

μ -Adipato- $\kappa^2O^1:O^4$ -bis[[2,6-bis(1H-benzimidazol-2-yl- κN^3)pyridine- κN]- (nitrate- κO)lead(II)]

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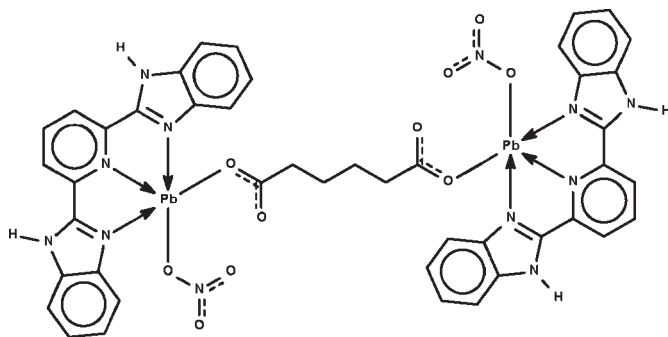
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.012$ Å; R factor = 0.041; wR factor = 0.099; data-to-parameter ratio = 14.9.

The dinuclear title compound, $[Pb_2(C_6H_8O_4)(NO_3)_2(C_{19}H_{13}N_5)_2]$, lies with the mid-point of the butyl chain of the bridging adipate unit on a center of inversion. The Pb^{II} ion is covalently bonded to the nitrate anion and is bonded to a carboxylate group of the adipate unit by another covalent bond. The N -heterocycle functions in a chelating tridentate mode. The metal atom exists in a Ψ -octahedral coordination environment. When weaker $Pb \cdots O$ interactions are also considered, the geometry is a Ψ -tricapped trigonal prism in which the lone-pair electrons occupy one face of the trigonal prism. Adjacent molecules are linked into a layer structure by $N-H \cdots O$ hydrogen bonds.

Related literature

For the structure of a related Pb^{II} complex and its lone-pair stereochemistry, see: Meng *et al.* (2009).



Experimental

Crystal data

$[Pb_2(C_6H_8O_4)(NO_3)_2(C_{19}H_{13}N_5)_2]$
 $M_r = 1305.21$
 Triclinic, $P\bar{1}$
 $a = 9.3470$ (7) Å
 $b = 10.6433$ (8) Å
 $c = 11.3776$ (8) Å
 $\alpha = 106.696$ (1)°
 $\beta = 95.343$ (1)°
 $\gamma = 99.117$ (1)°
 $V = 1058.9$ (1) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 8.02$ mm⁻¹
 $T = 293$ K
 $0.26 \times 0.12 \times 0.08$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.230$, $T_{max} = 0.566$
 8299 measured reflections
 4561 independent reflections
 3586 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.099$
 $S = 1.02$
 4561 reflections
 307 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.93$ e Å⁻³
 $\Delta\rho_{min} = -1.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2 \cdots O1^i$	0.86	1.95	2.744 (8)	152
$N5-H5 \cdots O3^{ii}$	0.86	2.10	2.891 (9)	153

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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: *pubCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5131).

References

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 Meng, F.-Y., Zhou, Y.-L., Zou, H.-H., Zeng, M.-H. & Liang, H. (2009). *J. Mol. Struct.* **920**, 238–241.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supplementary materials

Acta Cryst. (2010). E66, m56 [doi:10.1107/S1600536809052647]

μ -Adipato- $\kappa^2O^1:O^4$ -bis{[2,6-bis(1*H*-benzimidazol-2-yl- κN^3)pyridine- κN](nitrato- κO)lead(II)}

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Experimental

Lead nitrate (0.250 mmol), 2-(6-(1*H*-benzo[*d*]imidazol-2-yl)pyridin-2-yl)-1*H*-benzo[*d*]imidazole (0.250 mmol), adipic acid (0.125 mmol) and water (10 ml) were sealed in a 25 ml Teflon-lined, stainless-steel Parr bomb. The bomb was heated at 413 K for 4 days and cooled to room temperature. Brown block-shaped crystals were collected and washed in water; the yield was 25%.

Refinement

Hydrogen atoms were generated geometrically and were constrained to ride on their parent atoms [C–H = 0.93, N–H 0.86 Å; $U_{iso}(H) = 1.2U_{eq}(C,N)$].

The final difference Fourier map had a peak near C14 and a hole near H2a.

Figures

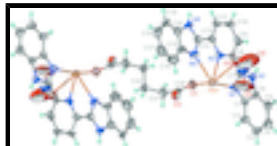


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $Pb_2(NO_3)_2(C_6H_8O_4)(C_{19}H_{13}N_5)_2$ at the 70% probability level; hydrogen atoms are drawn as sphere of arbitrary radius.

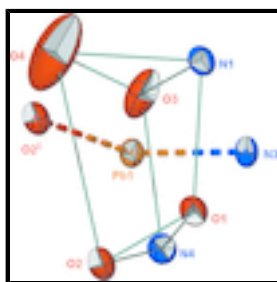


Fig. 2. Detail of the coordination environment of the Pb^{II} centre.

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Crystal data

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 $M_r = 1305.21$
 Triclinic, $P\bar{1}$
 Hall symbol: -P 1
 $a = 9.3470(7)$ Å

$Z = 1$
 $F(000) = 626$
 $D_x = 2.047$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 3150 reflections

supplementary materials

$b = 10.6433 (8) \text{ \AA}$
 $c = 11.3776 (8) \text{ \AA}$
 $\alpha = 106.696 (1)^\circ$
 $\beta = 95.343 (1)^\circ$
 $\gamma = 99.117 (1)^\circ$
 $V = 1058.9 (1) \text{ \AA}^3$

$\theta = 2.2\text{--}24.8^\circ$
 $\mu = 8.02 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
Block, brown
 $0.26 \times 0.12 \times 0.08 \text{ mm}$

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube graphite
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Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.230$, $T_{\max} = 0.566$
8299 measured reflections

4561 independent reflections
3586 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 $\theta_{\max} = 27.1^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -11 \rightarrow 11$
 $k = -13 \rightarrow 13$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.099$
 $S = 1.02$
4561 reflections
307 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
 $w = 1/[\sigma^2(F_o^2) + (0.0524P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.93 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.17 \text{ e \AA}^{-3}$

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	1.07669 (3)	0.71714 (3)	0.65491 (3)	0.02682 (11)
O1	0.8637 (6)	0.6980 (5)	0.5092 (5)	0.0341 (13)
O2	0.8304 (6)	0.4985 (5)	0.5330 (5)	0.0381 (13)
O3	1.2560 (7)	0.8902 (7)	0.8623 (6)	0.0579 (18)
O4	1.3952 (11)	0.7543 (10)	0.8022 (10)	0.126 (5)
O5	1.4055 (12)	0.8554 (14)	0.9916 (9)	0.141 (5)
N1	1.1854 (7)	0.8782 (6)	0.5449 (5)	0.0286 (14)
N2	1.2263 (6)	1.0797 (6)	0.5237 (5)	0.0274 (14)
H2	1.2215	1.1621	0.5343	0.033*
N3	1.0091 (7)	0.9473 (6)	0.7236 (5)	0.0251 (13)
N4	0.8962 (7)	0.7470 (6)	0.8149 (6)	0.0329 (15)
N5	0.7760 (7)	0.8747 (6)	0.9451 (6)	0.0352 (16)

H5	0.7435	0.9440	0.9839	0.042*
N6	1.3504 (9)	0.8307 (8)	0.8859 (7)	0.052 (2)
C1	1.2754 (8)	0.8763 (7)	0.4564 (7)	0.0262 (16)
C2	1.3328 (9)	0.7741 (8)	0.3826 (7)	0.0324 (18)
H2A	1.3132	0.6882	0.3893	0.039*
C3	1.4197 (9)	0.8036 (8)	0.2989 (7)	0.0349 (19)
H3	1.4600	0.7366	0.2490	0.042*
C4	1.4490 (9)	0.9331 (9)	0.2873 (7)	0.0369 (19)
H4	1.5085	0.9499	0.2303	0.044*
C5	1.3918 (8)	1.0343 (8)	0.3581 (7)	0.0350 (19)
H5A	1.4106	1.1200	0.3508	0.042*
C6	1.3046 (8)	1.0032 (7)	0.4412 (7)	0.0278 (16)
C7	1.1608 (8)	1.0009 (7)	0.5828 (6)	0.0258 (16)
C8	1.0701 (7)	1.0443 (7)	0.6764 (6)	0.0208 (14)
C9	1.0481 (8)	1.1737 (7)	0.7213 (8)	0.0344 (18)
H9	1.0887	1.2392	0.6882	0.041*
C10	0.9640 (9)	1.2052 (8)	0.8172 (7)	0.038 (2)
H10	0.9509	1.2926	0.8495	0.045*
C11	0.9004 (9)	1.1077 (8)	0.8642 (7)	0.0340 (18)
H11	0.8428	1.1276	0.9269	0.041*
C12	0.9248 (8)	0.9783 (7)	0.8148 (7)	0.0263 (16)
C13	0.8642 (8)	0.8677 (8)	0.8563 (7)	0.0299 (17)
C14	0.7477 (9)	0.7502 (8)	0.9616 (8)	0.0345 (18)
C15	0.6696 (9)	0.7026 (9)	1.0431 (8)	0.041 (2)
H15	0.6169	0.7550	1.0960	0.049*
C16	0.6744 (9)	0.5751 (10)	1.0410 (8)	0.046 (2)
H16	0.6258	0.5401	1.0958	0.056*
C17	0.7503 (11)	0.4942 (10)	0.9588 (9)	0.056 (3)
H17	0.7483	0.4066	0.9590	0.067*
C18	0.8266 (11)	0.5409 (9)	0.8793 (9)	0.050 (2)
H18	0.8782	0.4876	0.8261	0.060*
C19	0.8245 (9)	0.6720 (8)	0.8805 (7)	0.0333 (18)
C20	0.7885 (8)	0.5807 (7)	0.4878 (7)	0.0264 (16)
C21	0.6450 (8)	0.5467 (8)	0.4015 (8)	0.039 (2)
H21A	0.6606	0.4989	0.3187	0.047*
H21B	0.6159	0.6292	0.3982	0.047*
C22	0.5208 (9)	0.4628 (8)	0.4384 (7)	0.038 (2)
H22A	0.5500	0.3811	0.4443	0.045*
H22B	0.4361	0.4383	0.3746	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.02973 (17)	0.02289 (16)	0.03042 (16)	0.00981 (11)	0.00830 (11)	0.00846 (11)
O1	0.030 (3)	0.025 (3)	0.046 (3)	0.003 (2)	0.003 (3)	0.013 (2)
O2	0.041 (3)	0.027 (3)	0.051 (4)	0.009 (3)	0.010 (3)	0.016 (3)
O3	0.053 (4)	0.060 (4)	0.052 (4)	0.031 (4)	-0.009 (3)	-0.001 (3)
O4	0.127 (9)	0.126 (9)	0.097 (7)	0.085 (7)	-0.009 (6)	-0.034 (6)

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O5	0.122 (9)	0.244 (14)	0.055 (6)	0.098 (9)	-0.008 (6)	0.017 (7)
N1	0.035 (4)	0.022 (3)	0.030 (3)	0.007 (3)	0.011 (3)	0.008 (3)
N2	0.030 (3)	0.022 (3)	0.031 (3)	0.006 (3)	0.007 (3)	0.008 (3)
N3	0.031 (3)	0.019 (3)	0.025 (3)	0.009 (3)	0.003 (3)	0.004 (2)
N4	0.038 (4)	0.029 (4)	0.036 (4)	0.011 (3)	0.016 (3)	0.010 (3)
N5	0.033 (4)	0.033 (4)	0.039 (4)	0.010 (3)	0.019 (3)	0.004 (3)
N6	0.057 (5)	0.062 (5)	0.037 (4)	0.029 (4)	0.006 (4)	0.005 (4)
C1	0.022 (4)	0.025 (4)	0.028 (4)	0.002 (3)	-0.002 (3)	0.007 (3)
C2	0.042 (5)	0.027 (4)	0.032 (4)	0.014 (4)	0.011 (4)	0.010 (3)
C3	0.036 (5)	0.042 (5)	0.027 (4)	0.014 (4)	0.010 (3)	0.006 (3)
C4	0.036 (5)	0.050 (5)	0.027 (4)	0.007 (4)	0.007 (4)	0.015 (4)
C5	0.033 (4)	0.033 (4)	0.040 (5)	-0.003 (4)	0.002 (4)	0.019 (4)
C6	0.022 (4)	0.030 (4)	0.028 (4)	0.004 (3)	0.000 (3)	0.005 (3)
C7	0.025 (4)	0.024 (4)	0.024 (4)	0.000 (3)	0.001 (3)	0.004 (3)
C8	0.009 (3)	0.027 (4)	0.020 (3)	0.002 (3)	-0.007 (3)	0.002 (3)
C9	0.032 (4)	0.022 (4)	0.045 (5)	0.000 (3)	-0.005 (4)	0.012 (3)
C10	0.050 (5)	0.023 (4)	0.039 (5)	0.018 (4)	0.011 (4)	-0.001 (3)
C11	0.034 (4)	0.034 (4)	0.031 (4)	0.009 (4)	0.013 (3)	0.001 (3)
C12	0.029 (4)	0.019 (4)	0.030 (4)	0.010 (3)	0.003 (3)	0.003 (3)
C13	0.028 (4)	0.029 (4)	0.029 (4)	0.005 (3)	0.002 (3)	0.005 (3)
C14	0.034 (5)	0.027 (4)	0.042 (5)	0.004 (3)	0.005 (4)	0.011 (4)
C15	0.027 (4)	0.049 (5)	0.048 (5)	0.003 (4)	0.018 (4)	0.015 (4)
C16	0.038 (5)	0.060 (6)	0.047 (5)	-0.003 (4)	0.012 (4)	0.029 (5)
C17	0.068 (7)	0.047 (6)	0.046 (6)	-0.006 (5)	0.008 (5)	0.013 (5)
C18	0.070 (7)	0.032 (5)	0.054 (6)	0.016 (5)	0.027 (5)	0.014 (4)
C19	0.033 (4)	0.032 (4)	0.035 (4)	0.009 (4)	0.012 (4)	0.007 (3)
C20	0.026 (4)	0.019 (4)	0.031 (4)	0.003 (3)	0.012 (3)	0.002 (3)
C21	0.036 (5)	0.036 (5)	0.041 (5)	-0.005 (4)	0.004 (4)	0.012 (4)
C22	0.032 (4)	0.035 (5)	0.036 (5)	0.000 (4)	0.006 (4)	-0.001 (4)

Geometric parameters (Å, °)

Pb1—O1	2.411 (5)	C4—C5	1.364 (11)
Pb1—N1	2.541 (6)	C4—H4	0.9300
Pb1—N3	2.548 (6)	C5—C6	1.380 (11)
Pb1—N4	2.583 (6)	C5—H5A	0.9300
Pb1—O3	2.749 (6)	C7—C8	1.441 (10)
Pb1—O2	2.914 (6)	C8—C9	1.381 (10)
Pb1—O2 ⁱ	2.958 (5)	C9—C10	1.397 (11)
Pb1—O4	3.185 (10)	C9—H9	0.9300
O1—C20	1.275 (9)	C10—C11	1.378 (11)
O2—C20	1.231 (9)	C10—H10	0.9300
O3—N6	1.217 (9)	C11—C12	1.393 (10)
O4—N6	1.216 (11)	C11—H11	0.9300
O5—N6	1.200 (11)	C12—C13	1.445 (11)
N1—C7	1.317 (9)	C14—C15	1.389 (11)
N1—C1	1.369 (9)	C14—C19	1.389 (11)
N2—C7	1.330 (9)	C15—C16	1.359 (12)
N2—C6	1.399 (9)	C15—H15	0.9300

N2—H2	0.8600	C16—C17	1.405 (13)
N3—C12	1.358 (9)	C16—H16	0.9300
N3—C8	1.367 (9)	C17—C18	1.356 (13)
N4—C13	1.327 (9)	C17—H17	0.9300
N4—C19	1.382 (10)	C18—C19	1.394 (12)
N5—C13	1.356 (9)	C18—H18	0.9300
N5—C14	1.379 (10)	C20—C21	1.513 (11)
N5—H5	0.8600	C21—C22	1.516 (11)
C1—C2	1.386 (10)	C21—H21A	0.9700
C1—C6	1.399 (10)	C21—H21B	0.9700
C2—C3	1.378 (11)	C22—C22 ⁱⁱ	1.519 (14)
C2—H2A	0.9300	C22—H22A	0.9700
C3—C4	1.408 (11)	C22—H22B	0.9700
C3—H3	0.9300		
O1—Pb1—N1	81.15 (19)	C3—C4—H4	119.3
O1—Pb1—N3	76.12 (18)	C4—C5—C6	116.6 (7)
N1—Pb1—N3	65.32 (19)	C4—C5—H5A	121.7
O1—Pb1—N4	83.9 (2)	C6—C5—H5A	121.7
N1—Pb1—N4	129.70 (19)	C5—C6—C1	123.5 (7)
N3—Pb1—N4	64.51 (19)	C5—C6—N2	131.7 (7)
O1—Pb1—O3	142.75 (18)	C1—C6—N2	104.8 (6)
N1—Pb1—O3	84.8 (2)	N1—C7—N2	112.8 (6)
N3—Pb1—O3	66.66 (19)	N1—C7—C8	123.6 (7)
N4—Pb1—O3	78.9 (2)	N2—C7—C8	123.6 (7)
O1—Pb1—O2	47.51 (16)	N3—C8—C9	120.6 (6)
N1—Pb1—O2	121.65 (18)	N3—C8—C7	114.8 (6)
N3—Pb1—O2	114.54 (17)	C9—C8—C7	124.5 (7)
N4—Pb1—O2	77.49 (18)	C8—C9—C10	119.2 (7)
O3—Pb1—O2	152.3 (2)	C8—C9—H9	120.4
O1—Pb1—O2 ⁱ	89.14 (17)	C10—C9—H9	120.4
N1—Pb1—O2 ⁱ	87.79 (17)	C11—C10—C9	120.6 (7)
N3—Pb1—O2 ⁱ	150.76 (17)	C11—C10—H10	119.7
N4—Pb1—O2 ⁱ	139.77 (18)	C9—C10—H10	119.7
O3—Pb1—O2 ⁱ	124.72 (17)	C10—C11—C12	118.0 (7)
O2—Pb1—O2 ⁱ	68.94 (18)	C10—C11—H11	121.0
O1—Pb1—O4	167.8 (3)	C12—C11—H11	121.0
N1—Pb1—O4	88.3 (3)	N3—C12—C11	121.9 (7)
N3—Pb1—O4	105.0 (2)	N3—C12—C13	114.9 (6)
N4—Pb1—O4	107.6 (2)	C11—C12—C13	123.2 (7)
O3—Pb1—O4	40.80 (19)	N4—C13—N5	111.9 (7)
O2—Pb1—O4	137.4 (2)	N4—C13—C12	122.8 (7)
O2 ⁱ —Pb1—O4	84.36 (19)	N5—C13—C12	125.2 (7)
C20—O1—Pb1	106.6 (5)	N5—C14—C15	131.9 (8)
C20—O2—Pb1	83.5 (4)	N5—C14—C19	105.6 (7)
N6—O3—Pb1	105.7 (5)	C15—C14—C19	122.4 (8)
N6—O4—Pb1	84.3 (6)	C16—C15—C14	116.2 (8)
C7—N1—C1	106.2 (6)	C16—C15—H15	121.9

supplementary materials

C7—N1—Pb1	116.8 (4)	C14—C15—H15	121.9
C1—N1—Pb1	136.9 (5)	C15—C16—C17	122.1 (8)
C7—N2—C6	107.1 (6)	C15—C16—H16	118.9
C7—N2—H2	126.5	C17—C16—H16	118.9
C6—N2—H2	126.5	C18—C17—C16	121.6 (9)
C12—N3—C8	119.6 (6)	C18—C17—H17	119.2
C12—N3—Pb1	120.8 (5)	C16—C17—H17	119.2
C8—N3—Pb1	119.3 (4)	C17—C18—C19	117.3 (9)
C13—N4—C19	105.6 (6)	C17—C18—H18	121.3
C13—N4—Pb1	116.7 (5)	C19—C18—H18	121.3
C19—N4—Pb1	137.6 (5)	N4—C19—C14	109.5 (7)
C13—N5—C14	107.4 (6)	N4—C19—C18	130.0 (7)
C13—N5—H5	126.3	C14—C19—C18	120.4 (8)
C14—N5—H5	126.3	O2—C20—O1	122.3 (7)
O5—N6—O4	120.5 (10)	O2—C20—C21	121.4 (7)
O5—N6—O3	119.2 (9)	O1—C20—C21	116.4 (7)
O4—N6—O3	120.1 (9)	C20—C21—C22	114.5 (7)
N1—C1—C2	131.7 (7)	C20—C21—H21A	108.6
N1—C1—C6	109.1 (6)	C22—C21—H21A	108.6
C2—C1—C6	119.2 (7)	C20—C21—H21B	108.6
C3—C2—C1	118.0 (8)	C22—C21—H21B	108.6
C3—C2—H2A	121.0	H21A—C21—H21B	107.6
C1—C2—H2A	121.0	C21—C22—C22 ⁱⁱ	111.7 (8)
C2—C3—C4	121.4 (7)	C21—C22—H22A	109.3
C2—C3—H3	119.3	C22 ⁱⁱ —C22—H22A	109.3
C4—C3—H3	119.3	C21—C22—H22B	109.3
C5—C4—C3	121.3 (7)	C22 ⁱⁱ —C22—H22B	109.3
C5—C4—H4	119.3	H22A—C22—H22B	107.9
N1—Pb1—O1—C20	151.2 (5)	Pb1—N1—C1—C2	7.0 (13)
N3—Pb1—O1—C20	-142.2 (5)	C7—N1—C1—C6	-0.2 (8)
N4—Pb1—O1—C20	-77.0 (5)	Pb1—N1—C1—C6	-175.5 (5)
O3—Pb1—O1—C20	-139.6 (5)	N1—C1—C2—C3	178.9 (8)
O2—Pb1—O1—C20	1.6 (4)	C6—C1—C2—C3	1.6 (11)
O2 ⁱ —Pb1—O1—C20	63.3 (5)	C1—C2—C3—C4	-0.5 (12)
O4—Pb1—O1—C20	120.9 (10)	C2—C3—C4—C5	-0.3 (13)
O1—Pb1—O2—C20	-1.6 (4)	C3—C4—C5—C6	0.1 (12)
N1—Pb1—O2—C20	-37.5 (5)	C4—C5—C6—C1	1.0 (12)
N3—Pb1—O2—C20	37.6 (5)	C4—C5—C6—N2	-177.8 (8)
N4—Pb1—O2—C20	91.7 (4)	N1—C1—C6—C5	-179.8 (7)
O3—Pb1—O2—C20	123.7 (5)	C2—C1—C6—C5	-1.9 (12)
O2 ⁱ —Pb1—O2—C20	-110.9 (5)	N1—C1—C6—N2	-0.7 (8)
O4—Pb1—O2—C20	-165.8 (4)	C2—C1—C6—N2	177.2 (7)
O1—Pb1—O3—N6	-178.2 (5)	C7—N2—C6—C5	-179.7 (8)
N1—Pb1—O3—N6	-110.1 (6)	C7—N2—C6—C1	1.3 (8)
N3—Pb1—O3—N6	-175.4 (7)	C1—N1—C7—N2	1.1 (9)
N4—Pb1—O3—N6	117.7 (6)	Pb1—N1—C7—N2	177.5 (5)
O2—Pb1—O3—N6	85.9 (7)	C1—N1—C7—C8	179.9 (7)

O2 ⁱ —Pb1—O3—N6	-26.4 (7)	Pb1—N1—C7—C8	-3.7 (9)
O4—Pb1—O3—N6	-16.7 (6)	C6—N2—C7—N1	-1.6 (9)
O1—Pb1—O4—N6	130.1 (9)	C6—N2—C7—C8	179.7 (6)
N1—Pb1—O4—N6	100.2 (8)	C12—N3—C8—C9	0.7 (10)
N3—Pb1—O4—N6	36.4 (8)	Pb1—N3—C8—C9	-173.1 (5)
N4—Pb1—O4—N6	-31.1 (8)	C12—N3—C8—C7	178.2 (6)
O3—Pb1—O4—N6	16.2 (6)	Pb1—N3—C8—C7	4.4 (8)
O2—Pb1—O4—N6	-121.7 (7)	N1—C7—C8—N3	-0.4 (10)
O2 ⁱ —Pb1—O4—N6	-171.8 (8)	N2—C7—C8—N3	178.2 (6)
O1—Pb1—N1—C7	82.8 (5)	N1—C7—C8—C9	177.0 (7)
N3—Pb1—N1—C7	4.0 (5)	N2—C7—C8—C9	-4.4 (11)
N4—Pb1—N1—C7	8.3 (6)	N3—C8—C9—C10	0.8 (11)
O3—Pb1—N1—C7	-62.6 (5)	C7—C8—C9—C10	-176.4 (7)
O2—Pb1—N1—C7	108.7 (5)	C8—C9—C10—C11	-1.8 (12)
O2 ⁱ —Pb1—N1—C7	172.2 (5)	C9—C10—C11—C12	1.2 (12)
O4—Pb1—N1—C7	-103.4 (5)	C8—N3—C12—C11	-1.3 (11)
O1—Pb1—N1—C1	-102.3 (7)	Pb1—N3—C12—C11	172.4 (6)
N3—Pb1—N1—C1	179.0 (8)	C8—N3—C12—C13	179.1 (6)
N4—Pb1—N1—C1	-176.8 (6)	Pb1—N3—C12—C13	-7.3 (9)
O3—Pb1—N1—C1	112.3 (7)	C10—C11—C12—N3	0.4 (12)
O2—Pb1—N1—C1	-76.3 (7)	C10—C11—C12—C13	180.0 (8)
O2 ⁱ —Pb1—N1—C1	-12.8 (7)	C19—N4—C13—N5	0.0 (9)
O4—Pb1—N1—C1	71.6 (7)	Pb1—N4—C13—N5	-176.3 (5)
O1—Pb1—N3—C12	95.3 (6)	C19—N4—C13—C12	176.8 (7)
N1—Pb1—N3—C12	-178.2 (6)	Pb1—N4—C13—C12	0.5 (10)
N4—Pb1—N3—C12	5.5 (5)	C14—N5—C13—N4	-0.6 (9)
O3—Pb1—N3—C12	-83.0 (6)	C14—N5—C13—C12	-177.2 (7)
O2—Pb1—N3—C12	66.7 (6)	N3—C12—C13—N4	4.4 (11)
O2 ⁱ —Pb1—N3—C12	157.1 (5)	C11—C12—C13—N4	-175.2 (8)
O4—Pb1—N3—C12	-97.2 (6)	N3—C12—C13—N5	-179.3 (7)
O1—Pb1—N3—C8	-91.0 (5)	C11—C12—C13—N5	1.1 (12)
N1—Pb1—N3—C8	-4.5 (5)	C13—N5—C14—C15	177.1 (9)
N4—Pb1—N3—C8	179.2 (5)	C13—N5—C14—C19	0.8 (9)
O3—Pb1—N3—C8	90.7 (5)	N5—C14—C15—C16	-174.5 (9)
O2—Pb1—N3—C8	-119.6 (5)	C19—C14—C15—C16	1.2 (13)
O2 ⁱ —Pb1—N3—C8	-29.2 (7)	C14—C15—C16—C17	-1.8 (14)
O4—Pb1—N3—C8	76.5 (5)	C15—C16—C17—C18	1.9 (16)
O1—Pb1—N4—C13	-80.3 (6)	C16—C17—C18—C19	-1.2 (16)
N1—Pb1—N4—C13	-7.2 (7)	C13—N4—C19—C14	0.5 (9)
N3—Pb1—N4—C13	-2.9 (5)	Pb1—N4—C19—C14	175.6 (6)
O3—Pb1—N4—C13	66.4 (6)	C13—N4—C19—C18	-176.0 (9)
O2—Pb1—N4—C13	-128.1 (6)	Pb1—N4—C19—C18	-0.9 (15)
O2 ⁱ —Pb1—N4—C13	-161.8 (5)	N5—C14—C19—N4	-0.8 (9)
O4—Pb1—N4—C13	95.7 (6)	C15—C14—C19—N4	-177.5 (8)
O1—Pb1—N4—C19	104.9 (8)	N5—C14—C19—C18	176.1 (8)
N1—Pb1—N4—C19	178.1 (7)	C15—C14—C19—C18	-0.6 (13)
N3—Pb1—N4—C19	-177.6 (9)	C17—C18—C19—N4	176.8 (9)

supplementary materials

O3—Pb1—N4—C19	-108.3 (8)	C17—C18—C19—C14	0.6 (14)
O2—Pb1—N4—C19	57.2 (8)	Pb1—O2—C20—O1	2.6 (7)
O2 ⁱ —Pb1—N4—C19	23.5 (9)	Pb1—O2—C20—C21	-178.5 (7)
O4—Pb1—N4—C19	-79.0 (8)	Pb1—O1—C20—O2	-3.2 (8)
Pb1—O4—N6—O5	156.9 (12)	Pb1—O1—C20—C21	177.8 (5)
Pb1—O4—N6—O3	-28.4 (10)	O2—C20—C21—C22	39.6 (10)
Pb1—O3—N6—O5	-150.5 (10)	O1—C20—C21—C22	-141.5 (7)
Pb1—O3—N6—O4	34.7 (12)	C20—C21—C22—C22 ⁱⁱ	64.3 (12)
C7—N1—C1—C2	-177.7 (8)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots O1 ⁱⁱⁱ	0.86	1.95	2.744 (8)	152
N5—H5 \cdots O3 ^{iv}	0.86	2.10	2.891 (9)	153

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

Fig. 2

