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Poly[diaqua-μ_3-nitrato-[μ_2-5-(2-pyrazinyl)-5*H*-tetrazolato]lead(II)]

Ju-Tao Liu,[a] Sheng-Di Fan[a] and Seik Weng Ng[b]*

[a]School of Life Science, Dalian Nationalities University, Dalian 116600, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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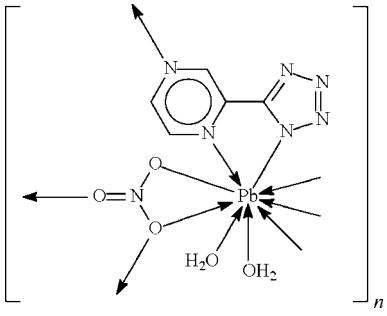
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.027; wR factor = 0.078; data-to-parameter ratio = 14.9.

In the crystal structure of the polymeric title compound, $[Pb(C_5H_3N_6)(NO_3)(H_2O)_2]_n$, pyrazinyltetrazolate and nitrate ligands chelate a water-coordinated Pb atom, while the heterocyclic ligand is additionally linked to an adjacent Pb atom and the nitrate ligand is linked to two other neighboring Pb atoms. Bridging by the two ligands leads to the formation of a layer architecture with adjacent layers connected into a three-dimensional network by O–H···N hydrogen bonds. The Pb atom has a bicapped square-antiprismatic coordination geometry.

Related literature

See Liu *et al.* (2007) for a report of the copper(II) pyrazinyltetrazolate derivative.



Experimental

Crystal data

$[Pb(C_5H_3N_6)(NO_3)(H_2O)_2]$
M_r = 452.37
Monoclinic, $C2/c$
a = 25.2969 (6) Å
b = 5.7523 (2) Å
c = 15.7938 (4) Å
β = 110.484 (1)°
V = 2152.9 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 15.70 mm^{-1}
T = 295 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.056, T_{max} = 0.188
8341 measured reflections
2475 independent reflections
2011 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.078
S = 1.04
2475 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pb1—O1	2.754 (3)	Pb1—O1*w*	2.483 (3)
Pb1—O1^{i}	3.105 (4)	Pb1—O2*w*	2.541 (3)
Pb1—O2	3.169 (4)	Pb1—N1	2.593 (3)
Pb1—O2^{ii}	3.033 (4)	Pb1—N5^{iii}	2.830 (3)
Pb1—O3^{i}	2.976 (4)	Pb1—N6	2.819 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H11···N2^{iv}	0.82	2.02	2.827 (5)	171
O1*w*—H12···N3^{v}	0.82	2.12	2.932 (5)	173
O2*w*—H21···N4^{v}	0.82	2.32	3.081 (4)	156
O2*w*—H22···N4^{vi}	0.82	2.23	2.846 (4)	132

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2384).

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supplementary materials

Acta Cryst. (2007). E**63**, m1652 [**doi:10.1107/S1600536807023781**]

Poly[diaqua-μ_3-nitrato-[μ_2-5-(2-pyrazinyl)-5*H*-tetrazolato]lead(II)]

J.-T. Liu, S.-D. Fan and S. W. Ng

Comment

The preceeding paper describes the structure of the copper derivative of 2-(1*H*-tetrazol-5-yl)pyrazine, which is the first report of a metal derivative (Liu *et al.*, 2007).

Experimental

Lead nitrate (33 mg, 0.1 mmol) and 2-(1*H*-tetrazol-5-yl)pyrazine (30 mg, 0.2 mmol) were dissolved in 10 ml of 1:1 methanol/water solution. The solution was filtered and set aside for crystals to grow. Colorless crystals were isolated in 50% yield after two weeks.

Refinement

H atoms were placed at calculated positions [C—H = 0.93, O–H = 0.82 Å; U(H) = 1.2U_{eq}(C,O)], as were included in the refinement in the riding model approximation. The hydrogen atoms of the water molecules were rotated to fit the electron density. The final difference Fourier map had a large peak at 1 Å and a deep hole at 1 Å from Pb1.

Figures

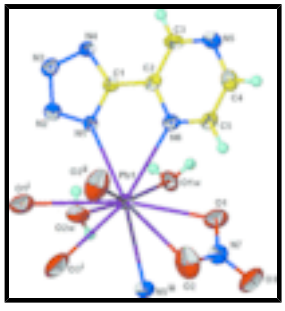

Fig. 1. **Figure 1**. Thermal ellipsoid plot of a part of the layer structure of the title compound with ellipsoids are drawn at the 70% probability level.

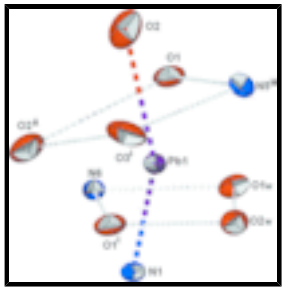

Fig. 2. **Figure 2**. A repesentation of the bicapped square-antiprismatic geometry of Pb1.

Poly[diaqua-μ$_3$-nitrato-[μ$_2$-5-(2-pyrazinyl)-5*H*-tetrazolato]lead(II)]

Crystal data

$[Pb(C_5H_3N_6)(NO_3)(H_2O)_2]$	F_{000} = 1664
M_r = 452.37	D_x = 2.791 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4180 reflections
a = 25.2969 (6) Å	θ = 2.2–28.3º
b = 5.7523 (2) Å	μ = 15.70 mm^{-1}
c = 15.7938 (4) Å	*T* = 295 (2) K
β = 110.484 (1)º	Block, colorless
V = 2152.9 (1) Å^3	0.22 × 0.20 × 0.16 mm
Z = 8	

Data collection

Bruker APEX area-detector diffractometer	2475 independent reflections
Radiation source: fine-focus sealed tube	2011 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 294(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan SADABS (Sheldrick, 1996)	*h* = −31→32
T_{min} = 0.056, T_{max} = 0.188	*k* = −7→7
8341 measured reflections	*l* = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 3.9882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.078	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 2.05 e Å^{-3}
2475 reflections	$\Delta\rho_{min}$ = −1.44 e Å^{-3}
166 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00140 (8)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pb1	0.64631 (1)	0.75580 (3)	0.70393 (1)	0.0202 (1)
O1	0.6691 (2)	0.2869 (6)	0.7253 (3)	0.035 (1)
O2	0.7463 (2)	0.4286 (7)	0.8195 (3)	0.050 (1)
O3	0.7162 (2)	0.0889 (7)	0.8421 (3)	0.050 (1)
O1w	0.5588 (1)	0.5188 (6)	0.6531 (2)	0.028 (1)
O2w	0.5674 (1)	0.9748 (6)	0.7340 (2)	0.030 (1)
N1	0.5892 (1)	0.9584 (6)	0.5529 (2)	0.019 (1)
N2	0.5576 (2)	1.1515 (7)	0.5335 (2)	0.023 (1)
N3	0.5363 (2)	1.1800 (7)	0.4459 (2)	0.024 (1)
N4	0.5536 (1)	1.0045 (6)	0.4050 (2)	0.022 (1)
N5	0.6433 (2)	0.3878 (7)	0.3736 (2)	0.026 (1)
N6	0.6472 (1)	0.5581 (6)	0.5411 (2)	0.020 (1)
N7	0.7111 (2)	0.2686 (6)	0.7966 (3)	0.026 (1)
C1	0.5856 (2)	0.8710 (8)	0.4729 (2)	0.017 (1)
C2	0.6164 (2)	0.6626 (9)	0.4636 (3)	0.018 (1)
C3	0.6142 (2)	0.5754 (8)	0.3806 (3)	0.026 (1)
C4	0.6739 (2)	0.2854 (8)	0.4513 (4)	0.024 (1)
C5	0.6757 (2)	0.3700 (8)	0.5335 (3)	0.023 (1)
H11	0.5608	0.4219	0.6163	0.033*
H12	0.5315	0.6036	0.6296	0.033*
H21	0.5407	0.9907	0.6865	0.036*
H22	0.5572	0.9013	0.7700	0.036*
H3	0.5916	0.6501	0.3282	0.032*
H4	0.6946	0.1530	0.4495	0.029*
H5	0.6977	0.2930	0.5858	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.0189 (2)	0.0236 (2)	0.0159 (2)	−0.0001 (1)	0.0034 (1)	0.0014 (1)
O1	0.028 (2)	0.042 (2)	0.027 (2)	0.009 (2)	0.001 (2)	0.006 (1)
O2	0.033 (2)	0.044 (3)	0.071 (3)	−0.013 (2)	0.015 (2)	−0.012 (2)
O3	0.059 (3)	0.038 (2)	0.044 (2)	0.002 (2)	0.005 (2)	0.019 (2)
O1w	0.025 (2)	0.024 (2)	0.028 (2)	0.002 (1)	0.000 (1)	−0.006 (1)
O2w	0.030 (2)	0.040 (2)	0.020 (2)	0.006 (2)	0.007 (1)	0.000 (1)
N1	0.021 (2)	0.016 (2)	0.018 (2)	0.002 (2)	0.003 (1)	−0.001 (1)
N2	0.025 (2)	0.022 (2)	0.022 (2)	−0.003 (2)	0.008 (2)	0.000 (2)
N3	0.020 (2)	0.022 (2)	0.025 (2)	−0.001 (2)	0.003 (2)	0.004 (2)
N4	0.026 (2)	0.019 (2)	0.017 (2)	0.005 (2)	0.003 (1)	0.001 (1)
N5	0.031 (2)	0.026 (2)	0.021 (2)	0.000 (2)	0.009 (2)	−0.002 (2)
N6	0.019 (2)	0.022 (2)	0.018 (2)	0.002 (2)	0.005 (1)	0.001 (1)
N7	0.024 (2)	0.028 (3)	0.028 (2)	0.002 (2)	0.011 (2)	0.002 (2)
C1	0.017 (2)	0.019 (2)	0.015 (2)	−0.001 (2)	0.005 (2)	0.001 (2)
C2	0.017 (2)	0.019 (2)	0.021 (2)	−0.001 (2)	0.010 (2)	0.005 (2)

C3	0.033 (2)	0.028 (3)	0.015 (2)	0.004 (2)	0.005 (2)	0.001 (2)
C4	0.020 (2)	0.021 (2)	0.032 (3)	0.002 (2)	0.010 (2)	−0.004 (2)
C5	0.023 (2)	0.020 (2)	0.022 (2)	0.003 (2)	0.005 (2)	0.003 (2)

Geometric parameters (Å, °)

Pb1—O1	2.754 (3)	N3—N4	1.351 (5)
Pb1—O1^{i}	3.105 (4)	N4—C1	1.337 (5)
Pb1—O2	3.169 (4)	N5—C3	1.333 (6)
Pb1—O2^{ii}	3.033 (4)	N5—C4	1.337 (6)
Pb1—O3^{i}	2.976 (4)	N6—C5	1.330 (5)
Pb1—O1w	2.483 (3)	N6—C2	1.341 (5)
Pb1—O2w	2.541 (3)	C1—C2	1.466 (7)
Pb1—N1	2.593 (3)	C2—C3	1.386 (6)
Pb1—N5^{iii}	2.830 (3)	C4—C5	1.373 (7)
Pb1—N6	2.819 (3)	O1w—H11	0.8200
O1—N7	1.253 (6)	O1w—H12	0.8200
O2—N7	1.243 (5)	O2w—H21	0.8200
O3—N7	1.240 (5)	O2w—H22	0.8200
N1—C1	1.334 (5)	C3—H3	0.9300
N1—N2	1.340 (5)	C4—H4	0.9300
N2—N3	1.307 (5)	C5—H5	0.9300
O1w—Pb1—O2w	70.3 (1)	N5^{iii}—Pb1—O2	64.0 (1)
O1w—Pb1—N1	78.6 (1)	O3^{i}—Pb1—O2	79.1 (1)
O2w—Pb1—N1	74.2 (1)	O2^{ii}—Pb1—O2	72.3 (1)
O1w—Pb1—O1	68.1 (1)	O1^{i}—Pb1—O2	116.2 (1)
O2w—Pb1—O1	127.4 (1)	N7—O1—Pb1	105.5 (3)
N1—Pb1—O1	125.3 (1)	N7—O2—Pb1	85.7 (3)
O1w—Pb1—N6	77.0 (1)	C1—N1—N2	105.0 (3)
O2w—Pb1—N6	128.9 (1)	C1—N1—Pb1	122.3 (3)
N1—Pb1—N6	61.4 (1)	N2—N1—Pb1	132.8 (2)
O1—Pb1—N6	69.4 (1)	N3—N2—N1	109.8 (4)
O1w—Pb1—N5^{iii}	80.2 (1)	N2—N3—N4	109.2 (4)
O2w—Pb1—N5^{iii}	71.6 (1)	C1—N4—N3	104.6 (3)
N1—Pb1—N5^{iii}	144.2 (1)	C3—N5—C4	116.1 (4)
O1—Pb1—N5^{iii}	70.9 (1)	C5—N6—C2	116.2 (3)
N6—Pb1—N5^{iii}	139.2 (1)	C5—N6—Pb1	126.0 (2)
O1w—Pb1—O3^{i}	145.5 (1)	C2—N6—Pb1	117.7 (3)
O2w—Pb1—O3^{i}	81.2 (1)	O3—N7—O2	122.0 (5)
N1—Pb1—O3^{i}	112.5 (1)	O3—N7—O1	118.3 (4)
O1—Pb1—O3^{i}	119.7 (1)	O2—N7—O1	119.7 (4)
N6—Pb1—O3^{i}	137.5 (1)	N1—C1—N4	111.4 (4)
N5^{iii}—Pb1—O3^{i}	72.5 (1)	N1—C1—C2	122.7 (3)
O1w—Pb1—O2^{ii}	151.2 (1)	N4—C1—C2	125.8 (3)
O2w—Pb1—O2^{ii}	131.0 (1)	N6—C2—C3	121.4 (4)

N1—Pb1—O2^{ii}	88.6 (1)	N6—C2—C1	115.8 (3)
O1—Pb1—O2^{ii}	100.2 (1)	C3—C2—C1	122.9 (4)
N6—Pb1—O2^{ii}	74.2 (1)	N5—C3—C2	122.0 (4)
N5^{iii}—Pb1—O2^{ii}	122.2 (1)	N5—C4—C5	121.9 (4)
O3^{i}—Pb1—O2^{ii}	63.3 (1)	N6—C5—C4	122.3 (4)
O1w—Pb1—O1^{i}	133.3 (1)	Pb1—O1w—H11	109.5
O2w—Pb1—O1^{i}	67.7 (1)	Pb1—O1w—H12	109.5
N1—Pb1—O1^{i}	71.4 (1)	H11—O1w—H12	109.5
O1—Pb1—O1^{i}	158.0 (2)	Pb1—O2w—H21	109.5
N6—Pb1—O1^{i}	115.8 (1)	Pb1—O2w—H22	109.5
N5^{iii}—Pb1—O1^{i}	104.5 (1)	H21—O2w—H22	109.5
O3^{i}—Pb1—O1^{i}	41.2 (1)	N5—C3—H3	119.0
O2^{ii}—Pb1—O1^{i}	63.3 (1)	C2—C3—H3	119.0
O1w—Pb1—O2	107.6 (1)	N5—C4—H4	119.0
O2w—Pb1—O2	135.1 (1)	C5—C4—H4	119.0
N1—Pb1—O2	150.7 (1)	N6—C5—H5	118.8
O1—Pb1—O2	42.0 (1)	C4—C5—H5	118.8
N6—Pb1—O2	91.5 (1)		
O1w—Pb1—O1—N7	−144.1 (3)	N1—Pb1—N6—C5	178.1 (4)
O2w—Pb1—O1—N7	−104.0 (3)	O1—Pb1—N6—C5	−26.7 (3)
N1—Pb1—O1—N7	159.0 (3)	N5^{iii}—Pb1—N6—C5	−40.4 (4)
N6—Pb1—O1—N7	132.2 (3)	O3^{i}—Pb1—N6—C5	85.2 (4)
N5^{iii}—Pb1—O1—N7	−57.3 (3)	O2^{ii}—Pb1—N6—C5	80.9 (3)
O3^{i}—Pb1—O1—N7	−1.6 (4)	O1^{i}—Pb1—N6—C5	130.0 (3)
O2^{ii}—Pb1—O1—N7	63.4 (3)	O2—Pb1—N6—C5	9.8 (3)
O1^{i}—Pb1—O1—N7	24.0 (7)	O1w—Pb1—N6—C2	82.6 (3)
O2—Pb1—O1—N7	14.8 (3)	O2w—Pb1—N6—C2	31.8 (3)
O1w—Pb1—O2—N7	6.0 (3)	N1—Pb1—N6—C2	−1.4 (3)
O2w—Pb1—O2—N7	85.4 (3)	O1—Pb1—N6—C2	153.8 (3)
N1—Pb1—O2—N7	−92.1 (3)	N5^{iii}—Pb1—N6—C2	140.1 (3)
O1—Pb1—O2—N7	−14.4 (3)	O3^{i}—Pb1—N6—C2	−94.2 (3)
N6—Pb1—O2—N7	−70.8 (3)	O2^{ii}—Pb1—N6—C2	−98.5 (3)
N5^{iii}—Pb1—O2—N7	75.3 (3)	O1^{i}—Pb1—N6—C2	−49.5 (3)
O3^{i}—Pb1—O2—N7	151.0 (3)	O2—Pb1—N6—C2	−169.7 (3)
O2^{ii}—Pb1—O2—N7	−143.7 (3)	Pb1—O2—N7—O3	−155.2 (5)
O1^{i}—Pb1—O2—N7	169.4 (3)	Pb1—O2—N7—O1	25.0 (4)
O1w—Pb1—N1—C1	−78.5 (3)	Pb1—O1—N7—O3	150.0 (4)
O2w—Pb1—N1—C1	−151.0 (3)	Pb1—O1—N7—O2	−30.2 (5)
O1—Pb1—N1—C1	−26.0 (4)	N2—N1—C1—N4	0.8 (4)
N6—Pb1—N1—C1	2.7 (3)	Pb1—N1—C1—N4	179.5 (3)
N5^{iii}—Pb1—N1—C1	−133.2 (3)	N2—N1—C1—C2	177.2 (4)
O3^{i}—Pb1—N1—C1	135.8 (3)	Pb1—N1—C1—C2	−4.2 (6)
O2^{ii}—Pb1—N1—C1	75.5 (3)	N3—N4—C1—N1	−0.8 (5)

O1^{i}—Pb1—N1—C1	137.7 (3)	N3—N4—C1—C2	−177.1 (4)
O2—Pb1—N1—C1	27.2 (4)	C5—N6—C2—C3	1.1 (6)
O1w—Pb1—N1—N2	99.7 (4)	Pb1—N6—C2—C3	−179.4 (3)
O2w—Pb1—N1—N2	27.2 (3)	C5—N6—C2—C1	−179.4 (4)
O1—Pb1—N1—N2	152.2 (3)	Pb1—N6—C2—C1	0.1 (5)
N6—Pb1—N1—N2	−179.0 (4)	N1—C1—C2—N6	2.6 (6)
N5^{iii}—Pb1—N1—N2	45.0 (4)	N4—C1—C2—N6	178.4 (4)
O3^{i}—Pb1—N1—N2	−46.0 (4)	N1—C1—C2—C3	−177.9 (4)
O2^{ii}—Pb1—N1—N2	−106.3 (4)	N4—C1—C2—C3	−2.1 (7)
O1^{i}—Pb1—N1—N2	−44.0 (3)	C4—N5—C3—C2	1.4 (7)
O2—Pb1—N1—N2	−154.5 (3)	N6—C2—C3—N5	−1.7 (7)
C1—N1—N2—N3	−0.5 (4)	C1—C2—C3—N5	178.8 (4)
Pb1—N1—N2—N3	−178.9 (3)	C3—N5—C4—C5	−0.6 (7)
N1—N2—N3—N4	0.0 (5)	C2—N6—C5—C4	−0.3 (6)
N2—N3—N4—C1	0.5 (4)	Pb1—N6—C5—C4	−179.8 (3)
O1w—Pb1—N6—C5	−97.9 (3)	N5—C4—C5—N6	0.1 (7)
O2w—Pb1—N6—C5	−148.7 (3)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iii) *x*, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···N2^{iv}	0.82	2.02	2.827 (5)	171
O1w—H12···N3^{v}	0.82	2.12	2.932 (5)	173
O2w—H21···N4^{v}	0.82	2.32	3.081 (4)	156
O2w—H22···N4^{vi}	0.82	2.23	2.846 (4)	132

Symmetry codes: (iv) *x*, *y*−1, *z*; (v) −*x*+1, −*y*+2, −*z*+1; (vi) *x*, −*y*+2, *z*+1/2.

Fig. 1

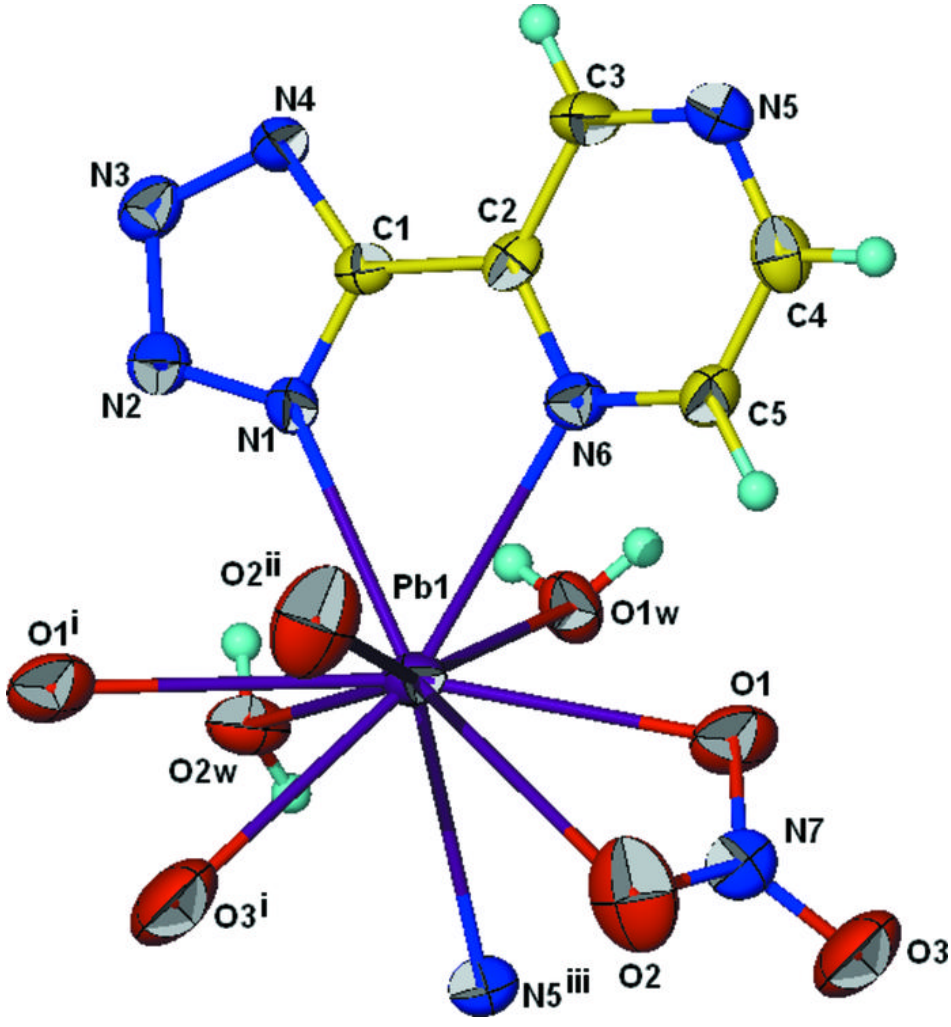
C3
N4
N5
N3
C1
C2
C4
N2
N1
N6
C5
O2ii
Pb1
O1w
O1i
O1
O2w
N7
O3i
O3
N5iii
O2

Fig. 2