Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[μ-aqua-di-μ-benzoato-lead(II)]

Jiantong Li and Juan Yang*

Department of Physical Chemistry, Henan Polytechnic University, Jiaozuo 454003, People's Republic of China
Correspondence e-mail: yangjuan0302@yahoo.cn

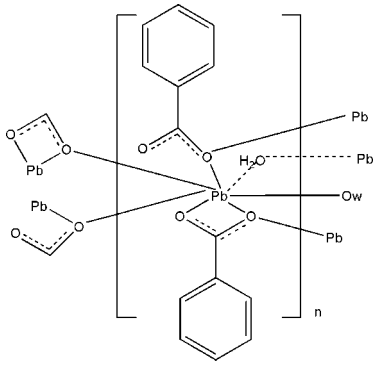
Received 11 July 2009; accepted 20 July 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.010 Å; R factor = 0.034; wR factor = 0.087; data-to-parameter ratio = 14.7.

The reaction of lead(II) nitrate and benzoic acid in aqueous solution yields the title polymer, $[Pb(C_7H_5O_2)_2(H_2O)]_n$. The asymmetric unit contains one Pb^{II} ion, two benzoate ligands and one water molecule. The Pb—O bond distances are in the range 2.494 (4)–2.735 (4) Å. The Pb···Pb distance is 4.0683 (4) Å, indicating an insignificant metal–metal interaction. The Pb^{II} atom has a distorted pentagonal-bipyramidal geometry chelated by two carboxylate O atoms. The Pb atoms are bridged through a coordinating water molecule and two carboxylate O atoms from another two benzoate ligands, giving an infinite three-dimensional supramolecular structure. O—H···O hydrogen-bonding interactions involved the coordinating water and carboxylate O atoms enhance the stability of the supramolecular arrangement.

Related literature

For general background to lead(II) compounds, see: Shi *et al.* (2007); Fan & Zhu (2006); Wang *et al.* (2006); Kim *et al.* (2001). For related structures, see: Shi *et al.* (2007).



Experimental

Crystal data

$[Pb(C_7H_5O_2)_2(H_2O)]$
M_r = 467.43
Monoclinic, $P2_1/c$
a = 15.4118 (12) Å
b = 7.5122 (6) Å
c = 11.4856 (9) Å
β = 91.2930 (10)°
V = 1329.42 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 12.71 mm^{-1}
T = 295 K
0.40 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.1, T_{max} = 0.247
(expected range = 0.146–0.362)
13406 measured reflections
2664 independent reflections
2315 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
S = 1.09
2664 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.35 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pb1—O3	2.494 (4)	Pb1—O3^{ii}	2.677 (4)
Pb1—O1	2.499 (4)	Pb1—O5	2.735 (4)
Pb1—O2	2.515 (5)	Pb1—C1^{ii}	2.867 (6)
Pb1—O5^{i}	2.639 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O4^{iii}	0.85	1.90	2.734 (7)	168
O5—H5B···O4	0.85	1.96	2.740 (7)	152

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the Doctoral Foundation of Henan Polytechnic University (B2008–58 648265).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2238).

References

Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fan, S. R. & Zhu, L. G. (2006). *Inorg. Chem.* **45**, 7935–7942.
Kim, J., Chen, B., Reneke, T. M., Li, H., Eddaoudi, M., Moler, D. B., O'Keeffe, M. & Yaghi, O. M. (2001). *J. Am. Chem. Soc.* **123**, 8239–8247.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shi, J., Xu, J.-N., Zhang, P., Fan, Y., Wang, L., Bi, M.-H., Ma, K.-R. & Song, T.-Y. (2007). *Chem. J. Chin. Univ.* **28**, 1617–1621.
Wang, X. L., Qin, C. & Wang, E. B. (2006). *Cryst. Growth. Des.* **6**, 439–443.

supporting information

Acta Cryst. (2009). E**65**, m989 [doi:10.1107/S1600536809028542]

Poly[μ-aqua-di-μ-benzoato-lead(II)]

Jiantong Li and Juan Yang

S1. Comment

Lead(II) compounds have been increasingly studied (Shi *et al.* 2007; Fan *et al.* 2006) owing to their possible applications in different fields, especially in environmental protection due to the toxicity of lead and in biological systems for its diverse interactions with biological molecules. As an important family of multidentate O-donor ligands, aromatic carboxylate ligands have been extensively employed in the preparation of metal-organic complexes because of their potential properties and intriguing structural topologies (Wang *et al.* 2006; Kim *et al.* 2001). Herein, we report the structure of the title complex.

The asymmetric unit of the title complex, $[Pb(C_7H_5O_2)_2(H_2O)]_n$, contains a Pb^{II} cation, two BA ligands and one water molecule, as illustrated in Fig. 1. The Pb^{II} atom is heptacoordinated and chelated by two carboxylate O atoms. The Pb atoms are bridged through a coordinating water and two carboxylate O atoms from another two BA ligands. The Pb—O bond lengths are in the range of 2.494 (4) to 2.735 (4) Å. The inter-distance of Pb···Pb is 4.0683 (4) Å, indicating the weak metal-metal interaction. The Pb^{II} atom has a distorted pentagonal bipyramidal geometry and the complexes extend infinitely to three-dimensional supramolecular structure. The coordinating water molecule and carboxylate O atoms are involved in extensive O—H···O hydrogen-bonding interactions (Table 2).

S2. Experimental

A mixture of $Pb(NO_3)_2$ $3H_2O$ (0.172 g, 0.52 mmol), BA (0.102 g, 0.84 mmol), melamine (0.026 g, 0.20 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave (Shi *et al.* 2007). The mixture was heated at 403 K for 6 days to give the colorless stick crystals suitable for X-ray diffraction analysis.

S3. Refinement

All H atoms bounded to C atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93 Å. The positions of the water H atoms were found from a difference Fourier map and refined with distance restraints O—H = 0.85 Å, U_{iso}(H) = 1.5Ueq(O).

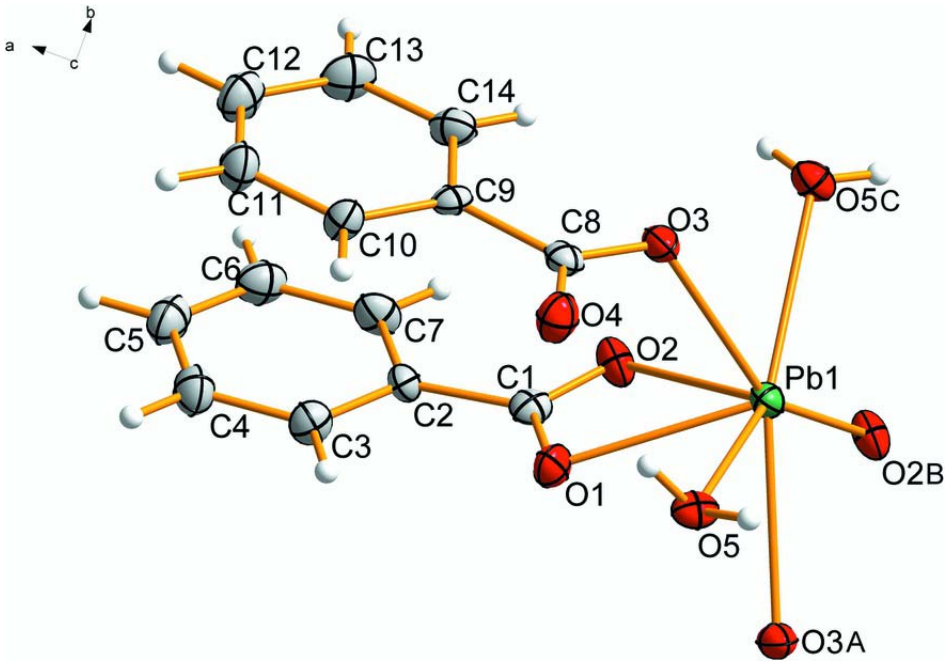


Figure 1

The coordination environment around Pb(II) in the title complex with the atom-labeling scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

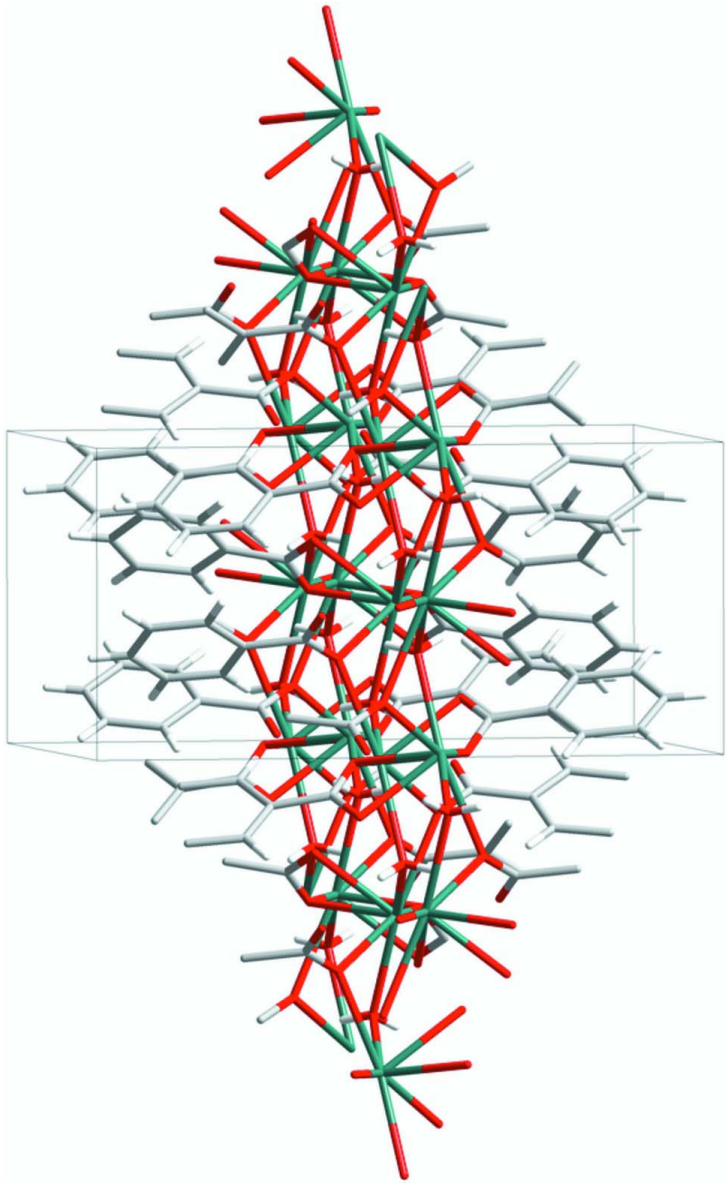


Figure 2

The three-dimensional structure of the title compound.

Poly[μ-aqua-di-μ-benzoato-lead(II)]

Crystal data

$[Pb(C_7H_5O_2)_2(H_2O)]$
$M_r = 467.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.4118\ (12)$ Å
$b = 7.5122\ (6)$ Å
$c = 11.4856\ (9)$ Å
$\beta = 91.293\ (1)°$
$V = 1329.42\ (18)$ Å^3
$Z = 4$
$F(000) = 872$
$D_x = 2.335$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4827 reflections
$\theta = 2.6–28.5°$
$\mu = 12.71$ mm^{-1}
$T = 295$ K
Block, colorless
0.4 × 0.1 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.1, T_{max} = 0.247
13406 measured reflections
2664 independent reflections
2315 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 26.2°, θ_{min} = 3.2°
h = −19→18
k = −9→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
S = 1.09
2664 reflections
181 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 3.35 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0.082

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pb1	0.478855 (16)	0.52214 (3)	0.311202 (19)	0.02834 (12)
O1	0.6082 (3)	0.3213 (6)	0.3120 (4)	0.0390 (11)
O2	0.5947 (4)	0.4879 (5)	0.4674 (4)	0.0401 (12)
O3	0.5875 (3)	0.6929 (5)	0.1986 (4)	0.0372 (11)
O4	0.6356 (4)	0.5476 (7)	0.0428 (4)	0.0453 (13)
O5	0.4960 (3)	0.3455 (6)	0.1048 (3)	0.0349 (10)
H5A	0.4562	0.3648	0.0539	0.052*
H5B	0.5374	0.3865	0.0651	0.052*
C1	0.6397 (4)	0.3861 (8)	0.4045 (5)	0.0310 (14)
C2	0.7318 (4)	0.3531 (8)	0.4365 (5)	0.0286 (13)
C3	0.7840 (5)	0.2548 (9)	0.3639 (5)	0.0370 (15)
H3A	0.7596	0.1994	0.2986	0.044*
C4	0.8716 (5)	0.2383 (10)	0.3876 (6)	0.0469 (18)
H4A	0.9062	0.1732	0.3378	0.056*
C5	0.9082 (5)	0.3177 (10)	0.4847 (6)	0.0495 (19)
H5C	0.9675	0.3082	0.4996	0.059*
C6	0.8567 (5)	0.4114 (10)	0.5599 (6)	0.0470 (18)
H6A	0.8810	0.4624	0.6268	0.056*
C7	0.7695 (5)	0.4291 (9)	0.5356 (6)	0.0405 (16)
H7A	0.7351	0.4930	0.5863	0.049*
C8	0.6480 (4)	0.6270 (8)	0.1387 (5)	0.0309 (14)
C9	0.7395 (4)	0.6483 (7)	0.1816 (5)	0.0270 (13)
C10	0.8062 (4)	0.5691 (9)	0.1224 (5)	0.0346 (14)
H10A	0.7938	0.5033	0.0554	0.042*

C11	0.8914 (5)	0.5869 (11)	0.1619 (6)	0.0462 (17)
H11A	0.9361	0.5359	0.1203	0.055*
C12	0.9098 (5)	0.6794 (11)	0.2623 (6)	0.0503 (19)
H12A	0.9668	0.6896	0.2898	0.060*
C13	0.8433 (5)	0.7573 (10)	0.3222 (6)	0.050 (2)
H13A	0.8560	0.8209	0.3899	0.060*
C14	0.7587 (5)	0.7427 (9)	0.2838 (6)	0.0408 (17)
H14A	0.7144	0.7952	0.3254	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.02962 (19)	0.02363 (16)	0.03171 (17)	0.00173 (9)	−0.00073 (11)	0.00129 (8)
O1	0.030 (3)	0.042 (3)	0.044 (3)	0.001 (2)	−0.010 (2)	−0.004 (2)
O2	0.039 (3)	0.041 (3)	0.041 (3)	0.015 (2)	0.005 (2)	0.0009 (19)
O3	0.036 (3)	0.027 (2)	0.049 (3)	0.0032 (19)	0.011 (2)	0.0011 (19)
O4	0.037 (3)	0.056 (3)	0.043 (3)	−0.001 (2)	−0.004 (2)	−0.006 (2)
O5	0.043 (3)	0.033 (2)	0.028 (2)	−0.005 (2)	−0.0034 (19)	0.0054 (17)
C1	0.035 (4)	0.030 (3)	0.028 (3)	−0.003 (3)	−0.001 (3)	0.009 (2)
C2	0.027 (4)	0.026 (3)	0.032 (3)	0.004 (2)	−0.002 (3)	0.003 (2)
C3	0.039 (4)	0.041 (4)	0.031 (3)	0.001 (3)	−0.005 (3)	−0.003 (3)
C4	0.037 (5)	0.053 (5)	0.051 (4)	0.005 (3)	0.008 (3)	0.003 (3)
C5	0.034 (4)	0.057 (5)	0.057 (5)	−0.003 (4)	−0.006 (4)	0.012 (4)
C6	0.052 (5)	0.045 (4)	0.044 (4)	−0.006 (4)	−0.011 (4)	−0.002 (3)
C7	0.048 (5)	0.038 (4)	0.035 (4)	0.005 (3)	−0.010 (3)	−0.008 (3)
C8	0.037 (4)	0.021 (3)	0.035 (3)	0.002 (3)	0.001 (3)	0.006 (2)
C9	0.031 (4)	0.022 (3)	0.028 (3)	−0.006 (2)	0.000 (2)	0.006 (2)
C10	0.029 (4)	0.041 (4)	0.034 (3)	−0.003 (3)	0.002 (3)	−0.003 (3)
C11	0.033 (4)	0.055 (5)	0.051 (4)	0.003 (4)	0.006 (3)	−0.004 (4)
C12	0.039 (5)	0.060 (5)	0.052 (4)	−0.004 (4)	−0.012 (4)	0.002 (4)
C13	0.057 (6)	0.053 (5)	0.039 (4)	−0.008 (4)	−0.012 (4)	−0.007 (3)
C14	0.048 (5)	0.033 (4)	0.041 (4)	−0.004 (3)	0.008 (3)	−0.005 (3)

Geometric parameters (Å, º)

Pb1—O3	2.494 (4)	C4—C5	1.374 (10)
Pb1—O1	2.499 (4)	C4—H4A	0.9300
Pb1—O2	2.515 (5)	C5—C6	1.379 (10)
Pb1—O5^{i}	2.639 (4)	C5—H5C	0.9300
Pb1—O3^{ii}	2.677 (4)	C6—C7	1.374 (10)
Pb1—O5	2.735 (4)	C6—H6A	0.9300
Pb1—C1	2.867 (6)	C7—H7A	0.9300
O1—C1	1.256 (7)	C8—C9	1.493 (8)
O2—C1	1.269 (8)	C9—C10	1.379 (9)
O3—C8	1.271 (7)	C9—C14	1.397 (8)
O3—Pb1^{i}	2.677 (4)	C10—C11	1.386 (10)
O4—C8	1.264 (7)	C10—H10A	0.9300
O5—Pb1^{ii}	2.639 (4)	C11—C12	1.370 (10)

O5—H5A	0.8500	C11—H11A	0.9300
O5—H5B	0.8500	C12—C13	1.378 (10)
C1—C2	1.479 (8)	C12—H12A	0.9300
C2—C3	1.385 (8)	C13—C14	1.371 (10)
C2—C7	1.389 (8)	C13—H13A	0.9300
C3—C4	1.377 (10)	C14—H14A	0.9300
C3—H3A	0.9300		

O3—Pb1—O1	76.58 (15)	C3—C2—C1	120.5 (5)
O3—Pb1—O2	87.06 (16)	C7—C2—C1	121.1 (6)
O1—Pb1—O2	51.87 (14)	C4—C3—C2	120.6 (6)
O3—Pb1—O5^{i}	67.76 (13)	C4—C3—H3A	119.7
O1—Pb1—O5^{i}	116.34 (14)	C2—C3—H3A	119.7
O2—Pb1—O5^{i}	74.78 (13)	C5—C4—C3	120.2 (7)
O3—Pb1—O3^{ii}	135.53 (10)	C5—C4—H4A	119.9
O1—Pb1—O3^{ii}	75.30 (14)	C3—C4—H4A	119.9
O2—Pb1—O3^{ii}	101.51 (14)	C4—C5—C6	119.9 (7)
O5^{i}—Pb1—O3^{ii}	156.67 (12)	C4—C5—H5C	120.0
O3—Pb1—O5	73.78 (13)	C6—C5—H5C	120.0
O1—Pb1—O5	67.52 (13)	C7—C6—C5	119.7 (7)
O2—Pb1—O5	119.18 (14)	C7—C6—H6A	120.1
O5^{i}—Pb1—O5	138.36 (11)	C5—C6—H6A	120.1
O3^{ii}—Pb1—O5	63.89 (12)	C6—C7—C2	121.1 (7)
O3—Pb1—C1	78.02 (15)	C6—C7—H7A	119.5
O1—Pb1—C1	25.93 (15)	C2—C7—H7A	119.5
O2—Pb1—C1	26.25 (15)	O4—C8—O3	123.8 (6)
O5^{i}—Pb1—C1	94.18 (15)	O4—C8—C9	117.5 (6)
O3^{ii}—Pb1—C1	90.71 (16)	O3—C8—C9	118.7 (5)
O5—Pb1—C1	92.94 (15)	C10—C9—C14	119.2 (6)
C1—O1—Pb1	93.6 (4)	C10—C9—C8	120.0 (5)
C1—O2—Pb1	92.5 (4)	C14—C9—C8	120.8 (6)
C8—O3—Pb1	126.1 (4)	C9—C10—C11	120.5 (6)
C8—O3—Pb1^{i}	128.4 (4)	C9—C10—H10A	119.8
Pb1—O3—Pb1^{i}	103.70 (15)	C11—C10—H10A	119.8
Pb1^{ii}—O5—Pb1	98.38 (12)	C12—C11—C10	120.1 (7)
Pb1^{ii}—O5—H5A	120.4	C12—C11—H11A	119.9
Pb1—O5—H5A	115.5	C10—C11—H11A	119.9
Pb1^{ii}—O5—H5B	115.0	C11—C12—C13	119.5 (7)
Pb1—O5—H5B	112.2	C11—C12—H12A	120.3
H5A—O5—H5B	96.3	C13—C12—H12A	120.3
O1—C1—O2	120.6 (6)	C14—C13—C12	121.2 (7)
O1—C1—C2	119.7 (6)	C14—C13—H13A	119.4
O2—C1—C2	119.5 (6)	C12—C13—H13A	119.4
O1—C1—Pb1	60.5 (3)	C13—C14—C9	119.5 (7)
O2—C1—Pb1	61.2 (4)	C13—C14—H14A	120.3

C2—C1—Pb1	165.8 (4)	C9—C14—H14A	120.3
C3—C2—C7	118.3 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O4^{iii}	0.85	1.90	2.734 (7)	168
O5—H5*B*···O4	0.85	1.96	2.740 (7)	152

Symmetry code: (iii) −*x*+1, −*y*+1, −*z*.