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Bis(μ_2-quinoline-2-carboxylato)-$\kappa^3N,O^1:O^1;\kappa^3O^1:N,O^1$-bis[(acetato-$\kappa O$)(ethanol-$\kappa O$)lead(II)]

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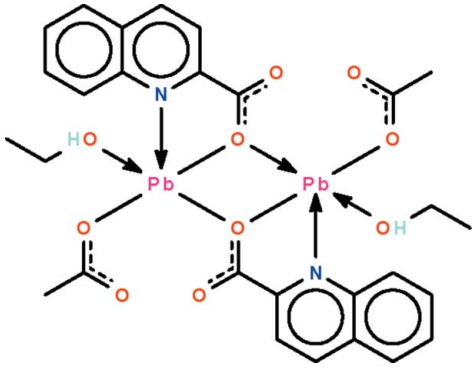
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.029; wR factor = 0.073; data-to-parameter ratio = 17.3.

In the centrosymmetric dinuclear title compound, $[Pb_2(C_{10}H_6NO_2)_2(CH_3COO)_2(C_2H_5OH)_2]$, one O atom of the carboxylate group of the quinoline-2-carboxylate anion connects the two Pb^{II} atoms. The Pb^{II} atom is surrounded by four O atoms and one N atom in a Ψ-octahedral PbO_4NE geometry (E is the electron lone pair). Two longer Pb···O interactions distort the geometry towards a Ψ-square-antiprism. Intermolecular O—H···O hydrogen bonds link the molecules.

Related literature

For the analogous methanol-coordinated compound, see: Mohammadnezhad *et al.* (2010).



Experimental

Crystal data

$[Pb_2(C_{10}H_6NO_2)_2(C_2H_3O_2)_2(C_2H_6O)_2]$
M_r = 968.92
Monoclinic, $P2_1/c$
a = 7.3419 (1) Å
b = 8.4004 (1) Å
c = 23.8008 (4) Å
β = 93.722 (1)°
V = 1464.82 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.54 mm^{-1}
T = 100 K
0.20 × 0.20 × 0.05 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
T_{min} = 0.206, T_{max} = 0.596
12668 measured reflections
3314 independent reflections
3010 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 1.08
3314 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pb1—O1	2.377 (4)	Pb1—O5	2.694 (4)
Pb1—O3	2.384 (4)	Pb1—O4	2.763 (3)
Pb1—O1^{i}	2.500 (3)	Pb1—O2^{ii}	3.096 (4)
Pb1—N1	2.645 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O3^{i}	0.84	2.36	2.710 (5)	106

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

Data collection: *CrysAlis PRO* (Agilent Technologies, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5469).

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supporting information

Acta Cryst. (2011). E**67**, m264 [doi:10.1107/S1600536811002509]

Bis(μ_2-quinoline-2-carboxylato)-$\kappa^3N,O^1:O^1;\kappa^3O^1:N,O^1$-bis[(acetato-$\kappa O$)(ethanol-$\kappa O$)lead(II)]

Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng

S1. Comment

A previous study of the methanol adduct of the title dinuclear compound, $[Pb(C_{10}H_6NO_2)(C_2H_3O_2)(CH_3OH)_2]_2$, has found a Ψ-octahedral geometry for the lead(II) atom. Two longer Pb···O interactions distort the geometry towards a Ψ-square-antiprism (Mohammadnezhad *et al.*, 2010). Replacing the methanol solvent system by ethanol leads to the analogous ethanol adduct (Scheme I, Fig. 1), which has a similar structure.

S2. Experimental

Lead(II) acetate (1 mmol) and quinoline-2-carboxylic acid (1 mmol) were loaded into a convection tube; the tube was filled with dry ethanol and kept at 333 K. Colorless crystals were collected from the side arm after several days.

S3. Refinement

H atoms were placed in calculated positions [C—H 0.95 to 0.98, O—H 0.84 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C, O)] and were included in the refinement in the riding model approximation.

The final difference Fourier map had a peak/hole in the vicinity of Pb1.

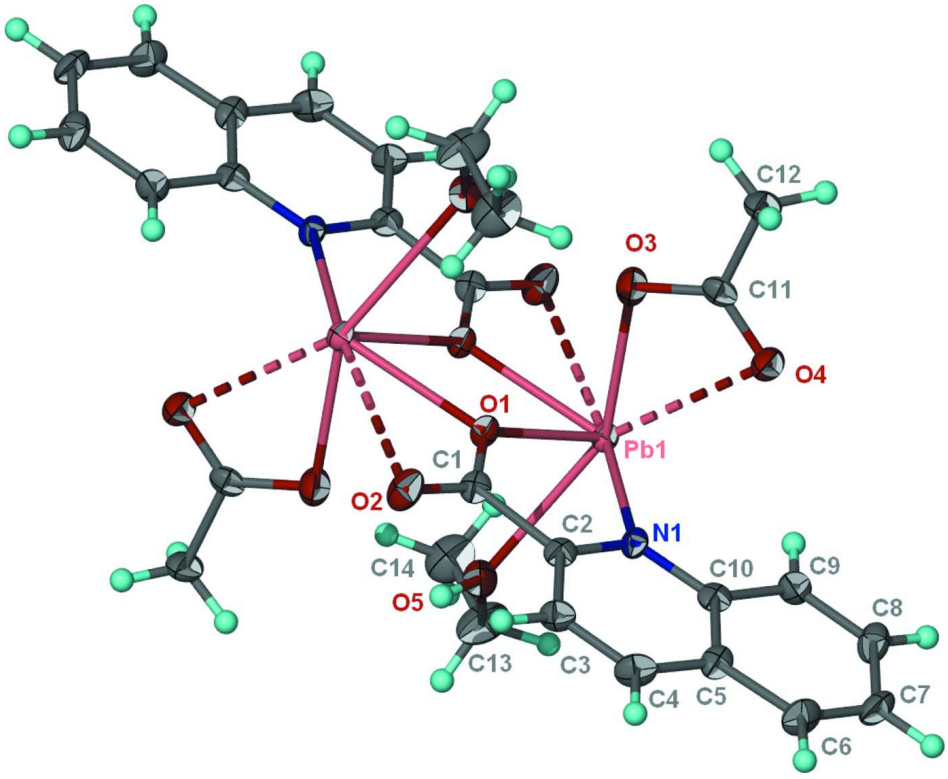

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The longer interactions that raise the coordination number are shown as dashed lines.

Bis(μ_2-quinoline-2-carboxylato)-$\kappa^3N,O^1:O^1$; $\kappa^3O^1:N,O^1$-bis[(acetato-κO)(ethanol- κO)lead(II)]

Crystal data

$[Pb_2(C_{10}H_6NO_2)_2(C_2H_3O_2)_2(C_2H_6O)_2]$
M_r = 968.92
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.3419 (1) Å
b = 8.4004 (1) Å
c = 23.8008 (4) Å
β = 93.722 (1)°
V = 1464.82 (4) Å^3
Z = 2
$F(000)$ = 912
D_x = 2.197 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7627 reflections
θ = 2.4–29.3°
μ = 11.54 mm^{-1}
T = 100 K
Prim, colorless
0.20 × 0.20 × 0.05 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
T_{min} = 0.206, T_{max} = 0.596
12668 measured reflections
3314 independent reflections
3010 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −9→9
k = −10→10
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.073$
$S = 1.08$
3314 reflections
192 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
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 1.3471P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.21$ e Å^{-3}
$\Delta\rho_{min} = -1.57$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pb1	0.72555 (2)	0.46532 (2)	0.554759 (7)	0.01208 (8)
O1	0.4023 (5)	0.4525 (4)	0.54078 (14)	0.0149 (7)
O2	0.1288 (5)	0.3557 (5)	0.55875 (15)	0.0225 (8)
O3	0.6357 (5)	0.7354 (5)	0.56638 (14)	0.0225 (8)
O4	0.7982 (5)	0.6708 (4)	0.64405 (14)	0.0215 (8)
O5	0.6307 (5)	0.1781 (4)	0.51184 (13)	0.0206 (8)
H5	0.5230	0.1444	0.5119	0.031*
N1	0.5510 (5)	0.3454 (5)	0.63884 (16)	0.0134 (8)
C1	0.2921 (7)	0.3768 (6)	0.57117 (19)	0.0144 (10)
C2	0.3771 (7)	0.3126 (6)	0.62685 (19)	0.0145 (10)
C3	0.2694 (7)	0.2289 (6)	0.66278 (19)	0.0168 (10)
H3	0.1453	0.2066	0.6518	0.020*
C4	0.3433 (7)	0.1795 (7)	0.7138 (2)	0.0199 (11)
H4	0.2712	0.1234	0.7390	0.024*
C5	0.5280 (7)	0.2127 (6)	0.72855 (19)	0.0162 (10)
C6	0.6171 (7)	0.1640 (7)	0.7808 (2)	0.0211 (11)
H6	0.5501	0.1091	0.8076	0.025*
C7	0.7974 (7)	0.1958 (6)	0.7925 (2)	0.0206 (11)
H7	0.8559	0.1611	0.8271	0.025*
C8	0.8983 (7)	0.2801 (6)	0.7536 (2)	0.0208 (11)
H8	1.0239	0.3017	0.7624	0.025*
C9	0.8177 (7)	0.3308 (6)	0.70336 (19)	0.0168 (10)
H9	0.8862	0.3887	0.6777	0.020*
C10	0.6310 (7)	0.2963 (6)	0.68997 (19)	0.0155 (10)
C11	0.7125 (7)	0.7694 (6)	0.61446 (19)	0.0155 (10)
C12	0.6856 (8)	0.9361 (6)	0.6361 (2)	0.0225 (12)
H12A	0.8021	0.9774	0.6524	0.034*
H12B	0.5964	0.9343	0.6650	0.034*
H12C	0.6406	1.0049	0.6050	0.034*
C13	0.7704 (9)	0.0864 (8)	0.4891 (2)	0.0311 (14)
H13A	0.7238	−0.0224	0.4810	0.037*
H13B	0.8746	0.0775	0.5175	0.037*
C14	0.8359 (8)	0.1573 (8)	0.4361 (2)	0.0315 (14)
H14A	0.9244	0.0853	0.4204	0.047*

H14B	0.8941	0.2602	0.4448	0.047*
H14C	0.7319	0.1727	0.4087	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.00993 (11)	0.01418 (12)	0.01215 (12)	0.00129 (7)	0.00073 (7)	0.00054 (6)
O1	0.0135 (18)	0.0172 (19)	0.0138 (17)	0.0006 (14)	−0.0009 (14)	0.0015 (13)
O2	0.0117 (18)	0.032 (2)	0.0239 (18)	0.0019 (16)	−0.0002 (14)	0.0063 (16)
O3	0.024 (2)	0.022 (2)	0.0209 (18)	0.0037 (17)	−0.0060 (15)	−0.0039 (16)
O4	0.028 (2)	0.0179 (19)	0.0179 (17)	0.0039 (17)	−0.0045 (15)	−0.0008 (15)
O5	0.0188 (19)	0.0208 (19)	0.0218 (18)	0.0037 (16)	−0.0012 (14)	−0.0045 (15)
N1	0.013 (2)	0.014 (2)	0.0129 (19)	0.0040 (17)	−0.0012 (15)	−0.0020 (16)
C1	0.012 (2)	0.016 (3)	0.015 (2)	0.004 (2)	0.0023 (18)	−0.0019 (19)
C2	0.016 (2)	0.013 (2)	0.015 (2)	0.004 (2)	0.0026 (18)	−0.0019 (19)
C3	0.015 (2)	0.016 (3)	0.020 (2)	−0.001 (2)	0.0040 (19)	0.002 (2)
C4	0.020 (3)	0.020 (3)	0.021 (2)	0.000 (2)	0.008 (2)	0.005 (2)
C5	0.018 (3)	0.017 (3)	0.014 (2)	0.006 (2)	0.0017 (19)	−0.0030 (19)
C6	0.028 (3)	0.024 (3)	0.012 (2)	0.002 (2)	0.005 (2)	0.003 (2)
C7	0.026 (3)	0.021 (3)	0.014 (2)	0.006 (2)	−0.002 (2)	0.004 (2)
C8	0.018 (3)	0.025 (3)	0.019 (2)	0.007 (2)	−0.003 (2)	−0.004 (2)
C9	0.018 (3)	0.018 (3)	0.015 (2)	−0.002 (2)	0.0029 (19)	0.000 (2)
C10	0.019 (3)	0.011 (2)	0.017 (2)	0.005 (2)	0.0023 (19)	−0.0042 (19)
C11	0.014 (2)	0.013 (2)	0.020 (2)	−0.004 (2)	0.0050 (19)	0.000 (2)
C12	0.032 (3)	0.012 (3)	0.023 (3)	0.003 (2)	−0.002 (2)	−0.003 (2)
C13	0.030 (3)	0.031 (3)	0.034 (3)	0.019 (3)	0.007 (3)	0.003 (3)
C14	0.024 (3)	0.039 (4)	0.032 (3)	0.009 (3)	0.008 (2)	0.003 (3)

Geometric parameters (Å, º)

Pb1—O1	2.377 (4)	C4—H4	0.9500
Pb1—O3	2.384 (4)	C5—C10	1.414 (7)
Pb1—O1^{i}	2.500 (3)	C5—C6	1.427 (7)
Pb1—N1	2.645 (4)	C6—C7	1.362 (8)
Pb1—O5	2.694 (4)	C6—H6	0.9500
Pb1—O4	2.763 (3)	C7—C8	1.413 (7)
Pb1—O2^{ii}	3.096 (4)	C7—H7	0.9500
O1—C1	1.288 (6)	C8—C9	1.367 (7)
O1—Pb1^{i}	2.500 (3)	C8—H8	0.9500
O2—C1	1.229 (6)	C9—C10	1.417 (7)
O3—C11	1.275 (6)	C9—H9	0.9500
O4—C11	1.233 (6)	C11—C12	1.510 (7)
O5—C13	1.418 (6)	C12—H12A	0.9800
O5—H5	0.8400	C12—H12B	0.9800
N1—C2	1.319 (6)	C12—H12C	0.9800
N1—C10	1.380 (6)	C13—C14	1.502 (8)
C1—C2	1.526 (7)	C13—H13A	0.9900
C2—C3	1.392 (7)	C13—H13B	0.9900

C3—C4	1.362 (7)	C14—H14A	0.9800
C3—H3	0.9500	C14—H14B	0.9800
C4—C5	1.407 (7)	C14—H14C	0.9800

O1—Pb1—O3	77.18 (12)	C3—C4—H4	120.5
O1—Pb1—O1^{i}	64.70 (14)	C5—C4—H4	120.5
O3—Pb1—O1^{i}	75.67 (11)	C4—C5—C10	119.0 (4)
O1—Pb1—N1	63.92 (12)	C4—C5—C6	122.7 (5)
O3—Pb1—N1	97.09 (12)	C10—C5—C6	118.3 (5)
O1^{i}—Pb1—N1	128.43 (12)	C7—C6—C5	120.4 (5)
O1—Pb1—O5	71.05 (11)	C7—C6—H6	119.8
O3—Pb1—O5	146.07 (12)	C5—C6—H6	119.8
O1^{i}—Pb1—O5	80.20 (11)	C6—C7—C8	120.5 (5)
N1—Pb1—O5	79.62 (11)	C6—C7—H7	119.7
O1—Pb1—O4	106.08 (11)	C8—C7—H7	119.7
O3—Pb1—O4	50.00 (11)	C9—C8—C7	120.9 (5)
O1^{i}—Pb1—O4	124.72 (10)	C9—C8—H8	119.5
N1—Pb1—O4	74.61 (11)	C7—C8—H8	119.5
O5—Pb1—O4	152.06 (10)	C8—C9—C10	119.4 (5)
O1—Pb1—O2^{ii}	159.18 (11)	C8—C9—H9	120.3
O3—Pb1—O2^{ii}	123.42 (12)	C10—C9—H9	120.3
O1^{i}—Pb1—O2^{ii}	114.32 (10)	N1—C10—C5	120.4 (4)
N1—Pb1—O2^{ii}	111.89 (10)	N1—C10—C9	119.2 (4)
O5—Pb1—O2^{ii}	88.18 (11)	C5—C10—C9	120.4 (4)
O4—Pb1—O2^{ii}	91.48 (10)	O4—C11—O3	122.8 (5)
C1—O1—Pb1	127.0 (3)	O4—C11—C12	120.1 (4)
C1—O1—Pb1^{i}	115.8 (3)	O3—C11—C12	117.0 (4)
Pb1—O1—Pb1^{i}	115.30 (14)	C11—C12—H12A	109.5
C11—O3—Pb1	102.0 (3)	C11—C12—H12B	109.5
C11—O4—Pb1	85.1 (3)	H12A—C12—H12B	109.5
C13—O5—Pb1	117.1 (4)	C11—C12—H12C	109.5
C13—O5—H5	121.4	H12A—C12—H12C	109.5
Pb1—O5—H5	121.4	H12B—C12—H12C	109.5
C2—N1—C10	118.6 (4)	O5—C13—C14	112.5 (5)
C2—N1—Pb1	115.2 (3)	O5—C13—H13A	109.1
C10—N1—Pb1	125.6 (3)	C14—C13—H13A	109.1
O2—C1—O1	125.1 (4)	O5—C13—H13B	109.1
O2—C1—C2	119.7 (4)	C14—C13—H13B	109.1
O1—C1—C2	115.2 (4)	H13A—C13—H13B	107.8
N1—C2—C3	123.6 (4)	C13—C14—H14A	109.5
N1—C2—C1	116.7 (4)	C13—C14—H14B	109.5
C3—C2—C1	119.7 (4)	H14A—C14—H14B	109.5
C4—C3—C2	119.5 (5)	C13—C14—H14C	109.5
C4—C3—H3	120.3	H14A—C14—H14C	109.5
C2—C3—H3	120.3	H14B—C14—H14C	109.5
C3—C4—C5	118.9 (5)		

O3—Pb1—O1—C1	−116.7 (4)	O4—Pb1—N1—C10	−60.4 (4)

O1^{i}—Pb1—O1—C1	163.3 (4)	O2^{ii}—Pb1—N1—C10	24.9 (4)
N1—Pb1—O1—C1	−12.1 (3)	Pb1—O1—C1—O2	−170.1 (4)
O5—Pb1—O1—C1	75.4 (4)	Pb1^{i}—O1—C1—O2	−6.8 (6)
O4—Pb1—O1—C1	−75.4 (4)	Pb1—O1—C1—C2	10.8 (6)
O2^{ii}—Pb1—O1—C1	71.1 (5)	Pb1^{i}—O1—C1—C2	174.0 (3)
O3—Pb1—O1—Pb1^{i}	80.02 (15)	C10—N1—C2—C3	−0.8 (7)
O1^{i}—Pb1—O1—Pb1^{i}	0.0	Pb1—N1—C2—C3	170.7 (4)
N1—Pb1—O1—Pb1^{i}	−175.37 (19)	C10—N1—C2—C1	176.9 (4)
O5—Pb1—O1—Pb1^{i}	−87.89 (15)	Pb1—N1—C2—C1	−11.6 (5)
O4—Pb1—O1—Pb1^{i}	121.29 (13)	O2—C1—C2—N1	−177.0 (4)
O2^{ii}—Pb1—O1—Pb1^{i}	−92.2 (3)	O1—C1—C2—N1	2.2 (6)
O1—Pb1—O3—C11	126.0 (3)	O2—C1—C2—C3	0.8 (7)
O1^{i}—Pb1—O3—C11	−167.2 (3)	O1—C1—C2—C3	180.0 (4)
N1—Pb1—O3—C11	64.9 (3)	N1—C2—C3—C4	1.2 (8)
O5—Pb1—O3—C11	146.8 (3)	C1—C2—C3—C4	−176.4 (5)
O4—Pb1—O3—C11	1.8 (3)	C2—C3—C4—C5	−0.8 (7)
O2^{ii}—Pb1—O3—C11	−57.3 (3)	C3—C4—C5—C10	0.0 (7)
O1—Pb1—O4—C11	−59.0 (3)	C3—C4—C5—C6	−179.4 (5)
O3—Pb1—O4—C11	−1.9 (3)	C4—C5—C6—C7	178.4 (5)
O1^{i}—Pb1—O4—C11	11.1 (3)	C10—C5—C6—C7	−0.9 (8)
N1—Pb1—O4—C11	−115.3 (3)	C5—C6—C7—C8	1.2 (8)
O5—Pb1—O4—C11	−138.7 (3)	C6—C7—C8—C9	−0.3 (8)
O2^{ii}—Pb1—O4—C11	132.4 (3)	C7—C8—C9—C10	−0.9 (8)
O1—Pb1—O5—C13	164.3 (3)	C2—N1—C10—C5	−0.1 (7)
O3—Pb1—O5—C13	142.8 (3)	Pb1—N1—C10—C5	−170.6 (3)
O1^{i}—Pb1—O5—C13	97.8 (3)	C2—N1—C10—C9	180.0 (4)
N1—Pb1—O5—C13	−129.9 (3)	Pb1—N1—C10—C9	9.4 (6)
O4—Pb1—O5—C13	−107.0 (4)	C4—C5—C10—N1	0.4 (7)
O2^{ii}—Pb1—O5—C13	−17.3 (3)	C6—C5—C10—N1	179.8 (4)
O1—Pb1—N1—C2	11.7 (3)	C4—C5—C10—C9	−179.6 (5)
O3—Pb1—N1—C2	83.6 (3)	C6—C5—C10—C9	−0.2 (7)
O1^{i}—Pb1—N1—C2	6.3 (4)	C8—C9—C10—N1	−178.9 (5)
O5—Pb1—N1—C2	−62.2 (3)	C8—C9—C10—C5	1.1 (7)
O4—Pb1—N1—C2	128.7 (3)	Pb1—O4—C11—O3	3.2 (5)
O2^{ii}—Pb1—N1—C2	−146.0 (3)	Pb1—O4—C11—C12	179.6 (4)
O1—Pb1—N1—C10	−177.5 (4)	Pb1—O3—C11—O4	−3.8 (5)
O3—Pb1—N1—C10	−105.5 (4)	Pb1—O3—C11—C12	179.7 (4)
O1^{i}—Pb1—N1—C10	177.2 (3)	Pb1—O5—C13—C14	−68.5 (6)
O5—Pb1—N1—C10	108.7 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O3^{i}	0.84	2.36	2.710 (5)	106

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