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Crystallographic report

Crystal structure of bis[dipyrido[3,2,-*a*:2′,3′-*c*]phenazine]lead(II)diiodide

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The mononuclear lead(II) complex of formula $[PbI_2(DPPZ)_2]$ (*DPPZ* = *dipyrido*[3,2,-*a*:2′,3′-*c*]phenazine) has two-fold symmetry and features a distorted octahedral geometry for lead defined by an N_4I_2 donor set. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: mononuclear lead(II) complex; DPPZ; single-crystal; $\pi-\pi$ stacking

COMMENT

Metal polypyridyl coordination compounds, such as ruthenium polypyridyl complexes, have been extensively studied in the past few years, as their unusual binding properties combined with their general photoactivity make them suitable candidates as DNA secondary structure probes, photocleavers and antitumor drugs.[1] It is of note that despite the interesting properties and the large amount of work that has been performed on complexes with dipyrido[3,2,-*a*:2′,3′-*c*]phenazine (DPPZ),[2] there are relatively few crystal structures available for these complexes. The mononuclear lead(II) complex $[PbI_2(DPPZ)_2]$ (**I**) crystallizes in space group $C2/c$ and has two fold symmetry (Fig. 1). The six-coordinated lead atom is surrounded by four nitrogen atoms from two ligands and two iodides to form a distorted octahedral geometry. The Pb–I distance is 3.1331(4) Å, which is 0.06 Å shorter than that of $[PbI_2(4,4'\text{-bipy})]_n$.[3] The Pb–N distances are 2.612(4) and 2.621(4) Å, and these are about 0.09 Å longer than those in $[PbI_2(2,2'\text{-bipy})]$ and $[PbI_2(1,10\text{-phen})]$.[4,5] The N(1)–Pb–N(2) bite angle in **I** is only 62.57(12)°, whereas the bite angles in other DPPZ complexes are in the range of 74–82°.[6,7]

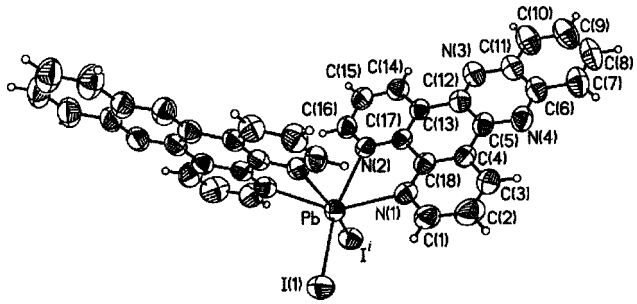

Figure 1. Molecular structure of **I**. Selected bond distances (Å) and angles (°): Pb–I 3.1331(4), Pb–N(1) 2.621(4), Pb–N(2) 2.612(4), I–Pb–N(1) 102.75(9), I–Pb–N(2) 85.56(9), I–Pb–I(1)^i 108.04(2), I–Pb–N(1)^i 96.05(9), I–Pb–N(2)^i 157.27(8), N(2)–Pb–N(2)^i 88.06(2), N(1)–Pb–N(2) 62.57(1), N(1)–Pb–N(1)^i 147.78(2), N(1)–Pb–N(2)^i 93.53(1). Symmetry operation *i*: $-x$, y, $3/2-z$.

EXPERIMENTAL

A dimethylformamide (DMF) solution containing 0.5 mmol PbI_2 was put on one side of a H-type tube and a DMF solution containing 1.0 mmol DPPZ on the other side, single crystals of **I** appeared after slow diffusion. Intensity data for **I** were collected at 293 K on a Bruker AXS SMART CCD diffractometer for a red block $0.15 \times 0.20 \times 0.30$ mm^3. $C_{36}H_{20}I_2N_8Pb$, $M = 1025.59$, monoclinic, $C2/c$, $a = 8.6715(9)$, $b = 13.1956(1)$, $c = 28.629(3)$ Å, $\beta = 93.538(2)°$, $V = 3269.6(6)$ Å^3, $Z = 4$, 3776 unique data (θ_{max} 28.0°), $R = 0.035$ [$I > 2\sigma(I)$], $wR = 0.084$ (all data), $\rho_{max} = 1.13$ e $-$ Å^{-3} (near lead). Programs used: teXsan, SHELXL and ORTEP. CCDC deposition number: 195974.

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