenyltin(IV)

Yan-Qiu Dang

Department of Chemistry & Chemical Engineering, Binzhou University, Binzhou 256600, People's Republic of China
Correspondence e-mail: yanqiudang@163.com

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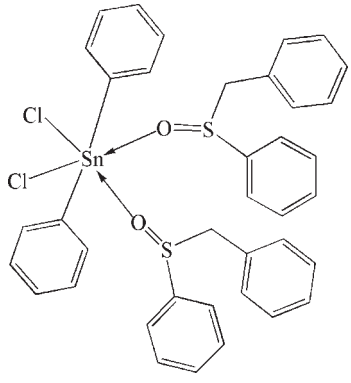
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.076; data-to-parameter ratio = 17.2.

The molecule of the title compound, $[Sn(C_6H_5)_2Cl_2(C_{13}H_{12}OS)_2]$, has crystallographic twofold symmetry. The Sn^{IV} atom is six-coordinate within a distored octahedral geometry defined by a $C_2Cl_2O_2$ donor set.

Related literature

For general background to organotin compounds and their applications, see: Davies (2004); Tian *et al.* (2005); Hadjikakou & Hadjiliadis (2009). For related structures, see: Ng & Rheingold (1989); Boa *et al.* (1995); Tian *et al.* (1998); Sadiq-ur-Rehman *et al.* (2007).



Experimental

Crystal data

$[Sn(C_6H_5)_2Cl_2(C_{13}H_{12}OS)_2]$
M_r = 776.40
Monoclinic, $C2/c$
a = 22.7485 (19) Å
b = 11.5478 (14) Å
c = 16.984 (2) Å
β = 126.633 (6)°
V = 3580.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 295 K
0.25 × 0.22 × 0.11 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.786, T_{max} = 0.897
9821 measured reflections
3512 independent reflections
3003 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.076
S = 1.03
3512 reflections
204 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2538).

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supporting information

Acta Cryst. (2009). E**65**, m1306 [https://doi.org/10.1107/S1600536809039269]

Bis(benzyl phenyl sulfoxide-*κO*)dichloridodiphenyltin(IV)

Yan-Qiu Dang

S1. Comment

Organotin compounds have received considerable attention due to their structural diversity as well as due to their industrial, agricultural and biological applications (Davies, 2004; Hadjikakou & Hadjiliadis, 2009; Tian *et al.*, 2005). Several structures of organotin sulfoxide complexes, such as dichlorobis(dimethylsulfoxide-*O*)diphenyltin (Rehman *et al.*, 2007), dichlorodimethyl(dibenzylsulfoxide-O)tin (Ng & Rheingold, 1989), [bis(phenylsulfinyl)ethane-*O*,*O*]dichlorodiphenyltin (Boa *et al.*, 1995), and trichloro(dibutylsulfoxide)(ethoxycarbonylethyl)tin (Tian *et al.*, 1998) have been reported. As a continuation of these studies, the structure of the title compound, (I), is described herein.

The molecule of (I), Fig. 1, has crystallographic twofold symmetry. The Sn atom is six-coordinate within a distorted $C_2Cl_2O_2$ octahedral geometry with *trans* phenyl groups, *cis* sulfoxides-O atoms, and *cis* chlorides. The Sn—C and Sn—Cl bond distances are similar to those found in dichlorobis(dimethylsulfoxide-*O*)diphenyltin (Rehman *et al.*, 2007), but the Sn—O length is longer. The C1—Sn1—C1^{i} and O1—Sn1—Cl^{i} angles are 162.98 (14) and 172.95 (5)°, respectively; i: 2 - *x*, *y*, 1/2 - *z*. The dihedral angle between the phenyl rings in the sulfoxide ligand is 46.8 (3)°.

S2. Experimental

Benzylphenylsulfoxide (0.865 g, 4 mmol) and diphenyltin dichloride (0.687 g, 2 mmol) in ethanol (30 ml) were refluxed for 1 h, and then the colourless solution was condensed and cooled. The solid product was filtered off and recrystallized from methanol. The colourless crystals suitable for X-ray analysis were obtained from the same solvent by slow evaporation (yield 72%; m.p. 383–384 K).

S3. Refinement

H atoms were placed at calculated positions with C—H = 0.93—0.93 Å, and refined in the riding model approximation with U_{iso}(H) = 1.2U_{eq}(C).

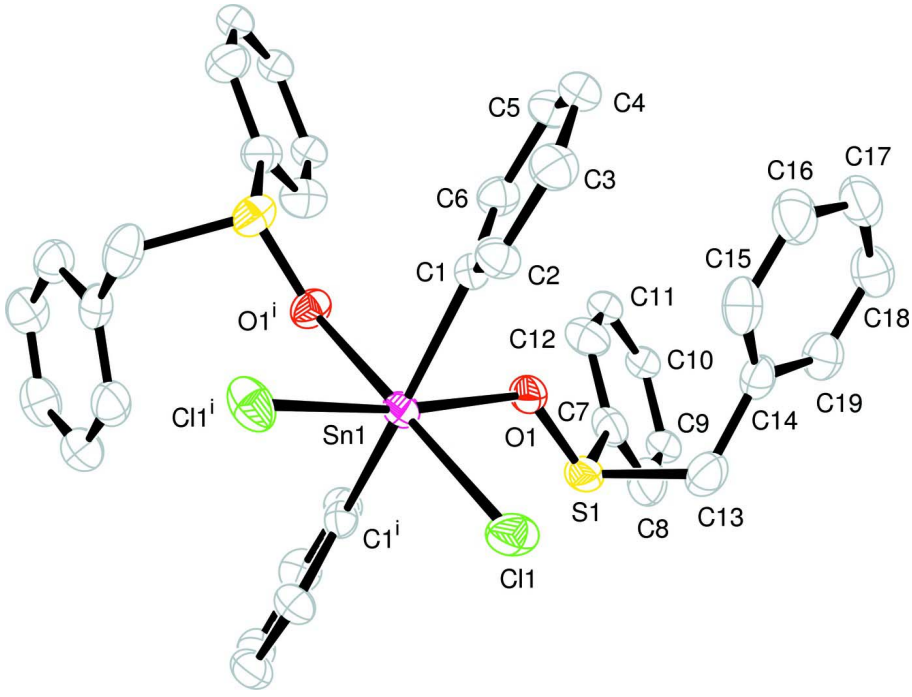

Figure 1

The structure of (I) with displacement ellipsoids are drawn at the 30% probability level. The H atoms have been omitted for clarity. The molecule has crystallographic twofold symmetry. Symmetry operation i: 2 - *x*, *y*, 1/2 - *z*.

Bis(benzyl phenyl sulfoxide-*κO*)dichloridodiphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_2Cl_2(C_{13}H_{12}OS)_2]$
M_r = 776.40
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 22.7485 (19) Å
b = 11.5478 (14) Å
c = 16.984 (2) Å
β = 126.633 (6)°
V = 3580.3 (7) Å^3
Z = 4
F(000) = 1576
D_x = 1.440 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3086 reflections
θ = 2.7–24.9°
μ = 1.01 mm^{-1}
T = 295 K
Block, colourless
0.25 × 0.22 × 0.11 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.786, T_{max} = 0.897
9821 measured reflections
3512 independent reflections
3003 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −24→28
k = −14→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.076$
$S = 1.03$
3512 reflections
204 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 1.727P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	1.0000	0.87434 (2)	0.2500	0.03980 (10)
Cl1	0.90700 (5)	1.01568 (7)	0.21844 (6)	0.0683 (2)
S1	0.84234 (4)	0.71126 (7)	0.15603 (5)	0.0544 (2)
O1	0.92338 (10)	0.72512 (16)	0.23458 (13)	0.0499 (5)
C1	1.04788 (14)	0.8471 (2)	0.40104 (18)	0.0396 (6)
C2	1.06132 (16)	0.9415 (2)	0.45947 (19)	0.0489 (7)
H2	1.0526	1.0158	0.4334	0.059*
C3	1.08741 (18)	0.9272 (3)	0.5554 (2)	0.0600 (8)
H3	1.0954	0.9916	0.5936	0.072*
C4	1.10169 (17)	0.8184 (3)	0.5954 (2)	0.0589 (8)
H4	1.1197	0.8089	0.6605	0.071*
C5	1.08941 (18)	0.7241 (3)	0.5389 (2)	0.0585 (8)
H5	1.0989	0.6502	0.5658	0.070*
C6	1.06288 (16)	0.7378 (2)	0.4418 (2)	0.0493 (7)
H6	1.0552	0.6732	0.4040	0.059*
C7	0.82742 (17)	0.5595 (3)	0.1480 (2)	0.0558 (8)
C8	0.7599 (2)	0.5161 (4)	0.0741 (3)	0.0748 (10)
H8	0.7222	0.5655	0.0287	0.090*
C9	0.7489 (3)	0.3981 (4)	0.0682 (4)	0.0967 (15)
H9	0.7028	0.3680	0.0198	0.116*
C10	0.8041 (3)	0.3252 (4)	0.1318 (4)	0.0978 (15)
H10	0.7960	0.2457	0.1265	0.117*
C11	0.8722 (3)	0.3686 (3)	0.2041 (3)	0.0867 (13)
H11	0.9103	0.3184	0.2472	0.104*
C12	0.8842 (2)	0.4863 (3)	0.2131 (2)	0.0645 (9)

H12	0.9301	0.5161	0.2624	0.077*
C13	0.79848 (19)	0.7551 (3)	0.2128 (3)	0.0685 (9)
H13A	0.8046	0.8381	0.2236	0.082*
H13B	0.7464	0.7400	0.1666	0.082*
C14	0.82573 (17)	0.6978 (2)	0.3077 (2)	0.0537 (7)
C15	0.8879 (2)	0.7370 (3)	0.3947 (3)	0.0699 (10)
H15	0.9147	0.7972	0.3940	0.084*
C16	0.9109 (2)	0.6882 (4)	0.4823 (3)	0.0849 (12)
H16	0.9526	0.7160	0.5407	0.102*
C17	0.8720 (2)	0.5978 (3)	0.4837 (3)	0.0789 (11)
H17	0.8873	0.5646	0.5431	0.095*
C18	0.8116 (2)	0.5575 (3)	0.3988 (3)	0.0715 (10)
H18	0.7855	0.4963	0.4000	0.086*
C19	0.7882 (2)	0.6056 (3)	0.3109 (3)	0.0637 (9)
H19	0.7469	0.5762	0.2529	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04550 (17)	0.04045 (16)	0.03513 (15)	0.000	0.02496 (13)	0.000
Cl1	0.0833 (6)	0.0662 (5)	0.0587 (5)	0.0318 (4)	0.0441 (5)	0.0117 (4)
S1	0.0453 (4)	0.0608 (5)	0.0503 (4)	−0.0038 (3)	0.0249 (4)	0.0146 (3)
O1	0.0448 (11)	0.0542 (12)	0.0485 (11)	−0.0061 (9)	0.0266 (10)	0.0059 (9)
C1	0.0386 (15)	0.0442 (15)	0.0390 (14)	0.0034 (11)	0.0248 (13)	0.0039 (11)
C2	0.0582 (19)	0.0468 (16)	0.0419 (15)	0.0056 (14)	0.0301 (15)	0.0013 (12)
C3	0.062 (2)	0.070 (2)	0.0458 (17)	0.0032 (17)	0.0311 (16)	−0.0098 (16)
C4	0.0514 (19)	0.086 (2)	0.0390 (16)	0.0066 (17)	0.0267 (15)	0.0091 (16)
C5	0.061 (2)	0.0587 (19)	0.0521 (18)	0.0103 (15)	0.0313 (17)	0.0199 (15)
C6	0.0501 (17)	0.0461 (16)	0.0485 (16)	0.0052 (13)	0.0277 (15)	−0.0004 (13)
C7	0.059 (2)	0.065 (2)	0.0481 (17)	−0.0162 (16)	0.0346 (16)	−0.0010 (15)
C8	0.058 (2)	0.100 (3)	0.065 (2)	−0.026 (2)	0.0362 (19)	−0.015 (2)
C9	0.105 (4)	0.110 (4)	0.095 (3)	−0.063 (3)	0.070 (3)	−0.043 (3)
C10	0.156 (5)	0.071 (3)	0.108 (4)	−0.045 (3)	0.101 (4)	−0.023 (3)
C11	0.123 (4)	0.064 (2)	0.074 (3)	−0.012 (2)	0.060 (3)	0.0100 (19)
C12	0.074 (2)	0.058 (2)	0.0545 (19)	−0.0076 (17)	0.0350 (19)	0.0064 (16)
C13	0.058 (2)	0.059 (2)	0.095 (3)	0.0126 (16)	0.049 (2)	0.0185 (18)
C14	0.0533 (19)	0.0466 (17)	0.075 (2)	0.0061 (14)	0.0458 (18)	0.0034 (15)
C15	0.076 (2)	0.065 (2)	0.094 (3)	−0.0187 (18)	0.064 (2)	−0.019 (2)
C16	0.078 (3)	0.121 (3)	0.066 (2)	−0.013 (2)	0.049 (2)	−0.020 (2)
C17	0.097 (3)	0.086 (3)	0.080 (3)	0.005 (2)	0.067 (3)	0.005 (2)
C18	0.088 (3)	0.060 (2)	0.086 (3)	−0.0102 (19)	0.063 (2)	−0.0022 (19)
C19	0.063 (2)	0.058 (2)	0.077 (2)	−0.0051 (16)	0.046 (2)	−0.0049 (16)

Geometric parameters (Å, º)

Sn1—C1	2.129 (2)	C8—H8	0.9300
Sn1—C1^{i}	2.129 (2)	C9—C10	1.355 (7)
Sn1—O1	2.3519 (18)	C9—H9	0.9300

Sn1—O1^{i}	2.3519 (18)	C10—C11	1.375 (6)
Sn1—Cl1^{i}	2.4645 (8)	C10—H10	0.9300
Sn1—Cl1	2.4645 (8)	C11—C12	1.376 (4)
S1—O1	1.506 (2)	C11—H11	0.9300
S1—C7	1.775 (3)	C12—H12	0.9300
S1—C13	1.824 (3)	C13—C14	1.492 (4)
C1—C6	1.380 (4)	C13—H13A	0.9700
C1—C2	1.381 (4)	C13—H13B	0.9700
C2—C3	1.372 (4)	C14—C15	1.377 (5)
C2—H2	0.9300	C14—C19	1.386 (4)
C3—C4	1.372 (4)	C15—C16	1.370 (5)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.364 (4)	C16—C17	1.379 (5)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.387 (4)	C17—C18	1.349 (5)
C5—H5	0.9300	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.369 (5)
C7—C8	1.374 (4)	C18—H18	0.9300
C7—C12	1.379 (4)	C19—H19	0.9300
C8—C9	1.379 (5)		

C1—Sn1—C1^{i}	162.98 (14)	C7—C8—C9	118.8 (4)
C1—Sn1—O1	80.68 (8)	C7—C8—H8	120.6
C1^{i}—Sn1—O1	86.85 (8)	C9—C8—H8	120.6
C1—Sn1—O1^{i}	86.85 (8)	C10—C9—C8	121.0 (4)
C1^{i}—Sn1—O1^{i}	80.68 (8)	C10—C9—H9	119.5
O1—Sn1—O1^{i}	85.78 (10)	C8—C9—H9	119.5
C1—Sn1—Cl1^{i}	94.61 (7)	C9—C10—C11	120.0 (4)
C1^{i}—Sn1—Cl1^{i}	96.64 (7)	C9—C10—H10	120.0
O1—Sn1—Cl1^{i}	172.95 (5)	C11—C10—H10	120.0
O1^{i}—Sn1—Cl1^{i}	88.74 (6)	C10—C11—C12	120.2 (4)
C1—Sn1—Cl1	96.64 (7)	C10—C11—H11	119.9
C1^{i}—Sn1—Cl1	94.61 (7)	C12—C11—H11	119.9
O1—Sn1—Cl1	88.74 (6)	C11—C12—C7	119.2 (4)
O1^{i}—Sn1—Cl1	172.95 (5)	C11—C12—H12	120.4
Cl1^{i}—Sn1—Cl1	97.05 (5)	C7—C12—H12	120.4
O1—S1—C7	104.46 (13)	C14—C13—S1	116.2 (2)
O1—S1—C13	105.59 (14)	C14—C13—H13A	108.2
C7—S1—C13	100.05 (14)	S1—C13—H13A	108.2
S1—O1—Sn1	127.62 (10)	C14—C13—H13B	108.2
C6—C1—C2	118.6 (2)	S1—C13—H13B	108.2
C6—C1—Sn1	122.35 (19)	H13A—C13—H13B	107.4
C2—C1—Sn1	118.93 (18)	C15—C14—C19	118.2 (3)
C3—C2—C1	120.8 (3)	C15—C14—C13	120.8 (3)
C3—C2—H2	119.6	C19—C14—C13	121.0 (3)
C1—C2—H2	119.6	C16—C15—C14	120.8 (3)
C4—C3—C2	120.3 (3)	C16—C15—H15	119.6
C4—C3—H3	119.9	C14—C15—H15	119.6

C2—C3—H3	119.9	C15—C16—C17	119.9 (4)
C5—C4—C3	119.7 (3)	C15—C16—H16	120.1
C5—C4—H4	120.2	C17—C16—H16	120.1
C3—C4—H4	120.2	C18—C17—C16	119.8 (3)
C4—C5—C6	120.4 (3)	C18—C17—H17	120.1
C4—C5—H5	119.8	C16—C17—H17	120.1
C6—C5—H5	119.8	C17—C18—C19	120.7 (3)
C1—C6—C5	120.2 (3)	C17—C18—H18	119.6
C1—C6—H6	119.9	C19—C18—H18	119.6
C5—C6—H6	119.9	C18—C19—C14	120.5 (3)
C8—C7—C12	120.8 (3)	C18—C19—H19	119.7
C8—C7—S1	119.2 (3)	C14—C19—H19	119.7
C12—C7—S1	119.9 (2)		

C7—S1—O1—Sn1	151.62 (14)	C13—S1—C7—C8	78.8 (3)
C13—S1—O1—Sn1	−103.37 (15)	O1—S1—C7—C12	5.1 (3)
C1—Sn1—O1—S1	143.25 (16)	C13—S1—C7—C12	−104.0 (3)
C1^{i}—Sn1—O1—S1	−48.38 (15)	C12—C7—C8—C9	2.5 (5)
O1^{i}—Sn1—O1—S1	−129.25 (17)	S1—C7—C8—C9	179.7 (3)
Cl1—Sn1—O1—S1	46.31 (14)	C7—C8—C9—C10	−2.3 (6)
O1—Sn1—C1—C6	45.7 (2)	C8—C9—C10—C11	0.6 (7)
O1^{i}—Sn1—C1—C6	−40.5 (2)	C9—C10—C11—C12	0.9 (6)
Cl1^{i}—Sn1—C1—C6	−129.0 (2)	C10—C11—C12—C7	−0.7 (6)
Cl1—Sn1—C1—C6	133.3 (2)	C8—C7—C12—C11	−1.0 (5)
C1^{i}—Sn1—C1—C2	−174.6 (2)	S1—C7—C12—C11	−178.2 (3)
O1—Sn1—C1—C2	−131.2 (2)	O1—S1—C13—C14	−52.3 (3)
O1^{i}—Sn1—C1—C2	142.6 (2)	C7—S1—C13—C14	55.9 (3)
Cl1^{i}—Sn1—C1—C2	54.1 (2)	S1—C13—C14—C15	82.2 (4)
Cl1—Sn1—C1—C2	−43.6 (2)	S1—C13—C14—C19	−99.3 (3)
C6—C1—C2—C3	−1.5 (4)	C19—C14—C15—C16	−1.9 (5)
Sn1—C1—C2—C3	175.5 (2)	C13—C14—C15—C16	176.6 (3)
C1—C2—C3—C4	1.1 (5)	C14—C15—C16—C17	0.9 (6)
C2—C3—C4—C5	−0.4 (5)	C15—C16—C17—C18	0.2 (6)
C3—C4—C5—C6	0.2 (5)	C16—C17—C18—C19	−0.2 (6)
C2—C1—C6—C5	1.4 (4)	C17—C18—C19—C14	−0.9 (5)
Sn1—C1—C6—C5	−175.6 (2)	C15—C14—C19—C18	1.9 (5)
C4—C5—C6—C1	−0.7 (5)	C13—C14—C19—C18	−176.6 (3)
O1—S1—C7—C8	−172.1 (2)		

Symmetry code: (i) −*x*+2, *y*, −*z*+1/2.