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Crystallographic report

Bis(indole-3-acetato)(1,10-phenanthroline)lead(II)

Zhen-Feng Chen[1]*, Ling Huang[1], Rui-Xiang Hu[1], Shao-Ming Shi[1], Hong Liang[1] and Yan Li[2]**

[1]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China
[2]Institute of Chemistry Chinese Academic Science, Beijing 10080, People's Republic of China

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The lead atom in Pb(phen)(IA)$_2$ is in a heavily distorted square pyramidal geometry surrounded by an N_2O_3 donor set with Pb–O distances ranging from 2.354(5) to 2.726(5) Å. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; lead; indole-3-acetic acid

COMMENT

Indole-3-acetic acid (IAH), a phytohormone of the auxin series, is a substance of multifunctional biological significance, and has been established as an essential component of associative plant–microbe interactions[1]. Although a few crystallographic studies on indole-3-acetate complexes are available, such as on $[Pd(IA)(py)]_2{\cdot}4CHCl_3$,[2] $[Pt(bpm)(L\text{–}Ala)](IA){\cdot}7H_2O$,[3] and Cd(phen)$(IA)_2$,[4] thus far, IA complexes with the toxic heavy-metal ion lead(II) have not yet been characterized in this way. Pb(phen)$(IA)_2$ (Fig. 1) is different from its Cd(phen)(indole-3-acetato)$_2$ analogue[4] by virtue of the presence of both chelating and monodentate IA ligands; the Pb···O4 separation is 2.914(5) Å. The lead(II) ion is in a heavily distorted square-pyramidal environment defined by an N_2O_3 donor set. Centrosymmetric pairs are loosely associated via Pb···O2^i interactions of 3.271(5) Å. These, in turn, are connected into a double helical chain via N–H···O interactions.

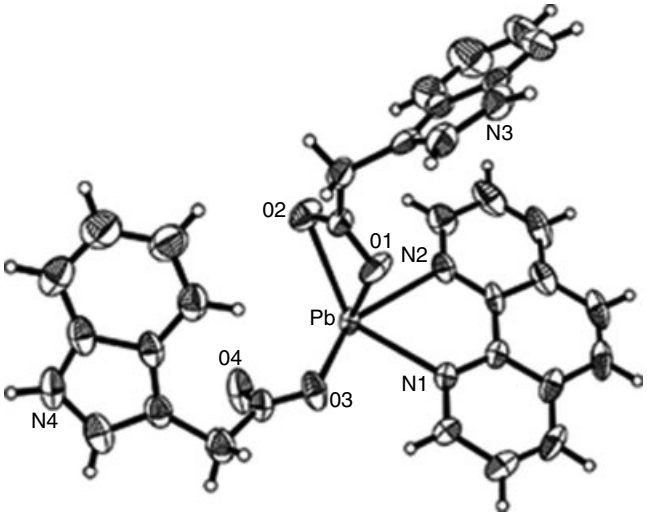

Figure 1. Molecular structure of Pb(phen)$(IA)_2$. Key geometric parameters: Pb–O1 2.354(5), Pb–O2 2.726(5), Pb–O3 2.403(5), Pb–N1 2.509(5), Pb–N2 2.620(5) Å; O1–Pb–O2 50.04(14), O1–Pb–O3 76.51(19), O1–Pb–N1 83.57(15), O1–Pb–N2 80.66(18), O2–Pb–O3 98.90(18), O2–Pb–N1 131.23(15), O2–Pb–N2 90.19(18), O3–Pb–N1 80.95(16), O3–Pb–N2 140.64(16), N1–Pb–N2 64.86(18)°.

EXPERIMENTAL

Pb(phen)$(IA)_2$ was prepared by a method similar to that for Cd(phen)$(IA)_2$,[4] with $Pb(OAc)_2$ replacing $Cd(OAc)_2$. Yield 50% (based on IAH). Anal. Found: C, 52.35; H, 3.34; N, 7.52. Calc. for $C_{32}H_{24}N_4O_4Pb$: C, 52.24; H, 3.29; N, 7.62%. Data were collected at 293(2) K on a Rigaku R-axis RAPID IP diffractometer using graphite-monochromated Mo Kα radiation on a block 0.15 × 0.21 × 0.23 mm^3.

*Correspondence to: Zhen-Feng Chen, Department of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China.
E-mail: chenzfgxnu@yahoo.com
**Correspondence to: Hong Liang, Department of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China.
E-mail: chenzfgxnu@yahoo.com
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$C_{32}H_{24}N_4O_4Pb$, $M = 735.74$, monoclinic, $P2_1/n$, $a = 12.8592(19)$, $b = 13.0736(16)$, $c = 17.064(3)$ Å, $\beta = 105.504(4)°$, $V = 2764.4(7)$ Å^3, $Z = 4$, $D_c = 1.768$ g cm^{-3}, $R = 0.040$ (3654 data with $I > 2\sigma(I)$), $\theta_{max} = 27.4°$), $wR = 0.080$ (all 6205 data), $\rho_{max} = 1.15$ e$^-$ Å^{-3} (near lead). Programs used: SHELXTL97, ORTEP. CCDC deposition number: 239616.

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