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Bis(4,4′-bipyridine-κN)tetrakis(nitrato-$\kappa^2 O,O'$)tin(IV)

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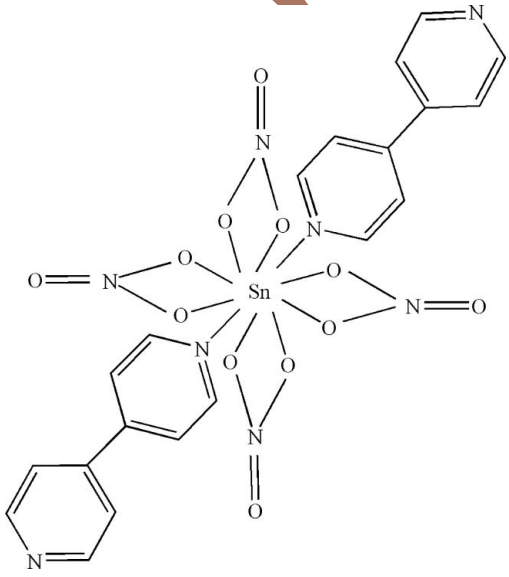
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.011 Å; R factor = 0.034; wR factor = 0.120; data-to-parameter ratio = 12.2.

The Sn^{IV} atom in the title complex, $[Sn(NO_3)_4(C_{10}H_8N_2)_2]$, is ten-coordinated by two N atoms of 4,4′-bipyridine ligands and eight O atoms of four NO_3^- ligands. The Sn atom lies on a crystallographic twofold rotation axis. The Sn—O bond lengths are in the range 2.378 (5)–2.538 (5) Å. The Sn—N bond length is 2.601 (5) Å. C—H···O hydrogen bonds link mononuclear complex molecules into a supramolecular network structure.

Related literature

For related literature, see: Allen *et al.* (1987); Bandoli *et al.* (1992); Bandoli *et al.* (1993); Barone *et al.* (2002); Hencher *et al.* (1982); Jiang & Ozin (1998); Nair & Nair (1991); Valiukonis *et al.* (1986).



Experimental

Crystal data

$[Sn(NO_3)_4(C_{10}H_8N_2)_2]$
M_r = 679.10
Monoclinic, $C2/c$
a = 20.112 (6) Å
b = 7.813 (4) Å
c = 17.302 (9) Å
β = 117.991 (7)°
V = 2400.9 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 273 (2) K
0.40 × 0.33 × 0.21 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.656, T_{max} = 0.797
7607 measured reflections
2286 independent reflections
2249 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.120
S = 1.08
2286 reflections
187 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O6	0.93	2.37	3.021 (8)	127
C1—H1···O1	0.93	2.74	3.111 (9)	105

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2281).

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supplementary materials

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Bis(4,4'-bipyridine-κN)tetrakis(nitrato-$\kappa^2 O,O'$)tin(IV)

H. Zhong, X.-R. Zeng, X.-M. Yang and Q.-Y. Luo

Comment

In recent years, the researches on tin complexes draw increasing attention owning to their potential applications as photovoltaic materials, holographic recording system and biological activities (Jiang & Ozin, 1998; Valiukonis *et al.*, 1986; Hencher *et al.*, 1982; Bandoli *et al.*, 1992, 1993), solar control devices (Nair & Nair, 1991) and semiconductor materials. Mononuclear or binuclear tin materials are important candidates as molecular precursors to prepare tin film materials by chemical vapour deposition (CVD)(Barone *et al.*, 2002). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The ten-coordinate environment of the Sn atom is completed by two N atoms of 4,4'-bipyridine ligands and eight O atoms of four NO_3^- ligands (Table 1). The Sn—O bond lengths are in the range 2.378 (5) to 2.538 (5) Å. The Sn—N bond length is 2.601 (5) Å. The C—H···O hydrogen bonds link the mononuclear complex into a supramolecular network structure (Fig. 2).

Experimental

Crystals of the title compound (I) were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Tin dioxide (30.1 mg, 0.2 mmol), 4,4'-bipyridine (93.6 mg, 0.6 mmol), nitric acid (0.2 mol/l, 4 ml) and distilled water (2 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 7 d at 413 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature. Powder X-ray diffraction was conducted on the sample.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

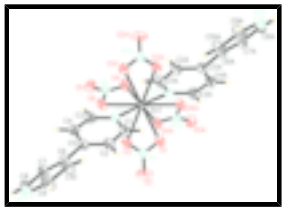

Fig. 1. The molecular structure of the title molecule (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $2-x, y, 1-z$].

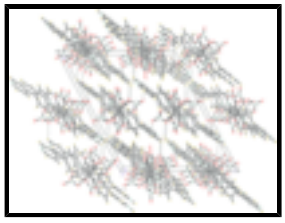

Fig. 2. Packing diagram for (I) showing hydrogen bonds as dashed lines.

Bis(4,4'-bipyridine-κ*N*)tetrakis(nitrato-κ^2*O*,*O*')tin(IV)

Crystal data

$[Sn(NO_3)_4(C_{10}H_8N_2)_2]$	F_{000} = 1352
M_r = 679.10	D_x = 1.879 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 8336 reflections
a = 20.112 (6) Å	θ = 2.4–29.3º
b = 7.813 (4) Å	μ = 1.15 mm^{-1}
c = 17.302 (9) Å	*T* = 273 (2) K
β = 117.991 (7)º	Plate, colourless
V = 2400.9 (18) Å^3	0.40 × 0.33 × 0.21 mm
Z = 4	

Data collection

Bruker APEX II area-detector diffractometer	2286 independent reflections
Radiation source: fine-focus sealed tube	2249 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.014
T = 273(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −24→24
T_{min} = 0.656, T_{max} = 0.797	*k* = −9→9
7607 measured reflections	*l* = −21→21

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 18.0815P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.120	$(\Delta/\sigma)_{max} < 0.001$
S = 1.08	$\Delta\rho_{max}$ = 0.91 e Å^{-3}
2286 reflections	$\Delta\rho_{min}$ = −0.48 e Å^{-3}

187 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0039 (4)

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	1.0000	0.33854 (5)	0.7500	0.0270 (2)
O1	1.0922 (3)	0.4420 (6)	0.8899 (3)	0.0648 (12)
O2	1.0826 (4)	0.4128 (9)	1.0030 (3)	0.0938 (19)
O3	0.9970 (3)	0.3044 (6)	0.8849 (3)	0.0653 (12)
O4	0.9294 (3)	0.0723 (7)	0.6688 (4)	0.0745 (14)
O5	0.8183 (3)	−0.0051 (7)	0.6530 (4)	0.0817 (15)
O6	0.8783 (3)	0.2147 (6)	0.7288 (3)	0.0650 (12)
N1	1.0580 (3)	0.3864 (7)	0.9290 (4)	0.0600 (13)
N2	0.8730 (3)	0.0901 (7)	0.6819 (3)	0.0558 (12)
N3	0.9364 (3)	0.6015 (7)	0.7804 (3)	0.0552 (12)
C1	0.9745 (4)	0.7368 (8)	0.8256 (4)	0.0563 (15)
H1	1.0232	0.7527	0.8338	0.068*
C2	0.9464 (4)	0.8529 (8)	0.8606 (5)	0.0543 (15)
H2	0.9751	0.9465	0.8915	0.065*
C3	0.8638 (4)	0.5856 (9)	0.7678 (4)	0.0612 (16)
H3	0.8352	0.4939	0.7344	0.073*
C4	0.8315 (4)	0.6930 (8)	0.8003 (4)	0.0571 (15)
H4	0.7823	0.6765	0.7903	0.068*
C5	0.8742 (4)	0.8304 (7)	0.8496 (4)	0.0501 (14)
C6	0.8428 (3)	0.9443 (8)	0.8911 (4)	0.0498 (13)
C7	0.7946 (4)	0.8782 (9)	0.9187 (4)	0.0549 (14)
H7	0.7825	0.7624	0.9124	0.066*
C8	0.7653 (4)	0.9862 (9)	0.9554 (4)	0.0604 (15)
H8	0.7324	0.9431	0.9745	0.073*
N4	0.7817 (4)	1.1533 (7)	0.9655 (4)	0.0616 (15)
C9	0.8274 (5)	1.2168 (10)	0.9397 (6)	0.075 (2)
H9	0.8378	1.3334	0.9464	0.090*
C10	0.8605 (5)	1.1178 (9)	0.9031 (5)	0.0685 (19)

H10	0.8942	1.1648	0.8863	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0322 (3)	0.0257 (3)	0.0323 (3)	0.000	0.0227 (2)	0.000
O1	0.063 (3)	0.072 (3)	0.067 (3)	−0.012 (2)	0.037 (2)	0.000 (2)
O2	0.128 (5)	0.098 (4)	0.043 (3)	−0.012 (4)	0.029 (3)	−0.005 (3)
O3	0.072 (3)	0.073 (3)	0.063 (3)	−0.018 (2)	0.041 (2)	−0.006 (2)
O4	0.084 (4)	0.067 (3)	0.092 (4)	−0.002 (3)	0.058 (3)	−0.015 (3)
O5	0.079 (3)	0.078 (3)	0.082 (3)	−0.034 (3)	0.033 (3)	−0.017 (3)
O6	0.077 (3)	0.059 (3)	0.075 (3)	−0.011 (2)	0.049 (3)	−0.018 (2)
N1	0.070 (4)	0.058 (3)	0.054 (3)	−0.001 (3)	0.031 (3)	0.002 (2)
N2	0.063 (3)	0.052 (3)	0.057 (3)	−0.006 (2)	0.031 (3)	−0.005 (2)
N3	0.065 (3)	0.056 (3)	0.057 (3)	0.002 (2)	0.039 (3)	−0.003 (2)
C1	0.063 (4)	0.051 (3)	0.070 (4)	−0.005 (3)	0.044 (3)	−0.006 (3)
C2	0.061 (4)	0.051 (3)	0.064 (4)	−0.006 (3)	0.041 (3)	−0.008 (3)
C3	0.062 (4)	0.062 (4)	0.064 (4)	−0.002 (3)	0.033 (3)	−0.015 (3)
C4	0.054 (4)	0.063 (4)	0.058 (3)	0.001 (3)	0.030 (3)	−0.011 (3)
C5	0.059 (4)	0.051 (3)	0.050 (3)	0.004 (2)	0.033 (3)	0.001 (2)
C6	0.054 (3)	0.052 (3)	0.051 (3)	0.002 (3)	0.031 (3)	−0.002 (2)
C7	0.061 (4)	0.055 (3)	0.060 (3)	−0.003 (3)	0.038 (3)	−0.007 (3)
C8	0.063 (4)	0.068 (4)	0.065 (4)	−0.004 (3)	0.042 (3)	−0.007 (3)
N4	0.070 (4)	0.064 (4)	0.067 (3)	0.005 (3)	0.046 (3)	−0.009 (2)
C9	0.103 (6)	0.055 (4)	0.098 (6)	−0.007 (4)	0.073 (5)	−0.014 (4)
C10	0.094 (6)	0.052 (3)	0.090 (5)	−0.007 (3)	0.069 (5)	−0.012 (3)

Geometric parameters (Å, °)

Sn1—O1	2.396 (5)	C1—H1	0.9300
Sn1—O3	2.378 (5)	C2—C5	1.384 (9)
Sn1—O4	2.538 (5)	C2—H2	0.9300
Sn1—O6	2.495 (5)	C3—C4	1.335 (9)
Sn1—N3	2.601 (5)	C3—H3	0.9300
Sn1—O3^{i}	2.378 (5)	C4—C5	1.389 (9)
Sn1—O1^{i}	2.396 (5)	C4—H4	0.9300
Sn1—O6^{i}	2.495 (5)	C5—C6	1.460 (8)
Sn1—O4^{i}	2.538 (5)	C6—C7	1.367 (9)
O1—N1	1.247 (7)	C6—C10	1.392 (9)
O2—N1	1.154 (7)	C7—C8	1.347 (9)
O3—N1	1.272 (8)	C7—H7	0.9300
O4—N2	1.265 (7)	C8—N4	1.338 (9)
O5—N2	1.223 (7)	C8—H8	0.9300
O6—N2	1.240 (7)	N4—C9	1.294 (10)
N3—C1	1.324 (9)	C9—C10	1.355 (10)
N3—C3	1.378 (9)	C9—H9	0.9300
C1—C2	1.353 (8)	C10—H10	0.9300
O1—Sn1—O3	53.85 (16)	O2—N1—O1	118.7 (7)

O1—Sn1—O4	143.36 (18)	O2—N1—O3	123.1 (6)
O1—Sn1—O6	121.36 (15)	O1—N1—O3	118.2 (5)
O3—Sn1—O4	100.75 (17)	O5—N2—O6	122.0 (6)
O3—Sn1—O6	68.01 (16)	O5—N2—O4	124.7 (6)
O4—Sn1—O6	49.13 (15)	O6—N2—O4	113.3 (5)
O1—Sn1—N3	75.55 (18)	C1—N3—C3	116.2 (5)
O3—Sn1—N3	69.45 (17)	C1—N3—Sn1	123.2 (4)
O4—Sn1—N3	123.99 (18)	C3—N3—Sn1	118.9 (4)
O6—Sn1—N3	78.13 (17)	N3—C1—C2	123.5 (6)
O3—Sn1—O3^{i}	167.1 (2)	N3—C1—H1	118.2
O3—Sn1—O1^{i}	131.72 (17)	C2—C1—H1	118.2
O3^{i}—Sn1—O1^{i}	53.85 (16)	C1—C2—C5	119.0 (6)
O3^{i}—Sn1—O1	131.72 (18)	C1—C2—H2	120.5
O1^{i}—Sn1—O1	140.6 (2)	C5—C2—H2	120.5
O3^{i}—Sn1—O6	106.71 (17)	C4—C3—N3	124.4 (6)
O1^{i}—Sn1—O6	75.01 (17)	C4—C3—H3	117.8
O3—Sn1—O6^{i}	106.70 (17)	N3—C3—H3	117.8
O3^{i}—Sn1—O6^{i}	68.01 (16)	C3—C4—C5	117.5 (7)
O1^{i}—Sn1—O6^{i}	121.36 (15)	C3—C4—H4	121.2
O1—Sn1—O6^{i}	75.01 (17)	C5—C4—H4	121.2
O6—Sn1—O6^{i}	134.3 (2)	C2—C5—C4	119.2 (6)
O3^{i}—Sn1—O4	68.27 (18)	C2—C5—C6	121.6 (6)
O1^{i}—Sn1—O4	75.55 (18)	C4—C5—C6	119.2 (6)
O6^{i}—Sn1—O4	91.07 (17)	C7—C6—C10	119.3 (6)
O3—Sn1—O4^{i}	68.28 (18)	C7—C6—C5	118.9 (6)
O3^{i}—Sn1—O4^{i}	100.75 (17)	C10—C6—C5	121.8 (6)
O1^{i}—Sn1—O4^{i}	143.36 (18)	C8—C7—C6	117.8 (6)
O1—Sn1—O4^{i}	75.55 (18)	C8—C7—H7	121.1
O6—Sn1—O4^{i}	91.07 (17)	C6—C7—H7	121.1
O6^{i}—Sn1—O4^{i}	49.12 (15)	N4—C8—C7	122.5 (6)
O4—Sn1—O4^{i}	69.9 (3)	N4—C8—H8	118.8
O3^{i}—Sn1—N3	121.88 (16)	C7—C8—H8	118.8
O1^{i}—Sn1—N3	73.54 (16)	C9—N4—C8	120.0 (6)
O6^{i}—Sn1—N3	144.95 (18)	N4—C9—C10	121.7 (7)
O4^{i}—Sn1—N3	137.37 (17)	N4—C9—H9	119.1
N1—O1—Sn1	93.9 (4)	C10—C9—H9	119.1
N1—O3—Sn1	94.0 (3)	C9—C10—C6	118.6 (7)
N2—O4—Sn1	97.3 (4)	C9—C10—H10	120.7
N2—O6—Sn1	100.2 (4)	C6—C10—H10	120.7

Symmetry codes: (i) −*x*+2, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C3—H3···O6	0.93	2.37	3.021 (8)	127
C1—H1···O1	0.93	2.74	3.111 (9)	105

Fig. 1

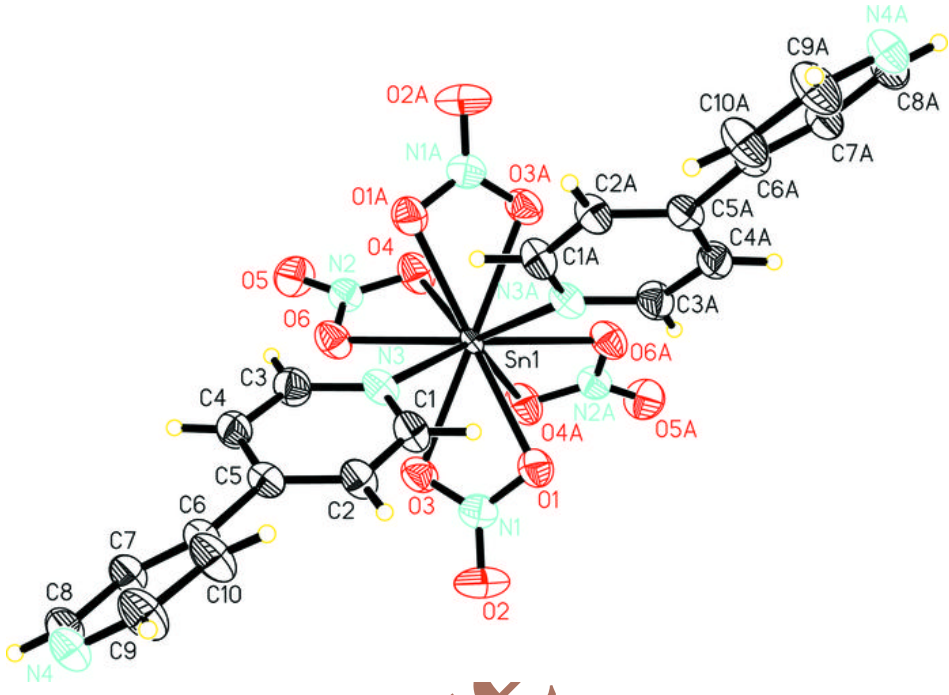

Fig. 2