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Bis(μ-4-nitrophenolato-κ^2O:O')bis[(2,2′-bipyridine-κ^2N,N')nitratolead(**II**)]

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Key indicators

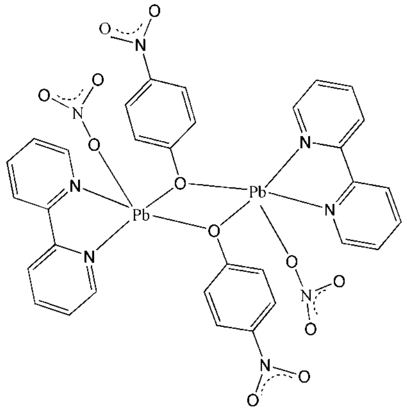
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.024
wR factor = 0.052
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Pb_2(C_6H_4NO_3)_2(C_{10}H_8N_2)_2(NO_3)_2]$, each Pb^{II} ion is surrounded by two N atoms from a 2,2′-bipyridine ligand, two O atoms from two bridging p-nitrophenolate anions and one O atom from a nitrate anion, so forming a centrosymmetric dimeric complex.

Comment

Among the many metal–p-nitrophenolate complexes that exist, the p-nitrophenolate anion usually coordinates in a monodenate fashion or exists as a free p-nitrophenolate anion to balance charges (Brahadeeswaran *et al.*, 2002; Camus *et al.*, 2003; Davies *et al.*, 2000; Facchinetti *et al.*, 2001). The title complex, $[Pb_2(bipy)_2(pnp)_2(NO_3)_2]$, (I) (where bipy is 2,2′-bipyridine and pnp is p-nitrophenolate), was obtained by hydrothermal synthesis, and the coordination mode of the p-nitrophenolate anion is very different from that observed in the above reported complexes.


(I)

In (I), each Pb^{II} cation has a five-coordinate environment, completed by two N atoms from a 2,2′-bipyridine ligand, two O atoms from two bridging p-nitrophenolate anions and one O atom from a nitrate anion (Fig. 1). Selected bond distances and angles are given in Table 1. The Pb1—O4 bond is longer than the bridging Pb1—O1 and Pb1—O1^{i} [symmetry code: (i) $2-x$, $2-y$, $-z$] bonds. The p-nitrophenolate anion acts as a bridge between two Pb atoms and forms a dimeric complex. The Pb1···Pb1^{i} distance is 4.097 (3) Å and the complex possesses a centre of symmetry midway between the two Pb atoms.

In the crystal structure, a two-dimensional network is formed by π–π interactions between the 2,2′-bipyridine heterocycles, with a separation of *ca* 3.62 Å, and between the benzene rings of p-nitrophenolates belonging to adjacent dimeric units, with a separation of *ca* 3.55 Å.

Experimental

The title complex was synthesized by the hydrothermal method from *p*-nitrophenol (0.5 mmol), $Pb(NO_3)_2$ (0.5 mmol), 2,2′-bipyridine (1 mmol) and water (10.0 ml), in a 30.0 ml Telfon-lined stainless steel reactor. The solution was heated at 403 K for 3 d. The reaction system was then cooled slowly to room temperature, and yellow crystals were collected.

Crystal data

$[Pb_2(C_6H_4NO_3)_2(C_{10}H_8N_2)_2(NO_3)_2]$
$M_r = 1126.97$
Triclinic, $P\bar{1}$
$a = 8.646$ (5) Å
$b = 10.5079$ (6) Å
$c = 10.7934$ (6) Å
$\alpha = 91.477$ (1)°
$\beta = 111.107$ (1)°
$\gamma = 109.929$ (1)°
$V = 847.6$ (5) Å^3
$Z = 1$
$D_x = 2.208$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4967 reflections
$\theta = 2.7$–25.2°
$\mu = 10.00$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.31 × 0.27 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: by integration (*SHELXTL*; Bruker, 2000)
$T_{min} = 0.061$, $T_{max} = 0.210$
6259 measured reflections
3047 independent reflections
2909 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.2°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.052$
$S = 1.11$
3047 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 0.5091P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pb1—O1	2.333 (3)	Pb1—O1^i	2.590 (3)
Pb1—N3	2.526 (4)	Pb1—O4	2.692 (4)
Pb1—N2	2.554 (4)		
O1—Pb1—N3	78.42 (12)	N2—Pb1—O1^i	142.17 (11)
O1—Pb1—N2	84.12 (11)	O1—Pb1—O4	77.28 (13)
N3—Pb1—N2	64.26 (12)	N3—Pb1—O4	137.30 (12)
O1—Pb1—O1^i	67.41 (12)	N2—Pb1—O4	78.73 (12)
N3—Pb1—O1^i	85.27 (11)	O1^i—Pb1—O4	116.19 (12)

Symmetry code: (i) $2 - x, 2 - y, -z$.

All H atoms were included in the refinement in calculated positions in the riding model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXL*97.

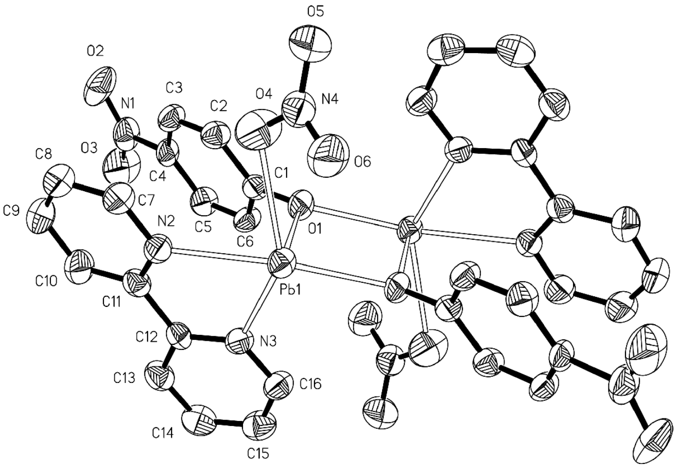


Figure 1
The molecular structure of (I), with the atom-numbering scheme, showing displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity.

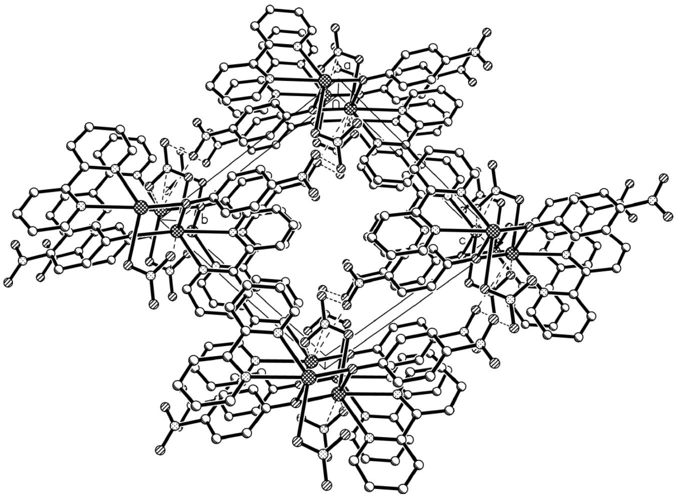


Figure 2
A view down the *a* axis of the two-dimensional network structure of (I) formed by π–π interactions.

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