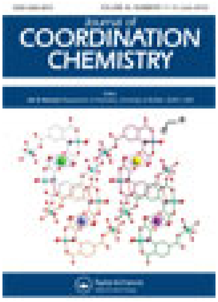
This article was downloaded by: [Renmin University of China]
On: 13 October 2013, At: 10:34
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Journal of Coordination Chemistry
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcoo20

1-D and 2-D coordination polymers of lead(II) thiocyanate with substituted 2,2′-bipyridine ligand

Farzin Marandi [a] , Javad Sartaji [a] , Giuseppe Bruno [b] & Hadi Amiri Rudbari [b]
[a] Chemistry Department , Payame Noor University , 19395-4697 Tehran, I.R. of IRAN
[b] Dipartimento di Chimica Inorganica , Vill. S. Agata, Salita Sperone 31, Università di Messina, 98166 Messina, Italy
Published online: 08 May 2012.

To cite this article: Farzin Marandi , Javad Sartaji , Giuseppe Bruno & Hadi Amiri Rudbari (2012) 1-D and 2-D coordination polymers of lead(II) thiocyanate with substituted 2,2′-bipyridine ligand, Journal of Coordination Chemistry, 65:11, 1872-1881, DOI: 10.1080/00958972.2012.683866

To link to this article: http://dx.doi.org/10.1080/00958972.2012.683866

PLEASE SCROLL DOWN FOR ARTICLE

Taylor & Francis makes every effort to ensure the accuracy of all the information (the "Content") contained in the publications on our platform. However, Taylor & Francis, our agents, and our licensors make no representations or warranties whatsoever as to the accuracy, completeness, or suitability for any purpose of the Content. Any opinions and views expressed in this publication are the opinions and views of the authors, and are not the views of or endorsed by Taylor & Francis. The accuracy of the Content should not be relied upon and should be independently verified with primary sources of information. Taylor and Francis shall not be liable for any losses, actions, claims, proceedings, demands, costs, expenses, damages, and other liabilities whatsoever or howsoever caused arising directly or indirectly in connection with, in relation to or arising out of the use of the Content.

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden. Terms &

Conditions of access and use can be found at http://www.tandfonline.com/page/terms-and-conditions

Downloaded by [Renmin University of China] at 10:34 13 October 2013

Journal of Coordination Chemistry
Vol. 65, No. 11, 10 June 2012, 1872–1881

Downloaded by [Renmin University of China] at 10:34 13 October 2013

1-D and 2-D coordination polymers of lead(II) thiocyanate with substituted 2,2′-bipyridine ligand

FARZIN MARANDI*†, JAVAD SARTAJI†, GIUSEPPE BRUNO‡ and HADI AMIRI RUDBARI‡

†Chemistry Department, Payame Noor University, 19395-4697 Tehran, I.R. of IRAN
‡Dipartimento di Chimica Inorganica, Vill. S. Agata, Salita Sperone 31,
Università di Messina, 98166 Messina, Italy

(*Received 28 November 2011; in final form 17 February 2012*)

Two lead(II)-thiocyanato coordination polymers with 5,5′-dimethyl-2,2′-bipyridine (5,5′-dm-2,2′-bpy) and 4,4′-dimethoxy-2,2′-bipyridine (4,4′-dmo-2,2′-bpy) as chelating ligands were synthesized and characterized by elemental analysis, IR and ^{1}H-NMR spectroscopy, thermal behavior, and X-ray crystallography. These complexes have formulas $[\mathrm{Pb}(5,5'\text{-dm-}2,2'\text{-bpy})(\mathrm{NCS})_2]_n$ (**1**) and $[\mathrm{Pb}(4,4'\text{-dmo-}2,2'\text{-bpy})(\mathrm{NCS})_2]_n$ (**2**). The coordination numbers of Pb$^{\mathrm{II}}$ in **1** and **2** are four, PbN$_4$, with "stereo-chemically active" electron pairs and hemidirected coordination spheres. Considering Pb···S as weak bonds, **1** and **2** are 1- and 2-D coordination polymers, respectively. The supramolecular features in these complexes are guided/controlled by weak directional intermolecular interactions.

Keywords: Coordination polymers; Substituted 2,2′-bipyridine; Lead(II)

1. Introduction

Metal–organic frameworks (MOFs) have achieved considerable progress in crystal engineering and supramolecular chemistry due to their fascinating structures and interesting functional properties [1–10]. Some publications have reviewed various MOFs built by transition metals [5–8] or main-group metals [9, 10].

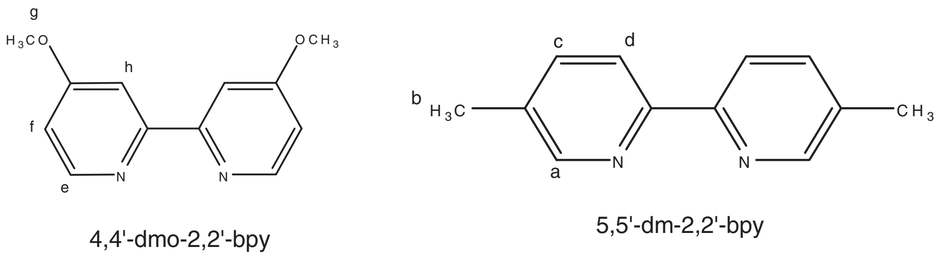
The structures and properties of coordination polymers depend on coordination and geometries of metal ions and connecting ligands, as well as on the influence of secondary interactions such as hydrogen bonding and π–π stacking interactions [11]. Several factors, including coordination bonds and secondary interactions, metal-to-ligand molar ratio, the coordination of ligands, the type of metal ions, the presence of solvent, counterions, and organic guest molecules affect the design and synthesis of metal-coordination polymers [12, 13].

Lead(II) contains the 6s^2 lone pair, which can cause distortion in coordination sphere [14–16] and frequently discussed in "stereo-chemical activity" of valence shell electron lone pairs [17–19]. In 1998, Shimoni-Livny discussed the possible stereo-chemical

---

*Corresponding author. Email: fmarandi2004@yahoo.com

Journal of Coordination Chemistry
ISSN 0095-8972 print/ISSN 1029-0389 online © 2012 Taylor & Francis
http://dx.doi.org/10.1080/00958972.2012.683866



Scheme 1. Schematic representation of employed ligands.

Downloaded by [Renmin University of China] at 10:34 13 October 2013

activity of the lone pair of lead(II) compounds based on a thorough review of crystal data available in the CSD. They classify lead coordination as holodirected which refers to complexes in which the bonds to ligand atoms are directed throughout the surface of encompassing sphere, while hemidirected refers to those cases where the bonds to ligands are directed only to a part of the coordination sphere, leaving a gap in the distribution of bonds to the ligand [20].

We have synthesized several $[Pb(L)_2(anion)_2]$ complexes (L = substituted 2,2′-bipyridine) [21]. In particular, research has concentrated on 5,5′-dimethyl-2,2′-bipyridine and 4,4′-dimethoxy-2,2′-bipyridine ligands (scheme 1) with thiocyanate for new lead(II) coordination polymers.

2. Experimental

2.1. *Materials and measurements*

All chemicals were of reagent grade and used without purification. FT-IR spectra were collected on a Mattson 1000 spectrophotometer using KBr pellets from 4000 to 450 cm^{-1}. Elemental analyses (C, H, and N) were performed using a Carlo ERBA model EA 1108 analyzer; ^1H NMR spectra were obtained with a Bruker spectrometer at 250 MHz in [D6]DMSO. Thermal analyses were carried out on a Perkin-Elmer instrument (Seiko Instruments).

2.2. *Preparation of [Pb(5,5′-dm-2,2′-bpy)(NCS)$_2$]$_n$ (1)*

5,5′-Dimethyl-2,2′-bipyridine (0.184 g, 1 m mol) was placed in one arm of a branched tube [21d], lead(II) acetate (0.190 g, 0.5 m mol) and potassium thiocyanate (0.097 g, 1 m mol) in the other. Methanol and water ratio (3 : 2) was carefully added to fill both arms; the tube was then sealed and the ligand-containing arm was immersed in a bath at 60°C while the other was at ambient temperature. After 3 days, crystals deposited in the cooler arm were filtered off, washed with acetone and ether, and dried in air; yield: 56%. Analysis: Found (%): C: 33.34, H: 2.20, N: 11.24. Calcd for $C_{14}H_{12}N_4PbS_2$ (%): C: 33.10, H: 2.36, N, 11.03. IR (cm^{-1}) selected bands: 670(s), 800(vs) (C–H), 1050(vs), 1230(vs) 1340, 1430, 1580 (s, aromatic ring), 2030–2050 (br, thiocyanate), 2880 (w, C–H aliphatic), 3020 (w, C–H aromatic). ^{1}H NMR (DMSO, δ): 8.49 (s, 2H, a), 8.23 (d, 2H, d), 7.73 (d, 2H, c), 2.32 (s, 6H, b) ppm.

2.3. *Preparation of [Pb(4,4′-dmo-2,2′-bpy)(NCS)$_2$]$_n$ (2)*

Complex **2** was synthesized in the same way as **1** using 4,4′-dimethoxy-2,2′-bipyridine instead of 5,5′-dimethyl-2,2′-bipyridine; yield: 68%. Analysis: Found (%): C: 31.43, H: 2.45, N: 10.69. Calcd for $C_{14}H_{12}N_4O_2PbS_2$ (%): C: 31.13, H: 2.22, N, 10.38. IR (cm^{-1}) selected bands: 780(s), 820(vs) (C–H), 1000(vs), 1250(vs) 1330, 1450, 1600 (s, aromatic ring), 2030–2050 (br, thiocyanate), 2910, 2940 (w, C–H aliphatic), 3030 (w, C–H aromatic). ^{1}H NMR (DMSO, δ): 8.56 (s, 2H, e), 7.96 (s, 2H, h), 7.13 (d, 2H, f), 3.90 (s, 6H, g) ppm.

2.4. *Crystallography*

Data were collected at room temperature with a Bruker APEX II CCD area-detector diffractometer using Mo-Kα radiation ($\lambda = 0.71073$ Å). Data collection, cell refinement, data reduction, and absorption corrections were performed using multiscan methods with Bruker software [22]. The structures were solved by direct methods using SIR2004 [23].

Non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using SHELXL-97 [24]. All hydrogen atoms were placed at calculated positions and constrained to ride on their parent atoms. Details concerning collection and analysis are reported in table 1.

3. Results and discussion

3.1. *Spectroscopic studies*

The reaction of lead(II) thiocyanate with 5,5′-dimethyl-2,2′-bipyridine (5,5′-dm-2,2′-bpy) and 4,4′-dimethoxy-2,2′-bipyridine (4,4′-dmo-2,2′-bpy) yielded crystalline materials, **1** and **2**. Infrared (IR) spectra display characteristic absorptions for chelating ligands and thiocyanate. Relatively weak absorptions at 3020 and 3030 cm^{-1} are due to C–H aromatic rings of **1** and **2**, respectively. C–H modes involving aliphatic hydrogen atoms of 5,5′-dm-2,2′-bpy and 4,4′-dmo-2,2′-bpy are at 2880, 2910, and 2940 cm^{-1}. Absorptions with variable intensity at 1400–1620 cm^{-1} correspond to aromatic ring vibrations of 5,5′-dm-2,2′-bpy and 4,4′-dmo-2,2′-bpy. IR spectra display very strong absorptions at 2050 cm^{-1} due to asymmetric stretching vibration, ν(C≡N) of coordinated thiocyanate. The ν(C≡N) are most consistent with N-bonded thiocyanate (for S-bonded thiocyanate the ν(C≡N) frequencies range from 2110 to 2140 cm^{-1}, whereas in N-bonded the $\nu(C{\equiv}N) < 2110$ cm^{-1} [25, 26]). This is also confirmed by X-ray (section 3.3). ^{1}H NMR spectra of the DMSO solutions of **1** and **2** at 6.59–8.51 ppm display three different protons of py groups of the substituted 2,2′-bipyridines. In spectra of the compounds, bands at 2.33 for **1** and 3.91 for **2** ppm are assigned to protons of $-CH_3$ groups of substituted 2,2′-bipyridines.

Downloaded by [Renmin University of China] at 10:34 13 October 2013

Downloaded by [Renmin University of China] at 10:34 13 October 2013

Table 1. Crystal data and structure refinement for **1** and **2**.

	1	**2**
Identification code	$[Pb(5,5'\text{-dm-}2,2'\text{-bpy})(NCS)_2]_n$	$[Pb(4,4'\text{-dmo-}2,2'\text{-bpy})(NCS)_2]_n$
Empirical formula	$C_{14}H_{12}N_4PbS_2$	$C_{14}H_{12}N_4O_2PbS_2$
Formula weight	507.59	539.59
Crystal system	Monoclinic	Monoclinic
Space group	$C2/c$	$P2_1/c$
Unit cell dimensions (Å, °)		
a	22.412(6)	10.381(2)
b	7.343(2)	13.677(2)
c	21.271(6)	11.979(3)
α	90.00	90.00
β	114.29(2)	109.03 (1)
γ	90.00	90.00
Volume (Å^3), Z	3190.7, 8	1607.84, 4
Calculated density (g cm^{-3})	2.113	2.229
Absorption coefficient (mm^{-1})	10.834	10.766
$F(000)$	1904	1016
θ range for data collection (°)	2.95–27.00	2.55–27.64
Limiting indices	$-28 \le h \le 28$ $-9 \le k \le 9$ $-27 \le l \le 27$	$-13 \le h \le 13$ $-17 \le k \le 17$ $-15 \le l \le 15$
Reflections collected	58,286	47,309
Independent reflections	3479 [R(int) = 0.0371]	3701 [R(int) = 0.0409]
Completeness to $\theta = 25.02$ (%)	99.7	98.9
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	3479/0/190	3701/0/204
Goodness-of-fit on F^2	1.177	1.037
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0147$, $wR_2 = 0.0387$	$R_1 = 0.0652$, $wR_2 = 0.1824$
R indices (all data)	$R_1 = 0.0163$, $wR_2 = 0.0396$	$R_1 = 0.0674$, $wR_2 = 0.1840$
Largest difference peak and hole (e Å^{-3})	0.93 and −0.72	9.66 and −4.95

3.2. *Thermal studies*

Thermogravimetric analyses (TGA) for these complexes were performed on polycrystalline samples under nitrogen. Compounds **1** (see, e.g., figure 1S) and **2** are thermally stable till 180°C. The thermal decompositions follow three steps in the temperature range 180–420°C corresponding to exothermic decomposition. The mass loss calculations as well as microanalyses suggest that the residue at 600°C is PbO and total mass loss of 47.10% for **1** (Calcd 44.20%) and 42.14% for **2** (Calcd 41.3%), respectively, agrees well with the structures. These compounds are potential precursors for lead oxides materials.

3.3. *Crystal structures of 1 and 2*

Compounds **1** and **2** were shown by single crystal X-ray diffraction to crystallize with the monoclinic space groups $C2/c$ and $P2_1/c$, respectively. ORTEP diagrams of **1** and **2** are shown in figures 1 and 2, respectively. Selected bond distances and angles are listed in table 2.

Each Pb^{2+} is coordinated by two nitrogen atoms of "5,5′-dm-2,2′-bpy" in **1**, "4,4′-dmo-2,2′-bpy" in **2**, and two nitrogen atoms of two "NCS^-". The thiocyanates are *trans* in **1**, but *cis* in **2** (figures 1a and 2a). Each Pb in these structures have four "normal"

Downloaded by [Renmin University of China] at 10:34 13 October 2013

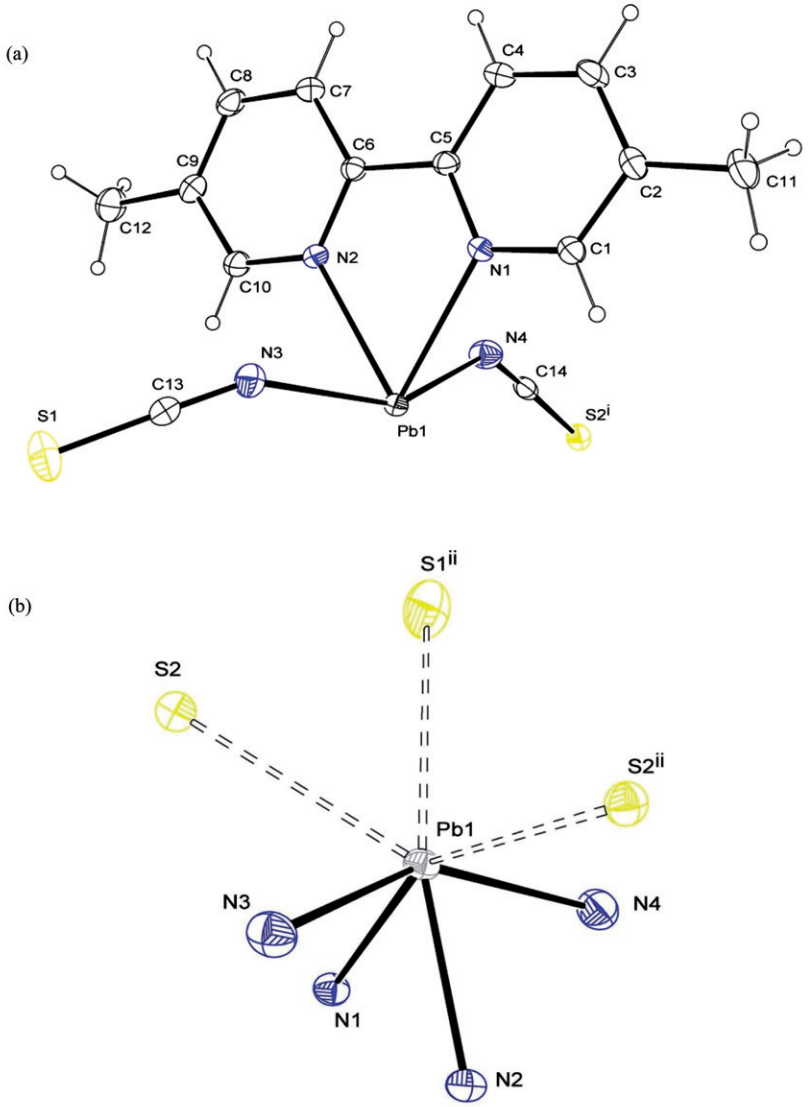
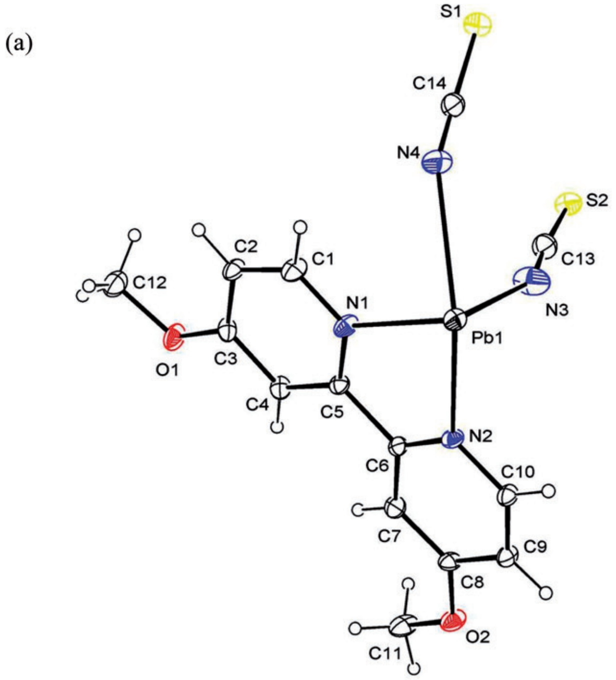


Figure 1. (a) ORTEP drawing of **1**; (b) representation of the hole in the coordination sphere of **1**.

Pb–N bonds and three "weak" Pb···S bonds, with distances $\mathrm{Pb1\cdots S2^{ii}} = 3.234(1)$, $\mathrm{Pb1\cdots S2} = 3.269(1)$, and $\mathrm{Pb1\cdots S1^{ii}} = 3.694(2)$ Å for **1** and $\mathrm{Pb1\cdots S1^{i}} = 3.304(5)$, $\mathrm{Pb1\cdots S2^{ii}} = 3.320(4)$, and $\mathrm{Pb1\cdots S1^{ii}} = 3.428(2)$ Å for **2** (table 2). These Pb···S interactions are significantly shorter than those found in other lead(II) thiocyanate complexes [25, 27]. The coordination number of $\mathrm{Pb^{II}}$ is seven (two nitrogen atoms of dmbpy, two nitrogen atoms, and three sulfur atoms of thiocyanates (figures 1b and 2b)). Lengths of four Pb–N bonds are different from the three Pb–S bonds, suggesting the existence of a stereochemically active lone pair . The shortening of the Pb–X bonds on the side of $\mathrm{Pb^{II}}$ ion opposite to the putative lone pair supports its presence [28, 29].

Downloaded by [Renmin University of China] at 10:34 13 October 2013



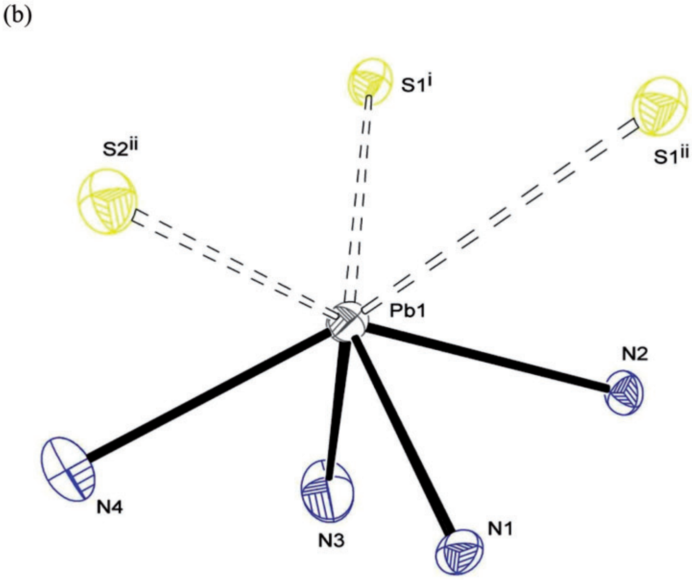


Figure 2. (a) ORTEP drawing of **2**; (b) representation of the hole in the coordination sphere of **2**.

Table 2. Selected bond lengths (Å) and angles (°) for **1** and **2**.

1		**2**	
Pb1–N1	2.459(2)	Pb1–N3	2.390(1)
Pb1–N3	2.463(3)	Pb1–N1	2.470(1)
Pb1–N2	2.469(3)	Pb1–N2	2.511(9)
Pb1–N4	2.680(3)	Pb1–N4	2.652(1)
Pb1···S2^{i}	3.234(1)	Pb1···S1^{i}	3.304(5)
Pb1···S2	3.269(1)	Pb1···S2^{ii}	3.320(4)
Pb1···S1^{ii}	3.694(2)	Pb1···S1^{ii}	3.428(2)
N1–Pb1–N3	93.08(8)	N3–Pb1–N1	87.2(5)
N1–Pb1–N2	66.12(7)	N3–Pb1–N2	77.0(4)
N3–Pb1–N2	75.00(8)	N1–Pb1–N2	65.1(3)
N1–Pb1–N4	78.07(8)	N3–Pb1–N4	73.3(5)
N3–Pb1–N4	149.85(9)	N1–Pb1–N4	83.7(4)
N2–Pb1–N4	75.07(8)	N2–Pb1–N4	137.5(4)

Symmetry codes for **1**: $^{i}x, 1 + y, z$; $^{ii}0.5 - x, 0.5 + y, 1.5 - z$; for **2**: $^{i}x, 0.5 - y, -0.5 + z$; ^{ii}**2** $- x, -0.5 + y, 0.5 - z$.

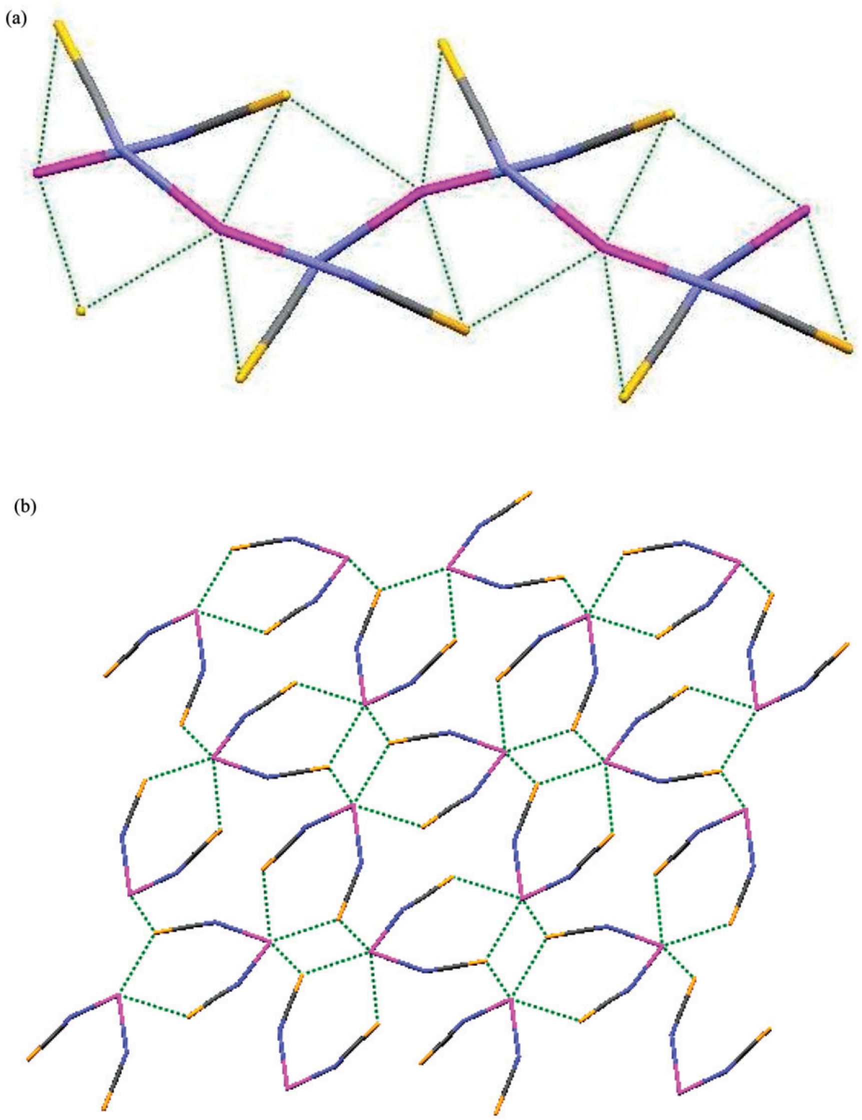


Figure 3. Coordination mode of thiocyanate in (a) **1** and (b) **2**.

Downloaded by [Renmin University of China] at 10:34 13 October 2013

Table 3. Intermolecular interactions for **1** and **2**.

A···H–B	A···H (Å)	A···B (Å)	A···H–B (°)
1			
S2···H1–C1 (x, $1+y$, z)	2.929	3.597	129.81
S2···H10–C10 ($0.5-x$, $0.5+y$, $1.5-z$)	2.856	3.668	146.74
N3···H4–C4 ($0.5-x$, $0.5-y$, $2-z$)	2.658	3.472	146.59
π–π stacking (slipped face-to-face)		3.481	
S2···S1 ($0.5-x$, $1.5+y$, $1.5-z$)		3.514	
H11B···H12C ($0.5-x$, $0.5-y$, $2-z$)		2.201	
2			
O1···H11B–C11 (x, $1/2-y$, $1/2+z$)	2.709	3.517	142.11
S1···H4–C4 ($1+x$, $1/2-y$, $1/2+z$)	2.842	3.733	160.97
S1···N2 ($2-x$, $1.5+y$, $1.5-z$)		3.211	
S2···N4 ($2-x$, $1.5+y$, $1.5-z$)		3.229	
π–π stacking (slipped face-to-face)		3.401	
H11B···H12C (x, $0.5-y$, $-1/2+z$)		2.201	

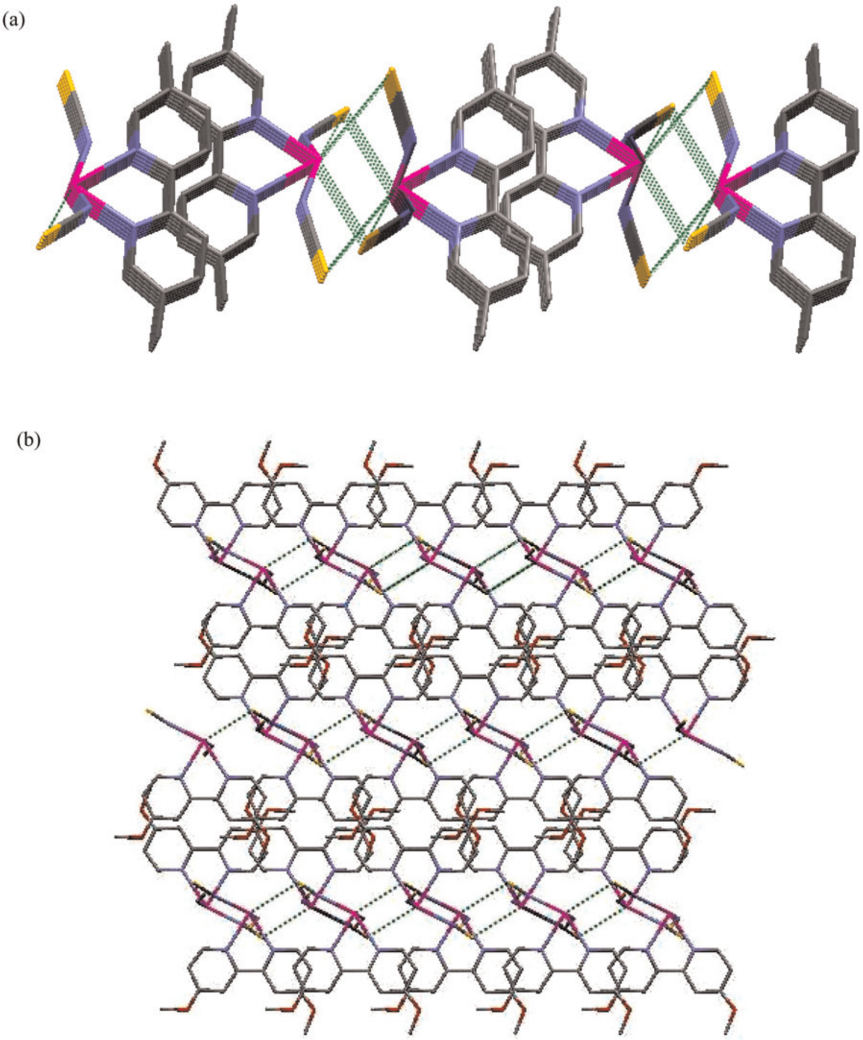


Figure 4. (a) Packing of 1-D chains of **1** to form 2-D supramolecular layers *via* $\pi\cdots\pi$ interactions (table 3); (b) Packing of 2-D layers of **2** to form 3-D supramolecular layers *via* intermolecular interactions (table 3).

Downloaded by [Renmin University of China] at 10:34 13 October 2013

Downloaded by [Renmin University of China] at 10:34 13 October 2013

In **1**, lead(II) is bridged by three thiocyanates in two fashions: one thiocyanate is a $\mu_{1,3}$-SCN− [30] and the other two are $\mu_{1,1,3}$-SCN− bridges with each neighboring lead building an extended 1-D chain along the *b*-axis. Two neighboring Pb^{II} ions in the bridging head of one Pb^{II} are in the same phase and these three Pb^{II} ions extend to an angular arrangement of 107.23°. The Pb···Pb separations are 4.561 and 7.343 Å. In **2**, lead(II) ions are bridged by $\mu_{1,1,3}$-SCN− and $\mu_{1,3}$-SCN− to form an eight-membered ring $Pb(SCN)_2Pb$ and a four-membered ring Pb_2S_2 with Pb···Pb separations of 7.277 and 4.517 Å, respectively [31]. These units construct a 2-D network along the crystallographic direction [0 1 1] (figure 3).

A useful comparison with **1** and **2** is provided by recent structural study of $Pb(SCN)_2$ with 2,2′-bipyridine [25, 32]. In $[Pb(bpy)(SCN)_2]_n$ [32], Pb^{II} is eight-coordinate and there is only one kind of thiocyanate, but in **1** and [Pb(4,4′-dm-2,2′-bpy)$(SCN)_2$] [25], Pb^{II} is seven-coordinate and there are two kinds of thiocyanate in a 1-D coordination polymer. In **2**, in spite of Pb^{II} being seven-coordinate, there are two kinds of thiocyanate in a 2-D network. Position of different substituents on 2,2′-bpy results in interesting intermolecular interactions in the structures of **1** and **2** (table 3). Relatively strong interactions within this class of weak non-covalent contacts [33] form hybrid 2-D and 3-D frameworks in **1** and **2**, respectively (figure 4).

Supplementary material

Full cif depositions, excluding structure factor amplitudes, reside with the Cambridge Crystallographic Data Center, CCDC-853948 for **1** and CCDC-853949 for **2**. Copies of the data can be obtained, free of charge, on application from CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033 or Email: deposit@ccdc.cam.ac.uk).

Acknowledgments

The authors acknowledge financial support by Payame Noor University and Università di Messina.

References

[1] O.K. Farha, J.T. Hupp. *Acc. Chem. Res.*, **43**, 1166 (2010).
[2] Y.H. Hu, L. Zhang. *Adv. Mater.*, **22**, E117 (2010).
[3] S. Natarajan, P. Mahata. *Chem. Soc. Rev.*, **38**, 2304 (2009).
[4] A.M. Spokoyny, M. Alexander, D. Kim, A. Sumrein, C.A. Mirkin. *Chem. Soc. Rev.*, **38**, 218 (2009).
[5] S. Noro, S. Kitagawa, T. Akutagawa, T. Nakamura. *Prog. Polym. Sci.*, **34**, 240 (2009).
[6] A. Morsali, M.Y. Masoomi. *Coord. Chem. Rev.*, **253**, 1882 (2009).
[7] A. Erxleben. *Coord. Chem. Rev.*, **246**, 203 (2003).
[8] R. Peng, M. Li, D. Li. *Coord. Chem. Rev.*, **254**, 1 (2010).
[9] R.L. Davidovich, V. Stavila, D.V. Marinin, E.I. Voit, K.H. Whitmire. *Coord. Chem. Rev.*, **253**, 1316 (2009).
[10] K.M. Fromm. *Coord. Chem. Rev.*, **252**, 856 (2008).
[11] X. Zhang, S. Gao, L. Huo, H. Zhao. *Acta Crystallogr. Sect. C: Cryst. Struct. Commun.*, **62**, m617 (2006).

[12] J. Yang, J.F. Ma, Y.Y. Liu, J.C. Ma, S.R. Batten. *Inorg. Chem.*, **46**, 6542 (2007).

[13] S.R. Fan, L.G. Zhu. *Inorg. Chem.*, **46**, 6785 (2007).

[14] K.L. Zhang, W. Liang, Y. Chang, L.M. Yuan, S.W. Ng. *Polyhedron*, **28**, 647 (2009).

[15] H. Ahmadzadi, F. Marandi, A. Morsali. *J. Organomet. Chem.*, **694**, 3565 (2009).

[16] F. Marandi, A. Morsali, A.A. Soudi. *Z. Anorg. Allg. Chem.*, **633**, 661 (2007).

[17] F. Marandi, B. Mirtamizdoust, S. Chantrapromma, H.-K. Fun. *Z. Anorg. Allg. Chem.*, **633**, 1329 (2007).

[18] J. Abedini, A. Morsali, M. Zeller. *Z. Anorg. Allg. Chem.*, **634**, 2659 (2008).

[19] F. Marandi, B. Mirtamizdoust, A.A. Soudi, V.T. Yilmaz, C. Kazak. *Z. Anorg. Allg. Chem.*, **632**, 2380 (2006).

[20] L. Shimoni-Livny, J.P. Glusker, C.W. Bock. *Inorg. Chem.*, **37**, 1853 (1998).

[21] (a) F. Marandi, Z. Nikpey, M. Khosravi, H.-K. Fun, M. Hemamalini. *J. Coord. Chem.*, **64**, 3012 (2011); (b) F. Marandi, R. Rutvand, M. Rafiee, J. H. Goh, H.-K. Fun. *Inorg. Chim. Acta*, **363**, 4000 (2010); (c) F. Marandi, Z. Nikpey, J.H. Goh, H.-K. Fun. *Z. Naturforsch.*, **65b**, 128 (2010); (d) F. Marandi, F. Amoopour, I. Pantenburg, G. Meyer. *J. Mol. Struct.*, **973**, 124 (2010); (e) F. Marandi, I. Pantenburg, G. Meyer. *Z. Anorg. Allg. Chem.*, **635**, 2558 (2009); (f) F. Marandi, A. Aslani, A. Morsali. *J. Coord. Chem.*, **61**, 882 (2008).

[22] (a) *COSMO* (*version 1.60*), Bruker AXS Inc., Madison, Wisconsin (2005); (b) *SAINT* (*version 7.06A*), Bruker AXS Inc., Madison, Wisconsin (2005); (c) *SADABS* (*version 2.10*), Bruker AXS Inc., Madison, Wisconsin (2005).

[23] M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Spagna. *SIR2004*. *J. Appl. Crystallogr.*, **38**, 381 (2005).

[24] G.M. Sheldrick. *SHELXL-97, University of Göttingen*, Göttingen, Germany (1997).

[25] F. Marandi, M. Mottaghi, G. Meyer, I. Pantenburg. *Z. Anorg. Allg. Chem.*, **635**, 165 (2009).

[26] K. Nakamoto. *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 4th Edn, Wiley, New York (1986) and Part B 5th Edn. (1997).

[27] A. Aslani, A. Morsali, M. Zeller. *Solid State Sci.*, **10**, 1591 (2008).

[28] F. Marandi, A. Morsali. *Inorg. Chim. Acta*, **370**, 526 (2011).

[29] H. Sadeghzadeh, A. Morsali. *J. Coord. Chem.*, **63**, 713 (2010).

[30] D.-M. Xian, Z.-L. You, M. Zhang, P. Hous, X.-H. Li. *J. Coord. Chem.*, **64**, 3265 (2011).

[31] B. Machura, I. Nawrot, K. Michalik. *Polyhedron*, **30**, 2619 (2011).

[32] A. Morsali, M. Payeghader, S. Salehi, M. Moradi. *J. Coord. Chem.*, **56**, 761 (2003).

[33] (a) C.-L. Ma, Z.-F. Guo, R.-F. Zhang. *Polyhedron*, **27**, 420 (2008); (b) Y.-Y. Liu, Y.-Q. Huang, W. Shi, P. Cheng, D.-Z. Liao, S.-P. Yan. *Cryst. Growth Des.*, **7**, 1483 (2007).

Downloaded by [Renmin University of China] at 10:34 13 October 2013