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Bis(μ-4-hydroxybenzoato-κ²O:O′)bis[(2,9-dimethyl-1,10-phenanthroline-κ²N,N′)(4-hydroxybenzoato-κ²O,O′)-lead(II)]

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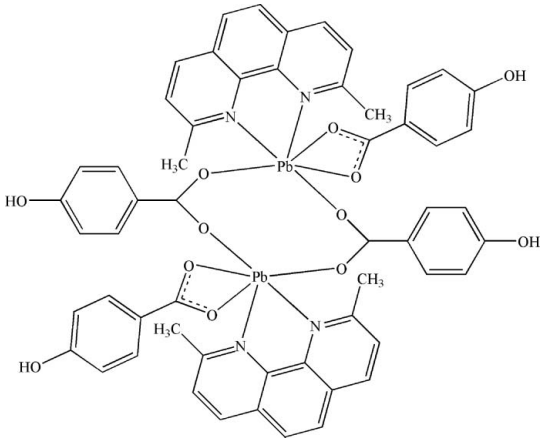
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.018; wR factor = 0.042; data-to-parameter ratio = 14.1.

In the centrosymmetric binuclear title complex, $[Pb_2(C_7H_5O_3)_4(C_{14}H_{12}N_2)_2]$, each Pb^{II} ion is coordinated by two N atoms from a 2,9-dimethyl-1,10-phenanthroline (dmphen) ligand and four O atoms from three 4-hydroxybenzoate anions in a distorted octahedral environment. The 4-hydroxybenzoate groups coordinate to each Pb^{II} atom in two different ways. Two 4-hydroxybenzoate ions behave as chelating ligands to a single Pb atom, and the other two form bridges between the two Pb atoms, forming a centrosymmetric eight-membered ring in the binuclear structure. Molecules are linked into a two-dimensional framework by O—H···O hydrogen bonds. The packing is further stabilized by π–π interactions between the dmphen rings of neighboring molecules, with a distance of 3.327 Å between the planes of the dmphen ligands.

Related literature

For the background to lead coordination chemistry, see: Shimoni-Livny *et al.* (1998). For related structures, see: Li *et al.* (2005); Mahjoub & Morsali (2002); Morsali, Mahjoub *et al.* (2003); Morsali, Payeghader *et al.* (2003); Xuan & Zhao (2007); Zhang & Lu (2005).



Experimental

Crystal data

$[Pb_2(C_7H_5O_3)_4(C_{14}H_{12}N_2)_2]$
M_r = 1379.35
Monoclinic, $P2_1/c$
a = 11.0539 (9) Å
b = 20.9060 (16) Å
c = 11.2905 (9) Å
β = 101.667 (1)°
V = 2555.2 (4) Å³
Z = 2
Mo $K\alpha$ radiation
μ = 6.65 mm⁻¹
T = 293 (2) K
0.26 × 0.21 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.277, T_{max} = 0.396
(expected range = 0.226–0.323)
17442 measured reflections
4760 independent reflections
4180 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.042
S = 1.03
4760 reflections
338 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å⁻³
$\Delta\rho_{min}$ = −0.56 e Å⁻³

Table 1
Selected bond lengths (Å).

Pb1—N2	2.464 (2)	Pb1—O4	2.5291 (18)
Pb1—N1	2.4818 (19)	Pb1—O1	2.6298 (18)
Pb1—O2	2.4851 (17)	Pb1—O5^{i}	2.767 (2)

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{ii}	0.82	1.84	2.652 (3)	172
O6—H6···O4^{iii}	0.82	1.82	2.619 (3)	165

Symmetry codes: (ii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: SJ2410).

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supplementary materials

Acta Cryst. (2007). E**63**, m3042-m3043 [**doi:10.1107/S1600536807057868**]

Bis(μ-4-hydroxybenzoato-κ^2O:O')bis[(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')(4-hydroxybenzoato-κ^2O,O')lead(II)]

P.-Z. Zhao, X.-P. Xuan and Q.-H. Tang

Comment

The coordination chemistry of lead(II) with N and O donor ligands has been investigated in the past decade and is frequently discussed as lead is an environmental pollutant with severe toxic effects (Shimoni-Livny *et al.*, 2003). Because of its electronic configuration and size, Pb(II) exhibits various coordination numbers and geometries. A number of lead(II) complexes with different donor ligands have been synthesized and studied by X-ray crystallography (Mahjoub & Morsali, 2002; Morsali *et al.*, 2003; Li *et al.*, 2005; Zhang *et al.*, 2005; Xuan & Zhao, 2007). The title complex, (I), was recently obtained from the reaction of lead acetate, sodium 4-hydroxybenzoate and dmphen in an ethanol/water mixture, and its crystal structure is reported here.

Each Pb^{II} ion is six-coordinated by the two N atoms from a dmphen ligand, and four carbonyl O atoms from three 4-hydroxybenzoate ligands (Fig.1). The four Pb—O bond lengths are significantly different, as are the two Pb—N bond lengths and each Pb^{II} cation lies at the center of a distorted octahedron. The Pb—O—C—O bridging interaction, forms a centrosymmetric eight-membered $Pb_2O_4C_2$ ring with a Pb···Pb distance of 4.2639 (3) Å.

In the crystal structure, molecules are linked into a two dimensional framework by intermolecular O—H···O hydrogen (Fig.2). The packing is further stabilized by π-π interactions between the dmphen rings of neighboring molecules. The distance between the parallel planes (N1/C1—C10/ N2/C11/C12) [symmetry code: $-x + 1, -y + 2, -z + 1$] of neighboring molecules is 3.3272 Å. This combination of hydrogen bonds and π-π stacking interactions builds a three-dimensional network architecture.

Experimental

4-hydroxybenzoic acid (0.0691 g, 0.5 mmol) and NaOH (0.0182 g, 0.5 > mmol) were dissolved in distilled water (10 ml) and $Pb(CH_3COOH)_2{\cdot}3H_2O$ (0.1897 g, 0.5 mmol) was added. This solution was added to a solution of 2,9-dimethyl-1,10-phenanthroline hemihydrate ($C_{14}H_{12}N_2{\cdot}0.5H_2O$, 0.1090 g, 0.5 mmol) in ethanol (10 ml). The mixture was stirred at 323 K and then refluxed for 4 h, cooled to room temperature and filtered. Bright colorless single crystals of (I) appeared over a period of four days by slow evaporation at room temperature.

Refinement

Methyl H and hydroxy H atoms were placed in calculated positions,with C—H = 0.96 and O—H = 0.82 Å, and refined with free torsion angles to fit the electron density; U_{iso}(H) = 1.5U_{eq}(carrier). Other H atoms were placed in calculated positions, with C—H=0.93 Å, and refined using the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C).

Figures

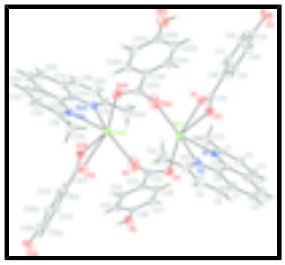


Fig. 1. The molecular structure of the title complex(I), with atom labels and 30% probability displacement ellipsoids. [Symmetry codes:(A)-*x* + 1, −*y* + 2, −*z* + 1]

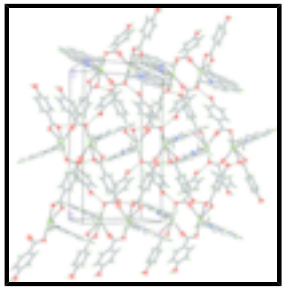


Fig. 2. The hydrogen-bonding motifs in the crystal structure of (I). Dashed lines indicate the hydrogen bonds.

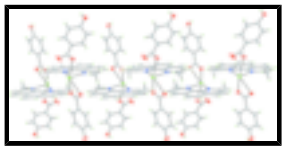


Fig. 3. π-π interactions between the dmphen rings of neighboring molecules in the crystal structure of (I).

Bis(μ-4-hydroxybenzoato-κ^2O:O')bis[(2,9-dimethyl-1,10- phenanthroline-κ^2N,N')(4-hydroxybenzoato-κ^2O,O')lead(II)]

Crystal data

$[Pb_2(C_7H_5O_3)_4(C_{14}H_{12}N_2)_2]$	F_{000} = 1336
M_r = 1379.35	D_x = 1.793 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8418 reflections
a = 11.0539 (9) Å	θ = 2.6–28.1°
b = 20.9060 (16) Å	μ = 6.65 mm^{-1}
c = 11.2905 (9) Å	T = 293 (2) K
β = 101.667 (1)°	Block, colorless
V = 2555.2 (4) Å^3	0.26 × 0.21 × 0.17 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	4760 independent reflections
Radiation source: fine-focus sealed tube	4180 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 293(2) K	θ_{max} = 25.5°

φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −13→13
T_{min} = 0.277, T_{max} = 0.396	k = −25→25
17442 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.018	H-atom parameters constrained
$wR(F^2)$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2 + 1.4405P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.008
4760 reflections	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
338 parameters	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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	0.348130 (9)	1.006948 (4)	0.350408 (8)	0.03245 (3)
O1	0.20574 (17)	1.10887 (8)	0.32230 (17)	0.0458 (5)
O2	0.32361 (17)	1.09044 (8)	0.19066 (16)	0.0407 (4)
O3	0.1365 (2)	1.37068 (9)	0.03074 (19)	0.0613 (6)
H3	0.1626	1.3744	−0.0320	0.092*
O4	0.3130 (2)	0.89345 (9)	0.41329 (18)	0.0572 (6)
O5	0.4729 (3)	0.90298 (13)	0.5611 (3)	0.1133 (11)
O6	0.17088 (18)	0.68062 (9)	0.75700 (18)	0.0509 (5)
H6	0.2228	0.6634	0.8095	0.076*
N1	0.16493 (18)	0.96424 (9)	0.20827 (18)	0.0304 (5)
N2	0.40432 (19)	0.95256 (10)	0.17560 (19)	0.0370 (5)
C1	0.0516 (2)	0.96366 (12)	0.2313 (2)	0.0381 (6)
C2	−0.0479 (3)	0.94005 (15)	0.1465 (3)	0.0536 (8)
H2	−0.1265	0.9398	0.1642	0.064*
C3	−0.0309 (3)	0.91738 (15)	0.0379 (3)	0.0554 (8)
H3A	−0.0982	0.9029	−0.0191	0.066*
C4	0.0881 (3)	0.91577 (13)	0.0120 (2)	0.0427 (7)
C5	0.1137 (3)	0.89075 (15)	−0.0979 (3)	0.0563 (9)
H5	0.0490	0.8762	−0.1578	0.068*
C6	0.2297 (3)	0.88786 (15)	−0.1160 (3)	0.0571 (9)
H6A	0.2441	0.8722	−0.1890	0.068*
C7	0.3317 (3)	0.90852 (13)	−0.0251 (2)	0.0464 (7)
C8	0.4554 (3)	0.90407 (16)	−0.0384 (3)	0.0640 (9)
H8	0.4740	0.8895	−0.1104	0.077*
C9	0.5475 (3)	0.92142 (18)	0.0556 (3)	0.0691 (10)
H9	0.6294	0.9174	0.0482	0.083*
C10	0.5203 (3)	0.94512 (16)	0.1627 (3)	0.0547 (8)
C11	0.3103 (2)	0.93440 (11)	0.0837 (2)	0.0349 (6)
C12	0.1850 (2)	0.93923 (11)	0.1022 (2)	0.0334 (6)
C13	0.0322 (3)	0.98732 (14)	0.3514 (3)	0.0518 (8)
H13A	0.1085	0.9846	0.4096	0.078*
H13B	−0.0292	0.9615	0.3777	0.078*
H13C	0.0050	1.0310	0.3439	0.078*
C14	0.6209 (3)	0.9627 (2)	0.2687 (3)	0.0871 (13)
H14A	0.6186	1.0079	0.2830	0.131*
H14B	0.6997	0.9514	0.2516	0.131*
H14C	0.6085	0.9401	0.3393	0.131*
C15	0.2559 (2)	1.12721 (11)	0.2362 (2)	0.0337 (6)
C16	0.2293 (2)	1.19281 (11)	0.1859 (2)	0.0327 (6)
C17	0.1416 (2)	1.23151 (12)	0.2226 (2)	0.0398 (7)
H17	0.1018	1.2171	0.2827	0.048*
C18	0.1123 (3)	1.29088 (13)	0.1716 (3)	0.0471 (7)
H18	0.0533	1.3161	0.1973	0.057*
C19	0.1709 (3)	1.31292 (12)	0.0819 (2)	0.0416 (7)
C20	0.2618 (3)	1.27543 (13)	0.0469 (3)	0.0455 (7)
H20	0.3039	1.2905	−0.0110	0.055*
C21	0.2892 (2)	1.21626 (12)	0.0979 (2)	0.0406 (7)
H21	0.3491	1.1913	0.0730	0.049*
C22	0.3756 (3)	0.87749 (13)	0.5160 (3)	0.0523 (8)

C23	0.3240 (2)	0.82471 (12)	0.5819 (2)	0.0390 (6)
C24	0.3987 (3)	0.78902 (14)	0.6709 (3)	0.0503 (8)
H24	0.4828	0.7979	0.6909	0.060*
C25	0.3509 (3)	0.74027 (13)	0.7308 (3)	0.0495 (8)
H25	0.4027	0.7164	0.7897	0.059*
C26	0.2253 (3)	0.72726 (12)	0.7024 (2)	0.0393 (6)
C27	0.1495 (3)	0.76263 (13)	0.6135 (3)	0.0450 (7)
H27	0.0653	0.7539	0.5937	0.054*
C28	0.1986 (3)	0.81074 (13)	0.5542 (2)	0.0439 (7)
H28	0.1468	0.8342	0.4946	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.03696 (5)	0.03192 (5)	0.02734 (5)	−0.00627 (4)	0.00379 (4)	−0.00068 (4)
O1	0.0582 (12)	0.0384 (10)	0.0471 (11)	−0.0025 (9)	0.0258 (10)	0.0015 (8)
O2	0.0481 (11)	0.0396 (9)	0.0362 (10)	0.0098 (8)	0.0129 (9)	0.0037 (8)
O3	0.0839 (15)	0.0490 (11)	0.0582 (13)	0.0280 (11)	0.0313 (12)	0.0177 (10)
O4	0.0853 (15)	0.0409 (11)	0.0417 (12)	−0.0202 (10)	0.0037 (11)	0.0067 (9)
O5	0.0940 (18)	0.1016 (19)	0.119 (2)	−0.0676 (16)	−0.0374 (17)	0.0441 (17)
O6	0.0571 (12)	0.0458 (11)	0.0524 (12)	0.0004 (9)	0.0171 (10)	0.0133 (9)
N1	0.0313 (11)	0.0301 (10)	0.0303 (11)	−0.0027 (8)	0.0073 (9)	−0.0012 (8)
N2	0.0334 (11)	0.0411 (12)	0.0372 (12)	0.0016 (9)	0.0088 (10)	−0.0015 (9)
C1	0.0340 (14)	0.0372 (14)	0.0449 (16)	−0.0034 (11)	0.0121 (12)	−0.0010 (11)
C2	0.0318 (15)	0.0667 (19)	0.063 (2)	−0.0111 (14)	0.0100 (14)	−0.0072 (16)
C3	0.0367 (16)	0.068 (2)	0.0544 (19)	−0.0132 (14)	−0.0071 (14)	−0.0123 (16)
C4	0.0445 (16)	0.0451 (15)	0.0353 (15)	−0.0074 (13)	0.0004 (13)	−0.0056 (12)
C5	0.063 (2)	0.0629 (19)	0.0377 (17)	−0.0111 (16)	−0.0027 (15)	−0.0139 (14)
C6	0.076 (2)	0.0606 (19)	0.0351 (16)	−0.0031 (17)	0.0124 (16)	−0.0158 (14)
C7	0.0543 (17)	0.0501 (16)	0.0375 (16)	0.0035 (13)	0.0159 (14)	−0.0070 (12)
C8	0.065 (2)	0.076 (2)	0.057 (2)	0.0112 (18)	0.0280 (17)	−0.0155 (17)
C9	0.0449 (17)	0.095 (3)	0.073 (2)	0.0104 (18)	0.0258 (17)	−0.017 (2)
C10	0.0366 (16)	0.071 (2)	0.057 (2)	0.0050 (15)	0.0116 (14)	−0.0066 (16)
C11	0.0398 (14)	0.0318 (12)	0.0337 (14)	0.0011 (11)	0.0086 (12)	−0.0012 (10)
C12	0.0376 (14)	0.0294 (12)	0.0324 (14)	−0.0006 (10)	0.0052 (11)	−0.0025 (10)
C13	0.0436 (15)	0.0598 (18)	0.0589 (19)	−0.0091 (14)	0.0262 (14)	−0.0120 (14)
C14	0.0338 (18)	0.147 (4)	0.079 (3)	0.002 (2)	0.0060 (18)	−0.025 (3)
C15	0.0351 (14)	0.0349 (13)	0.0299 (14)	−0.0031 (11)	0.0039 (11)	−0.0029 (10)
C16	0.0318 (13)	0.0343 (13)	0.0310 (14)	−0.0007 (10)	0.0041 (11)	−0.0017 (10)
C17	0.0413 (15)	0.0450 (15)	0.0358 (15)	0.0022 (12)	0.0141 (12)	0.0016 (11)
C18	0.0500 (16)	0.0501 (16)	0.0451 (17)	0.0173 (13)	0.0190 (14)	0.0022 (13)
C19	0.0489 (16)	0.0375 (14)	0.0390 (16)	0.0085 (12)	0.0104 (13)	0.0035 (11)
C20	0.0471 (16)	0.0473 (15)	0.0470 (17)	0.0077 (13)	0.0211 (13)	0.0105 (12)
C21	0.0405 (15)	0.0437 (14)	0.0402 (16)	0.0109 (12)	0.0146 (13)	0.0035 (12)
C22	0.061 (2)	0.0396 (15)	0.0538 (19)	−0.0162 (14)	0.0057 (16)	−0.0010 (13)
C23	0.0444 (15)	0.0355 (13)	0.0347 (15)	−0.0069 (12)	0.0020 (12)	−0.0004 (11)
C24	0.0398 (16)	0.0552 (17)	0.0509 (19)	−0.0105 (13)	−0.0027 (14)	0.0063 (14)
C25	0.0502 (17)	0.0466 (16)	0.0474 (18)	0.0056 (13)	−0.0006 (14)	0.0118 (13)

C26	0.0518 (16)	0.0323 (13)	0.0361 (15)	0.0008 (12)	0.0138 (13)	0.0017 (11)
C27	0.0411 (15)	0.0503 (16)	0.0440 (17)	−0.0035 (13)	0.0099 (13)	0.0066 (13)
C28	0.0457 (16)	0.0446 (15)	0.0385 (16)	0.0038 (13)	0.0017 (13)	0.0074 (12)

Geometric parameters (Å, °)

Pb1—N2	2.464 (2)	C8—C9	1.363 (5)
Pb1—N1	2.4818 (19)	C8—H8	0.9300
Pb1—O2	2.4851 (17)	C9—C10	1.394 (4)
Pb1—O4	2.5291 (18)	C9—H9	0.9300
Pb1—O1	2.6298 (18)	C10—C14	1.506 (4)
Pb1—O5^{i}	2.767 (2)	C11—C12	1.445 (3)
Pb1—C15	2.914 (2)	C13—H13A	0.9600
O1—C15	1.271 (3)	C13—H13B	0.9600
O2—C15	1.254 (3)	C13—H13C	0.9600
O3—C19	1.359 (3)	C14—H14A	0.9600
O3—H3	0.8200	C14—H14B	0.9600
O4—C22	1.269 (3)	C14—H14C	0.9600
O5—C22	1.216 (4)	C15—C16	1.491 (3)
O5—Pb1^{i}	2.767 (2)	C16—C17	1.389 (3)
O6—C26	1.357 (3)	C16—C21	1.390 (3)
O6—H6	0.8200	C17—C18	1.379 (4)
N1—C1	1.330 (3)	C17—H17	0.9300
N1—C12	1.365 (3)	C18—C19	1.386 (4)
N2—C10	1.329 (3)	C18—H18	0.9300
N2—C11	1.365 (3)	C19—C20	1.393 (4)
C1—C2	1.394 (4)	C20—C21	1.372 (4)
C1—C13	1.499 (4)	C20—H20	0.9300
C2—C3	1.363 (4)	C21—H21	0.9300
C2—H2	0.9300	C22—C23	1.506 (4)
C3—C4	1.405 (4)	C23—C24	1.383 (4)
C3—H3A	0.9300	C23—C28	1.389 (4)
C4—C12	1.409 (3)	C24—C25	1.386 (4)
C4—C5	1.427 (4)	C24—H24	0.9300
C5—C6	1.340 (4)	C25—C26	1.387 (4)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.430 (4)	C26—C27	1.385 (4)
C6—H6A	0.9300	C27—C28	1.379 (4)
C7—C11	1.406 (4)	C27—H27	0.9300
C7—C8	1.408 (4)	C28—H28	0.9300
N2—Pb1—N1	67.72 (7)	N2—C11—C7	122.3 (2)
N2—Pb1—O2	75.58 (6)	N2—C11—C12	118.4 (2)
N1—Pb1—O2	80.12 (6)	C7—C11—C12	119.3 (2)
N2—Pb1—O4	82.52 (7)	N1—C12—C4	122.2 (2)
N1—Pb1—O4	72.09 (7)	N1—C12—C11	119.0 (2)
O2—Pb1—O4	149.58 (6)	C4—C12—C11	118.8 (2)
N2—Pb1—O1	121.26 (6)	C1—C13—H13A	109.5
N1—Pb1—O1	79.82 (6)	C1—C13—H13B	109.5

O2—Pb1—O1	50.84 (6)	H13A—C13—H13B	109.5
O4—Pb1—O1	132.21 (7)	C1—C13—H13C	109.5
N2—Pb1—O5^{i}	109.00 (9)	H13A—C13—H13C	109.5
N1—Pb1—O5^{i}	155.30 (7)	H13B—C13—H13C	109.5
O2—Pb1—O5^{i}	75.47 (7)	C10—C14—H14A	109.5
O4—Pb1—O5^{i}	132.55 (7)	C10—C14—H14B	109.5
O1—Pb1—O5^{i}	81.89 (8)	H14A—C14—H14B	109.5
N2—Pb1—C15	99.56 (7)	C10—C14—H14C	109.5
N1—Pb1—C15	81.81 (6)	H14A—C14—H14C	109.5
O2—Pb1—C15	25.29 (6)	H14B—C14—H14C	109.5
O4—Pb1—C15	150.90 (7)	O2—C15—O1	121.2 (2)
O1—Pb1—C15	25.87 (6)	O2—C15—C16	119.7 (2)
O5^{i}—Pb1—C15	74.53 (7)	O1—C15—C16	119.1 (2)
C15—O1—Pb1	89.65 (14)	O2—C15—Pb1	57.86 (12)
C15—O2—Pb1	96.86 (15)	O1—C15—Pb1	64.48 (13)
C19—O3—H3	109.5	C16—C15—Pb1	170.63 (17)
C22—O4—Pb1	114.65 (17)	C17—C16—C21	118.0 (2)
C22—O5—Pb1^{i}	163.1 (3)	C17—C16—C15	121.2 (2)
C26—O6—H6	109.5	C21—C16—C15	120.8 (2)
C1—N1—C12	119.6 (2)	C18—C17—C16	121.2 (3)
C1—N1—Pb1	123.69 (16)	C18—C17—H17	119.4
C12—N1—Pb1	116.66 (15)	C16—C17—H17	119.4
C10—N2—C11	119.1 (2)	C17—C18—C19	120.0 (3)
C10—N2—Pb1	123.19 (18)	C17—C18—H18	120.0
C11—N2—Pb1	117.42 (16)	C19—C18—H18	120.0
N1—C1—C2	120.8 (3)	O3—C19—C18	118.3 (2)
N1—C1—C13	119.1 (2)	O3—C19—C20	122.4 (3)
C2—C1—C13	120.1 (2)	C18—C19—C20	119.4 (2)
C3—C2—C1	120.5 (3)	C21—C20—C19	119.9 (3)
C3—C2—H2	119.8	C21—C20—H20	120.0
C1—C2—H2	119.8	C19—C20—H20	120.0
C2—C3—C4	120.1 (3)	C20—C21—C16	121.4 (2)
C2—C3—H3A	119.9	C20—C21—H21	119.3
C4—C3—H3A	119.9	C16—C21—H21	119.3
C3—C4—C12	116.6 (3)	O5—C22—O4	122.7 (3)
C3—C4—C5	123.3 (3)	O5—C22—C23	120.3 (3)
C12—C4—C5	120.1 (3)	O4—C22—C23	117.0 (3)
C6—C5—C4	120.9 (3)	C24—C23—C28	118.2 (2)
C6—C5—H5	119.5	C24—C23—C22	121.6 (3)
C4—C5—H5	119.5	C28—C23—C22	120.2 (2)
C5—C6—C7	121.1 (3)	C23—C24—C25	121.4 (3)
C5—C6—H6A	119.4	C23—C24—H24	119.3
C7—C6—H6A	119.4	C25—C24—H24	119.3
C11—C7—C8	117.2 (3)	C24—C25—C26	119.6 (3)
C11—C7—C6	119.7 (3)	C24—C25—H25	120.2
C8—C7—C6	123.0 (3)	C26—C25—H25	120.2
C9—C8—C7	119.2 (3)	O6—C26—C27	117.0 (2)

C9—C8—H8	120.4	O6—C26—C25	123.4 (2)
C7—C8—H8	120.4	C27—C26—C25	119.6 (2)
C8—C9—C10	120.8 (3)	C28—C27—C26	120.1 (3)
C8—C9—H9	119.6	C28—C27—H27	119.9
C10—C9—H9	119.6	C26—C27—H27	119.9
N2—C10—C9	121.2 (3)	C27—C28—C23	121.1 (3)
N2—C10—C14	117.2 (3)	C27—C28—H28	119.4
C9—C10—C14	121.5 (3)	C23—C28—H28	119.4
N2—Pb1—O1—C15	−36.24 (16)	C10—N2—C11—C12	176.3 (2)
N1—Pb1—O1—C15	−92.21 (15)	Pb1—N2—C11—C12	−9.2 (3)
O2—Pb1—O1—C15	−6.72 (13)	C8—C7—C11—N2	−2.4 (4)
O4—Pb1—O1—C15	−146.43 (14)	C6—C7—C11—N2	177.3 (3)
O5^{i}—Pb1—O1—C15	71.10 (16)	C8—C7—C11—C12	−179.2 (3)
N2—Pb1—O2—C15	161.08 (16)	C6—C7—C11—C12	0.5 (4)
N1—Pb1—O2—C15	91.73 (15)	C1—N1—C12—C4	3.7 (4)
O4—Pb1—O2—C15	115.79 (18)	Pb1—N1—C12—C4	−177.46 (19)
O1—Pb1—O2—C15	6.86 (14)	C1—N1—C12—C11	−173.9 (2)
O5^{i}—Pb1—O2—C15	−84.47 (16)	Pb1—N1—C12—C11	4.9 (3)
N2—Pb1—O4—C22	122.6 (2)	C3—C4—C12—N1	−2.0 (4)
N1—Pb1—O4—C22	−168.4 (2)	C5—C4—C12—N1	179.3 (2)
O2—Pb1—O4—C22	166.60 (19)	C3—C4—C12—C11	175.6 (2)
O1—Pb1—O4—C22	−111.4 (2)	C5—C4—C12—C11	−3.1 (4)
O5^{i}—Pb1—O4—C22	13.7 (3)	N2—C11—C12—N1	2.8 (3)
C15—Pb1—O4—C22	−141.1 (2)	C7—C11—C12—N1	179.8 (2)
N2—Pb1—N1—C1	172.1 (2)	N2—C11—C12—C4	−174.9 (2)
O2—Pb1—N1—C1	−109.56 (19)	C7—C11—C12—C4	2.1 (4)
O4—Pb1—N1—C1	82.97 (19)	Pb1—O2—C15—O1	−12.9 (3)
O1—Pb1—N1—C1	−57.88 (19)	Pb1—O2—C15—C16	169.45 (19)
O5^{i}—Pb1—N1—C1	−100.7 (3)	Pb1—O1—C15—O2	12.1 (2)
C15—Pb1—N1—C1	−84.01 (19)	Pb1—O1—C15—C16	−170.2 (2)
N2—Pb1—N1—C12	−6.72 (15)	N2—Pb1—C15—O2	−18.57 (15)
O2—Pb1—N1—C12	71.63 (16)	N1—Pb1—C15—O2	−84.19 (15)
O4—Pb1—N1—C12	−95.83 (17)	O4—Pb1—C15—O2	−110.36 (18)
O1—Pb1—N1—C12	123.32 (17)	O1—Pb1—C15—O2	−167.7 (2)
O5^{i}—Pb1—N1—C12	80.5 (3)	O5^{i}—Pb1—C15—O2	88.64 (16)
C15—Pb1—N1—C12	97.19 (17)	N2—Pb1—C15—O1	149.17 (14)
N1—Pb1—N2—C10	−177.5 (2)	N1—Pb1—C15—O1	83.54 (14)
O2—Pb1—N2—C10	97.4 (2)	O2—Pb1—C15—O1	167.7 (2)
O4—Pb1—N2—C10	−103.9 (2)	O4—Pb1—C15—O1	57.4 (2)
O1—Pb1—N2—C10	120.7 (2)	O5^{i}—Pb1—C15—O1	−103.62 (16)
O5^{i}—Pb1—N2—C10	28.7 (2)	O2—C15—C16—C17	171.0 (2)
C15—Pb1—N2—C10	105.5 (2)	O1—C15—C16—C17	−6.7 (4)
N1—Pb1—N2—C11	8.24 (16)	O2—C15—C16—C21	−7.0 (4)
O2—Pb1—N2—C11	−76.82 (17)	O1—C15—C16—C21	175.3 (2)
O4—Pb1—N2—C11	81.90 (18)	C21—C16—C17—C18	1.5 (4)
O1—Pb1—N2—C11	−53.58 (19)	C15—C16—C17—C18	−176.6 (2)
O5^{i}—Pb1—N2—C11	−145.56 (17)	C16—C17—C18—C19	0.0 (4)

C15—Pb1—N2—C11	−68.75 (18)	C17—C18—C19—O3	177.7 (3)
C12—N1—C1—C2	−2.5 (4)	C17—C18—C19—C20	−1.9 (4)
Pb1—N1—C1—C2	178.8 (2)	O3—C19—C20—C21	−177.2 (3)
C12—N1—C1—C13	176.0 (2)	C18—C19—C20—C21	2.4 (4)
Pb1—N1—C1—C13	−2.7 (3)	C19—C20—C21—C16	−1.0 (4)
N1—C1—C2—C3	−0.3 (4)	C17—C16—C21—C20	−0.9 (4)
C13—C1—C2—C3	−178.8 (3)	C15—C16—C21—C20	177.1 (2)
C1—C2—C3—C4	2.0 (5)	Pb1^{i}—O5—C22—O4	52.9 (11)
C2—C3—C4—C12	−0.8 (4)	Pb1^{i}—O5—C22—C23	−127.0 (8)
C2—C3—C4—C5	177.8 (3)	Pb1—O4—C22—O5	−25.3 (4)
C3—C4—C5—C6	−177.1 (3)	Pb1—O4—C22—C23	154.6 (2)
C12—C4—C5—C6	1.4 (5)	O5—C22—C23—C24	−22.2 (5)
C4—C5—C6—C7	1.3 (5)	O4—C22—C23—C24	157.9 (3)
C5—C6—C7—C11	−2.2 (5)	O5—C22—C23—C28	157.7 (3)
C5—C6—C7—C8	177.5 (3)	O4—C22—C23—C28	−22.2 (4)
C11—C7—C8—C9	3.5 (5)	C28—C23—C24—C25	0.4 (4)
C6—C7—C8—C9	−176.2 (3)	C22—C23—C24—C25	−179.6 (3)
C7—C8—C9—C10	−1.9 (5)	C23—C24—C25—C26	−0.8 (5)
C11—N2—C10—C9	2.4 (4)	C24—C25—C26—O6	−179.7 (3)
Pb1—N2—C10—C9	−171.7 (2)	C24—C25—C26—C27	0.8 (4)
C11—N2—C10—C14	−177.0 (3)	O6—C26—C27—C28	−179.9 (3)
Pb1—N2—C10—C14	8.9 (4)	C25—C26—C27—C28	−0.4 (4)
C8—C9—C10—N2	−1.2 (5)	C26—C27—C28—C23	0.0 (4)
C8—C9—C10—C14	178.2 (4)	C24—C23—C28—C27	0.0 (4)
C10—N2—C11—C7	−0.6 (4)	C22—C23—C28—C27	−180.0 (3)
Pb1—N2—C11—C7	173.90 (19)		

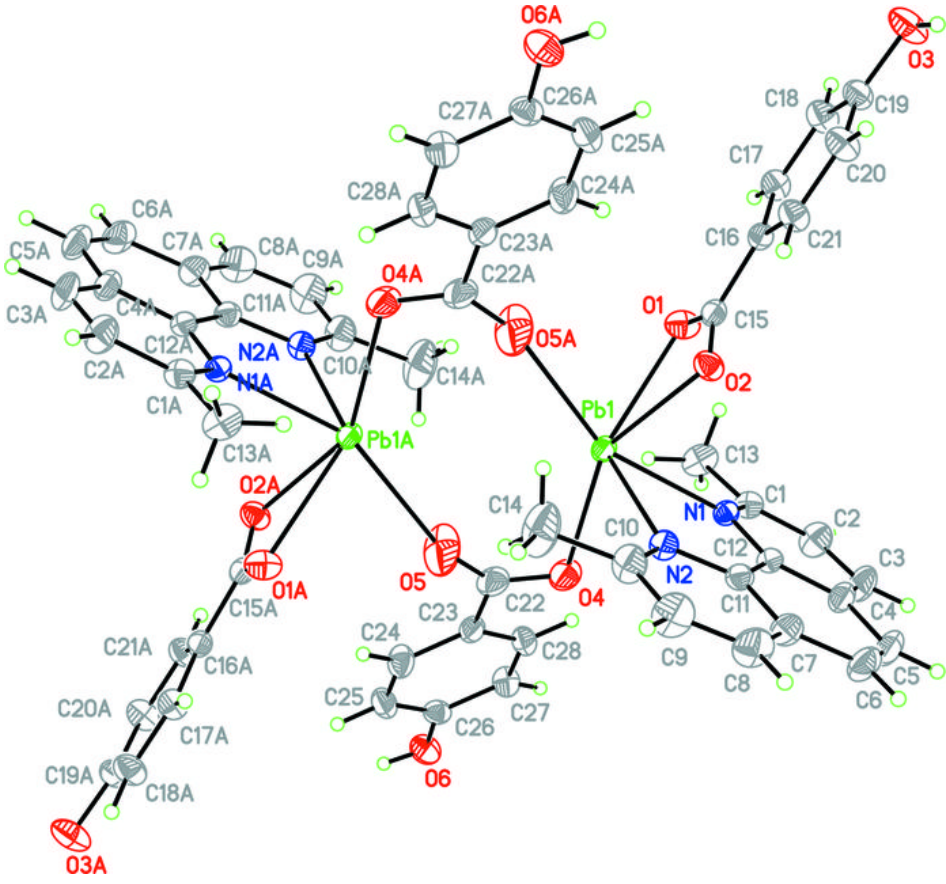
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{ii}	0.82	1.84	2.652 (3)	172
O6—H6···O4^{iii}	0.82	1.82	2.619 (3)	165

Symmetry codes: (ii) *x*, −*y*+5/2, *z*−1/2; (iii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1


O6A
O3
C27A
C26A
C18
C19
C25A
C17
C20
C28A
C24A
C6A
C16
C21
C5A
C7A
C8A
C9A
C23A
O4A
C22A
O1
C3A
C4A
C11A
C15
C12A
N2A
C10A
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O2
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C14
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C10
C12
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C22
C11
C4
C23
C24
C28
C9
C7
C21A
C16A
C25
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C26
C6
C19A
C18A
O6
O3A

Fig. 2

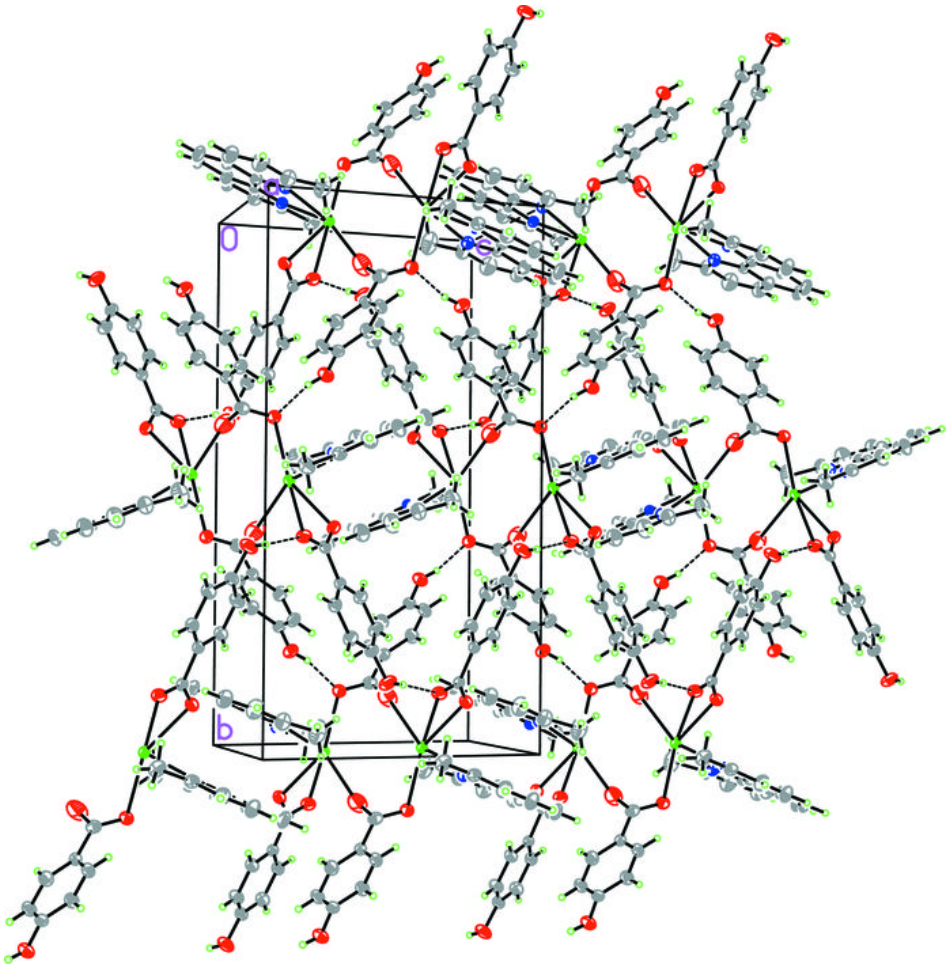

Fig. 3