

catena-Poly[[[bis[4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol- $\kappa^2 N^7, N^8$]]lead(II)]- μ -4,4'-oxydibenzoato- $\kappa^3 O, O': O''$] dihydrate]

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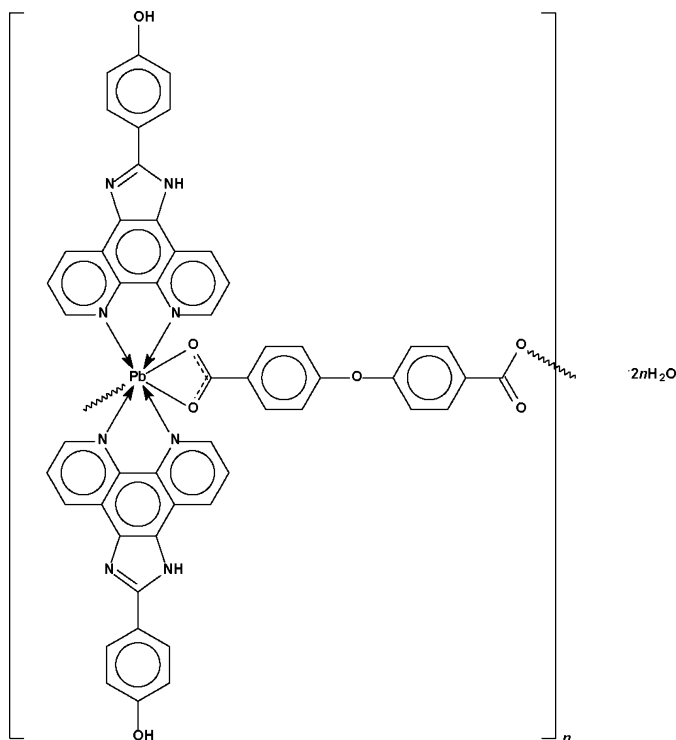
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Key indicators: single-crystal X-ray study; *T* = 295 K; mean $\sigma(C-C)$ = 0.012 Å; *R* factor = 0.055; *wR* factor = 0.168; data-to-parameter ratio = 15.8.

The carboxylate dianion in the title compound, [Pb(C₁₄H₈O₅)(C₁₉H₁₂N₄O)₂]-2H₂O, uses one carboxylate group to *O, O'*-chelate a bis[4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol]-chelated Pb^{II} atom and uses its other carboxylate group to bind to another Pb^{II} atom in an irregular seven-coordinate geometry in the chain structure; the lone pair is stereochemically active. Adjacent chains are linked by intermolecular O—H...N, N—H...O and O—H...O hydrogen bonds that involve the uncoordinated water molecules to form a three-dimensional network.

Related literature

For a transition metal dicarboxylate adduct of 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol, see: Xu *et al.* (2008).



Experimental

Crystal data

[Pb(C₁₄H₈O₅)(C₁₉H₁₂N₄O)₂]-2H₂O
M_r = 1124.08
 Monoclinic, *P*2₁/*n*
a = 10.767 (4) Å
b = 29.916 (7) Å
c = 13.688 (4) Å
 β = 97.70 (1)°

V = 4369 (2) Å³
Z = 4
 Mo *K*α radiation
 μ = 3.93 mm⁻¹
T = 295 (2) K
 0.33 × 0.24 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.188, *T_{max}* = 0.492
 (expected range = 0.167–0.438)

42355 measured reflections
 9977 independent reflections
 6235 reflections with *I* > 2σ(*I*)
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
 $wR(F^2)$ = 0.168
S = 1.02
 9977 reflections

631 parameters
 H-atom parameters constrained
 $\Delta\rho_{max}$ = 1.51 e Å⁻³
 $\Delta\rho_{min}$ = -1.09 e Å⁻³

Table 1

Selected bond lengths (Å).

Pb1—O1	2.582 (5)	Pb1—N2	2.570 (6)
Pb1—O2	2.824 (5)	Pb1—N5	2.612 (6)
Pb1—O5 ⁱ	2.818 (6)	Pb1—N6	2.506 (6)
Pb1—N1	2.672 (6)		

Symmetry code: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H3N\cdots O2^{ii}$	0.86	1.98	2.82 (1)	166
$N7-H7N\cdots O4^{iii}$	0.86	1.97	2.81 (1)	166
$O1W-H1W1\cdots N4$	0.82	2.00	2.82 (1)	174
$O1W-H1W2\cdots O6^{iv}$	0.82	2.37	2.57 (1)	95
$O2W-H2W1\cdots N8$	0.82	2.00	2.79 (1)	160
$O2W-H2W2\cdots O3^v$	0.82	2.27	3.06 (1)	160

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2072).

References

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 Xu, M.-L., Zhao, R., Wang, G.-Y. & Ng, S. W. (2008). *Acta Cryst.* **E64**, m710–m711.

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Acta Cryst. (2008). E64, m712-m713 [doi:10.1107/S1600536808010805]

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Comment

The 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol *N*-heterocycle furnishes adducts with metal dicarboxylates (Xu *et al.*, 2008).

The carboxylate dianion in the title chain compound uses one carboxyl $-\text{CO}_2$ group to *O, O'*-chelate to the lead(II) atom and uses its other carboxyl end to bind to another lead atom in a unidentate manner. The lead atom exists in an undefined seven-coordinate geometry; the Pb—O distances range between 2.582 (5) and 2.824 (5) Å, and the Pb—N distances vary between 2.506 (6) and 2.672 (6) Å (Table 1). The lone-pair is stereochemically active. Adjacent chains are linked by intermolecular O—H \cdots N, N—H \cdots O and O—H \cdots O hydrogen bonds (Table 2) that involve the lattice water molecules to form a three-dimensional network.

Experimental

Lead(II) nitrate (0.1 mmol), 1,4-oxobis(benzoic acid), 4-(1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthren-2-yl)phenol (0.1 mmol) and water (14 ml) were heated in a 23 ml, Teflon-lined, stainless-steel Parr bomb at 458 K for 3 days. Crystals were obtained in 30% yield.

Refinement

The carbon- and nitrogen-bound H atoms were placed in calculated positions [C—H 0.93, N—H 0.86, O—H 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C, N, O})$], and were included in the refinement in the riding-model approximation.

Figures

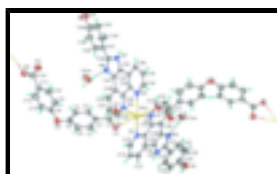


Fig. 1. Thermal ellipsoid plot of a portion of the chain structure of $\text{Pb}(\text{C}_{19}\text{H}_{12}\text{N}_4\text{O})_2(\text{C}_{14}\text{H}_8\text{O}_5)_2\cdot 2\text{H}_2\text{O}$; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. Symmetry codes are given in Table 1.

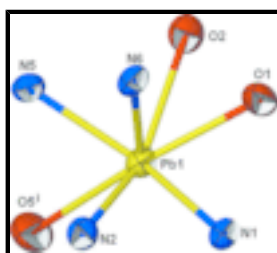


Fig. 2. Seven-coordinate environment of lead.

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Crystal data

[Pb(C₁₄H₈O₅)(C₁₉H₁₂N₄O)₂] \cdot 2H₂O

$M_r = 1124.08$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.767$ (4) Å

$b = 29.916$ (7) Å

$c = 13.688$ (4) Å

$\beta = 97.70$ (1)°

$V = 4369$ (2) Å³

$Z = 4$

$F_{000} = 2232$

$D_x = 1.709$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 24960 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 3.93$ mm⁻¹

$T = 295$ (2) K

Block, colorless

$0.33 \times 0.24 \times 0.21$ mm

Data collection

Rigaku R-AXIS RAPID
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10 pixels mm⁻¹

$T = 295$ (2) K

ω scans

Absorption correction: Multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.188$, $T_{\max} = 0.492$

42355 measured reflections

9977 independent reflections

6235 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.0$ °

$h = -13 \rightarrow 13$

$k = -38 \rightarrow 38$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.168$

$S = 1.02$

9977 reflections

631 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

$$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 9.1333P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.52$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.09$ e Å⁻³

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb1	0.22221 (3)	0.252248 (8)	0.632884 (19)	0.04982 (12)
O1	0.1768 (7)	0.31678 (17)	0.5080 (4)	0.0838 (19)
O2	0.1246 (6)	0.33913 (18)	0.6496 (4)	0.0704 (15)
O3	0.2197 (8)	0.5257 (2)	0.4374 (5)	0.099 (2)
O4	0.4930 (7)	0.6379 (2)	0.7966 (5)	0.094 (2)
O5	0.3496 (9)	0.6846 (2)	0.7428 (5)	0.114 (3)
O6	1.0871 (7)	0.0039 (2)	0.2469 (5)	0.092 (2)
H6O	1.0994	0.0068	0.1894	0.138*
O7	0.9813 (8)	0.5095 (3)	1.2543 (5)	0.124 (3)
H7O	1.0442	0.5223	1.2408	0.186*
O1W	0.8513 (7)	0.0694 (2)	0.6615 (5)	0.097 (2)
H1W1	0.8047	0.0778	0.6127	0.145*
H1W2	0.8102	0.0643	0.7066	0.145*
O2W	0.8223 (7)	0.4435 (3)	0.7773 (5)	0.128 (3)
H2W1	0.7757	0.4259	0.8005	0.191*
H2W2	0.7958	0.4477	0.7191	0.191*
N1	0.3196 (6)	0.2288 (2)	0.4707 (4)	0.0541 (15)
N2	0.4077 (6)	0.19747 (19)	0.6534 (4)	0.0560 (15)
N3	0.6337 (6)	0.13120 (19)	0.3461 (4)	0.0542 (15)
H3N	0.6276	0.1356	0.2836	0.065*
N4	0.7003 (6)	0.10439 (19)	0.4949 (4)	0.0554 (15)
N5	0.3031 (6)	0.27173 (18)	0.8164 (4)	0.0491 (14)
N6	0.4143 (6)	0.30027 (19)	0.6616 (4)	0.0512 (14)
N7	0.6079 (6)	0.36530 (19)	1.0242 (4)	0.0516 (14)
H7N	0.5899	0.3632	1.0834	0.062*
N8	0.7061 (6)	0.38671 (19)	0.8986 (4)	0.0536 (15)
C1	0.1535 (8)	0.3474 (3)	0.5655 (6)	0.065 (2)
C2	0.1686 (8)	0.3954 (3)	0.5314 (6)	0.061 (2)
C3	0.1180 (8)	0.4303 (2)	0.5783 (6)	0.066 (2)
H3	0.0716	0.4248	0.6297	0.079*
C4	0.1373 (9)	0.4749 (3)	0.5474 (6)	0.069 (2)
H4	0.1044	0.4988	0.5788	0.082*
C5	0.2045 (9)	0.4823 (3)	0.4712 (7)	0.072 (2)
C6	0.2548 (10)	0.4470 (3)	0.4242 (7)	0.084 (3)
H6	0.2991	0.4528	0.3717	0.101*
C7	0.2405 (9)	0.4042 (3)	0.4532 (6)	0.075 (3)
H7	0.2772	0.3808	0.4225	0.090*
C8	0.2650 (11)	0.5560 (3)	0.5087 (6)	0.079 (3)
C9	0.3789 (11)	0.5484 (3)	0.5651 (7)	0.098 (3)
H9	0.4252	0.5230	0.5548	0.117*
C10	0.4246 (11)	0.5793 (3)	0.6381 (7)	0.096 (3)
H10	0.5000	0.5737	0.6779	0.115*
C11	0.3572 (9)	0.6186 (3)	0.6515 (6)	0.070 (2)
C12	0.2442 (9)	0.6260 (4)	0.5880 (7)	0.084 (3)
H12	0.1993	0.6523	0.5934	0.101*

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C13	0.2011 (9)	0.5948 (3)	0.5191 (7)	0.077 (2)
H13	0.1264	0.6001	0.4781	0.093*
C14	0.4078 (11)	0.6516 (3)	0.7334 (7)	0.090 (3)
C15	0.2765 (9)	0.2453 (2)	0.3820 (6)	0.065 (2)
H15	0.2113	0.2659	0.3768	0.078*
C16	0.3252 (10)	0.2329 (3)	0.2974 (5)	0.072 (2)
H16	0.2946	0.2457	0.2371	0.086*
C17	0.4159 (8)	0.2026 (3)	0.3029 (5)	0.061 (2)
H17	0.4484	0.1937	0.2463	0.073*
C18	0.4623 (7)	0.1841 (2)	0.3943 (5)	0.0534 (18)
C19	0.4116 (7)	0.1985 (2)	0.4769 (5)	0.0478 (16)
C20	0.5610 (7)	0.1511 (2)	0.4104 (5)	0.0522 (17)
C21	0.7153 (8)	0.1039 (2)	0.3996 (6)	0.0575 (19)
C22	0.8102 (8)	0.0774 (3)	0.3582 (6)	0.060 (2)
C23	0.8326 (9)	0.0832 (2)	0.2636 (6)	0.066 (2)
H23	0.7873	0.1044	0.2240	0.079*
C24	0.9235 (9)	0.0574 (3)	0.2253 (6)	0.069 (2)
H24	0.9353	0.0603	0.1596	0.083*
C25	0.9933 (9)	0.0285 (3)	0.2840 (7)	0.076 (2)
C26	0.9773 (12)	0.0230 (4)	0.3790 (7)	0.116 (5)
H26	1.0265	0.0030	0.4194	0.139*
C27	0.8852 (12)	0.0481 (4)	0.4143 (8)	0.110 (4)
H27	0.8739	0.0447	0.4801	0.132*
C28	0.6054 (7)	0.1341 (2)	0.5018 (5)	0.0519 (17)
C29	0.5571 (8)	0.1494 (2)	0.5886 (5)	0.0532 (18)
C30	0.4597 (7)	0.1814 (2)	0.5749 (5)	0.0475 (16)
C31	0.5963 (9)	0.1339 (3)	0.6837 (6)	0.075 (3)
H31	0.6577	0.1119	0.6944	0.090*
C32	0.5450 (10)	0.1509 (3)	0.7599 (6)	0.088 (3)
H32	0.5733	0.1418	0.8240	0.106*
C33	0.4502 (9)	0.1819 (3)	0.7424 (6)	0.072 (2)
H33	0.4139	0.1925	0.7958	0.087*
C34	0.2457 (8)	0.2584 (2)	0.8911 (6)	0.0573 (19)
H34	0.1771	0.2394	0.8778	0.069*
C35	0.2824 (8)	0.2712 (3)	0.9875 (6)	0.062 (2)
H35	0.2385	0.2610	1.0372	0.074*
C36	0.3824 (7)	0.2986 (2)	1.0100 (5)	0.0542 (18)
H36	0.4086	0.3072	1.0749	0.065*
C37	0.4461 (6)	0.3140 (2)	0.9323 (5)	0.0439 (15)
C38	0.4027 (7)	0.2994 (2)	0.8353 (5)	0.0445 (15)
C39	0.5495 (7)	0.3434 (2)	0.9428 (5)	0.0487 (16)
C40	0.6998 (7)	0.3911 (2)	0.9936 (5)	0.0534 (18)
C41	0.7755 (7)	0.4217 (3)	1.0608 (6)	0.0593 (19)
C42	0.7432 (11)	0.4316 (4)	1.1507 (8)	0.116 (5)
H42	0.6739	0.4175	1.1707	0.140*
C43	0.8099 (13)	0.4621 (5)	1.2140 (9)	0.133 (6)
H43	0.7826	0.4698	1.2733	0.160*
C44	0.9163 (9)	0.4804 (3)	1.1872 (7)	0.083 (3)
C45	0.9535 (8)	0.4709 (3)	1.1008 (6)	0.073 (2)

H45	1.0265	0.4834	1.0834	0.087*
C46	0.8813 (8)	0.4416 (3)	1.0360 (6)	0.072 (2)
H46	0.9059	0.4356	0.9748	0.086*
C47	0.6115 (6)	0.3568 (2)	0.8667 (5)	0.0493 (16)
C48	0.5710 (7)	0.3414 (2)	0.7678 (5)	0.0496 (16)
C49	0.4643 (7)	0.3140 (2)	0.7525 (5)	0.0477 (16)
C50	0.6268 (8)	0.3542 (3)	0.6863 (6)	0.066 (2)
H50	0.6980	0.3722	0.6944	0.079*
C51	0.5767 (9)	0.3404 (3)	0.5946 (6)	0.074 (2)
H51	0.6132	0.3486	0.5394	0.089*
C52	0.4692 (9)	0.3134 (3)	0.5850 (6)	0.068 (2)
H52	0.4349	0.3043	0.5222	0.082*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.06011 (19)	0.04550 (16)	0.04314 (16)	-0.00172 (12)	0.00430 (12)	-0.00412 (12)
O1	0.151 (6)	0.047 (3)	0.056 (3)	0.019 (3)	0.023 (4)	0.001 (3)
O2	0.094 (4)	0.069 (3)	0.053 (3)	0.002 (3)	0.026 (3)	0.002 (3)
O3	0.154 (7)	0.065 (4)	0.074 (4)	-0.025 (4)	0.000 (4)	0.002 (3)
O4	0.112 (6)	0.090 (5)	0.074 (4)	-0.002 (4)	-0.007 (4)	-0.011 (4)
O5	0.199 (9)	0.065 (4)	0.080 (5)	0.022 (5)	0.032 (5)	-0.011 (4)
O6	0.108 (5)	0.098 (5)	0.077 (4)	0.016 (4)	0.039 (4)	-0.020 (4)
O7	0.129 (7)	0.160 (7)	0.088 (5)	-0.084 (6)	0.031 (5)	-0.058 (5)
O1W	0.109 (5)	0.111 (5)	0.067 (4)	0.035 (4)	0.003 (4)	-0.012 (4)
O2W	0.120 (6)	0.166 (8)	0.087 (5)	-0.080 (6)	-0.021 (4)	0.042 (5)
N1	0.075 (4)	0.050 (3)	0.036 (3)	-0.001 (3)	0.003 (3)	-0.004 (3)
N2	0.077 (4)	0.051 (3)	0.042 (3)	0.009 (3)	0.013 (3)	-0.001 (3)
N3	0.079 (4)	0.052 (3)	0.034 (3)	0.000 (3)	0.015 (3)	-0.004 (3)
N4	0.071 (4)	0.050 (3)	0.046 (3)	0.007 (3)	0.013 (3)	-0.007 (3)
N5	0.062 (4)	0.042 (3)	0.044 (3)	-0.008 (3)	0.012 (3)	-0.007 (3)
N6	0.065 (4)	0.052 (3)	0.036 (3)	-0.005 (3)	0.005 (3)	-0.007 (3)
N7	0.061 (4)	0.051 (3)	0.042 (3)	-0.005 (3)	0.004 (3)	-0.006 (3)
N8	0.056 (4)	0.052 (3)	0.053 (4)	-0.005 (3)	0.006 (3)	-0.002 (3)
C1	0.086 (6)	0.054 (4)	0.056 (5)	0.011 (4)	0.012 (4)	0.000 (4)
C2	0.067 (5)	0.058 (4)	0.054 (5)	-0.002 (4)	0.000 (4)	0.004 (4)
C3	0.084 (6)	0.053 (4)	0.060 (5)	0.008 (4)	0.004 (4)	-0.004 (4)
C4	0.088 (6)	0.057 (4)	0.060 (5)	0.005 (4)	0.005 (5)	-0.006 (4)
C5	0.088 (6)	0.055 (4)	0.072 (6)	-0.009 (4)	0.011 (5)	-0.001 (4)
C6	0.115 (8)	0.064 (5)	0.078 (6)	-0.008 (5)	0.027 (6)	0.006 (5)
C7	0.099 (7)	0.067 (5)	0.062 (5)	-0.014 (5)	0.027 (5)	-0.001 (4)
C8	0.124 (9)	0.062 (5)	0.049 (5)	-0.018 (5)	0.006 (5)	0.003 (4)
C9	0.135 (10)	0.073 (6)	0.076 (6)	0.026 (6)	-0.018 (6)	0.001 (5)
C10	0.128 (9)	0.074 (6)	0.077 (6)	0.021 (6)	-0.015 (6)	-0.018 (5)
C11	0.090 (7)	0.060 (5)	0.063 (5)	0.001 (4)	0.022 (5)	0.004 (4)
C12	0.081 (7)	0.091 (7)	0.079 (6)	0.008 (5)	0.007 (5)	0.002 (6)
C13	0.076 (6)	0.080 (6)	0.074 (6)	-0.007 (5)	0.003 (5)	-0.002 (5)
C14	0.133 (9)	0.078 (6)	0.050 (5)	0.044 (6)	-0.021 (5)	-0.011 (5)

supplementary materials

C15	0.083 (6)	0.062 (5)	0.047 (4)	0.009 (4)	-0.001 (4)	0.000 (4)
C16	0.109 (7)	0.069 (5)	0.032 (4)	0.008 (5)	-0.004 (4)	-0.003 (4)
C17	0.080 (6)	0.066 (5)	0.036 (4)	0.000 (4)	0.009 (4)	0.003 (3)
C18	0.073 (5)	0.051 (4)	0.039 (4)	-0.010 (3)	0.015 (4)	-0.006 (3)
C19	0.064 (5)	0.041 (3)	0.036 (3)	-0.004 (3)	0.001 (3)	-0.001 (3)
C20	0.073 (5)	0.046 (3)	0.039 (4)	-0.002 (3)	0.011 (3)	0.001 (3)
C21	0.076 (5)	0.051 (4)	0.048 (4)	0.004 (4)	0.014 (4)	-0.011 (3)
C22	0.077 (6)	0.056 (4)	0.049 (4)	0.000 (4)	0.017 (4)	-0.010 (4)
C23	0.091 (6)	0.051 (4)	0.058 (5)	-0.002 (4)	0.018 (4)	-0.012 (4)
C24	0.087 (6)	0.069 (5)	0.056 (5)	0.002 (5)	0.029 (5)	-0.012 (4)
C25	0.094 (7)	0.065 (5)	0.074 (6)	0.010 (5)	0.030 (5)	-0.015 (5)
C26	0.158 (12)	0.124 (9)	0.073 (7)	0.084 (8)	0.043 (7)	0.016 (6)
C27	0.160 (12)	0.112 (8)	0.066 (6)	0.057 (8)	0.042 (7)	0.001 (6)
C28	0.067 (5)	0.049 (4)	0.041 (4)	0.001 (3)	0.014 (3)	-0.005 (3)
C29	0.075 (5)	0.048 (4)	0.038 (4)	0.006 (3)	0.010 (3)	0.001 (3)
C30	0.065 (5)	0.045 (3)	0.033 (3)	-0.005 (3)	0.008 (3)	-0.003 (3)
C31	0.098 (7)	0.081 (6)	0.048 (5)	0.035 (5)	0.020 (4)	0.010 (4)
C32	0.117 (8)	0.102 (7)	0.045 (5)	0.047 (6)	0.013 (5)	0.018 (5)
C33	0.099 (7)	0.076 (5)	0.043 (4)	0.033 (5)	0.013 (4)	0.004 (4)
C34	0.062 (5)	0.053 (4)	0.058 (5)	-0.012 (3)	0.011 (4)	-0.011 (4)
C35	0.083 (6)	0.059 (4)	0.046 (4)	-0.005 (4)	0.020 (4)	0.002 (4)
C36	0.068 (5)	0.058 (4)	0.036 (4)	-0.002 (4)	0.004 (3)	-0.003 (3)
C37	0.049 (4)	0.044 (3)	0.038 (3)	0.004 (3)	0.003 (3)	0.003 (3)
C38	0.057 (4)	0.038 (3)	0.038 (3)	0.002 (3)	0.006 (3)	-0.004 (3)
C39	0.060 (4)	0.046 (3)	0.040 (4)	-0.003 (3)	0.005 (3)	-0.004 (3)
C40	0.059 (5)	0.051 (4)	0.048 (4)	-0.005 (3)	0.000 (3)	-0.004 (3)
C41	0.060 (5)	0.069 (5)	0.048 (4)	-0.011 (4)	0.002 (4)	-0.012 (4)
C42	0.128 (10)	0.151 (11)	0.077 (7)	-0.090 (8)	0.038 (7)	-0.027 (7)
C43	0.151 (12)	0.174 (12)	0.084 (8)	-0.102 (10)	0.049 (8)	-0.067 (8)
C44	0.076 (6)	0.101 (7)	0.070 (6)	-0.040 (5)	0.008 (5)	-0.024 (5)
C45	0.072 (6)	0.090 (6)	0.056 (5)	-0.027 (5)	0.005 (4)	-0.012 (5)
C46	0.083 (6)	0.079 (5)	0.052 (5)	-0.019 (5)	0.007 (4)	-0.007 (4)
C47	0.048 (4)	0.046 (3)	0.053 (4)	0.004 (3)	0.002 (3)	0.001 (3)
C48	0.061 (5)	0.046 (4)	0.043 (4)	0.000 (3)	0.011 (3)	0.001 (3)
C49	0.054 (4)	0.043 (3)	0.046 (4)	0.002 (3)	0.009 (3)	0.001 (3)
C50	0.073 (6)	0.064 (5)	0.059 (5)	-0.018 (4)	0.005 (4)	-0.002 (4)
C51	0.096 (7)	0.078 (6)	0.051 (5)	-0.023 (5)	0.021 (5)	0.000 (4)
C52	0.090 (6)	0.070 (5)	0.046 (4)	-0.017 (5)	0.014 (4)	-0.003 (4)

Geometric parameters (Å, °)

Pb1—O1	2.582 (5)	C13—H13	0.9300
Pb1—O2	2.824 (5)	C15—C16	1.384 (12)
Pb1—O5 ⁱ	2.818 (6)	C15—H15	0.9300
Pb1—N1	2.672 (6)	C16—C17	1.327 (11)
Pb1—N2	2.570 (6)	C16—H16	0.9300
Pb1—N5	2.612 (6)	C17—C18	1.398 (10)
Pb1—N6	2.506 (6)	C17—H17	0.9300
O1—C1	1.255 (9)	C18—C19	1.388 (9)

O2—C1	1.257 (9)	C18—C20	1.446 (10)
O3—C8	1.371 (10)	C19—C30	1.464 (9)
O3—C5	1.397 (9)	C20—C28	1.376 (9)
O4—C14	1.243 (10)	C21—C22	1.466 (11)
O5—C14	1.184 (10)	C22—C27	1.357 (12)
O6—C25	1.398 (10)	C22—C23	1.360 (10)
O6—H6O	0.8200	C23—C24	1.402 (11)
O7—C44	1.385 (10)	C23—H23	0.9300
O7—H7O	0.8201	C24—C25	1.339 (12)
O1W—H1W1	0.8199	C24—H24	0.9300
O1W—H1W2	0.8200	C25—C26	1.344 (12)
O2W—H2W1	0.8199	C26—C27	1.383 (13)
O2W—H2W2	0.8201	C26—H26	0.9300
N1—C15	1.335 (10)	C27—H27	0.9300
N1—C19	1.339 (9)	C28—C29	1.434 (9)
N2—C33	1.327 (9)	C29—C31	1.393 (10)
N2—C30	1.364 (9)	C29—C30	1.413 (10)
N3—C21	1.343 (10)	C31—C32	1.344 (11)
N3—C20	1.387 (9)	C31—H31	0.9300
N3—H3N	0.8600	C32—C33	1.377 (11)
N4—C21	1.335 (9)	C32—H32	0.9300
N4—C28	1.367 (9)	C33—H33	0.9300
N5—C34	1.325 (10)	C34—C35	1.381 (11)
N5—C38	1.353 (8)	C34—H34	0.9300
N6—C52	1.330 (9)	C35—C36	1.356 (10)
N6—C49	1.352 (8)	C35—H35	0.9300
N7—C40	1.364 (9)	C36—C37	1.417 (9)
N7—C39	1.371 (8)	C36—H36	0.9300
N7—H7N	0.8600	C37—C39	1.410 (9)
N8—C40	1.318 (9)	C37—C38	1.417 (9)
N8—C47	1.382 (9)	C38—C49	1.454 (9)
C1—C2	1.524 (11)	C39—C47	1.371 (10)
C2—C3	1.376 (11)	C40—C41	1.466 (10)
C2—C7	1.427 (11)	C41—C42	1.355 (12)
C3—C4	1.423 (11)	C41—C46	1.368 (11)
C3—H3	0.9300	C42—C43	1.390 (13)
C4—C5	1.364 (12)	C42—H42	0.9300
C4—H4	0.9300	C43—C44	1.363 (13)
C5—C6	1.383 (12)	C43—H43	0.9300
C6—C7	1.357 (11)	C44—C45	1.330 (12)
C6—H6	0.9300	C45—C46	1.405 (11)
C7—H7	0.9300	C45—H45	0.9300
C8—C13	1.369 (13)	C46—H46	0.9300
C8—C9	1.378 (13)	C47—C48	1.440 (9)
C9—C10	1.399 (13)	C48—C50	1.390 (11)
C9—H9	0.9300	C48—C49	1.404 (10)
C10—C11	1.407 (12)	C50—C51	1.363 (11)
C10—H10	0.9300	C50—H50	0.9300
C11—C12	1.415 (13)	C51—C52	1.403 (12)

supplementary materials

C11—C14	1.539 (12)	C51—H51	0.9300
C12—C13	1.364 (13)	C52—H52	0.9300
C12—H12	0.9300		
N6—Pb1—N2	74.7 (2)	N1—C19—C18	121.8 (6)
N6—Pb1—O1	75.8 (2)	N1—C19—C30	117.6 (6)
N2—Pb1—O1	128.6 (2)	C18—C19—C30	120.6 (7)
N6—Pb1—N5	63.86 (18)	C28—C20—N3	105.2 (6)
N2—Pb1—N5	83.28 (19)	C28—C20—C18	123.3 (6)
O1—Pb1—N5	118.63 (18)	N3—C20—C18	131.4 (6)
N6—Pb1—N1	82.70 (18)	N4—C21—N3	111.7 (6)
N2—Pb1—N1	62.47 (18)	N4—C21—C22	124.4 (7)
O1—Pb1—N1	72.93 (18)	N3—C21—C22	123.9 (7)
N5—Pb1—N1	137.72 (19)	C27—C22—C23	117.0 (8)
N6—Pb1—O5 ⁱ	127.2 (2)	C27—C22—C21	121.6 (8)
N2—Pb1—O5 ⁱ	75.4 (2)	C23—C22—C21	121.4 (8)
O1—Pb1—O5 ⁱ	153.4 (3)	C22—C23—C24	120.4 (8)
N5—Pb1—O5 ⁱ	70.28 (19)	C22—C23—H23	119.8
N1—Pb1—O5 ⁱ	118.9 (2)	C24—C23—H23	119.8
N6—Pb1—O2	76.57 (18)	C25—C24—C23	119.7 (8)
N2—Pb1—O2	150.48 (19)	C25—C24—H24	120.1
O1—Pb1—O2	47.62 (16)	C23—C24—H24	120.1
N5—Pb1—O2	78.26 (17)	C24—C25—C26	121.6 (9)
N1—Pb1—O2	120.01 (17)	C24—C25—O6	119.8 (8)
O5 ⁱ —Pb1—O2	118.49 (19)	C26—C25—O6	118.6 (9)
C1—O1—Pb1	99.6 (5)	C25—C26—C27	117.5 (10)
C1—O2—Pb1	88.1 (4)	C25—C26—H26	121.2
C8—O3—C5	115.1 (7)	C27—C26—H26	121.2
C25—O6—H6O	120.7	C22—C27—C26	123.6 (9)
C44—O7—H7O	120.1	C22—C27—H27	118.2
H1W1—O1W—H1W2	109.8	C26—C27—H27	118.2
H2W1—O2W—H2W2	108.8	N4—C28—C20	110.4 (6)
C15—N1—C19	118.1 (6)	N4—C28—C29	128.5 (7)
C15—N1—Pb1	122.1 (5)	C20—C28—C29	121.0 (7)
C19—N1—Pb1	119.7 (4)	C31—C29—C30	118.4 (7)
C33—N2—C30	118.1 (6)	C31—C29—C28	124.7 (7)
C33—N2—Pb1	119.4 (5)	C30—C29—C28	116.8 (6)
C30—N2—Pb1	122.3 (5)	N2—C30—C29	120.7 (6)
C21—N3—C20	107.3 (6)	N2—C30—C19	117.8 (6)
C21—N3—H3N	126.3	C29—C30—C19	121.5 (6)
C20—N3—H3N	126.3	C32—C31—C29	119.7 (8)
C21—N4—C28	105.4 (6)	C32—C31—H31	120.1
C34—N5—C38	118.5 (6)	C29—C31—H31	120.1
C34—N5—Pb1	123.0 (5)	C31—C32—C33	119.4 (8)
C38—N5—Pb1	118.3 (4)	C31—C32—H32	120.3
C52—N6—C49	118.1 (7)	C33—C32—H32	120.3
C52—N6—Pb1	119.4 (5)	N2—C33—C32	123.6 (8)
C49—N6—Pb1	122.5 (5)	N2—C33—H33	118.2

C40—N7—C39	107.1 (6)	C32—C33—H33	118.2
C40—N7—H7N	126.5	N5—C34—C35	123.4 (7)
C39—N7—H7N	126.5	N5—C34—H34	118.3
C40—N8—C47	104.0 (6)	C35—C34—H34	118.3
O2—C1—O1	121.6 (7)	C36—C35—C34	120.2 (7)
O2—C1—C2	121.0 (7)	C36—C35—H35	119.9
O1—C1—C2	117.3 (7)	C34—C35—H35	119.9
C3—C2—C7	119.9 (8)	C35—C36—C37	118.4 (6)
C3—C2—C1	120.5 (8)	C35—C36—H36	120.8
C7—C2—C1	119.5 (8)	C37—C36—H36	120.8
C2—C3—C4	119.3 (8)	C39—C37—C38	116.3 (6)
C2—C3—H3	120.3	C39—C37—C36	125.5 (6)
C4—C3—H3	120.3	C38—C37—C36	118.2 (6)
C5—C4—C3	119.5 (8)	N5—C38—C37	121.4 (6)
C5—C4—H4	120.2	N5—C38—C49	117.9 (6)
C3—C4—H4	120.2	C37—C38—C49	120.8 (6)
C4—C5—C6	120.9 (8)	N7—C39—C47	105.1 (6)
C4—C5—O3	120.1 (8)	N7—C39—C37	130.6 (6)
C6—C5—O3	119.0 (9)	C47—C39—C37	124.3 (6)
C7—C6—C5	121.1 (9)	N8—C40—N7	112.5 (6)
C7—C6—H6	119.4	N8—C40—C41	125.7 (7)
C5—C6—H6	119.4	N7—C40—C41	121.7 (7)
C6—C7—C2	119.2 (9)	C42—C41—C46	117.0 (8)
C6—C7—H7	120.4	C42—C41—C40	121.2 (8)
C2—C7—H7	120.4	C46—C41—C40	121.8 (7)
O3—C8—C13	119.9 (10)	C41—C42—C43	122.4 (9)
O3—C8—C9	119.8 (9)	C41—C42—H42	118.8
C13—C8—C9	120.2 (9)	C43—C42—H42	118.8
C8—C9—C10	119.6 (10)	C44—C43—C42	118.6 (10)
C8—C9—H9	120.2	C44—C43—H43	120.7
C10—C9—H9	120.2	C42—C43—H43	120.7
C9—C10—C11	120.4 (10)	C45—C44—C43	121.1 (9)
C9—C10—H10	119.8	C45—C44—O7	122.6 (8)
C11—C10—H10	119.8	C43—C44—O7	116.3 (9)
C10—C11—C12	117.9 (9)	C44—C45—C46	119.2 (8)
C10—C11—C14	119.6 (9)	C44—C45—H45	120.4
C12—C11—C14	122.5 (8)	C46—C45—H45	120.4
C13—C12—C11	120.2 (9)	C41—C46—C45	121.6 (8)
C13—C12—H12	119.9	C41—C46—H46	119.2
C11—C12—H12	119.9	C45—C46—H46	119.2
C8—C13—C12	121.6 (9)	C39—C47—N8	111.3 (6)
C8—C13—H13	119.2	C39—C47—C48	120.2 (6)
C12—C13—H13	119.2	N8—C47—C48	128.4 (7)
O5—C14—O4	123.5 (9)	C50—C48—C49	118.3 (7)
O5—C14—C11	118.2 (9)	C50—C48—C47	123.8 (7)
O4—C14—C11	116.7 (8)	C49—C48—C47	117.8 (6)
N1—C15—C16	122.5 (8)	N6—C49—C48	122.1 (6)
N1—C15—H15	118.7	N6—C49—C38	117.4 (6)
C16—C15—H15	118.7	C48—C49—C38	120.5 (6)

supplementary materials

C17—C16—C15	119.6 (8)	C51—C50—C48	119.7 (8)
C17—C16—H16	120.2	C51—C50—H50	120.2
C15—C16—H16	120.2	C48—C50—H50	120.2
C16—C17—C18	119.5 (7)	C50—C51—C52	118.8 (8)
C16—C17—H17	120.2	C50—C51—H51	120.6
C18—C17—H17	120.2	C52—C51—H51	120.6
C19—C18—C17	118.3 (7)	N6—C52—C51	123.0 (7)
C19—C18—C20	116.7 (6)	N6—C52—H52	118.5
C17—C18—C20	125.0 (7)	C51—C52—H52	118.5
N6—Pb1—O1—C1	-75.1 (6)	C19—C18—C20—N3	-177.2 (7)
N2—Pb1—O1—C1	-131.5 (6)	C17—C18—C20—N3	2.1 (13)
N5—Pb1—O1—C1	-26.1 (6)	C28—N4—C21—N3	-0.9 (9)
N1—Pb1—O1—C1	-161.7 (6)	C28—N4—C21—C22	178.3 (7)
O5 ⁱ —Pb1—O1—C1	77.3 (7)	C20—N3—C21—N4	0.3 (9)
O2—Pb1—O1—C1	9.6 (5)	C20—N3—C21—C22	-178.8 (7)
N6—Pb1—O2—C1	73.4 (5)	N4—C21—C22—C27	5.3 (14)
N2—Pb1—O2—C1	86.6 (6)	N3—C21—C22—C27	-175.7 (9)
O1—Pb1—O2—C1	-9.4 (5)	N4—C21—C22—C23	-170.4 (8)
N5—Pb1—O2—C1	139.0 (5)	N3—C21—C22—C23	8.6 (13)
N1—Pb1—O2—C1	0.2 (6)	C27—C22—C23—C24	4.4 (13)
O5 ⁱ —Pb1—O2—C1	-161.3 (5)	C21—C22—C23—C24	-179.8 (8)
N6—Pb1—N1—C15	-102.2 (6)	C22—C23—C24—C25	-3.5 (13)
N2—Pb1—N1—C15	-178.7 (6)	C23—C24—C25—C26	1.0 (16)
O1—Pb1—N1—C15	-24.9 (6)	C23—C24—C25—O6	-177.7 (8)
N5—Pb1—N1—C15	-139.0 (6)	C24—C25—C26—C27	0.5 (19)
O5 ⁱ —Pb1—N1—C15	129.1 (6)	O6—C25—C26—C27	179.1 (11)
O2—Pb1—N1—C15	-32.3 (6)	C23—C22—C27—C26	-3.0 (18)
N6—Pb1—N1—C19	80.2 (5)	C21—C22—C27—C26	-178.8 (11)
N2—Pb1—N1—C19	3.8 (5)	C25—C26—C27—C22	1(2)
O1—Pb1—N1—C19	157.5 (6)	C21—N4—C28—C20	1.1 (9)
N5—Pb1—N1—C19	43.4 (6)	C21—N4—C28—C29	-175.5 (8)
O5 ⁱ —Pb1—N1—C19	-48.5 (6)	N3—C20—C28—N4	-0.9 (8)
O2—Pb1—N1—C19	150.1 (5)	C18—C20—C28—N4	-178.6 (6)
N6—Pb1—N2—C33	90.8 (7)	N3—C20—C28—C29	176.0 (7)
O1—Pb1—N2—C33	147.7 (6)	C18—C20—C28—C29	-1.7 (11)
N5—Pb1—N2—C33	26.1 (6)	N4—C28—C29—C31	-4.0 (13)
N1—Pb1—N2—C33	-179.5 (7)	C20—C28—C29—C31	179.7 (8)
O5 ⁱ —Pb1—N2—C33	-45.2 (6)	N4—C28—C29—C30	178.4 (7)
O2—Pb1—N2—C33	77.5 (7)	C20—C28—C29—C30	2.2 (11)
N6—Pb1—N2—C30	-93.5 (6)	C33—N2—C30—C29	-0.8 (11)
O1—Pb1—N2—C30	-36.6 (6)	Pb1—N2—C30—C29	-176.5 (5)
N5—Pb1—N2—C30	-158.2 (6)	C33—N2—C30—C19	179.5 (7)
N1—Pb1—N2—C30	-3.8 (5)	Pb1—N2—C30—C19	3.8 (9)
O5 ⁱ —Pb1—N2—C30	130.5 (6)	C31—C29—C30—N2	1.7 (11)
O2—Pb1—N2—C30	-106.8 (6)	C28—C29—C30—N2	179.4 (7)
N6—Pb1—N5—C34	178.3 (6)	C31—C29—C30—C19	-178.6 (7)
N2—Pb1—N5—C34	-105.6 (6)	C28—C29—C30—C19	-0.9 (10)

O1—Pb1—N5—C34	123.7 (6)	N1—C19—C30—N2	0.0 (10)
N1—Pb1—N5—C34	-140.3 (5)	C18—C19—C30—N2	178.7 (7)
O5 ⁱ —Pb1—N5—C34	-28.7 (6)	N1—C19—C30—C29	-179.7 (7)
O2—Pb1—N5—C34	97.6 (6)	C18—C19—C30—C29	-1.0 (10)
N6—Pb1—N5—C38	3.3 (4)	C30—C29—C31—C32	-2.8 (14)
N2—Pb1—N5—C38	79.5 (5)	C28—C29—C31—C32	179.6 (9)
O1—Pb1—N5—C38	-51.2 (5)	C29—C31—C32—C33	3.0 (16)
N1—Pb1—N5—C38	44.7 (6)	C30—N2—C33—C32	1.0 (14)
O5 ⁱ —Pb1—N5—C38	156.4 (5)	Pb1—N2—C33—C32	176.8 (8)
O2—Pb1—N5—C38	-77.3 (5)	C31—C32—C33—N2	-2.1 (17)
N2—Pb1—N6—C52	88.8 (6)	C38—N5—C34—C35	-0.2 (11)
O1—Pb1—N6—C52	-48.7 (6)	Pb1—N5—C34—C35	-175.1 (6)
N5—Pb1—N6—C52	178.8 (7)	N5—C34—C35—C36	-0.4 (13)
N1—Pb1—N6—C52	25.4 (6)	C34—C35—C36—C37	0.8 (11)
O5 ⁱ —Pb1—N6—C52	146.4 (6)	C35—C36—C37—C39	178.4 (7)
O2—Pb1—N6—C52	-97.9 (6)	C35—C36—C37—C38	-0.7 (10)
N2—Pb1—N6—C49	-91.9 (5)	C34—N5—C38—C37	0.3 (10)
O1—Pb1—N6—C49	130.5 (6)	Pb1—N5—C38—C37	175.4 (5)
N5—Pb1—N6—C49	-1.9 (5)	C34—N5—C38—C49	-179.7 (6)
N1—Pb1—N6—C49	-155.3 (5)	Pb1—N5—C38—C49	-4.5 (8)
O5 ⁱ —Pb1—N6—C49	-34.3 (6)	C39—C37—C38—N5	-179.1 (6)
O2—Pb1—N6—C49	81.4 (5)	C36—C37—C38—N5	0.2 (10)
Pb1—O2—C1—O1	17.0 (9)	C39—C37—C38—C49	0.9 (9)
Pb1—O2—C1—C2	-159.6 (8)	C36—C37—C38—C49	-179.9 (6)
Pb1—O1—C1—O2	-18.9 (10)	C40—N7—C39—C47	0.9 (8)
Pb1—O1—C1—C2	157.8 (6)	C40—N7—C39—C37	-177.5 (7)
O2—C1—C2—C3	-18.4 (13)	C38—C37—C39—N7	175.5 (7)
O1—C1—C2—C3	164.8 (8)	C36—C37—C39—N7	-3.7 (12)
O2—C1—C2—C7	158.8 (8)	C38—C37—C39—C47	-2.6 (10)
O1—C1—C2—C7	-18.0 (12)	C36—C37—C39—C47	178.2 (7)
C7—C2—C3—C4	0.5 (13)	C47—N8—C40—N7	0.8 (8)
C1—C2—C3—C4	177.7 (7)	C47—N8—C40—C41	-175.6 (7)
C2—C3—C4—C5	0.7 (13)	C39—N7—C40—N8	-1.1 (9)
C3—C4—C5—C6	-0.4 (14)	C39—N7—C40—C41	175.5 (7)
C3—C4—C5—O3	177.3 (8)	N8—C40—C41—C42	164.3 (10)
C8—O3—C5—C4	52.7 (13)	N7—C40—C41—C42	-11.8 (13)
C8—O3—C5—C6	-129.6 (10)	N8—C40—C41—C46	-15.6 (13)
C4—C5—C6—C7	-1.1 (16)	N7—C40—C41—C46	168.3 (8)
O3—C5—C6—C7	-178.8 (9)	C46—C41—C42—C43	3.0 (19)
C5—C6—C7—C2	2.3 (15)	C40—C41—C42—C43	-177.0 (12)
C3—C2—C7—C6	-2.0 (14)	C41—C42—C43—C44	-4(2)
C1—C2—C7—C6	-179.2 (9)	C42—C43—C44—C45	3(2)
C5—O3—C8—C13	-126.1 (10)	C42—C43—C44—O7	-178.0 (12)
C5—O3—C8—C9	58.3 (13)	C43—C44—C45—C46	0.4 (18)
O3—C8—C9—C10	-179.7 (10)	O7—C44—C45—C46	-178.9 (10)
C13—C8—C9—C10	4.6 (16)	C42—C41—C46—C45	0.2 (15)
C8—C9—C10—C11	-2.4 (17)	C40—C41—C46—C45	-179.9 (8)
C9—C10—C11—C12	-1.1 (16)	C44—C45—C46—C41	-1.9 (15)

supplementary materials

C9—C10—C11—C14	178.9 (10)	N7—C39—C47—N8	-0.4 (8)
C10—C11—C12—C13	2.5 (14)	C37—C39—C47—N8	178.1 (6)
C14—C11—C12—C13	-177.5 (10)	N7—C39—C47—C48	-177.4 (6)
O3—C8—C13—C12	-178.9 (9)	C37—C39—C47—C48	1.0 (11)
C9—C8—C13—C12	-3.3 (16)	C40—N8—C47—C39	-0.2 (8)
C11—C12—C13—C8	-0.4 (15)	C40—N8—C47—C48	176.5 (7)
C10—C11—C14—O5	179.6 (11)	C39—C47—C48—C50	178.5 (7)
C12—C11—C14—O5	-0.4 (16)	N8—C47—C48—C50	2.0 (12)
C10—C11—C14—O4	-13.9 (15)	C39—C47—C48—C49	2.3 (10)
C12—C11—C14—O4	166.1 (10)	N8—C47—C48—C49	-174.1 (7)
C19—N1—C15—C16	-1.5 (12)	C52—N6—C49—C48	0.2 (11)
Pb1—N1—C15—C16	-179.1 (7)	Pb1—N6—C49—C48	-179.1 (5)
N1—C15—C16—C17	1.9 (14)	C52—N6—C49—C38	179.8 (7)
C15—C16—C17—C18	-1.0 (13)	Pb1—N6—C49—C38	0.5 (8)
C16—C17—C18—C19	-0.4 (12)	C50—C48—C49—N6	-0.7 (11)
C16—C17—C18—C20	-179.6 (8)	C47—C48—C49—N6	175.6 (6)
C15—N1—C19—C18	0.1 (11)	C50—C48—C49—C38	179.7 (7)
Pb1—N1—C19—C18	177.8 (5)	C47—C48—C49—C38	-4.0 (10)
C15—N1—C19—C30	178.8 (7)	N5—C38—C49—N6	2.7 (9)
Pb1—N1—C19—C30	-3.5 (8)	C37—C38—C49—N6	-177.2 (6)
C17—C18—C19—N1	0.8 (11)	N5—C38—C49—C48	-177.6 (6)
C20—C18—C19—N1	-179.8 (6)	C37—C38—C49—C48	2.4 (10)
C17—C18—C19—C30	-177.9 (7)	C49—C48—C50—C51	0.5 (12)
C20—C18—C19—C30	1.5 (10)	C47—C48—C50—C51	-175.6 (8)
C21—N3—C20—C28	0.3 (8)	C48—C50—C51—C52	0.1 (14)
C21—N3—C20—C18	177.8 (8)	C49—N6—C52—C51	0.5 (13)
C19—C18—C20—C28	-0.2 (11)	Pb1—N6—C52—C51	179.8 (7)
C17—C18—C20—C28	179.1 (7)	C50—C51—C52—N6	-0.7 (14)

Symmetry codes: (i) $-x+1/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3N \cdots O2 ⁱⁱ	0.86	1.98	2.82 (1)	166
N7—H7N \cdots O4 ⁱⁱⁱ	0.86	1.97	2.81 (1)	166
O1W—H1W1 \cdots N4	0.82	2.00	2.82 (1)	174
O1W—H1W2 \cdots O6 ^{iv}	0.82	2.37	2.57 (1)	95
O2W—H2W1 \cdots N8	0.82	2.00	2.79 (1)	160
O2W—H2W2 \cdots O3 ^v	0.82	2.27	3.06 (1)	160

Symmetry codes: (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y, -z+1$; (v) $-x+1, -y+1, -z+1$.

Fig. 1

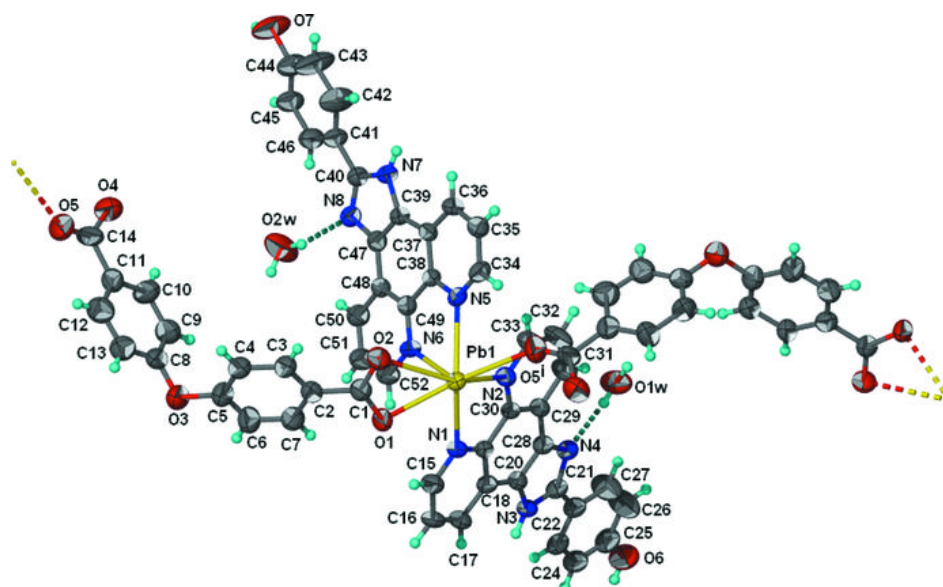


Fig. 2

