metal-organic papers

Bis(2-naphthoxy)[5,10,15,20-tetra-*p*-tolyl-porphyrinato]tin(IV)

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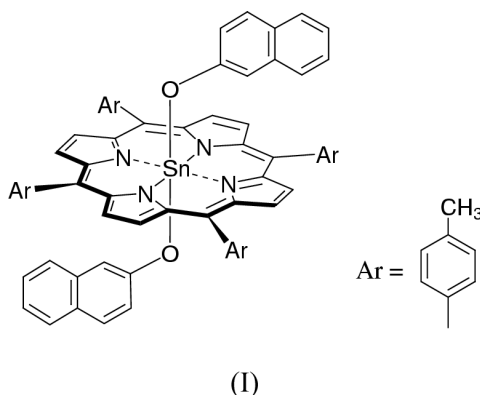
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The structure determination of the deep-red centrosymmetric tin(IV) complex, $[Sn(C_{48}H_{36}N_4)(C_{10}H_7O)_2]$, shows an octahedral Sn atom within a *trans*-N_4O_2 donor set.

Comment

As part of experiments directed towards the preparation of photosynthetic mimics, the title deep-red centrosymmetric tin(IV) complex, (I), was prepared.

(I)

The molecular structure of (I) is shown in Fig. 1. The Sn atom lies on a centre of symmetry. The geometry around the Sn atom is almost regular octahedral, with Sn—N bond lengths of 2.094 (1) and 2.099 (1) Å, and an Sn—O bond length of 2.062 (1) Å. The 2-naphthoxy groups adopt a diaxial and *anti* arrangement. Angles around the Sn atom fall within the range $90 \pm 1.7°$.

Experimental

(5,10,15,20-Tetra-*p*-tolylporphyrinato)tin(IV) dihydroxide was synthesized and purified by literature methods (Arnold, 1988). The title compound was formed by mixing 2-hydroxynaphthalene (6.4 mg, 4.44×10^{-2} mmol) with (5,10,15,20-tetra-*p*-tolylporphyrinato)tin(IV) dihydroxide (18.2 mg, 2.21×10^{-2} mmol) in base-washed $CHCl_3$ with stirring overnight. Deep-red crystals suitable for X-ray analysis were grown by vapour diffusion of hexane into a CH_2Cl_2 solution of the compound.

Crystal data

$[Sn(C_{48}H_{36}N_4)(C_{10}H_7O)_2]$	$Z = 1$
$M_r = 1073.9$	$D_x = 1.380$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 11.166$ (1) Å	Cell parameters from 34 660
$b = 11.409$ (1) Å	reflections
$c = 11.724$ (1) Å	$\theta = 2.8$–28.3°
$\alpha = 107.63$ (1)°	$\mu = 0.55$ mm^{-1}
$\beta = 110.44$ (1)°	$T = 123$ (2) K
$\gamma = 96.68$ (1)°	Prism, red
$V = 1291.9$ (2) Å^3	$0.12 \times 0.12 \times 0.05$ mm

Data collection

Nonius KappaCCD diffractometer	6331 independent reflections
CCD rotation images, thick-slice scans	6153 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.037$
Absorption correction: analytical (Alcock, 1970)	$\theta_{max} = 28.3°$
	$h = -14 \rightarrow 14$
$T_{min} = 0.898$, $T_{max} = 0.953$	$k = -15 \rightarrow 15$
22 917 measured reflections	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 0.91P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	
$wR(F^2) = 0.067$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
6331 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}
342 parameters	$\Delta\rho_{min} = -0.56$ e Å^{-3}
H-atom parameters constrained	

The H atoms were included in the riding-model approximation.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).
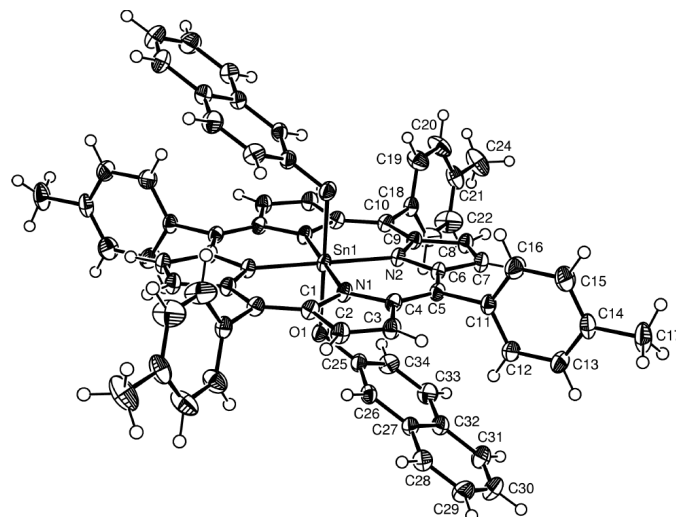
Figure 1
View of (I) shown with 50% probability displacement ellipsoids (Farrugia, 1997)

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