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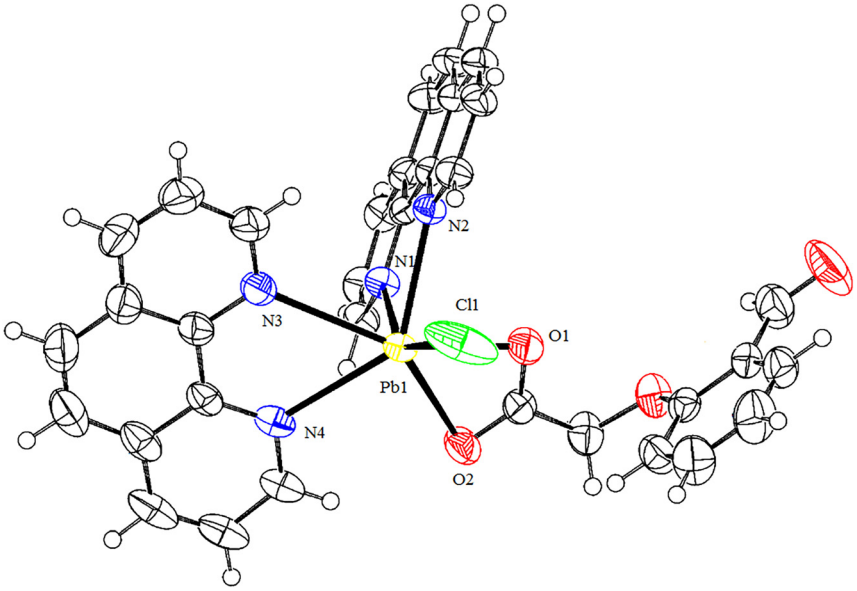
The crystal structure of chlorido-bis(1,10-phenantroline-κ^2N,N')-(2-formylphenoxyacetato-κ^2O,O) lead(II), $C_{33}H_{23}N_4O_4ClPb$



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Abstract

$C_{33}H_{23}N_4O_4ClPb$, monoclinic, $P2_1/n$ (no. 14), a = 11.0932(8) Å, b = 16.7331(10) Å, c = 16.1349(10) Å, β = 107.018(2)°, V = 2863.9(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0364, w$R_{ref}(F^2)$ = 0.0870, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Block, colourless
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	6.03 mm^{-1}
Diffractometer, scan mode:	Bruker D8, φ and ω-scans
θ_{max}, completeness:	27.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	78022, 6505, 0.093
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5367
$N(param)_{refined}$:	388
Programs:	Bruker programs[1], OLEX2[2], SHELX[3], DIAMOND[4]

1 Source of materials

Adding 0.2781 g $PbCl_2$ (1.0 mmol) to 30 ml ethanol-water (v:v = 1:1) solution containing 0.1802 g 2-formylphenoxyacetic acid (1.0 mmol), 0.1982 g 1,10-phenantroline (1.0 mmol) and 0.040 g sodium hydroxide (1.0 mmol) at room temperature. Then the aforementioned mixture was heated at 81 °C for 3 h with stirring. After cooling to room temperature the

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mixture was filtered. The colorless block crystals were received from the filtrate after 25 days.

2 Experimental details

Coordinates of hydrogen atoms were refined without any constraints or restraints. The hydrogen atoms were positioned geometrically. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms.

3 Comment

The synthesis and characterization of lead(II) complexes has been one of the interests of coordination chemistry, as they exhibited novel structure[5–7] and properties such as luminescent property,[8] selective potentiometric microsensor,[9] iodine capture and dye removel,[10] and so on. In this work, a new Pb(II) complex has been synthesized by the assembly of $PbCl_2$, 2-formylphenoxyacetic acid, 1,10-phenantroline and sodium hydroxide. The molecular structure of the title complex is shown in Figure 1. The single crystal X-ray diffraction shows that the Pb(II) complex is made up of one Pb(II) cation, two 1,10-phenantroline molecules, one 2-formylphenoxyacetate ligand, and one chloride ion. The Pb(II) ion is coordinated with four N atoms (N1, N2, N3, and N4) of two 1,10-phenantroline ligands, two O atoms (O1 and O2) of one coordinated H_2O molecules, and two N atoms (N1, N2) of one 2-formylphenoxyacetate ligand, and one chloride ion, which forms a seven-coordinated distorted pentagonal bipyramid coordination geometry (Figure 1). Both 1,10-phenantroline and 2-formylphenoxyacetate ligands are in a bidentate coordination mode. The bond angles of N–Pb1–N, N–Pb–O, O–Pb–O, O–Pb–Cl, and N–Pb–Cl are in the range of 59.30(12)–129.61(12)°, 73.68(13)–151.33(13)°, 49.80(10)°, 94.53(10)–117.41(10)°, and 83.98(9)–148.55(9)°. The lengths of Pb–O bonds, Pb–N bonds, and Pb–Cl bond are in the range of 2.501(4)–2.710(4) Å, 2.531(4)–2.774(4) Å, and 2.9471(17) Å, respectively which are agreement with those in refs. 11 and 12. The dihedral angle of two phenantroline rings is 86.53°. The Pb(II) complex molecules form 1D chained structure by π–π interactions.

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References

1. Bruker. SAINT and SADABS; Bruker AXS Inc.: Madison, Wisconsin, USA, 2000.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
3. Sheldrick, G. M. Crystal Structure Refinement with *SHELXL*. *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. Brandenburg, K. *DIAMOND*. Visual Crystal Structure Information System. Ver. 3.2; Crystal Impact: Bonn, Germany, 2012.
5. Darious, R. S.; Evangeline, H. G.; Perdih, F.; Vedha, S. A. Role of Tetrel Bonds in the Supramolecular Architecture of Tetranuclear Pb(ii) [LL-Thiophene Carboxylate] Complexes C an Experimental and Computational Study. *CrystEngComm* **2024**, *26*, 4098–4106.
6. Song, Y.; Yan, Y.; Zhang, H.; Wang, X. Y. Synthesis and Structural Characterization of a Novel 2D Supramolecular Lead Coordination Polymer with Phenanthroline Derivate and Adipic Acid. *Main Group Met. Chem.* **2021**, *44*, 239–242.
7. Zhang, L. L.; Tang, S. L.; Li, D. J.; Cheng, Y. Z.; Zhang, L. P. Synthesis and Crystal Structure of One New Pb(II) Complex Constructed by 1,10-Phenanthroline and Two Carboxylate Ligands. *Main Group Met. Chem.* **2021**, *44*, 157–164.
8. Cheng, M. L.; Yang, B. X.; Tang, L. Z. P.; Qin, M. N.; Liu, Q.; Tang, X. Y. Pb(II) Coordination Complexes Based on 5-Methyl-1*H*-Pyrazole-3-Carboxylic Acid: Syntheses, Structures and Luminescent Properties. *Chin. J. Inorg. Chem.* **2019**, *35*, 687–694.
9. Çıtlakoğlu, M.; Yolcu, Z. Dinuclear Pb(II) Monomer Complex: Synthesis, Characterization, and Application of Pb(II) Ion-Imprinted Polymer as a Selective Potentiometric Microsensor. *Polyhedron* **2023**, *243*, 116539.
10. Kamal, S.; Khalid, M.; Khan, M. S.; Shahid, M.; Ahmas, M. A Bifunctionalised Pb-Based MOF for Iodine Capture and Dye Removel. *Dalton Trans.* **2023**, *52*, 4501–4516.
11. Wang, L. H.; Tai, H. W.; Li, Q. S.; Xia, Y. P.; Tai, X. S. The Crystal Structure of Tetrakis(6-phenylpyridine-2-carboxylate- κ^2N,O)-bis(μ_2-6-phenylpyridine-2-carboxylate-$\kappa^2O:O'$)-bis(μ_2-6-phenylpyridine-2-carboxylate-$\kappa^3N,O:O$)tetralead(II), $C_{48}H_{32}N_4O_8Pb_2$. *Z. Kristallogr. N. Cryst. Struct.* **2022**, *237*, 1113–1116.
12. Tai, X. S.; Liang, L.; Li, X. T.; Cao, S. H.; Wang, L. H. Crystal Structure of Diaqua-bis(μ_2-6-phenylpyridine-2-carboxylate-$\kappa^3N,O:O$)-bis(6-phenylpyridine-2-carboxylato-κ^2N,O)lead(II)-*N,N*-dimethylformamide-water (1/2/4), $C_{54}H_{58}N_6O_{16}Pb_2$. *Z. Kristallogr. N. Cryst. Struct.* **2021**, *236*, 1199–1201.