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(2,2′-Bipyridine-κ^2N,N')bis(4-hydroxybenzoato-κ^2O,O')lead(II) monohydrate

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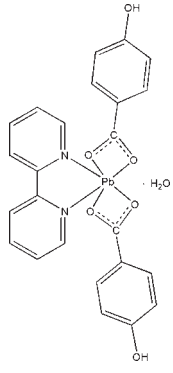
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.025; wR factor = 0.072; data-to-parameter ratio = 12.9.

The reaction of lead acetate, 4-hydroxybenzoic acid and 2,2′-bipyridine in aqueous solution gave the title complex, $[Pb(C_7H_5O_3)_2(C_{10}H_8N_2)]\cdot H_2O$. The asymmetric unit contains one Pb^{II} atom, two 4-hydroxybenzoate ligands, one 2,2′-bipyridine ligand and one uncoordinated water molecule. The Pb^{II} atom is hexacoordinated in a distorted tetragonal-bipyramidal geometry and is chelated by four carboxylate O atoms and two N atoms. O—H···O hydrogen-bonding interactions, involving the uncoordinated water, the carboxylate O atoms and hydroxy O atoms, produce a three-dimensional supramolecular structure.

Related literature

For general background to the potential applications of lead compounds, see: Fan & Zhu (2006); Hamilton *et al.* (2004); Shi *et al.* (2007). For the use of aromatic carboxylate ligands in the preparation of metal-organic complexes, see: Wang *et al.* (2006); Masaoka *et al.* (2001). For related lead structures, see: Shi *et al.* (2007).



Experimental

Crystal data

$[Pb(C_7H_5O_3)_2(C_{10}H_8N_2)]\cdot H_2O$
M_r = 655.61
Monoclinic, $P2_1/c$
a = 10.9483 (4) Å
b = 17.5194 (6) Å
c = 12.0479 (4) Å
β = 100.334 (2)°
V = 2273.39 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.47 mm^{-1}
T = 296 K
0.35 × 0.26 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.180, T_{max} = 0.303
18618 measured reflections
4067 independent reflections
3579 reflections with $I > \sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.072
S = 1.01
4067 reflections
315 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O1^{i}	0.82	1.90	2.671 (4)	157
O3—H3A···O1W	0.82	1.89	2.695 (5)	166
O1W—H1A···O5^{ii}	0.90 (3)	2.04 (3)	2.849 (4)	148 (5)
O1W—H1B···O4^{iii}	0.83 (3)	2.00 (3)	2.789 (4)	158 (5)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2224).

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supporting information

Acta Cryst. (2010). E**66**, m237 [https://doi.org/10.1107/S1600536810002941]

(2,2′-Bipyridine-κ^2N,N')bis(4-hydroxybenzoato-κ^2O,O')lead(II) monohydrate

Jun Dai and Juan Yang

S1. Comment

Recently, lead compounds have been increasingly studied owing to their possible applications in different fields (Fan & Zhu 2006; Hamilton *et al.* 2004; Shi *et al.* 2007), such as ion-exchange, non-linear optics and catalysis. Environmental and biological concerns are due to the toxicity of lead and its diverse interactions with biological systems. 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; Masaoka *et al.* 2001). Herein, we report the structure of the title complex.

The asymmetric unit of the title complex, $[Pb(C_{24}H_{18}O_6N_2)(H_2O)]$, contains a Pb^{II} cation, two 4-hydroxybenzonic acid ligands, one 2,2′-bipyridine and one free water molecule, as illustrated in Fig. 1. The Pb^{II} atom is hexacoordinate and chelated by four carboxylate O atoms from two 4-hydroxybenzoic acid and two N atoms from one 2,2′-bipyridine. The Pb—O bond lengths are in the range of 2.477 (3) to 2.625 (3) Å. The Pb—N bond lengths are 2.463 (3) to 2.562 (3) Å. The Pb^{II} atom has a distorted tetragonal bipyramidal geometry. The free water molecule, carboxylate O atoms and hydroxy O atoms are involved in extensive O—H···O hydrogen-bonding interactions (Table 1).

S2. Experimental

A mixture of $Pb(CH_3COO)_2\ 3H_2O$ (0.199 g, 0.52 mmol), 4-hydroxybenzoic acid (0.116 g, 0.84 mmol), 2,2′-bipyridine (0.033 g, 0.21 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave. The mixture was heated at 403 K for 5 days to give colorless crystals suitable for X-ray diffraction analysis.

S3. Refinement

All H atoms bonded to C atoms and the hydroxy H atoms were placed in calculated positions (C—H = 0.93 Å, O—H = 0.82 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2Ueq(C) or U_{iso}(H) = 1.5Ueq(O). The positions of the water H atoms were found in a difference Fourier map and refined with distance restraints O—H = 0.83 Å, U_{iso}(H) = 1.5Ueq(O).

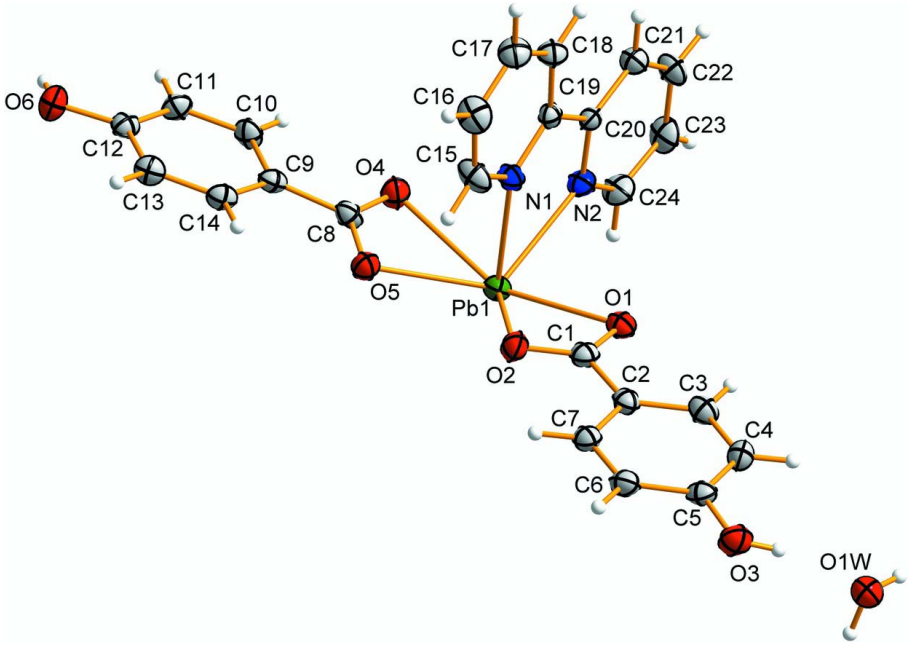

Figure 1

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.

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$c = 12.0479\ (4)$ Å
$\beta = 100.334\ (2)°$
$V = 2273.39\ (14)$ Å^3
$Z = 4$
$F(000) = 1264$
$D_x = 1.915$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9368 reflections
$\theta = 2.2–26.9°$
$\mu = 7.47$ mm^{-1}
$T = 296$ K
Block, colorless
0.35 × 0.26 × 0.21 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)
$T_{min} = 0.180$, $T_{max} = 0.303$
18618 measured reflections
4067 independent reflections
3579 reflections with $I > \sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.2°$
$h = -13\rightarrow13$
$k = -19\rightarrow20$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.072$
$S = 1.01$
4067 reflections
315 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.280P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pb1	0.261796 (15)	0.580074 (8)	0.261115 (12)	0.03852 (9)
O5	0.0806 (3)	0.64137 (15)	0.1348 (2)	0.0475 (7)
C7	0.4017 (5)	0.4162 (2)	−0.0512 (4)	0.0420 (11)
H7	0.3423	0.4505	−0.0863	0.050*
C20	0.1550 (3)	0.4657 (2)	0.4545 (3)	0.0320 (8)
O2	0.2797 (3)	0.50785 (17)	0.0880 (2)	0.0483 (7)
N2	0.2459 (3)	0.51668 (19)	0.4497 (3)	0.0404 (8)
O1	0.3906 (3)	0.45881 (15)	0.2420 (2)	0.0432 (7)
C19	0.0708 (4)	0.4488 (2)	0.3465 (3)	0.0315 (8)
C9	−0.0879 (4)	0.7114 (2)	0.1842 (3)	0.0356 (9)
C2	0.4263 (4)	0.4108 (2)	0.0654 (4)	0.0375 (9)
N1	0.0957 (3)	0.48437 (18)	0.2536 (2)	0.0380 (8)
O6	−0.3930 (3)	0.85265 (16)	0.0985 (2)	0.0482 (7)
H6A	−0.4058	0.8767	0.1536	0.072*
C21	0.1424 (5)	0.4314 (2)	0.5547 (4)	0.0408 (10)
H21	0.0775	0.3976	0.5575	0.049*
C1	0.3605 (4)	0.4621 (2)	0.1352 (3)	0.0409 (10)
C13	−0.2517 (4)	0.7641 (2)	0.0452 (3)	0.0419 (10)
H13	−0.2914	0.7679	−0.0296	0.050*
C14	−0.1501 (4)	0.7182 (2)	0.0728 (3)	0.0393 (9)
H14	−0.1217	0.6909	0.0163	0.047*
C3	0.5150 (4)	0.3590 (2)	0.1156 (3)	0.0462 (10)
H3	0.5318	0.3543	0.1937	0.055*
C10	−0.1360 (4)	0.7505 (2)	0.2682 (3)	0.0420 (10)
H10	−0.0986	0.7452	0.3435	0.050*
C12	−0.2965 (4)	0.8055 (2)	0.1294 (3)	0.0376 (9)
O4	0.0747 (3)	0.65607 (16)	0.3160 (2)	0.0503 (8)
C18	−0.0272 (4)	0.3996 (2)	0.3390 (4)	0.0424 (10)
H18	−0.0429	0.3752	0.4035	0.051*
C5	0.5550 (4)	0.3211 (2)	−0.0643 (3)	0.0399 (9)
C16	−0.0779 (5)	0.4215 (2)	0.1430 (4)	0.0555 (13)
H16	−0.1275	0.4132	0.0729	0.067*
O3	0.6169 (3)	0.2796 (2)	−0.1324 (2)	0.0587 (8)

H3A	0.6778	0.2594	−0.0940	0.088*
C17	−0.1021 (4)	0.3859 (2)	0.2378 (4)	0.0504 (11)
H17	−0.1691	0.3527	0.2332	0.061*
C4	0.5782 (4)	0.3146 (2)	0.0512 (3)	0.0461 (10)
H4	0.6371	0.2798	0.0859	0.055*
C8	0.0289 (4)	0.6673 (2)	0.2142 (3)	0.0389 (9)
C15	0.0219 (5)	0.4700 (2)	0.1548 (3)	0.0521 (12)
H15	0.0393	0.4941	0.0907	0.063*
C6	0.4647 (4)	0.3710 (2)	−0.1153 (3)	0.0466 (10)
H6	0.4462	0.3740	−0.1936	0.056*
C11	−0.2373 (4)	0.7962 (3)	0.2403 (3)	0.0447 (11)
H11	−0.2677	0.8219	0.2971	0.054*
C24	0.3265 (4)	0.5317 (2)	0.5439 (3)	0.0517 (11)
H24	0.3901	0.5662	0.5400	0.062*
C22	0.2272 (5)	0.4478 (2)	0.6510 (3)	0.0499 (11)
H22	0.2208	0.4242	0.7188	0.060*
C23	0.3208 (4)	0.4987 (3)	0.6463 (3)	0.0545 (12)
H23	0.3786	0.5107	0.7104	0.065*
O1W	0.8383 (3)	0.23234 (19)	−0.0179 (3)	0.0588 (8)
H1A	0.885 (5)	0.273 (2)	−0.030 (4)	0.088*
H1B	0.867 (5)	0.222 (3)	0.049 (3)	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.03782 (13)	0.03792 (13)	0.04067 (12)	−0.00251 (6)	0.00932 (8)	0.00471 (6)
O5	0.0479 (19)	0.0526 (17)	0.0440 (15)	0.0115 (14)	0.0139 (14)	0.0043 (13)
C7	0.034 (3)	0.048 (3)	0.044 (2)	−0.0059 (18)	0.005 (2)	0.0071 (17)
C20	0.025 (2)	0.036 (2)	0.0352 (19)	0.0043 (16)	0.0062 (17)	0.0005 (15)
O2	0.0394 (18)	0.0588 (18)	0.0450 (15)	0.0114 (15)	0.0032 (14)	0.0044 (13)
N2	0.035 (2)	0.0451 (19)	0.0393 (17)	−0.0048 (16)	0.0027 (16)	0.0004 (14)
O1	0.0461 (19)	0.0453 (17)	0.0382 (15)	−0.0017 (14)	0.0077 (13)	0.0033 (12)
C19	0.031 (2)	0.0262 (18)	0.038 (2)	0.0034 (16)	0.0068 (17)	−0.0005 (15)
C9	0.042 (2)	0.031 (2)	0.0369 (19)	−0.0055 (17)	0.0141 (19)	0.0000 (15)
C2	0.037 (3)	0.037 (2)	0.039 (2)	−0.0053 (17)	0.0064 (19)	0.0038 (15)
N1	0.039 (2)	0.0410 (19)	0.0329 (16)	−0.0028 (15)	0.0029 (15)	0.0047 (13)
O6	0.0435 (19)	0.0505 (17)	0.0480 (16)	0.0107 (14)	0.0009 (14)	−0.0065 (13)
C21	0.042 (3)	0.041 (2)	0.039 (2)	−0.0018 (19)	0.007 (2)	0.0018 (17)
C1	0.035 (3)	0.043 (2)	0.045 (2)	−0.008 (2)	0.008 (2)	0.0026 (18)
C13	0.045 (3)	0.044 (2)	0.037 (2)	−0.004 (2)	0.0056 (19)	−0.0038 (17)
C14	0.045 (3)	0.037 (2)	0.037 (2)	−0.0042 (19)	0.0129 (19)	−0.0047 (16)
C3	0.050 (3)	0.047 (2)	0.040 (2)	−0.002 (2)	0.006 (2)	0.0025 (18)
C10	0.053 (3)	0.045 (2)	0.0287 (18)	0.006 (2)	0.0087 (19)	0.0018 (16)
C12	0.037 (2)	0.033 (2)	0.043 (2)	−0.0050 (18)	0.0082 (19)	−0.0024 (16)
O4	0.059 (2)	0.0521 (17)	0.0410 (16)	0.0137 (15)	0.0124 (15)	0.0015 (13)
C18	0.039 (3)	0.040 (2)	0.047 (2)	−0.0064 (19)	0.006 (2)	−0.0003 (18)
C5	0.031 (2)	0.051 (2)	0.0372 (19)	−0.0068 (19)	0.0069 (18)	−0.0010 (17)
C16	0.060 (4)	0.056 (3)	0.044 (3)	−0.010 (2)	−0.008 (2)	−0.0073 (19)

O3	0.055 (2)	0.076 (2)	0.0473 (16)	0.0091 (17)	0.0158 (16)	0.0009 (16)
C17	0.046 (3)	0.047 (3)	0.056 (3)	−0.010 (2)	0.001 (2)	−0.004 (2)
C4	0.041 (3)	0.046 (2)	0.050 (2)	0.009 (2)	0.006 (2)	0.0039 (19)
C8	0.051 (3)	0.036 (2)	0.0320 (19)	−0.0002 (19)	0.013 (2)	0.0014 (15)
C15	0.065 (3)	0.054 (3)	0.034 (2)	−0.014 (2)	−0.001 (2)	0.0032 (18)
C6	0.042 (3)	0.059 (3)	0.039 (2)	−0.006 (2)	0.009 (2)	0.0073 (19)
C11	0.049 (3)	0.047 (3)	0.043 (2)	0.006 (2)	0.019 (2)	−0.0029 (17)
C24	0.041 (3)	0.060 (3)	0.051 (2)	−0.010 (2)	−0.003 (2)	0.000 (2)
C22	0.060 (3)	0.055 (3)	0.033 (2)	0.001 (2)	0.003 (2)	0.0090 (19)
C23	0.047 (3)	0.068 (3)	0.040 (2)	−0.002 (2)	−0.013 (2)	0.001 (2)
O1W	0.060 (2)	0.060 (2)	0.0592 (19)	0.0064 (17)	0.0169 (18)	0.0124 (16)

Geometric parameters (Å, º)

Pb1—N1	2.463 (3)	C13—H13	0.9300
Pb1—O2	2.477 (3)	C14—H14	0.9300
Pb1—O5	2.514 (3)	C3—C4	1.370 (6)
Pb1—N2	2.563 (3)	C3—H3	0.9300
Pb1—O1	2.583 (3)	C10—C11	1.359 (6)
Pb1—O4	2.625 (3)	C10—H10	0.9300
O5—C8	1.279 (4)	C12—C11	1.386 (5)
C7—C6	1.374 (6)	O4—C8	1.254 (4)
C7—C2	1.385 (6)	C18—C17	1.363 (6)
C7—H7	0.9300	C18—H18	0.9300
C20—N2	1.346 (5)	C5—O3	1.364 (5)
C20—C21	1.378 (5)	C5—C4	1.374 (5)
C20—C19	1.484 (5)	C5—C6	1.379 (6)
O2—C1	1.252 (5)	C16—C17	1.368 (6)
N2—C24	1.332 (5)	C16—C15	1.371 (6)
O1—C1	1.271 (5)	C16—H16	0.9300
C19—N1	1.351 (5)	O3—H3A	0.8200
C19—C18	1.366 (6)	C17—H17	0.9300
C9—C14	1.397 (5)	C4—H4	0.9300
C9—C10	1.402 (5)	C15—H15	0.9300
C9—C8	1.482 (6)	C6—H6	0.9300
C2—C3	1.387 (6)	C11—H11	0.9300
C2—C1	1.501 (6)	C24—C23	1.374 (6)
N1—C15	1.337 (5)	C24—H24	0.9300
O6—C12	1.341 (5)	C22—C23	1.368 (6)
O6—H6A	0.8200	C22—H22	0.9300
C21—C22	1.379 (6)	C23—H23	0.9300
C21—H21	0.9300	O1W—H1A	0.90 (3)
C13—C14	1.364 (6)	O1W—H1B	0.83 (3)
C13—C12	1.405 (5)		
N1—Pb1—O2	77.93 (10)	C13—C14—H14	119.3
N1—Pb1—O5	76.79 (10)	C9—C14—H14	119.3
O2—Pb1—O5	83.20 (9)	C4—C3—C2	120.7 (4)

N1—Pb1—N2	64.57 (10)	C4—C3—H3	119.7
O2—Pb1—N2	123.60 (11)	C2—C3—H3	119.7
O5—Pb1—N2	123.38 (10)	C11—C10—C9	120.3 (4)
N1—Pb1—O1	81.27 (11)	C11—C10—H10	119.9
O2—Pb1—O1	51.53 (9)	C9—C10—H10	119.9
O5—Pb1—O1	132.96 (8)	O6—C12—C11	123.3 (3)
N2—Pb1—O1	81.23 (9)	O6—C12—C13	118.6 (3)
N1—Pb1—O4	75.54 (10)	C11—C12—C13	118.2 (4)
O2—Pb1—O4	130.87 (9)	C8—O4—Pb1	91.5 (2)
O5—Pb1—O4	50.89 (8)	C17—C18—C19	120.6 (4)
N2—Pb1—O4	79.42 (10)	C17—C18—H18	119.7
O1—Pb1—O4	154.53 (9)	C19—C18—H18	119.7
C8—O5—Pb1	96.1 (2)	O3—C5—C4	122.9 (4)
C6—C7—C2	120.3 (4)	O3—C5—C6	117.6 (3)
C6—C7—H7	119.9	C4—C5—C6	119.5 (4)
C2—C7—H7	119.9	C17—C16—C15	117.7 (4)
N2—C20—C21	121.2 (4)	C17—C16—H16	121.1
N2—C20—C19	116.3 (3)	C15—C16—H16	121.1
C21—C20—C19	122.5 (4)	C5—O3—H3A	109.5
C1—O2—Pb1	95.8 (2)	C18—C17—C16	119.4 (4)
C24—N2—C20	118.4 (3)	C18—C17—H17	120.3
C24—N2—Pb1	122.0 (3)	C16—C17—H17	120.3
C20—N2—Pb1	119.6 (2)	C3—C4—C5	120.3 (4)
C1—O1—Pb1	90.4 (2)	C3—C4—H4	119.8
N1—C19—C18	120.6 (4)	C5—C4—H4	119.8
N1—C19—C20	116.6 (3)	O4—C8—O5	121.5 (4)
C18—C19—C20	122.7 (3)	O4—C8—C9	119.8 (3)
C14—C9—C10	118.1 (4)	O5—C8—C9	118.7 (3)
C14—C9—C8	122.0 (3)	N1—C15—C16	123.6 (4)
C10—C9—C8	119.9 (3)	N1—C15—H15	118.2
C7—C2—C3	118.7 (4)	C16—C15—H15	118.2
C7—C2—C1	120.2 (4)	C7—C6—C5	120.5 (4)
C3—C2—C1	121.1 (4)	C7—C6—H6	119.8
C15—N1—C19	118.1 (3)	C5—C6—H6	119.8
C15—N1—Pb1	119.0 (3)	C10—C11—C12	121.8 (4)
C19—N1—Pb1	122.8 (2)	C10—C11—H11	119.1
C12—O6—H6A	109.5	C12—C11—H11	119.1
C20—C21—C22	119.2 (4)	N2—C24—C23	123.5 (4)
C20—C21—H21	120.4	N2—C24—H24	118.2
C22—C21—H21	120.4	C23—C24—H24	118.2
O2—C1—O1	121.6 (4)	C23—C22—C21	119.9 (4)
O2—C1—C2	119.9 (4)	C23—C22—H22	120.1
O1—C1—C2	118.5 (4)	C21—C22—H22	120.1
C14—C13—C12	120.2 (4)	C22—C23—C24	117.8 (4)
C14—C13—H13	119.9	C22—C23—H23	121.1
C12—C13—H13	119.9	C24—C23—H23	121.1
C13—C14—C9	121.3 (4)	H1A—O1W—H1B	102 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O1^{i}	0.82	1.90	2.671 (4)	157
O3—H3*A*···O1*W*	0.82	1.89	2.695 (5)	166
O1*W*—H1*A*···O5^{ii}	0.90 (3)	2.04 (3)	2.849 (4)	148 (5)
O1*W*—H1*B*···O4^{iii}	0.83 (3)	2.00 (3)	2.789 (4)	158 (5)

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