Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Poly[lead(II)-μ-4,4-bipyridine-N:N'-di-μ-bromo]

Yong Cui *et al.*

Electronic paper
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Poly[lead(II)-μ-4,4-bipyridine-N:N'-di-μ-bromo]

Yong Cui,* Jing Ren, Gang Chen, Weichao Yu and Yitai Qian

Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China
Correspondence e-mail: ycui@ustc.edu.cn

Received 29 September 2000
Accepted 23 October 2000

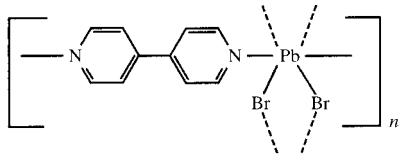
Data validation number: IUC0000303

The title complex, $[PbBr_2(bipy)]_n$ (bipy is 4,4′-bipyridine, $C_{10}H_8N_2$), was obtained by hydrothermal reaction of $Pb(O_2CCH_3)$, NaBr and bipy. The bipy group acts as a linear bifunctional bridge forming a planar $\{-[Pb(bipy)]-\}_n$ belt in the direction of the *b* axis. The remaining lead coordination sites are occupied by Br ions which link Pb centres in adjacent belts through double bridges to form extended two-dimensional layers.

Comment

In recent years, an increasing interest has been given to low-dimensional organic–inorganic hybrid compounds owing to their special magnetic, electronic and optoelectronic properties (Lacroix *et al.*, 1994; Chakravarthy & Guloy, 1997). Studies suggest that complex systems consisting of organic and inorganic components have great potential for the creation of functional materials utilizing the wide variety of properties associated with each component. Lead halide-based (PbX_3, PbX_4 and PbX_5) molecules with ionic-type hybrid compounds have been extensively studied (Conadi *et al.*, 1997; Chakravarthy & Guloy, 1997), because they form a stable exciton with a large binding energy of several hundred meV and exhibit attractive optical properties such as strong and sharp photoluminescence (Papavassiliou & Kontselas, 1995) and electroluminescence (Hattori *et al.*, 1996), and highly efficient nonlinear optical effects (Kondo *et al.*, 1998). However, the lead halide adducts $Pb(L)X_2$ (X = halide and L = ligand) with ligands coordinatively linked to the inorganic backbone have received little attention and structural information on this type of compounds is still rather scarce (Zhu *et al.*, 1999). Herein, the hydrothermal growth and crystal structure of the two-dimensional lead coordination polymer $[PbBr_2(bipy)]_n$ (bipy is 4,4′-bipyridine), (I), is reported.

Structural analysis of (I) reveals that the Pb centre has a distorted octahedral coordination with four μ_2-Br and two bridging 4,4′-bipy at *trans* positions. The Pb—Br bond lengths of 2.999 (2) and 3.008 (2) Å are comparable with those in the reported lead bromides (Klapotke *et al.*, 1999), while the Pb—N bond length of 2.659 (14) Å is significantly longer than those



(I)

in $[PbI_2(L)]_n$ [L is 2,2′-bipyridine; Pb—N = 2.516; L is 1,10-phenanthroline, Pb—N = 2.518 (8); Zhu *et al.*, 1999]. The crystal structure of compound (I) consists of two-dimensional $[PbBr_2(bipy)]$ networks built upon $PbBr_4(bipy)_2$ building blocks. The two-dimensional layers are formed in the *bc* plane by connecting metal centres through bridging Br and 4,4′-bipy ligands. The adjacent bipy ligands are parallel to each other at a distance of 3.74 Å. These layers stack on top of each other along the *c* axis at a distance of *c*/2 to complete the three dimensional structure. Therefore, the present crystal structure is very similar to those observed for $[MCl_2(bipy)]_n$ (M = Fe, Co; Lawandy *et al.*, 1999) and $[HgBr_2(bipy)]_n$ (Pan *et al.*, 1999).

Experimental

A solution of $Pb(O_2CCH_3)$ (1 mmol), NaBr (2 mmol), bipy (1 mmol) and water (10 ml) was heated at 393 K for 3 d in a 23 ml acid digestion bomb. After cooling to room temperature, triangular prismatic crystals of (I) were isolated.

Crystal data

$[PbBr_2(C_{10}H_8N_2)]$
M_r = 523.19
Monoclinic, *C*2/*m*
a = 12.282 (3) Å
b = 12.407 (3) Å
c = 4.2191 (8) Å
β = 95.55 (3)°
V = 639.9 (2) Å^3
Z = 2
D_x = 2.715 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.34–27.51°
μ = 19.397 mm^{-1}
T = 293 (2) K
Triangular prism, colourless
0.10 × 0.10 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (Fair, 1990)
T_{min} = 0.179, T_{max} = 0.212
721 measured reflections
721 independent reflections
709 reflections with $I > 2\sigma(I)$
θ_{max} = 27.51°
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 0$
$l = -5 \rightarrow 0$
3 standard reflections
every 265 reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.128
S = 1.108
721 reflections
39 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0797P)^2 + 7.2192P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.56 e Å^{-3}
$\Delta\rho_{min}$ = −3.85 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pb—N	2.659 (14)	Pb—Br^{i}	3.008 (2)
Pb—Br	2.9992 (18)		
Br^{ii}—Pb—Br^{iii}	89.22 (4)		

Symmetry codes: (i) $x, y, z-1$; (ii) $-1-x, 2-y, 1-z$; (iii) $-1-x, 2-y, 2-z$.

Data collection was curtailed after 93% completion, since the data at the end were very weak. The largest positive and negative features in the final difference synthesis are close to Pb.

Data collection and cell refinement: *CAD*-4 *Software* (Enraf–Noinus, 1989); data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

The authors thank the National Natural Science Foundation of China, China Postdoctoral Science Foundation and Wang Kuanchen Postdoctoral Science Foundation for financial support of this work.

References

Chakravarthy, V. & Guloy, A. M. (1997). *Chem. Commun.* pp. 697–698.
Conadi, A. B., Bruni, S., Cariati, F., Ferrari, A. M., Saccani, A., Sandrolini, F. & Sgaraboto, P (1997). *Inorg. Chim. Acta*, **254**, 137–143.
Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Fair, C. K. (1990). *MolEN*. Enraf–Nonius, Delft, The Netherlands.
Hattori, T., Taira, T., Era, M., Tsutsui, T. & Saito, S. (1996). *Chem. Phys. Lett.* **254**, 103–108.
Klapotke, T. M., Knizek, J., Noth, H. & Krumm, B. (1999). *Polyhedron*, **18**, 839–844.
Kondo, T., Iwamoto, S., Hayase, S., Tanaka, K., Ishi, J., Mizuno, M., Ema, K. & Ito, R. (1998). *Solid State Commun.* **105**, 503–504.
Lacroix, P. G., Clement, R., Nakatani, K., Zyss, J. & Ledoux, I. (1994). *Science*, **263**, 658–660.
Lawandy, M. A., Huang, X, Wang, R.-J., Li, J., Lu, J. Y., Yuen, T. & Lin, C. L. (1999). *Inorg. Chem.* **38**, 5410–5414.
Papavassiliou, G. C. & Kontselas, I. B. (1995). *Synth. Met.* **71**, 1713–1776.
Pan, L., Zheng, N., Wu, Y., Wu, S. & Huang, X. (1999). *Acta Cryst.* C**55**, 343–345.
Sheldrick, G. M. (1990). *Acta Cryst*. C**51**, 2277–2279.
Sheldrick, G. M. (1997). *SHELXL*97. University of Gottingen, Germany.
Zhu, H.-G., Xu, Y., Yu, Z., Wu, Q.-J., Fun, H.-K. & You, X.-Z. (1999). *Polyhedron*, **18**, 3491–3495.