Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis(μ_3-benzene-1,4-dicarboxylato-$\kappa^4O:O':O'',O'''$)bis(1-methylpyrrolidin-2-one-κO)dilead(II)]

Chao Du, Shi-Yao Yang* and Rong-Bin Huang

College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China
Correspondence e-mail: syyang@xmu.edu.cn

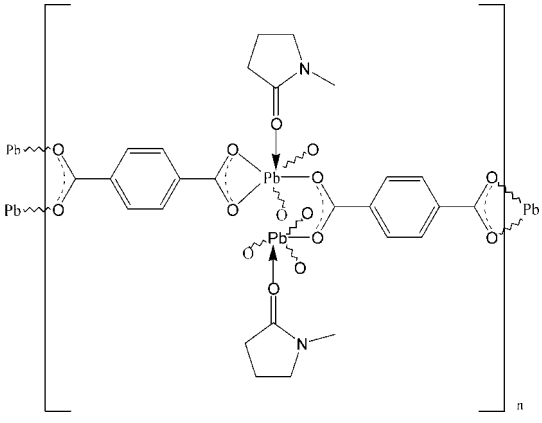
Received 3 March 2007; accepted 2 August 2007

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.009 Å; R factor = 0.033; wR factor = 0.079; data-to-parameter ratio = 17.0.

A new coordination polymer, $[Pb_2(C_8H_4O_4)_2(C_5H_9NO)_2]_n$, has been prepared by the reaction of $Pb(NO_3)_2$ with benzene-1,4-dicarboxylic acid (H_2bdc) in 1-methylpyrrolidin-2-one (nmp). There are two types of Pb ions in the crystal structure, one coordinated by five O atoms and the other by six O atoms, with severely distorted pyramidal and severely distorted octahedral coordination geometries, respectively.

Related literature

For related literature, see: Hancock *et al.* (1988); Li *et al.* (1999); Rosi *et al.* (2005); Schuy & Ruschewitz (2005); Zhou *et al.* (2006).



Experimental

Crystal data

$[Pb_2(C_8H_4O_4)_2(C_5H_9NO)_2]$
M_r = 940.87
Triclinic, $P\overline{1}$
a = 6.7327 (11) Å
b = 10.1503 (17) Å
c = 20.249 (3) Å
α = 78.521 (3)°
β = 83.357 (3)°
γ = 77.113 (3)°
V = 1318.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 12.82 mm^{-1}
T = 223 (2) K
0.18 × 0.10 × 0.03 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.206, T_{max} = 0.700
15362 measured reflections
6153 independent reflections
5400 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.079
S = 1.04
6153 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.38 e Å^{-3}
$\Delta\rho_{min}$ = −1.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pb1—O2	2.381 (4)	Pb2—O4^{ii}	2.494 (4)
Pb1—O5	2.410 (4)	Pb2—O1	2.552 (4)
Pb1—O6	2.461 (4)	Pb2—O10	2.657 (5)
Pb1—O3^{i}	2.486 (4)	Pb2—O3^{ii}	2.660 (4)
Pb1—O9	2.633 (5)	O3—Pb1^{iii}	2.486 (4)
Pb2—O7	2.434 (4)	O3—Pb2^{iv}	2.660 (4)
Pb2—O8	2.456 (4)	O4—Pb2^{iv}	2.494 (4)
O2—Pb1—O5	72.48 (14)	O7—Pb2—O1	72.97 (13)
O2—Pb1—O6	77.41 (15)	O8—Pb2—O1	125.62 (13)
O5—Pb1—O6	53.70 (13)	O4^{ii}—Pb2—O1	94.54 (13)
O2—Pb1—O3^{i}	79.52 (13)	O7—Pb2—O10	90.42 (15)
O5—Pb1—O3^{i}	72.31 (13)	O8—Pb2—O10	80.92 (15)
O6—Pb1—O3^{i}	125.39 (13)	O4^{ii}—Pb2—O10	159.02 (16)
O2—Pb1—O9	152.10 (16)	O1—Pb2—O10	91.84 (14)
O5—Pb1—O9	79.82 (16)	O7—Pb2—O3^{ii}	111.17 (13)
O6—Pb1—O9	83.63 (16)	O8—Pb2—O3^{ii}	78.39 (13)
O3^{i}—Pb1—O9	95.47 (15)	O4^{ii}—Pb2—O3^{ii}	50.44 (12)
O7—Pb2—O8	53.45 (13)	O1—Pb2—O3^{ii}	136.11 (13)
O7—Pb2—O4^{ii}	72.48 (14)	O10—Pb2—O3^{ii}	130.70 (13)
O8—Pb2—O4^{ii}	79.12 (15)		

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No. 20471049) and Xiamen University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2082).

References

Bruker (2001). *SAINT* (Version 6.22), *SMART* (Version 5.625) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hancock, R. D., Shaikjee, M. S., Dobson, S. M. & Boeyens, J. C. A. (1988). *Inorg. Chim. Acta*, **154**, 229–238.
Li, H. L., Eddaoudi, M., O'Keeffe, M. & Yaghi, O. M. (1999). *Nature (London)*, **402**, 276–279.
Rosi, N. L., Kim, J., Eddaoudi, M., Chen, B., O'Keeffe, M. & Yaghi, O. M. (2005). *J. Am. Chem. Soc.* **127**, 1504–1518.
Schuy, A. & Ruschewitz, U. (2005). *Z. Anorg. Allg. Chem.* **631**, 659–662.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhou, J., Yuan, Y.-Z., Liu, X., Li, D.-Q., Zhou, Z., Chen, Z.-F. & Yu, K.-B. (2006). *J. Coord. Chem.* **59**, 1477–1482.

  doi:10.1107/S1600536807037981

supplementary materials

Acta Cryst. (2007). E**63**, m2476 [**doi:10.1107/S1600536807037981**]

Poly[bis(μ_3-benzene-1,4-dicarboxylato-$\kappa^4O:O':O'',O'''$)bis(1-methylpyrrolidin-2-one-κO)dilead(II)\]

C. Du, S.-Y. Yang and R.-B. Huang

Comment

The three-dimensional coordination polymers have received much attention in recent years. However, most of the reported structures are transition metal compounds (Li *et al.*, 1999; Rosi *et al.*, 2005); compounds with main group metals such as Pb are seldom reported (Schuy & Ruschewitz, 2005; Zhou *et al.*, 2006). Herein the crystal structure of a three-dimensional lead coordination polymer $[Pb_2(C_8H_4O_4)_2(C_5H_9NO)_2]_n$, is reported.

In the title compound, $[Pb_2(C_8H_4O_4)_2(C_5H_9NO)_2]_n$, the two Pb atoms in the structure exist in different coordination geometries (Fig. 1). The Pb1 ion is coordinated by five O atoms, four of which are from three carboxyl groups and one is from a nmp molecule, with 'stereo-chemically active' electron lone pair, and the coordination sphere is hemi-directed (Hancock *et al.*, 1988). [Pb1—O2 2.381 (4) Å; Pb1—O5 2.410 (4) Å; Pb1—O6 2.461 (4) Å; Pb1—$O3^{i}$ 2.486 (4) Å; Pb1—O9 2.633 (5) Å]. The Pb2 ion is coordinated by six O atoms, five of which are from three carboxyl groups and one is from a nmp molecule. [Pb2—O7 2.434 (4) Å; Pb2—O8 2.456 (4) Å; Pb2—$O4^{ii}$ 2.494 (4) Å; Pb2—O1 2.552 (4) Å; Pb2—O10 2.657 (5) Å; Pb2—$O3^{ii}$ 2.660 (4) Å]. There are three coordination modes between Pb ions and carboxyl groups: (*a*) chelating/bridging bidentate, (*b*) chelating bidentate, (*c*) bidentate. The Pb ions are connected by carboxyl groups to form metal chains along *a* axis. Furthermore the bdc dianions connect each chain to four neighboring chains, resulting in a three-dimensional network with channels in which nmp molecules reside as coordinated ligands (Fig. 2).

Experimental

The title compound was synthesized with lead nitrate (0.331 g, 1 mmol) and H_2bdc (0.166 g, 1 mmol) in nmp (15 ml). The mixture was placed in a 25 ml conical flask, which was heated at 363 K for 3 days. The product was isolated in 55% yield. The elemental analysis for the title compound is almost in agreement with the theoretical values. (Found wt%: C, 32.88; H, 2.74; N, 2.99; calculated wt%: C, 33.19; H, 2.78; N, 2.98).

Refinement

H atoms were placed in calculated positions, C—H = 0.94 Å (aromatic), 0.98 Å (methylene), with U_{iso}(H) = 1.2U_{eq}(C) and 0.97 Å (methyl), with U_{iso}(H) = 1.5U_{eq}(C) and refined in riding mode.

Figures

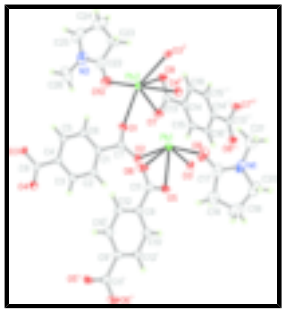


Fig. 1. The molecular structure of the title compound, shown with 50% probability displacement ellipsoids. [Symmetry codes: (i) *x*, *y* + 1, *z*; (ii) *x* − 1, *y* + 1, *z*, (v) 2 − *x*, 1 − *y*, 1 − *z*, (vi) 1 − *x*, 2 − *y*, −*z*.]

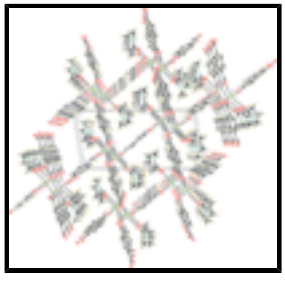


Fig. 2. Perspective view down the *a* axis showing the three-dimensional structrue of the title compound.

Poly[bis(μ$_3$-benzene-1,4-dicarboxylato-κ^4*O*:*O*':*O*'',*O*''')bis(1- methylpyrrolidin-2-one-κ*O*)dilead(II)]

Crystal data

$[Pb_2(C_8H_4O_4)_2(C_5H_9NO)_2]$	$Z = 2$
$M_r = 940.87$	$F_{000} = 880$
Triclinic, $P\overline{1}$	$D_x = 2.370$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 6.7327$ (11) Å	Cell parameters from 7207 reflections
$b = 10.1503$ (17) Å	θ = 2.5–28.6º
$c = 20.249$ (3) Å	μ = 12.82 mm^{-1}
α = 78.521 (3)º	$T = 223$ (2) K
β = 83.357 (3)º	Plate, light-yellow
γ = 77.113 (3)º	0.18 × 0.10 × 0.03 mm
$V = 1318.3$ (4) Å^3	

Data collection

Bruker APEX area-detector diffractometer	6153 independent reflections
Radiation source: fine-focus sealed tube	5400 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 223(2)$ K	$\theta_{max} = 28.6$º
φ and ω scans	$\theta_{min} = 1.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -8\rightarrow8$

T_{min} = 0.206, T_{max} = 0.700
15362 measured reflections
k = −13→13
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.079
S = 1.04
6153 reflections
361 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 2.0349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.38 e Å^{-3}
$\Delta\rho_{min}$ = −1.53 e Å^{-3}
Extinction correction: none

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}
Pb1	0.49390 (3)	0.79973 (2)	0.293309 (10)	0.01922 (7)
Pb2	0.07338 (3)	0.681658 (19)	0.205959 (10)	0.01888 (7)
O1	0.3686 (6)	0.5548 (4)	0.2779 (2)	0.0249 (9)
O2	0.6821 (6)	0.5951 (4)	0.2572 (2)	0.0245 (9)
O3	0.7606 (6)	−0.1078 (4)	0.2138 (2)	0.0220 (8)
O4	1.0651 (6)	−0.0907 (4)	0.2364 (2)	0.0294 (10)
O5	0.8092 (6)	0.7332 (4)	0.3482 (2)	0.0248 (9)
O6	0.5560 (6)	0.6398 (5)	0.4009 (2)	0.0306 (10)
O7	0.3786 (6)	0.7598 (4)	0.1514 (2)	0.0282 (9)
O8	0.1058 (6)	0.8232 (4)	0.0934 (2)	0.0294 (10)
O9	0.4368 (8)	0.9887 (5)	0.3696 (3)	0.0462 (13)
O10	0.1395 (8)	0.4857 (5)	0.1317 (3)	0.0397 (12)
C1	0.6404 (8)	0.3726 (5)	0.2533 (3)	0.0211 (12)
C2	0.8410 (9)	0.3127 (6)	0.2657 (3)	0.0257 (13)
H2A	0.9255	0.3641	0.2786	0.031*
C3	0.9179 (9)	0.1773 (6)	0.2592 (3)	0.0251 (13)

H3A	1.0531	0.1354	0.2690	0.030*
C4	0.7941 (8)	0.1038 (5)	0.2381 (3)	0.0191 (11)
C5	0.5969 (9)	0.1660 (6)	0.2233 (3)	0.0237 (12)
H5A	0.5155	0.1169	0.2072	0.028*
C6	0.5179 (9)	0.2987 (6)	0.2316 (3)	0.0241 (12)
H6A	0.3817	0.3394	0.2227	0.029*
C7	0.5572 (9)	0.5174 (5)	0.2632 (3)	0.0206 (11)
C8	0.8810 (9)	−0.0405 (6)	0.2293 (3)	0.0206 (11)
C9	0.8759 (9)	0.5726 (6)	0.4494 (3)	0.0211 (11)
C10	1.0735 (9)	0.5929 (6)	0.4484 (3)	0.0270 (13)
H10A	1.1236	0.6555	0.4133	0.032*
C11	0.7381 (9)	0.6534 (6)	0.3962 (3)	0.0231 (12)
C12	0.8054 (9)	0.4786 (6)	0.5013 (3)	0.0238 (12)
H12A	0.6722	0.4640	0.5018	0.029*
C13	0.2876 (9)	0.8267 (6)	0.1006 (3)	0.0228 (12)
C14	0.3981 (8)	0.9159 (5)	0.0480 (3)	0.0205 (11)
C15	0.5835 (8)	0.9424 (6)	0.0614 (3)	0.0216 (12)
H15A	0.6399	0.9026	0.1029	0.026*
C16	0.3171 (8)	0.9733 (6)	−0.0138 (3)	0.0226 (12)
H16A	0.1938	0.9544	−0.0230	0.027*
C17	0.5294 (12)	1.0507 (7)	0.3975 (3)	0.0365 (16)
C18	0.7348 (12)	0.9995 (7)	0.4256 (4)	0.0421 (17)
H18A	0.7333	0.9176	0.4605	0.050*
H18B	0.8398	0.9759	0.3897	0.050*
C19	0.7776 (14)	1.1124 (10)	0.4549 (5)	0.065 (3)
H19A	0.9021	1.1409	0.4325	0.079*
H19B	0.7954	1.0826	0.5033	0.079*
C20	0.5956 (13)	1.2285 (8)	0.4433 (4)	0.0471 (19)
H20A	0.5307	1.2525	0.4864	0.057*
H20B	0.6363	1.3099	0.4152	0.057*
C21	0.2615 (12)	1.2598 (8)	0.3909 (4)	0.0442 (18)
H21A	0.1928	1.2076	0.3691	0.066*
H21B	0.2799	1.3432	0.3600	0.066*
H21C	0.1795	1.2834	0.4311	0.066*
C22	−0.0052 (11)	0.4676 (7)	0.1046 (3)	0.0350 (15)
C23	−0.1965 (10)	0.5733 (7)	0.0896 (4)	0.0381 (16)
H23A	−0.2691	0.5997	0.1313	0.046*
H23B	−0.1648	0.6556	0.0595	0.046*
C24	−0.3207 (14)	0.5057 (10)	0.0563 (4)	0.060 (2)
H24A	−0.3416	0.5545	0.0099	0.072*
H24B	−0.4545	0.5058	0.0811	0.072*
C25	−0.2025 (14)	0.3580 (10)	0.0561 (4)	0.057 (2)
H25A	−0.2762	0.2916	0.0844	0.068*
H25B	−0.1780	0.3379	0.0101	0.068*
C26	0.1454 (15)	0.2341 (8)	0.0906 (5)	0.062 (3)
H26A	0.2605	0.2524	0.1094	0.093*
H26B	0.1886	0.2087	0.0466	0.093*
H26C	0.0950	0.1595	0.1205	0.093*
N1	0.4575 (9)	1.1788 (6)	0.4093 (3)	0.0355 (13)

N2	−0.0156 (11)	0.3562 (6)	0.0834 (3)	0.0448 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.01844 (12)	0.01974 (11)	0.01939 (12)	−0.00224 (8)	−0.00335 (8)	−0.00412 (8)
Pb2	0.01798 (12)	0.01763 (11)	0.02114 (12)	−0.00417 (8)	−0.00126 (8)	−0.00327 (8)
O1	0.019 (2)	0.024 (2)	0.028 (2)	0.0010 (16)	−0.0018 (17)	−0.0013 (17)
O2	0.023 (2)	0.0189 (19)	0.032 (2)	−0.0030 (16)	−0.0017 (17)	−0.0068 (17)
O3	0.024 (2)	0.0224 (19)	0.023 (2)	−0.0090 (17)	−0.0032 (16)	−0.0054 (16)
O4	0.024 (2)	0.022 (2)	0.043 (3)	−0.0011 (18)	−0.0036 (19)	−0.0104 (19)
O5	0.025 (2)	0.028 (2)	0.018 (2)	−0.0050 (17)	−0.0075 (16)	0.0043 (17)
O6	0.023 (2)	0.045 (3)	0.022 (2)	−0.010 (2)	−0.0072 (17)	0.0041 (19)
O7	0.025 (2)	0.033 (2)	0.021 (2)	−0.0061 (18)	−0.0024 (17)	0.0083 (18)
O8	0.025 (2)	0.038 (2)	0.025 (2)	−0.0110 (19)	−0.0041 (17)	0.0025 (19)
O9	0.056 (3)	0.043 (3)	0.050 (3)	−0.018 (3)	−0.002 (3)	−0.025 (3)
O10	0.042 (3)	0.047 (3)	0.035 (3)	−0.006 (2)	−0.010 (2)	−0.019 (2)
C1	0.020 (3)	0.019 (3)	0.022 (3)	0.000 (2)	0.000 (2)	−0.005 (2)
C2	0.023 (3)	0.024 (3)	0.032 (3)	−0.007 (2)	−0.004 (2)	−0.006 (3)
C3	0.020 (3)	0.026 (3)	0.029 (3)	−0.001 (2)	0.001 (2)	−0.008 (2)
C4	0.022 (3)	0.019 (3)	0.015 (3)	−0.004 (2)	−0.003 (2)	0.000 (2)
C5	0.025 (3)	0.025 (3)	0.025 (3)	−0.010 (2)	−0.005 (2)	−0.004 (2)
C6	0.026 (3)	0.023 (3)	0.023 (3)	−0.003 (2)	−0.006 (2)	−0.004 (2)
C7	0.024 (3)	0.019 (3)	0.017 (3)	−0.002 (2)	−0.003 (2)	−0.001 (2)
C8	0.022 (3)	0.022 (3)	0.016 (3)	−0.003 (2)	0.001 (2)	−0.003 (2)
C9	0.021 (3)	0.025 (3)	0.017 (3)	−0.005 (2)	−0.002 (2)	−0.005 (2)
C10	0.029 (3)	0.031 (3)	0.021 (3)	−0.011 (3)	−0.003 (2)	0.003 (2)
C11	0.026 (3)	0.029 (3)	0.016 (3)	−0.007 (2)	−0.002 (2)	−0.008 (2)
C12	0.019 (3)	0.031 (3)	0.022 (3)	−0.008 (2)	−0.006 (2)	0.000 (2)
C13	0.024 (3)	0.021 (3)	0.021 (3)	−0.001 (2)	0.002 (2)	−0.003 (2)
C14	0.020 (3)	0.019 (3)	0.020 (3)	−0.001 (2)	0.001 (2)	−0.001 (2)
C15	0.019 (3)	0.027 (3)	0.016 (3)	−0.001 (2)	−0.004 (2)	0.000 (2)
C16	0.016 (3)	0.028 (3)	0.024 (3)	−0.002 (2)	−0.005 (2)	−0.008 (2)
C17	0.056 (5)	0.036 (4)	0.021 (3)	−0.019 (3)	0.005 (3)	−0.006 (3)
C18	0.052 (5)	0.040 (4)	0.032 (4)	−0.005 (3)	0.004 (3)	−0.010 (3)
C19	0.049 (5)	0.086 (7)	0.076 (7)	−0.024 (5)	−0.003 (5)	−0.036 (6)
C20	0.063 (5)	0.052 (4)	0.039 (4)	−0.027 (4)	0.002 (4)	−0.023 (4)
C21	0.053 (5)	0.048 (4)	0.036 (4)	−0.017 (4)	0.008 (3)	−0.015 (3)
C22	0.046 (4)	0.038 (4)	0.023 (3)	−0.015 (3)	0.006 (3)	−0.007 (3)
C23	0.033 (4)	0.047 (4)	0.030 (4)	−0.001 (3)	−0.003 (3)	−0.004 (3)
C24	0.059 (6)	0.090 (7)	0.040 (5)	−0.023 (5)	−0.009 (4)	−0.024 (5)
C25	0.073 (6)	0.086 (7)	0.030 (4)	−0.050 (5)	0.005 (4)	−0.021 (4)
C26	0.089 (7)	0.036 (4)	0.050 (5)	0.004 (4)	0.005 (5)	−0.008 (4)
N1	0.045 (4)	0.036 (3)	0.032 (3)	−0.019 (3)	0.003 (3)	−0.014 (3)
N2	0.067 (4)	0.040 (3)	0.031 (3)	−0.016 (3)	0.000 (3)	−0.010 (3)

Geometric parameters (Å, °)

Pb1—O2	2.381 (4)	C10—C12^{v}	1.365 (8)
Pb1—O5	2.410 (4)	C10—H10A	0.9400
Pb1—O6	2.461 (4)	C12—C10^{v}	1.365 (8)
Pb1—O3^{i}	2.486 (4)	C12—H12A	0.9400
Pb1—O9	2.633 (5)	C13—C14	1.496 (8)
Pb1—C11	2.779 (6)	C14—C16	1.388 (8)
Pb2—O7	2.434 (4)	C14—C15	1.400 (8)
Pb2—O8	2.456 (4)	C15—C16^{vi}	1.374 (8)
Pb2—O4^{ii}	2.494 (4)	C15—H15A	0.9400
Pb2—O1	2.552 (4)	C16—C15^{vi}	1.374 (8)
Pb2—O10	2.657 (5)	C16—H16A	0.9400
Pb2—O3^{ii}	2.660 (4)	C17—N1	1.341 (8)
Pb2—C13	2.791 (6)	C17—C18	1.500 (10)
O1—C7	1.260 (7)	C18—C19	1.485 (11)
O2—C7	1.256 (7)	C18—H18A	0.9800
O3—C8	1.271 (7)	C18—H18B	0.9800
O3—Pb1^{iii}	2.486 (4)	C19—C20	1.503 (12)
O3—Pb2^{iv}	2.660 (4)	C19—H19A	0.9800
O4—C8	1.243 (7)	C19—H19B	0.9800
O4—Pb2^{iv}	2.494 (4)	C20—N1	1.445 (9)
O5—C11	1.257 (7)	C20—H20A	0.9800
O6—C11	1.255 (7)	C20—H20B	0.9800
O7—C13	1.256 (7)	C21—N1	1.437 (10)
O8—C13	1.259 (7)	C21—H21A	0.9700
O9—C17	1.224 (8)	C21—H21B	0.9700
O10—C22	1.236 (8)	C21—H21C	0.9700
C1—C2	1.381 (8)	C22—N2	1.306 (9)
C1—C6	1.388 (8)	C22—C23	1.499 (9)
C1—C7	1.496 (7)	C23—C24	1.482 (10)
C2—C3	1.384 (8)	C23—H23A	0.9800
C2—H2A	0.9400	C23—H23B	0.9800
C3—C4	1.386 (8)	C24—C25	1.533 (13)
C3—H3A	0.9400	C24—H24A	0.9800
C4—C5	1.377 (8)	C24—H24B	0.9800
C4—C8	1.488 (7)	C25—N2	1.427 (10)
C5—C6	1.369 (8)	C25—H25A	0.9800
C5—H5A	0.9400	C25—H25B	0.9800
C6—H6A	0.9400	C26—N2	1.448 (10)
C9—C10	1.388 (8)	C26—H26A	0.9700
C9—C12	1.388 (8)	C26—H26B	0.9700
C9—C11	1.495 (8)	C26—H26C	0.9700
O2—Pb1—O5	72.48 (14)	O6—C11—Pb1	62.3 (3)
O2—Pb1—O6	77.41 (15)	O5—C11—Pb1	60.0 (3)
O5—Pb1—O6	53.70 (13)	C9—C11—Pb1	177.6 (4)

O2—Pb1—O3^{i}	79.52 (13)	C10^{v}—C12—C9	121.0 (5)
O5—Pb1—O3^{i}	72.31 (13)	C10^{v}—C12—H12A	119.5
O6—Pb1—O3^{i}	125.39 (13)	C9—C12—H12A	119.5
O2—Pb1—O9	152.10 (16)	O7—C13—O8	122.0 (5)
O5—Pb1—O9	79.82 (16)	O7—C13—C14	118.7 (5)
O6—Pb1—O9	83.63 (16)	O8—C13—C14	119.3 (5)
O3^{i}—Pb1—O9	95.47 (15)	O7—C13—Pb2	60.6 (3)
O2—Pb1—C11	72.56 (15)	O8—C13—Pb2	61.6 (3)
O5—Pb1—C11	26.86 (15)	C14—C13—Pb2	174.3 (4)
O6—Pb1—C11	26.85 (15)	C16—C14—C15	119.8 (5)
O3^{i}—Pb1—C11	98.80 (15)	C16—C14—C13	120.4 (5)
O9—Pb1—C11	81.26 (17)	C15—C14—C13	119.8 (5)
O7—Pb2—O8	53.45 (13)	C16^{vi}—C15—C14	119.9 (5)
O7—Pb2—O4^{ii}	72.48 (14)	C16^{vi}—C15—H15A	120.1
O8—Pb2—O4^{ii}	79.12 (15)	C14—C15—H15A	120.1
O7—Pb2—O1	72.97 (13)	C15^{vi}—C16—C14	120.3 (5)
O8—Pb2—O1	125.62 (13)	C15^{vi}—C16—H16A	119.8
O4^{ii}—Pb2—O1	94.54 (13)	C14—C16—H16A	119.8
O7—Pb2—O10	90.42 (15)	O9—C17—N1	124.3 (7)
O8—Pb2—O10	80.92 (15)	O9—C17—C18	127.7 (7)
O4^{ii}—Pb2—O10	159.02 (16)	N1—C17—C18	108.0 (6)
O1—Pb2—O10	91.84 (14)	C19—C18—C17	106.8 (6)
O7—Pb2—O3^{ii}	111.17 (13)	C19—C18—H18A	110.4
O8—Pb2—O3^{ii}	78.39 (13)	C17—C18—H18A	110.4
O4^{ii}—Pb2—O3^{ii}	50.44 (12)	C19—C18—H18B	110.4
O1—Pb2—O3^{ii}	136.11 (13)	C17—C18—H18B	110.4
O10—Pb2—O3^{ii}	130.70 (13)	H18A—C18—H18B	108.6
O7—Pb2—C13	26.71 (15)	C18—C19—C20	106.0 (7)
O8—Pb2—C13	26.80 (15)	C18—C19—H19A	110.5
O4^{ii}—Pb2—C13	72.88 (16)	C20—C19—H19A	110.5
O1—Pb2—C13	99.48 (15)	C18—C19—H19B	110.5
O10—Pb2—C13	86.36 (16)	C20—C19—H19B	110.5
O3^{ii}—Pb2—C13	94.22 (14)	H19A—C19—H19B	108.7
C7—O1—Pb2	132.2 (4)	N1—C20—C19	105.6 (6)
C7—O2—Pb1	105.6 (3)	N1—C20—H20A	110.6
C8—O3—Pb1^{iii}	124.5 (4)	C19—C20—H20A	110.6
C8—O3—Pb2^{iv}	89.4 (3)	N1—C20—H20B	110.6
Pb1^{iii}—O3—Pb2^{iv}	106.20 (13)	C19—C20—H20B	110.6
C8—O4—Pb2^{iv}	97.9 (3)	H20A—C20—H20B	108.7
C11—O5—Pb1	93.2 (3)	N1—C21—H21A	109.5
C11—O6—Pb1	90.9 (3)	N1—C21—H21B	109.5
C13—O7—Pb2	92.7 (3)	H21A—C21—H21B	109.5
C13—O8—Pb2	91.6 (3)	N1—C21—H21C	109.5
C17—O9—Pb1	142.2 (5)	H21A—C21—H21C	109.5

C22—O10—Pb2	118.8 (4)	H21B—C21—H21C	109.5
C2—C1—C6	120.0 (5)	O10—C22—N2	126.1 (7)
C2—C1—C7	119.5 (5)	O10—C22—C23	124.7 (6)
C6—C1—C7	120.5 (5)	N2—C22—C23	109.2 (6)
C1—C2—C3	120.1 (5)	C24—C23—C22	104.9 (7)
C1—C2—H2A	119.9	C24—C23—H23A	110.8
C3—C2—H2A	119.9	C22—C23—H23A	110.8
C2—C3—C4	119.5 (5)	C24—C23—H23B	110.8
C2—C3—H3A	120.3	C22—C23—H23B	110.8
C4—C3—H3A	120.3	H23A—C23—H23B	108.8
C5—C4—C3	120.0 (5)	C23—C24—C25	107.0 (7)
C5—C4—C8	121.2 (5)	C23—C24—H24A	110.3
C3—C4—C8	118.8 (5)	C25—C24—H24A	110.3
C6—C5—C4	120.9 (5)	C23—C24—H24B	110.3
C6—C5—H5A	119.6	C25—C24—H24B	110.3
C4—C5—H5A	119.6	H24A—C24—H24B	108.6
C5—C6—C1	119.5 (5)	N2—C25—C24	102.9 (6)
C5—C6—H6A	120.3	N2—C25—H25A	111.2
C1—C6—H6A	120.3	C24—C25—H25A	111.2
O2—C7—O1	123.4 (5)	N2—C25—H25B	111.2
O2—C7—C1	117.4 (5)	C24—C25—H25B	111.2
O1—C7—C1	119.2 (5)	H25A—C25—H25B	109.1
O4—C8—O3	122.3 (5)	N2—C26—H26A	109.5
O4—C8—C4	120.4 (5)	N2—C26—H26B	109.5
O3—C8—C4	117.4 (5)	H26A—C26—H26B	109.5
C10—C9—C12	119.3 (5)	N2—C26—H26C	109.5
C10—C9—C11	120.5 (5)	H26A—C26—H26C	109.5
C12—C9—C11	120.1 (5)	H26B—C26—H26C	109.5
$C12^{v}$—C10—C9	119.6 (6)	C17—N1—C21	123.9 (6)
$C12^{v}$—C10—H10A	120.2	C17—N1—C20	113.6 (6)
C9—C10—H10A	120.2	C21—N1—C20	122.5 (6)
O6—C11—O5	122.3 (5)	C22—N2—C25	115.8 (7)
O6—C11—C9	119.2 (5)	C22—N2—C26	122.9 (7)
O5—C11—C9	118.6 (5)	C25—N2—C26	121.2 (7)
O7—Pb2—O1—C7	−29.7 (5)	C3—C4—C8—O3	176.0 (5)
O8—Pb2—O1—C7	−20.0 (5)	$C12—C9—C10—C12^{v}$	−0.7 (10)
$O4^{ii}$—Pb2—O1—C7	−99.9 (5)	$C11—C9—C10—C12^{v}$	177.8 (5)
O10—Pb2—O1—C7	60.1 (5)	Pb1—O6—C11—O5	2.2 (6)
$O3^{ii}$—Pb2—O1—C7	−132.8 (4)	Pb1—O6—C11—C9	−177.9 (5)
C13—Pb2—O1—C7	−26.5 (5)	Pb1—O5—C11—O6	−2.2 (6)
O5—Pb1—O2—C7	132.5 (4)	Pb1—O5—C11—C9	177.9 (4)
O6—Pb1—O2—C7	76.9 (4)	C10—C9—C11—O6	−175.2 (6)
$O3^{i}$—Pb1—O2—C7	−153.0 (4)	C12—C9—C11—O6	3.2 (8)
O9—Pb1—O2—C7	125.2 (4)	C10—C9—C11—O5	4.7 (8)
C11—Pb1—O2—C7	104.3 (4)	C12—C9—C11—O5	−176.8 (5)
O2—Pb1—O5—C11	−85.8 (3)	O2—Pb1—C11—O6	−96.6 (4)
O6—Pb1—O5—C11	1.2 (3)	O5—Pb1—C11—O6	177.9 (6)

O3^{i}—Pb1—O5—C11	−170.1 (4)	O3^{i}—Pb1—C11—O6	−172.6 (3)
O9—Pb1—O5—C11	90.7 (4)	O9—Pb1—C11—O6	93.2 (4)
O2—Pb1—O6—C11	76.2 (3)	O2—Pb1—C11—O5	85.5 (3)
O5—Pb1—O6—C11	−1.2 (3)	O6—Pb1—C11—O5	−177.9 (6)
O3^{i}—Pb1—O6—C11	9.0 (4)	O3^{i}—Pb1—C11—O5	9.5 (3)
O9—Pb1—O6—C11	−83.2 (4)	O9—Pb1—C11—O5	−84.7 (3)
O8—Pb2—O7—C13	2.7 (3)	C10—C9—C12—C10^{v}	0.7 (10)
O4^{ii}—Pb2—O7—C13	−86.6 (3)	C11—C9—C12—C10^{v}	−177.8 (6)
O1—Pb2—O7—C13	172.8 (4)	Pb2—O7—C13—O8	−5.0 (6)
O10—Pb2—O7—C13	81.0 (3)	Pb2—O7—C13—C14	173.6 (4)
O3^{ii}—Pb2—O7—C13	−53.6 (4)	Pb2—O8—C13—O7	4.9 (6)
O7—Pb2—O8—C13	−2.7 (3)	Pb2—O8—C13—C14	−173.6 (5)
O4^{ii}—Pb2—O8—C13	73.5 (3)	O8—Pb2—C13—O7	−175.2 (6)
O1—Pb2—O8—C13	−14.3 (4)	O4^{ii}—Pb2—C13—O7	84.9 (3)
O10—Pb2—O8—C13	−100.0 (4)	O1—Pb2—C13—O7	−6.9 (4)
O3^{ii}—Pb2—O8—C13	125.0 (4)	O10—Pb2—C13—O7	−98.2 (3)
O2—Pb1—O9—C17	33.1 (10)	O3^{ii}—Pb2—C13—O7	131.2 (3)
O5—Pb1—O9—C17	26.1 (8)	O7—Pb2—C13—O8	175.2 (6)
O6—Pb1—O9—C17	80.3 (8)	O4^{ii}—Pb2—C13—O8	−99.9 (4)
O3^{i}—Pb1—O9—C17	−44.8 (8)	O1—Pb2—C13—O8	168.3 (3)
C11—Pb1—O9—C17	53.3 (8)	O10—Pb2—C13—O8	77.0 (3)
O7—Pb2—O10—C22	−134.2 (5)	O3^{ii}—Pb2—C13—O8	−53.6 (3)
O8—Pb2—O10—C22	−81.4 (5)	O7—C13—C14—C16	169.3 (5)
O4^{ii}—Pb2—O10—C22	−99.5 (6)	O8—C13—C14—C16	−12.2 (8)
O1—Pb2—O10—C22	152.8 (5)	O7—C13—C14—C15	−11.3 (8)
O3^{ii}—Pb2—O10—C22	−15.4 (6)	O8—C13—C14—C15	167.3 (5)
C13—Pb2—O10—C22	−107.8 (5)	C16—C14—C15—C16^{vi}	1.0 (9)
C6—C1—C2—C3	−2.6 (9)	C13—C14—C15—C16^{vi}	−178.5 (5)
C7—C1—C2—C3	177.5 (5)	C15—C14—C16—C15^{vi}	−1.0 (9)
C1—C2—C3—C4	2.0 (9)	C13—C14—C16—C15^{vi}	178.5 (5)
C2—C3—C4—C5	0.6 (9)	Pb1—O9—C17—N1	150.4 (6)
C2—C3—C4—C8	178.1 (5)	Pb1—O9—C17—C18	−31.4 (12)
C3—C4—C5—C6	−2.6 (9)	O9—C17—C18—C19	−179.1 (8)
C8—C4—C5—C6	179.9 (5)	N1—C17—C18—C19	−0.6 (8)
C4—C5—C6—C1	2.0 (9)	C17—C18—C19—C20	0.0 (9)
C2—C1—C6—C5	0.6 (9)	C18—C19—C20—N1	0.6 (9)
C7—C1—C6—C5	−179.6 (5)	Pb2—O10—C22—N2	−159.4 (6)
Pb1—O2—C7—O1	7.5 (7)	Pb2—O10—C22—C23	22.1 (9)
Pb1—O2—C7—C1	−171.6 (4)	O10—C22—C23—C24	178.9 (7)
Pb2—O1—C7—O2	83.5 (7)	N2—C22—C23—C24	0.1 (8)
Pb2—O1—C7—C1	−97.5 (6)	C22—C23—C24—C25	3.0 (9)
C2—C1—C7—O2	26.5 (8)	C23—C24—C25—N2	−4.8 (9)
C6—C1—C7—O2	−153.3 (6)	O9—C17—N1—C21	0.0 (11)
C2—C1—C7—O1	−152.6 (6)	C18—C17—N1—C21	−178.5 (6)
C6—C1—C7—O1	27.6 (8)	O9—C17—N1—C20	179.6 (7)

Pb2^{iv}—O4—C8—O3	2.6 (6)	C18—C17—N1—C20	1.1 (8)
Pb2^{iv}—O4—C8—C4	−176.6 (4)	C19—C20—N1—C17	−1.1 (9)
Pb1^{iii}—O3—C8—O4	106.9 (6)	C19—C20—N1—C21	178.5 (7)
Pb2^{iv}—O3—C8—O4	−2.4 (6)	O10—C22—N2—C25	177.7 (7)
Pb1^{iii}—O3—C8—C4	−73.9 (6)	C23—C22—N2—C25	−3.6 (9)
Pb2^{iv}—O3—C8—C4	176.8 (4)	O10—C22—N2—C26	1.5 (12)
C5—C4—C8—O4	172.7 (6)	C23—C22—N2—C26	−179.8 (7)
C3—C4—C8—O4	−4.8 (8)	C24—C25—N2—C22	5.3 (9)
C5—C4—C8—O3	−6.5 (8)	C24—C25—N2—C26	−178.4 (7)

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*−1, *y*+1, *z*; (iii) *x*, *y*−1, *z*; (iv) *x*+1, *y*−1, *z*; (v) −*x*+2, −*y*+1, −*z*+1; (vi) −*x*+1, −*y*+2, −*z*.

Fig. 1

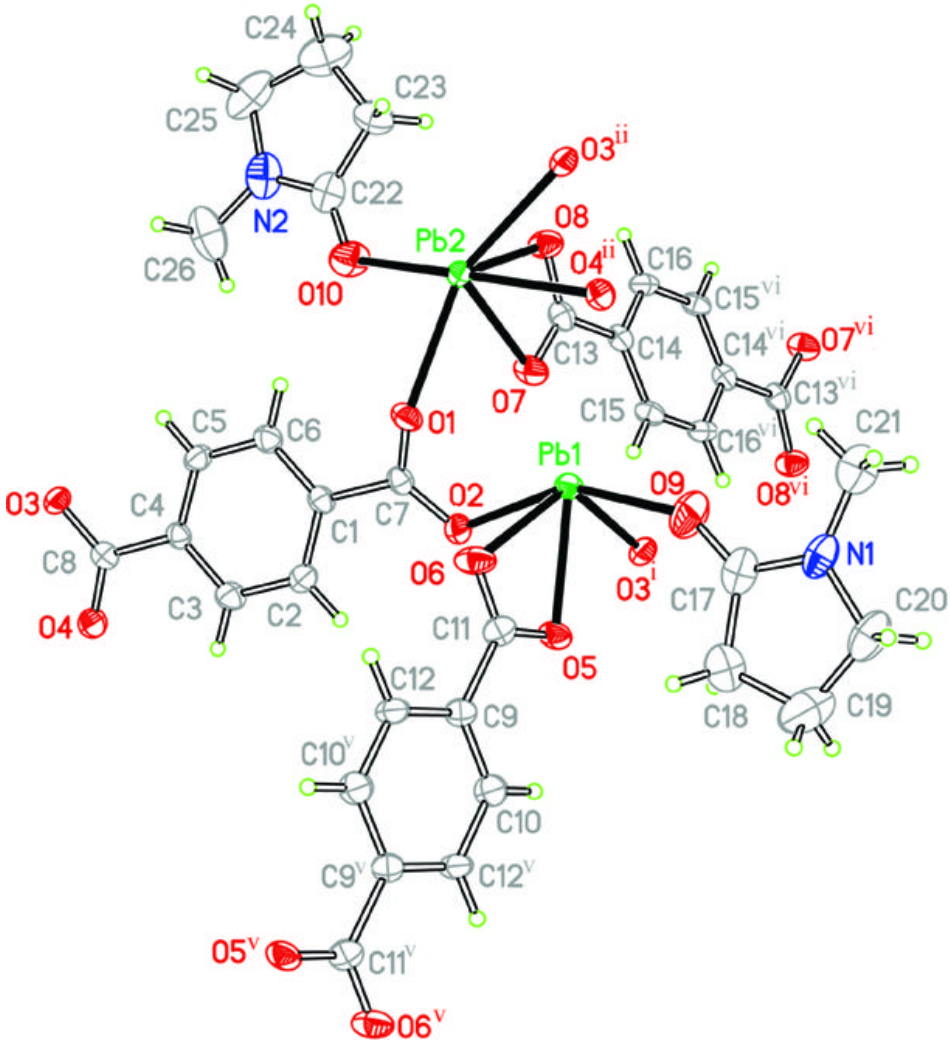

C24
C23
C25
C22
N2
C26
O10
Pb2
O3ii
O8
O4ii
C16
C15vi
C14
C14vi
O7vi
C13
C13vi
O7
C15
C16vi
O8vi
C21
O1
Pb1
O9
O2
O3
C4
C5
C6
C1
C7
C8
O4
C3
C2
O6
O3i
N1
C17
C20
C11
O5
C12
C9
C18
C19
C10v
C10
C9v
C12v
O5v
C11v
O6v

Fig. 2