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# (2,2′-Bipyridine-$\kappa^2N,N'$)bis(4-methylbenzoato-$\kappa^2O,O'$)lead(II)

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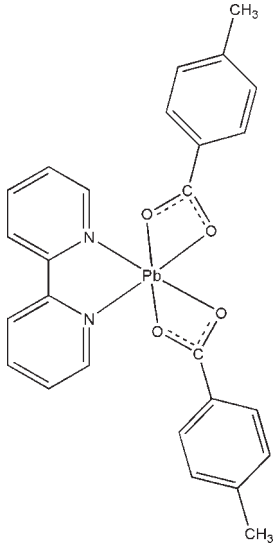
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.023; $wR$ factor = 0.051; data-to-parameter ratio = 18.5.

In the title compound, $[Pb(C_8H_7O_2)_2(C_{10}H_8N_2)]$, the $Pb^{II}$ ion is coordinated by two N atoms from one 2,2′-bipyridine ligand and four O atoms from two 4-methylbenzoate anions in a distorted pseudo-square-pyramidal environment, considering one of the carboxylate anions as an apical ligand. Pairs of complex molecules related by inversion centers are organized into dimers *via* pairs of Pb···O interactions [3.185 (2) Å] and stacking interactions between 2,2′-bipyridine and 4-methylbenzoate ligands, with a mean distance between their planes of 3.491 Å.

## Related literature

For potential applications of lead compounds, see: Fan & Zhu (2006); Hamilton *et al.* (2004). For the use of aromatic carboxylates and 2,2′-bipyridine-type ligands in the preparation of metal complexes, see: Wang *et al.* (2006); Masaoka *et al.* (2001).




## Experimental

### Crystal data

$[Pb(C_8H_7O_2)_2(C_{10}H_8N_2)]$
$M_r$ = 633.65
Triclinic, $P\overline{1}$
$a$ = 9.5510 (11) Å
$b$ = 10.0805 (12) Å
$c$ = 13.2483 (15) Å
$\alpha$ = 109.865 (1)°
$\beta$ = 97.322 (1)°
$\gamma$ = 90.643 (1)°
$V$ = 1187.8 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 7.14 mm$^{-1}$
$T$ = 296 K
0.35 × 0.26 × 0.18 mm

### Data collection

Bruker APEXII CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.124, $T_{max}$ = 0.277
14285 measured reflections
5555 independent reflections
4965 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.051
$S$ = 1.02
5555 reflections
300 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.76 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Pb1—O1 | 2.333 (2) | Pb1—O2 | 2.644 (2) |
| Pb1—O3 | 2.418 (2) | Pb1—N1 | 2.656 (3) |
| Pb1—N2 | 2.608 (3) | Pb1—O4 | 2.701 (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: GK2256).

## References

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# supporting information

*Acta Cryst.* (2010). E**66**, m298 [doi:10.1107/S1600536810005544]

## (2,2′-Bipyridine-$\kappa^2N,N'$)bis(4-methylbenzoato-$\kappa^2O,O'$)lead(II)

**Jun Dai, Juan Yang and Yingjie Li**

### S1. Comment

Recently, lead compounds have been increasingly studied owing to their possible applications in different fields (Fan *et al.*, 2006; Hamilton *et al.*, 2004), such as ion-exchange, nonlinear optics and catalysis, especially in environmental protection due to the toxicity of lead and in biological systems for its diverse interactions with biological molecules. 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, $[Pb(C_8H_7O_2)_2(C_{10}H_8N_2)]$, contains a $Pb^{II}$ cation, two 4-methylbenzoate ligands, one 2,2′-bipyridine ligand, as illustrated in Fig. 1. The $Pb^{II}$ atom is hexacoordinated being chelated by two carboxylate groups and one 2,2′-bipyridine. The Pb—O bond lengths are in the range of 2.333 (2) to 2.701 (2) Å. The Pb—N bond lengths are 2.608 (3) to 2.656 (3) Å. The $Pb^{II}$ atom has a distorted pseudo-square-pyramidal environment, considering one of the carboxylate anions as an apical ligand. The complex molecules related by inversion center are organized into dimeric units via a pair of Pb···O interactions of 3.185 (2) Å and stacking inteactions between 2,2′-bipyridine and 4-methylbenzoate ligands, with a mean distance between their planes of 3.491 Å.

### S2. Experimental

A mixture of $Pb(CH_3COO)_2{\cdot}3H_2O$ (0.199 g, 0.52 mmol), 4-methylbenzoic acid (0.114 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 7 days to give the colorless crystals suitable for X-ray diffraction analysis.

### S3. Refinement

All H atoms bounded to C atoms were placed in calculated positions and treated in a riding-model approximation, with C (aromatic)—H = 0.93 Å, *C*(methyl)—H = 0.96 Å and $U_{iso}(H_{aromatic}) = 1.2U_{eq}(C)$, $U_{iso}(H_{methyl}) = 1.5U_{eq}(C)$. Two rigid-bond restraints to Uij values (DELU) were imposed on bonded atoms Pb1—O4 and Pb1—O2.

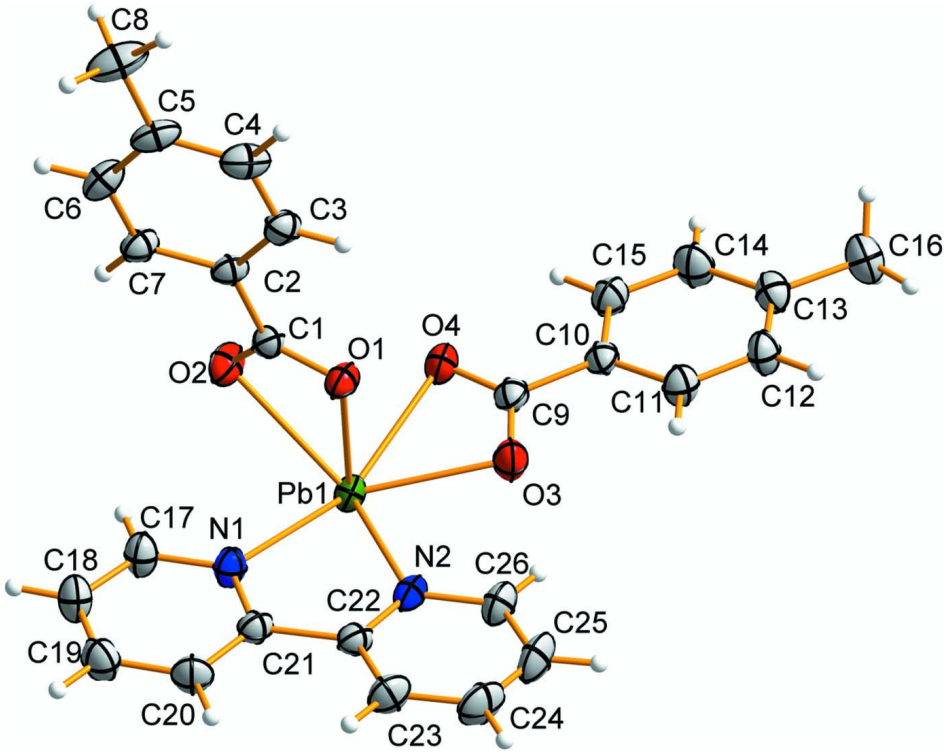


**Figure 1**

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.

**(2,2′-Bipyridine-$\kappa^2N,N'$)bis(4-methylbenzoato-$\kappa^2O,O'$)lead(II)**

*Crystal data*

$[Pb(C_8H_7O_2)_2(C_{10}H_8N_2)]$
$M_r = 633.65$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.5510$ (11) Å
$b = 10.0805$ (12) Å
$c = 13.2483$ (15) Å
$\alpha = 109.865$ (1)°
$\beta = 97.322$ (1)°
$\gamma = 90.643$ (1)°
$V = 1187.8$ (2) Å$^3$
$Z = 2$
$F(000) = 612$
$D_x = 1.772$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7017 reflections
$\theta = 2.2$–$26.6$°
$\mu = 7.14$ mm$^{-1}$
$T = 296$ K
Prism, colorless
0.35 × 0.26 × 0.18 mm

*Data collection*

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.124$, $T_{max} = 0.277$
14285 measured reflections
5555 independent reflections
4965 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.8°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.051$
$S = 1.02$
5555 reflections
300 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 0.140P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.77$ e Å$^{-3}$
$\Delta\rho_{min} = -0.76$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pb1 | 0.010726 (12) | 0.117736 (12) | 0.677133 (9) | 0.03988 (5) |
| O1 | 0.2108 (2) | 0.1792 (2) | 0.80800 (18) | 0.0483 (5) |
| O2 | 0.0648 (2) | 0.3523 (2) | 0.84728 (18) | 0.0543 (6) |
| O3 | 0.1789 (3) | 0.0320 (3) | 0.5511 (2) | 0.0601 (6) |
| O4 | 0.1595 (3) | 0.2603 (2) | 0.58236 (19) | 0.0556 (6) |
| N1 | −0.0850 (3) | 0.0481 (3) | 0.8332 (2) | 0.0468 (6) |
| N2 | 0.0489 (3) | −0.1362 (3) | 0.6814 (2) | 0.0454 (6) |
| C1 | 0.1748 (3) | 0.2982 (3) | 0.8699 (3) | 0.0413 (7) |
| C2 | 0.2682 (3) | 0.3698 (3) | 0.9753 (3) | 0.0409 (7) |
| C3 | 0.4063 (3) | 0.3339 (3) | 0.9934 (3) | 0.0488 (8) |
| H3A | 0.4430 | 0.2632 | 0.9395 | 0.059* |
| C4 | 0.4895 (4) | 0.4025 (4) | 1.0911 (3) | 0.0586 (10) |
| H4A | 0.5825 | 0.3781 | 1.1016 | 0.070* |
| C5 | 0.4386 (4) | 0.5062 (4) | 1.1735 (3) | 0.0559 (9) |
| C6 | 0.3003 (4) | 0.5395 (4) | 1.1556 (3) | 0.0576 (9) |
| H6A | 0.2630 | 0.6076 | 1.2108 | 0.069* |
| C7 | 0.2156 (4) | 0.4740 (3) | 1.0576 (3) | 0.0470 (7) |
| H7A | 0.1233 | 0.5000 | 1.0470 | 0.056* |
| C8 | 0.5337 (5) | 0.5824 (5) | 1.2781 (4) | 0.0861 (15) |
| H8A | 0.5932 | 0.5164 | 1.2977 | 0.129* |
| H8B | 0.4770 | 0.6244 | 1.3343 | 0.129* |
| H8C | 0.5913 | 0.6548 | 1.2687 | 0.129* |
| C9 | 0.2085 (3) | 0.1461 (4) | 0.5346 (3) | 0.0449 (7) |
| C10 | 0.3033 (3) | 0.1363 (3) | 0.4516 (2) | 0.0413 (7) |
| C11 | 0.3697 (4) | 0.0135 (4) | 0.4040 (3) | 0.0522 (8) |
| H11A | 0.3569 | −0.0640 | 0.4254 | 0.063* |
| C12 | 0.4548 (4) | 0.0043 (4) | 0.3251 (3) | 0.0571 (9) |
| H12A | 0.4985 | −0.0792 | 0.2947 | 0.068* |
| C13 | 0.4757 (4) | 0.1168 (4) | 0.2909 (3) | 0.0532 (8) |
| C14 | 0.4090 (4) | 0.2395 (4) | 0.3393 (3) | 0.0662 (11) |
| H14A | 0.4209 | 0.3168 | 0.3173 | 0.079* |
| C15 | 0.3258 (4) | 0.2498 (4) | 0.4188 (3) | 0.0584 (9) |
| H15A | 0.2844 | 0.3342 | 0.4508 | 0.070* |
| C16 | 0.5663 (5) | 0.1044 (5) | 0.2032 (3) | 0.0709 (11) |

| | | | | |
|---|---|---|---|---|
| H16A | 0.6455 | 0.0495 | 0.2118 | 0.106* |
| H16B | 0.5998 | 0.1970 | 0.2084 | 0.106* |
| H16C | 0.5113 | 0.0589 | 0.1335 | 0.106* |
| C17 | −0.1533 (4) | 0.1412 (4) | 0.9053 (3) | 0.0553 (9) |
| H17A | −0.1560 | 0.2331 | 0.9046 | 0.066* |
| C18 | −0.2200 (4) | 0.1079 (4) | 0.9806 (3) | 0.0599 (10) |
| H18A | −0.2657 | 0.1759 | 1.0301 | 0.072* |
| C19 | −0.2174 (4) | −0.0266 (4) | 0.9810 (3) | 0.0640 (10) |
| H19A | −0.2606 | −0.0521 | 1.0313 | 0.077* |
| C20 | −0.1495 (4) | −0.1250 (4) | 0.9053 (3) | 0.0600 (10) |
| H20A | −0.1487 | −0.2182 | 0.9032 | 0.072* |
| C21 | −0.0830 (3) | −0.0847 (3) | 0.8330 (3) | 0.0435 (7) |
| C22 | −0.0052 (3) | −0.1848 (3) | 0.7519 (3) | 0.0441 (7) |
| C23 | 0.0131 (5) | −0.3217 (4) | 0.7493 (4) | 0.0672 (11) |
| H23A | −0.0239 | −0.3531 | 0.7993 | 0.081* |
| C24 | 0.0856 (5) | −0.4114 (4) | 0.6734 (4) | 0.0755 (12) |
| H24A | 0.0987 | −0.5035 | 0.6713 | 0.091* |
| C25 | 0.1376 (5) | −0.3618 (4) | 0.6014 (4) | 0.0736 (12) |
| H25A | 0.1864 | −0.4203 | 0.5485 | 0.088* |
| C26 | 0.1179 (4) | −0.2249 (4) | 0.6073 (3) | 0.0600 (9) |
| H26A | 0.1542 | −0.1925 | 0.5575 | 0.072* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pb1 | 0.04568 (8) | 0.03734 (7) | 0.03350 (7) | 0.00681 (5) | 0.00661 (5) | 0.00766 (5) |
| O1 | 0.0490 (13) | 0.0417 (13) | 0.0455 (12) | 0.0100 (10) | 0.0040 (10) | 0.0047 (10) |
| O2 | 0.0543 (14) | 0.0485 (12) | 0.0465 (12) | 0.0145 (11) | −0.0036 (11) | 0.0024 (8) |
| O3 | 0.0754 (17) | 0.0499 (15) | 0.0603 (15) | 0.0102 (12) | 0.0314 (13) | 0.0178 (12) |
| O4 | 0.0650 (15) | 0.0465 (14) | 0.0517 (14) | 0.0039 (11) | 0.0230 (11) | 0.0069 (11) |
| N1 | 0.0555 (17) | 0.0416 (15) | 0.0474 (16) | 0.0116 (12) | 0.0152 (13) | 0.0175 (13) |
| N2 | 0.0493 (16) | 0.0372 (14) | 0.0425 (15) | 0.0101 (12) | 0.0068 (12) | 0.0041 (12) |
| C1 | 0.0449 (18) | 0.0384 (17) | 0.0400 (16) | 0.0004 (13) | 0.0069 (13) | 0.0122 (14) |
| C2 | 0.0449 (17) | 0.0317 (16) | 0.0451 (17) | −0.0002 (13) | 0.0026 (13) | 0.0132 (13) |
| C3 | 0.0450 (18) | 0.0385 (18) | 0.062 (2) | 0.0048 (14) | 0.0081 (16) | 0.0162 (16) |
| C4 | 0.047 (2) | 0.045 (2) | 0.082 (3) | −0.0008 (16) | −0.0102 (18) | 0.025 (2) |
| C5 | 0.067 (2) | 0.0364 (18) | 0.059 (2) | −0.0093 (16) | −0.0156 (18) | 0.0191 (17) |
| C6 | 0.076 (3) | 0.0364 (18) | 0.051 (2) | 0.0046 (17) | 0.0001 (18) | 0.0063 (15) |
| C7 | 0.0463 (18) | 0.0387 (18) | 0.0507 (19) | 0.0068 (14) | 0.0017 (15) | 0.0102 (15) |
| C8 | 0.100 (4) | 0.059 (3) | 0.082 (3) | −0.013 (2) | −0.036 (3) | 0.019 (2) |
| C9 | 0.0417 (17) | 0.0466 (19) | 0.0370 (16) | 0.0020 (14) | 0.0028 (13) | 0.0035 (14) |
| C10 | 0.0392 (16) | 0.0446 (18) | 0.0352 (15) | 0.0013 (13) | 0.0022 (12) | 0.0084 (13) |
| C11 | 0.056 (2) | 0.050 (2) | 0.055 (2) | 0.0112 (16) | 0.0145 (16) | 0.0217 (17) |
| C12 | 0.059 (2) | 0.056 (2) | 0.059 (2) | 0.0196 (17) | 0.0222 (18) | 0.0187 (19) |
| C13 | 0.0469 (19) | 0.066 (2) | 0.050 (2) | 0.0074 (17) | 0.0112 (15) | 0.0227 (18) |
| C14 | 0.076 (3) | 0.059 (2) | 0.075 (3) | 0.009 (2) | 0.031 (2) | 0.031 (2) |
| C15 | 0.066 (2) | 0.045 (2) | 0.063 (2) | 0.0092 (17) | 0.0198 (19) | 0.0133 (18) |
| C16 | 0.065 (2) | 0.090 (3) | 0.068 (3) | 0.015 (2) | 0.028 (2) | 0.033 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.068 (2) | 0.050 (2) | 0.053 (2) | 0.0179 (17) | 0.0216 (18) | 0.0189 (17) |
| C18 | 0.066 (2) | 0.066 (3) | 0.052 (2) | 0.0174 (19) | 0.0237 (18) | 0.0201 (19) |
| C19 | 0.066 (2) | 0.070 (3) | 0.064 (2) | 0.004 (2) | 0.023 (2) | 0.029 (2) |
| C20 | 0.071 (2) | 0.048 (2) | 0.068 (2) | 0.0028 (18) | 0.018 (2) | 0.0268 (19) |
| C21 | 0.0435 (18) | 0.0357 (17) | 0.0495 (18) | 0.0037 (13) | 0.0053 (14) | 0.0129 (14) |
| C22 | 0.0453 (18) | 0.0346 (17) | 0.0486 (18) | 0.0016 (13) | 0.0036 (14) | 0.0105 (14) |
| C23 | 0.080 (3) | 0.040 (2) | 0.082 (3) | 0.0076 (19) | 0.016 (2) | 0.019 (2) |
| C24 | 0.089 (3) | 0.036 (2) | 0.093 (3) | 0.015 (2) | 0.010 (3) | 0.011 (2) |
| C25 | 0.087 (3) | 0.050 (2) | 0.071 (3) | 0.030 (2) | 0.018 (2) | 0.001 (2) |
| C26 | 0.069 (2) | 0.048 (2) | 0.057 (2) | 0.0158 (18) | 0.0149 (18) | 0.0071 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pb1—O1 | 2.333 (2) | C10—C11 | 1.386 (4) |
| Pb1—O3 | 2.418 (2) | C11—C12 | 1.383 (5) |
| Pb1—N2 | 2.608 (3) | C11—H11A | 0.9300 |
| Pb1—O2 | 2.644 (2) | C12—C13 | 1.378 (5) |
| Pb1—N1 | 2.656 (3) | C12—H12A | 0.9300 |
| Pb1—O4 | 2.701 (2) | C13—C14 | 1.389 (5) |
| O1—C1 | 1.282 (4) | C13—C16 | 1.509 (5) |
| O2—C1 | 1.239 (4) | C14—C15 | 1.376 (5) |
| O3—C9 | 1.277 (4) | C14—H14A | 0.9300 |
| O4—C9 | 1.240 (4) | C15—H15A | 0.9300 |
| N1—C17 | 1.335 (4) | C16—H16A | 0.9600 |
| N1—C21 | 1.339 (4) | C16—H16B | 0.9600 |
| N2—C26 | 1.333 (4) | C16—H16C | 0.9600 |
| N2—C22 | 1.345 (4) | C17—C18 | 1.378 (5) |
| C1—C2 | 1.500 (4) | C17—H17A | 0.9300 |
| C2—C7 | 1.384 (4) | C18—C19 | 1.358 (5) |
| C2—C3 | 1.385 (4) | C18—H18A | 0.9300 |
| C3—C4 | 1.379 (5) | C19—C20 | 1.384 (5) |
| C3—H3A | 0.9300 | C19—H19A | 0.9300 |
| C4—C5 | 1.375 (5) | C20—C21 | 1.378 (5) |
| C4—H4A | 0.9300 | C20—H20A | 0.9300 |
| C5—C6 | 1.377 (5) | C21—C22 | 1.486 (5) |
| C5—C8 | 1.508 (5) | C22—C23 | 1.382 (5) |
| C6—C7 | 1.383 (5) | C23—C24 | 1.372 (6) |
| C6—H6A | 0.9300 | C23—H23A | 0.9300 |
| C7—H7A | 0.9300 | C24—C25 | 1.359 (6) |
| C8—H8A | 0.9600 | C24—H24A | 0.9300 |
| C8—H8B | 0.9600 | C25—C26 | 1.372 (5) |
| C8—H8C | 0.9600 | C25—H25A | 0.9300 |
| C9—C10 | 1.490 (4) | C26—H26A | 0.9300 |
| C10—C15 | 1.379 (5) | | |
| | | | |
| O1—Pb1—O3 | 84.31 (9) | C15—C10—C11 | 118.0 (3) |
| O1—Pb1—N2 | 83.74 (8) | C15—C10—C9 | 120.4 (3) |
| O3—Pb1—N2 | 77.33 (8) | C11—C10—C9 | 121.6 (3) |

| | | | |
|---|---|---|---|
| O1—Pb1—O2 | 52.25 (7) | C12—C11—C10 | 121.2 (3) |
| O3—Pb1—O2 | 121.72 (8) | C12—C11—H11A | 119.4 |
| N2—Pb1—O2 | 124.68 (8) | C10—C11—H11A | 119.4 |
| O1—Pb1—N1 | 79.77 (8) | C13—C12—C11 | 121.0 (3) |
| O3—Pb1—N1 | 137.27 (8) | C13—C12—H12A | 119.5 |
| N2—Pb1—N1 | 61.75 (8) | C11—C12—H12A | 119.5 |
| O2—Pb1—N1 | 77.17 (8) | C12—C13—C14 | 117.4 (3) |
| O1—Pb1—O4 | 82.72 (8) | C12—C13—C16 | 120.5 (3) |
| O3—Pb1—O4 | 50.77 (8) | C14—C13—C16 | 122.1 (3) |
| N2—Pb1—O4 | 127.29 (8) | C15—C14—C13 | 121.8 (4) |
| O2—Pb1—O4 | 83.26 (7) | C15—C14—H14A | 119.1 |
| N1—Pb1—O4 | 159.20 (9) | C13—C14—H14A | 119.1 |
| C1—O1—Pb1 | 99.27 (19) | C14—C15—C10 | 120.6 (3) |
| C1—O2—Pb1 | 85.80 (18) | C14—C15—H15A | 119.7 |
| C9—O3—Pb1 | 99.36 (19) | C10—C15—H15A | 119.7 |
| C9—O4—Pb1 | 87.0 (2) | C13—C16—H16A | 109.5 |
| C17—N1—C21 | 118.3 (3) | C13—C16—H16B | 109.5 |
| C17—N1—Pb1 | 119.9 (2) | H16A—C16—H16B | 109.5 |
| C21—N1—Pb1 | 121.1 (2) | C13—C16—H16C | 109.5 |
| C26—N2—C22 | 118.0 (3) | H16A—C16—H16C | 109.5 |
| C26—N2—Pb1 | 119.3 (2) | H16B—C16—H16C | 109.5 |
| C22—N2—Pb1 | 122.6 (2) | N1—C17—C18 | 123.3 (3) |
| O2—C1—O1 | 122.5 (3) | N1—C17—H17A | 118.4 |
| O2—C1—C2 | 119.8 (3) | C18—C17—H17A | 118.4 |
| O1—C1—C2 | 117.7 (3) | C19—C18—C17 | 118.5 (4) |
| C7—C2—C3 | 118.6 (3) | C19—C18—H18A | 120.7 |
| C7—C2—C1 | 119.6 (3) | C17—C18—H18A | 120.7 |
| C3—C2—C1 | 121.8 (3) | C18—C19—C20 | 118.9 (3) |
| C4—C3—C2 | 120.3 (3) | C18—C19—H19A | 120.5 |
| C4—C3—H3A | 119.9 | C20—C19—H19A | 120.5 |
| C2—C3—H3A | 119.9 | C21—C20—C19 | 119.8 (3) |
| C5—C4—C3 | 121.7 (3) | C21—C20—H20A | 120.1 |
| C5—C4—H4A | 119.2 | C19—C20—H20A | 120.1 |
| C3—C4—H4A | 119.2 | N1—C21—C20 | 121.1 (3) |
| C4—C5—C6 | 117.7 (3) | N1—C21—C22 | 116.7 (3) |
| C4—C5—C8 | 120.4 (4) | C20—C21—C22 | 122.2 (3) |
| C6—C5—C8 | 121.9 (4) | N2—C22—C23 | 120.9 (3) |
| C5—C6—C7 | 121.6 (3) | N2—C22—C21 | 117.2 (3) |
| C5—C6—H6A | 119.2 | C23—C22—C21 | 121.9 (3) |
| C7—C6—H6A | 119.2 | C24—C23—C22 | 120.4 (4) |
| C6—C7—C2 | 120.1 (3) | C24—C23—H23A | 119.8 |
| C6—C7—H7A | 120.0 | C22—C23—H23A | 119.8 |
| C2—C7—H7A | 120.0 | C25—C24—C23 | 118.1 (4) |
| C5—C8—H8A | 109.5 | C25—C24—H24A | 120.9 |
| C5—C8—H8B | 109.5 | C23—C24—H24A | 120.9 |
| H8A—C8—H8B | 109.5 | C24—C25—C26 | 119.6 (4) |
| C5—C8—H8C | 109.5 | C24—C25—H25A | 120.2 |
| H8A—C8—H8C | 109.5 | C26—C25—H25A | 120.2 |

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| H8B—C8—H8C | 109.5 | N2—C26—C25 | 122.9 (4) |
| O4—C9—O3 | 122.8 (3) | N2—C26—H26A | 118.6 |
| O4—C9—C10 | 120.4 (3) | C25—C26—H26A | 118.6 |
| O3—C9—C10 | 116.8 (3) | | |