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# Bis($\mu$-5-carboxybenzene-1,3-dicarboxylato)-$\kappa^3O^1,O^{1'}:O^3;\kappa^3O^3:O^1,O^{1'}$-bis[(2-phenyl-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene-$\kappa^2N^7,N^8$)lead(II)]

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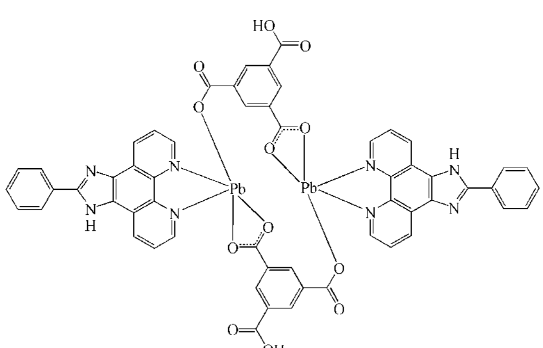
Key indicators: single-crystal X-ray study; $T$ = 292 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.024; $wR$ factor = 0.055; data-to-parameter ratio = 11.3.

In the title compound, $[Pb_2(C_9H_4O_6)_2(C_{19}H_{12}N_4)_2]$, the $Pb^{II}$ atom is five-coordinated by two N atoms from a chelating 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene (*L*) ligand and three O atoms from two Hbtc ligands ($H_3$btc is benzene-1,3,5-tricarboxylic acid), resulting in a distorted $PbN_2O_3$ coordination. Two $Pb^{II}$ atoms are bridged by the Hbtc ligands, forming a discrete centrosymmetric dinuclear complex. Intermolecular N—H⋯O and O—H⋯O hydrogen bonds and $\pi$–$\pi$ interactions between the pyridine and imidazole rings, and between the pyridyl rings of the *L* ligands [centroid–centroid distances = 3.600 (6) and 3.732 (6) Å] lead to a three-dimensional supramolecular structure.

## Related literature

For general background to the structures and potential applications of supramolecular architectures, see: Che *et al.* (2008). For a related structure, see: Liu *et al.* (2009). For the ligand synthesis, see: Steck & Day (1943).




## Experimental

*Crystal data*

| | |
|---|---|
| $[Pb_2(C_9H_4O_6)_2(C_{19}H_{12}N_4)_2]$ | $\gamma$ = 68.680 (4)° |
| $M_r$ = 1423.28 | $V$ = 1137.74 (9) Å$^3$ |
| Triclinic, $P\overline{1}$ | $Z$ = 1 |
| $a$ = 9.2776 (3) Å | Mo $K\alpha$ radiation |
| $b$ = 11.4409 (5) Å | $\mu$ = 7.47 mm$^{-1}$ |
| $c$ = 12.2764 (6) Å | $T$ = 292 K |
| $\alpha$ = 73.820 (4)° | 0.30 × 0.26 × 0.23 mm |
| $\beta$ = 72.754 (4)° | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R Ultra CCD diffractometer | 5399 measured reflections |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006) | 3979 independent reflections |
| $T_{min}$ = 0.122, $T_{max}$ = 0.179 | 3547 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.021 |

*Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.024 | 352 parameters |
| $wR(F^2)$ = 0.055 | H-atom parameters constrained |
| $S$ = 1.00 | $\Delta\rho_{max}$ = 0.82 e Å$^{-3}$ |
| 3979 reflections | $\Delta\rho_{min}$ = −1.28 e Å$^{-3}$ |

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

| | | | |
|---|---|---|---|
| Pb—N1 | 2.561 (4) | Pb—O3 | 2.530 (3) |
| Pb—N2 | 2.449 (3) | Pb—O6$^{i}$ | 2.903 (3) |
| Pb—O1$^{i}$ | 2.342 (3) | | |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N4—H4⋯O2$^{ii}$ | 0.86 | 1.97 | 2.815 (5) | 169 |
| O4—H4$A$⋯O6$^{iii}$ | 0.82 | 1.83 | 2.653 (4) | 177 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

The authors thank Jiangsu University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2360).

## References

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m1651-m1652 [ **doi:10.1107/S1600536810045812** ]

# Bis($\mu$-5-carboxybenzene-1,3-dicarboxylato)-$\kappa^3O^1,O^{1'}:O^3;\kappa^3O^3:O^1,O^{1'}$-bis[(2-phenyl-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene-$\kappa^2N^7,N^8$)lead(II)]

**J. Chen, X.-C. Wang and C.-X. Li**

## Comment

The design and construction of supramolecular architectures have received considerable attention in recent years, mostly motivated by their intriguing structural features and potential applications in catalysis, magnetism, molecular adsorption, non-linear optics and molecular sensing (Che *et al.*, 2008). 2-Phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene (*L*) as an important phenanthroline derivative possesses fruitful aromatic systems and is a good candidate for the construction of metal–organic supramolecular architectures (Liu *et al.*, 2009). In this paper, we selected benzene-1,3,5-tricarboxylic acid ($H_3$btc) as a linker and *L* as a secondary ligand, resulting in the title complex.

In the title compound, the $Pb^{II}$ atom is surrounded by two N atoms from one *L* ligand and three O atoms from two Hbtc ligands (Fig. 1). The neighboring two $Pb^{II}$ atoms are bridged by the two Hbtc ligands, forming a sixteen-membered ring with a long Pb···Pb distance of 8.3037 (5) Å. Adjacent dimers are further linked through intermolecular N—H···O and O—H···O hydrogen bonds and π–π interactions between the pyridyl and imidazole rings and between the pyridyl rings of the *L* ligands [centroid–centroid distances = 3.600 (6) and 3.732 (6) Å], leading to a three-dimensional supramolecular structure (Fig. 2).

## Experimental

The *L* ligand was synthesized according to the literature method (Steck & Day, 1943). The title compound was synthesized under hydrothermal conditions. A mixture of *L* (0.060 g, 0.2 mmol), $H_3$btc (0.042 g, 0.2 mmol), $Pb(NO_3)_2$ (0.066 g, 0.2 mmol) and water (10 ml) in a mole ratio of 1:1:1:5000 was placed in a 25 ml Teflon-lined autoclave and heated for 3 d at 433 K under autogenous pressure. Upon cooling and opening the bomb, yellow block-shaped crystals were obtained, washed with $H_2O$ and dried in air (yield: 65% based on Pb).

## Refinement

H atoms on C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C,N). H atom of the carboxyl group was located from a difference Fourier map and refined as riding, with O—H = 0.82 Å and $U_{iso}$(H) = 1.5$U_{eq}$(O).

## Figures

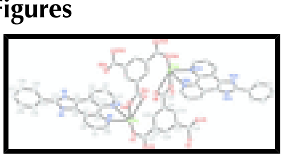

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (A) 1-*x*, 1-*y*, 1-*z*.]

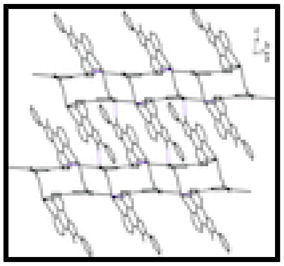

Fig. 2. Crystal packing of the title compound, with hydrogen bonds indicated by dotted lines.

## Bis(μ-5-carboxybenzene-1,3-dicarboxylato)-κ$^3$*O*$^1$,*O*$^{1'}$: *O*$^3$;κ$^3$*O*$^3$:*O*$^1$,*O*$^{1'}$-bis[(2-phenyl- 1,3,7,8-tetraazacyclopenta[*l*]phenanthrene- κ$^2$*N*$^7$,*N*$^8$)lead(II)]

### *Crystal data*

| | |
|---|---|
| $[Pb_2(C_9H_4O_6)_2(C_{19}H_{12}N_4)_2]$ | $Z = 1$ |
| $M_r = 1423.28$ | $F(000) = 684$ |
| Triclinic, $P\bar{1}$ | $D_x = 2.077$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo *K*α radiation, λ = 0.71073 Å |
| $a = 9.2776$ (3) Å | Cell parameters from 6223 reflections |
| $b = 11.4409$ (5) Å | θ = 4.3–29.1° |
| $c = 12.2764$ (6) Å | μ = 7.47 mm$^{-1}$ |
| α = 73.820 (4)° | $T = 292$ K |
| β = 72.754 (4)° | Block, yellow |
| γ = 68.680 (4)° | 0.30 × 0.26 × 0.23 mm |
| $V = 1137.74$ (9) Å$^3$ | |

### *Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R Ultra CCD diffractometer | 3979 independent reflections |
| Radiation source: fine-focus sealed tube | 3547 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.021$ |
| ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 4.3°$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006) | $h = -11 \rightarrow 11$ |
| $T_{min} = 0.122$, $T_{max} = 0.179$ | $k = -12 \rightarrow 13$ |
| 5399 measured reflections | $l = -14 \rightarrow 14$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.055$ | H-atom parameters constrained |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.0349P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| 3979 reflections | $(\Delta/\sigma)_{max} = 0.006$ |
| 352 parameters | $\Delta\rho_{max} = 0.82$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -1.28$ e Å$^{-3}$ |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.7189 (5) | 0.2900 (4) | 0.0863 (4) | 0.0311 (11) |
| H1 | 0.6208 | 0.3528 | 0.0892 | 0.037* |
| C2 | 0.8282 (6) | 0.2868 (5) | −0.0199 (4) | 0.0340 (11) |
| H2 | 0.8024 | 0.3455 | −0.0862 | 0.041* |
| C3 | 0.9727 (5) | 0.1970 (4) | −0.0252 (4) | 0.0284 (10) |
| H3 | 1.0473 | 0.1940 | −0.0952 | 0.034* |
| C4 | 1.0091 (5) | 0.1086 (4) | 0.0756 (4) | 0.0230 (9) |
| C5 | 1.1546 (5) | 0.0094 (4) | 0.0827 (4) | 0.0235 (9) |
| C6 | 1.1849 (5) | −0.0717 (4) | 0.1856 (4) | 0.0219 (9) |
| C7 | 1.0700 (4) | −0.0637 (4) | 0.2914 (3) | 0.0183 (8) |
| C8 | 1.0944 (5) | −0.1447 (4) | 0.3980 (4) | 0.0236 (9) |
| H8 | 1.1921 | −0.2058 | 0.4036 | 0.028* |
| C9 | 0.9727 (5) | −0.1323 (4) | 0.4929 (4) | 0.0257 (10) |
| H9 | 0.9871 | −0.1848 | 0.5643 | 0.031* |
| C10 | 0.8272 (5) | −0.0415 (4) | 0.4835 (4) | 0.0239 (9) |
| H10 | 0.7448 | −0.0361 | 0.5491 | 0.029* |
| C11 | 0.9200 (5) | 0.0296 (4) | 0.2884 (3) | 0.0188 (8) |
| C12 | 0.8917 (5) | 0.1180 (4) | 0.1795 (3) | 0.0207 (9) |
| C13 | 1.3926 (5) | −0.1295 (4) | 0.0540 (4) | 0.0251 (9) |
| C14 | 1.5482 (5) | −0.2019 (4) | −0.0049 (4) | 0.0248 (9) |
| C19 | 1.6161 (5) | −0.1588 (5) | −0.1198 (4) | 0.0335 (11) |
| H19 | 1.5631 | −0.0815 | −0.1614 | 0.040* |
| C18 | 1.7622 (6) | −0.2314 (5) | −0.1714 (4) | 0.0407 (13) |
| H18 | 1.8074 | −0.2031 | −0.2483 | 0.049* |
| C17 | 1.8423 (6) | −0.3458 (6) | −0.1105 (5) | 0.0493 (15) |
| H17 | 1.9410 | −0.3941 | −0.1462 | 0.059* |
| C26 | 0.2977 (4) | 0.2718 (4) | 0.6601 (3) | 0.0183 (8) |
| C24 | 0.1360 (5) | 0.3197 (4) | 0.6642 (3) | 0.0219 (9) |
| H24 | 0.0784 | 0.2638 | 0.6764 | 0.026* |
| C23 | 0.0600 (5) | 0.4498 (4) | 0.6502 (4) | 0.0206 (9) |
| C22 | 0.1453 (5) | 0.5317 (4) | 0.6363 (4) | 0.0223 (9) |
| H22 | 0.0948 | 0.6194 | 0.6255 | 0.027* |
| C21 | 0.3059 (4) | 0.4849 (4) | 0.6381 (4) | 0.0203 (9) |
| C25 | 0.3821 (4) | 0.3546 (4) | 0.6483 (3) | 0.0191 (9) |
| H25 | 0.4901 | 0.3226 | 0.6472 | 0.023* |
| C27 | 0.3789 (5) | 0.1300 (4) | 0.6694 (4) | 0.0204 (9) |
| C28 | −0.1124 (5) | 0.5072 (4) | 0.6481 (4) | 0.0230 (9) |
| C20 | 0.3893 (5) | 0.5775 (4) | 0.6332 (4) | 0.0224 (9) |
| C16 | 1.7755 (6) | −0.3883 (6) | 0.0038 (5) | 0.0504 (15) |
| H16 | 1.8298 | −0.4651 | 0.0452 | 0.060* |
| C15 | 1.6285 (6) | −0.3171 (5) | 0.0564 (4) | 0.0380 (12) |

| | | | | |
|---|---|---|---|---|
| H15 | 1.5834 | −0.3462 | 0.1330 | 0.046* |
| N1 | 0.7482 (4) | 0.2074 (3) | 0.1833 (3) | 0.0232 (8) |
| N2 | 0.8010 (4) | 0.0378 (3) | 0.3847 (3) | 0.0191 (7) |
| N4 | 1.2883 (4) | −0.0273 (3) | −0.0012 (3) | 0.0244 (8) |
| H4 | 1.3037 | 0.0068 | −0.0739 | 0.029* |
| N3 | 1.3343 (4) | −0.1584 (4) | 0.1674 (3) | 0.0259 (8) |
| O3 | 0.4905 (4) | 0.0925 (3) | 0.5863 (3) | 0.0346 (8) |
| O2 | 0.3312 (4) | 0.0561 (3) | 0.7562 (3) | 0.0312 (7) |
| O1 | 0.3317 (3) | 0.6937 (3) | 0.5876 (3) | 0.0281 (7) |
| O6 | 0.5074 (3) | 0.5389 (3) | 0.6780 (3) | 0.0380 (8) |
| O5 | −0.1757 (3) | 0.6197 (3) | 0.6241 (3) | 0.0371 (8) |
| O4 | −0.1880 (3) | 0.4204 (3) | 0.6780 (3) | 0.0395 (8) |
| H4A | −0.2815 | 0.4561 | 0.6755 | 0.059* |
| Pb | 0.537207 (17) | 0.188377 (15) | 0.371460 (14) | 0.02330 (7) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.032 (2) | 0.023 (2) | 0.035 (3) | −0.0044 (19) | −0.012 (2) | 0.000 (2) |
| C2 | 0.042 (3) | 0.029 (3) | 0.024 (2) | −0.007 (2) | −0.014 (2) | 0.007 (2) |
| C3 | 0.036 (2) | 0.028 (2) | 0.017 (2) | −0.011 (2) | −0.0024 (19) | 0.000 (2) |
| C4 | 0.026 (2) | 0.023 (2) | 0.020 (2) | −0.0090 (18) | −0.0063 (18) | −0.0022 (18) |
| C5 | 0.024 (2) | 0.024 (2) | 0.023 (2) | −0.0074 (18) | −0.0021 (18) | −0.0083 (19) |
| C6 | 0.022 (2) | 0.024 (2) | 0.021 (2) | −0.0061 (18) | −0.0059 (18) | −0.0061 (19) |
| C7 | 0.020 (2) | 0.021 (2) | 0.016 (2) | −0.0078 (16) | −0.0030 (17) | −0.0051 (17) |
| C8 | 0.026 (2) | 0.018 (2) | 0.022 (2) | −0.0015 (17) | −0.0045 (18) | −0.0030 (18) |
| C9 | 0.031 (2) | 0.024 (2) | 0.015 (2) | −0.0024 (19) | −0.0059 (19) | −0.0004 (18) |
| C10 | 0.027 (2) | 0.024 (2) | 0.016 (2) | −0.0069 (18) | −0.0001 (18) | −0.0027 (19) |
| C11 | 0.022 (2) | 0.020 (2) | 0.017 (2) | −0.0097 (17) | −0.0022 (17) | −0.0051 (17) |
| C12 | 0.028 (2) | 0.019 (2) | 0.016 (2) | −0.0071 (17) | −0.0076 (18) | −0.0024 (17) |
| C13 | 0.022 (2) | 0.029 (2) | 0.022 (2) | −0.0086 (18) | −0.0009 (18) | −0.007 (2) |
| C14 | 0.023 (2) | 0.032 (3) | 0.021 (2) | −0.0108 (19) | 0.0004 (18) | −0.010 (2) |
| C19 | 0.030 (2) | 0.039 (3) | 0.027 (2) | −0.006 (2) | −0.002 (2) | −0.009 (2) |
| C18 | 0.031 (3) | 0.059 (4) | 0.026 (3) | −0.010 (2) | 0.003 (2) | −0.013 (3) |
| C17 | 0.033 (3) | 0.056 (4) | 0.050 (4) | 0.003 (3) | −0.003 (3) | −0.027 (3) |
| C26 | 0.020 (2) | 0.020 (2) | 0.013 (2) | −0.0057 (16) | −0.0014 (16) | −0.0024 (17) |
| C24 | 0.023 (2) | 0.023 (2) | 0.022 (2) | −0.0109 (18) | −0.0027 (18) | −0.0046 (18) |
| C23 | 0.019 (2) | 0.022 (2) | 0.022 (2) | −0.0048 (17) | −0.0064 (17) | −0.0042 (18) |
| C22 | 0.022 (2) | 0.017 (2) | 0.024 (2) | −0.0020 (17) | −0.0048 (18) | −0.0033 (18) |
| C21 | 0.018 (2) | 0.018 (2) | 0.023 (2) | −0.0045 (16) | −0.0051 (17) | −0.0022 (18) |
| C25 | 0.0150 (19) | 0.018 (2) | 0.020 (2) | −0.0027 (16) | −0.0007 (16) | −0.0034 (17) |
| C27 | 0.020 (2) | 0.019 (2) | 0.025 (2) | −0.0054 (17) | −0.0094 (19) | −0.0044 (19) |
| C28 | 0.017 (2) | 0.026 (2) | 0.024 (2) | −0.0057 (18) | −0.0034 (18) | −0.0049 (19) |
| C20 | 0.017 (2) | 0.024 (2) | 0.025 (2) | −0.0067 (17) | 0.0019 (18) | −0.0089 (19) |
| C16 | 0.044 (3) | 0.046 (3) | 0.047 (3) | 0.006 (3) | −0.010 (3) | −0.014 (3) |
| C15 | 0.039 (3) | 0.036 (3) | 0.027 (3) | 0.003 (2) | −0.007 (2) | −0.008 (2) |
| N1 | 0.0248 (18) | 0.0207 (19) | 0.0231 (19) | −0.0057 (15) | −0.0088 (15) | −0.0008 (16) |
| N2 | 0.0187 (16) | 0.0216 (18) | 0.0160 (18) | −0.0080 (14) | −0.0015 (14) | −0.0024 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N4 | 0.0246 (18) | 0.027 (2) | 0.0182 (19) | −0.0072 (15) | 0.0006 (15) | −0.0051 (16) |
| N3 | 0.0224 (18) | 0.030 (2) | 0.021 (2) | −0.0047 (16) | −0.0026 (15) | −0.0052 (17) |
| O3 | 0.0308 (17) | 0.0241 (17) | 0.0301 (18) | 0.0034 (14) | 0.0087 (14) | −0.0088 (15) |
| O2 | 0.0413 (18) | 0.0236 (17) | 0.0254 (17) | −0.0120 (14) | −0.0078 (14) | 0.0033 (14) |
| O1 | 0.0315 (16) | 0.0210 (16) | 0.0350 (18) | −0.0103 (13) | −0.0128 (14) | −0.0013 (14) |
| O6 | 0.0233 (16) | 0.0293 (18) | 0.067 (2) | −0.0096 (14) | −0.0204 (17) | −0.0045 (17) |
| O5 | 0.0235 (16) | 0.0238 (18) | 0.060 (2) | −0.0008 (13) | −0.0140 (16) | −0.0062 (16) |
| O4 | 0.0156 (14) | 0.0305 (18) | 0.071 (2) | −0.0068 (13) | −0.0128 (16) | −0.0040 (17) |
| Pb | 0.01918 (9) | 0.02098 (10) | 0.02834 (11) | −0.00717 (6) | −0.00471 (7) | −0.00173 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.328 (6) | C18—H18 | 0.9300 |
| C1—C2 | 1.394 (7) | C17—C16 | 1.383 (8) |
| C1—H1 | 0.9300 | C17—H17 | 0.9300 |
| C2—C3 | 1.357 (6) | C26—C25 | 1.388 (6) |
| C2—H2 | 0.9300 | C26—C24 | 1.388 (5) |
| C3—C4 | 1.403 (6) | C26—C27 | 1.508 (5) |
| C3—H3 | 0.9300 | C24—C23 | 1.382 (6) |
| C4—C12 | 1.412 (6) | C24—H24 | 0.9300 |
| C4—C5 | 1.421 (6) | C23—C22 | 1.379 (6) |
| C5—N4 | 1.371 (5) | C23—C28 | 1.497 (5) |
| C5—C6 | 1.380 (6) | C22—C21 | 1.393 (5) |
| C6—N3 | 1.377 (5) | C22—H22 | 0.9300 |
| C6—C7 | 1.416 (6) | C21—C25 | 1.386 (5) |
| C7—C8 | 1.404 (6) | C21—C20 | 1.502 (6) |
| C7—C11 | 1.416 (5) | C25—H25 | 0.9300 |
| C8—C9 | 1.359 (6) | C27—O2 | 1.239 (5) |
| C8—H8 | 0.9300 | C27—O3 | 1.262 (5) |
| C9—C10 | 1.386 (6) | C28—O5 | 1.196 (5) |
| C9—H9 | 0.9300 | C28—O4 | 1.327 (5) |
| C10—N2 | 1.324 (5) | C20—O6 | 1.253 (5) |
| C10—H10 | 0.9300 | C20—O1 | 1.269 (5) |
| C11—N2 | 1.356 (5) | C16—C15 | 1.380 (7) |
| C11—C12 | 1.463 (6) | C16—H16 | 0.9300 |
| C12—N1 | 1.350 (5) | C15—H15 | 0.9300 |
| C13—N3 | 1.330 (6) | Pb—N1 | 2.561 (4) |
| C13—N4 | 1.374 (5) | Pb—N2 | 2.449 (3) |
| C13—C14 | 1.462 (6) | Pb—O1$^{i}$ | 2.342 (3) |
| C14—C15 | 1.387 (6) | Pb—O3 | 2.530 (3) |
| C14—C19 | 1.394 (6) | Pb—O6$^{i}$ | 2.903 (3) |
| C19—C18 | 1.376 (6) | O4—H4A | 0.8200 |
| C19—H19 | 0.9300 | N4—H4 | 0.8600 |
| C18—C17 | 1.379 (8) | | |
| N1—C1—C2 | 123.1 (4) | C23—C24—C26 | 120.5 (4) |
| N1—C1—H1 | 118.5 | C23—C24—H24 | 119.8 |
| C2—C1—H1 | 118.5 | C26—C24—H24 | 119.8 |
| C3—C2—C1 | 119.1 (4) | C22—C23—C24 | 119.3 (4) |

| | | | |
|---|---|---|---|
| C3—C2—H2 | 120.4 | C22—C23—C28 | 117.9 (4) |
| C1—C2—H2 | 120.4 | C24—C23—C28 | 122.8 (4) |
| C2—C3—C4 | 119.6 (4) | C23—C22—C21 | 121.0 (4) |
| C2—C3—H3 | 120.2 | C23—C22—H22 | 119.5 |
| C4—C3—H3 | 120.2 | C21—C22—H22 | 119.5 |
| C3—C4—C12 | 117.7 (4) | C25—C21—C22 | 119.2 (4) |
| C3—C4—C5 | 125.7 (4) | C25—C21—C20 | 122.2 (3) |
| C12—C4—C5 | 116.5 (4) | C22—C21—C20 | 118.6 (4) |
| N4—C5—C6 | 106.2 (3) | C21—C25—C26 | 120.1 (3) |
| N4—C5—C4 | 131.0 (4) | C21—C25—H25 | 119.9 |
| C6—C5—C4 | 122.8 (4) | C26—C25—H25 | 119.9 |
| N3—C6—C5 | 110.6 (4) | O2—C27—O3 | 123.3 (4) |
| N3—C6—C7 | 127.5 (4) | O2—C27—C26 | 118.9 (4) |
| C5—C6—C7 | 121.8 (4) | O3—C27—C26 | 117.7 (4) |
| C8—C7—C11 | 118.2 (4) | O5—C28—O4 | 123.7 (4) |
| C8—C7—C6 | 124.0 (4) | O5—C28—C23 | 123.3 (4) |
| C11—C7—C6 | 117.8 (3) | O4—C28—C23 | 113.0 (4) |
| C9—C8—C7 | 118.9 (4) | O6—C20—O1 | 122.8 (4) |
| C9—C8—H8 | 120.6 | O6—C20—C21 | 119.3 (4) |
| C7—C8—H8 | 120.6 | O1—C20—C21 | 117.8 (3) |
| C8—C9—C10 | 120.1 (4) | C17—C16—C15 | 120.1 (5) |
| C8—C9—H9 | 119.9 | C17—C16—H16 | 120.0 |
| C10—C9—H9 | 119.9 | C15—C16—H16 | 120.0 |
| N2—C10—C9 | 122.6 (4) | C16—C15—C14 | 120.0 (5) |
| N2—C10—H10 | 118.7 | C16—C15—H15 | 120.0 |
| C9—C10—H10 | 118.7 | C14—C15—H15 | 120.0 |
| N2—C11—C7 | 121.1 (3) | C1—N1—C12 | 118.4 (4) |
| N2—C11—C12 | 119.2 (3) | C1—N1—Pb | 123.8 (3) |
| C7—C11—C12 | 119.7 (4) | C12—N1—Pb | 117.3 (3) |
| N1—C12—C4 | 122.0 (4) | C10—N2—C11 | 119.1 (3) |
| N1—C12—C11 | 116.8 (4) | C10—N2—Pb | 120.9 (3) |
| C4—C12—C11 | 121.2 (3) | C11—N2—Pb | 119.9 (2) |
| N3—C13—N4 | 112.4 (4) | C5—N4—C13 | 106.3 (3) |
| N3—C13—C14 | 123.3 (4) | C5—N4—H4 | 126.9 |
| N4—C13—C14 | 124.3 (4) | C13—N4—H4 | 126.9 |
| C15—C14—C19 | 119.8 (4) | C13—N3—C6 | 104.5 (3) |
| C15—C14—C13 | 118.3 (4) | C27—O3—Pb | 130.6 (3) |
| C19—C14—C13 | 121.9 (4) | C20—O1—$Pb^{i}$ | 107.3 (2) |
| C18—C19—C14 | 119.5 (5) | C28—O4—H4A | 109.5 |
| C18—C19—H19 | 120.3 | $O1^{i}$—Pb—N2 | 75.71 (10) |
| C14—C19—H19 | 120.3 | $O1^{i}$—Pb—O3 | 86.66 (11) |
| C19—C18—C17 | 120.8 (5) | N2—Pb—O3 | 79.48 (10) |
| C19—C18—H18 | 119.6 | $O1^{i}$—Pb—N1 | 78.54 (11) |
| C17—C18—H18 | 119.6 | N2—Pb—N1 | 66.07 (10) |
| C18—C17—C16 | 119.8 (5) | O3—Pb—N1 | 144.85 (10) |
| C18—C17—H17 | 120.1 | $O6^{i}$—Pb—N1 | 79.58 (10) |
| C16—C17—H17 | 120.1 | $O6^{i}$—Pb—N2 | 119.29 (10) |

| | | | |
|---|---|---|---|
| C25—C26—C24 | 119.8 (4) | $O6^{i}$—Pb—$O1^{i}$ | 48.50 (10) |
| C25—C26—C27 | 121.0 (3) | $O6^{i}$—Pb—O3 | 113.57 (10) |
| C24—C26—C27 | 119.3 (4) | | |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H4···$O2^{ii}$ | 0.86 | 1.97 | 2.815 (5) | 169 |
| O4—H4A···$O6^{iii}$ | 0.82 | 1.83 | 2.653 (4) | 177 |

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

**Fig. 1**

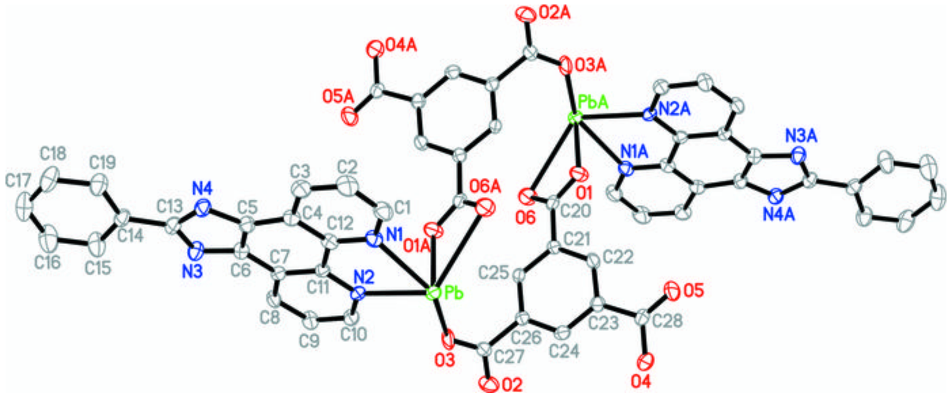
O2A
O4A
O3A
O5A
PbA
N2A
C18
C19
N3A
N1A
C17
C3
C2
O1
06A
C13
N4
C5
C1
O6
C20
C4
C12
N4A
C14
N1
O1A
C21
C22
C16
C15
N3
C6
C7
C11
N2
C25
Pb
O5
C8
C9
C10
C26
C23
C28
O3
C27
C24
O2
O4

Fig. 2