



A One-Dimensional Compound $[\text{HgCl}_2(2,2'\text{-bipy})]_n$ (bipy = bipyridine): Synthesis and Crystal Structure

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A mercury chloride bipyridine compound $[\text{HgCl}_2(2,2'\text{-bipy})]_n$ (**1**) (bipy = bipyridine) has been synthesized through hydrothermal reaction and structurally characterized by single-crystal X-ray diffraction. The title compound features a one-dimensional (1-D) infinite chain-like structure with the mercury ion showing a slightly distorted octahedral geometry. The 1-D chains pile up together through van der Waals interaction to complete three-dimensional (3-D) packing motif.

Keywords: Bipyridine, Chloride, Crystal structure, Hydrothermal, Mercury.

INTRODUCTION

In recent years, coordination compounds have attracted more and more interest because of their abundant and interesting properties, such as catalysis¹, solar energy conversion², chemical sensors³, molecular sieves⁴, light emitting diodes⁵, *etc.* Nowadays, a number of building units have been applied to design and synthesize new coordination compounds⁶⁻⁸. Among the various building blocks, many are N-containing ligands such as 2,2'-bipyridine isonicotinic acid, nicotinic acid, imidazole and 4,4'-bipyridine⁹⁻¹⁴. The 2,2'-bipyridine can act as a bidentate ligand and have been adopted to synthesize new coordination compounds. The 2,2'-bipyridine has delocalized π -electrons of the pyridyl rings and, therefore, it is a good candidate to prepare light-emitting coordination compounds. Recently, preparation of new 2,2'-bipyridine-containing coordination compounds are focussed. We report herein the synthesis and crystal structure of mercury chloride bipyridine compound $[\text{HgCl}_2(2,2'\text{-bipy})]_n$ (**1**) (bipy = bipyridine) which features 1-D infinite chain-like structure.

EXPERIMENTAL

Synthesis of $[\text{HgCl}_2(2,2'\text{-bipy})]_n$ (1**):** All chemicals were of analytical grade and used as received. Loading HgCl_2 (0.2 mmol, 54 mg), 2,2'-bipyridine (0.2 mmol, 31 mg), 1 mL ethanol and 9 mL distilled water into a 25 mL Teflon-lined stainless steel autoclave, then heated it to 453 K and kept for 10 days. Finally on cooling it down to room temperature and power off. Colourless crystals were obtained after filtrating.

X-ray structural determination: A crystal with dimensions of 0.18 mm \times 0.13 mm \times 0.11 mm was mounted on a Rigaku Mercury CCD X-ray area-detector diffractometer equipped with a graphite-monochromatic MoK_α radiation ($\lambda = 0.71073\text{\AA}$) at 296(2) K. Data reduction and cell refinement were performed by the Crystal Clear software. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares using all unique data with Siemens SHELXTLTM Version 5 package of crystallographic software. Non-hydrogen atoms were treated as anisotropic. Hydrogen atoms were generated theoretically and refined as a riding mode. Table-1 lists the summary of the crystallographic data and Table-2 shows the selected bond lengths and bond angles of compound **1**.

RESULTS AND DISCUSSION

Compound **1** is crystallized in the space group $C2/c$ of the monoclinic system. The asymmetric unit of **1** is comprised of $1/2\text{Hg}^{2+}$ ion, one chloride ion and $1/2$ bipy molecule. All crystallographically independent atoms reside at general positions, except for the Hg^{2+} ion. Its crystal structure features 1-D chain-like coordination polymer comprising of HgCl_2 (2,2'-bipyridine) building units. As depicted in Fig. 1, the coordination geometry of the Hg^{2+} ion can be approximately described as a slightly distorted octahedron. The basal plane of the octahedron is formed by two chlorine atoms and two nitrogen atoms of the 2,2'-bipyridine ligand, while two apical positions are occupied by other two chlorine atoms.

The distances of Hg-N and Hg-Cl in basal plane are 2.367(3) \AA and 2.5912(8) \AA , respectively. The apical Hg-Cl

TABLE-1
 SUMMARY OF THE CRYSTALLOGRAPHIC DATA OF **1**

Formula	$C_{10}H_8N_2HgCl_2$	$2\lambda_{max}$ (°)	50
Formula weight	427.67	Index ranges	$-20 \leq h \leq 20, -11 \leq k \leq 7, -8 \leq l \leq 8$
Colour	Colourless	Reflections collected	1978
Crystal size/mm ³	0.18 0.13 0.11	Independent, observed reflections (R_{int})	740, 386 (0.1984)
Crystal system	Monoclinic	$d_{calcd.}$ (g/cm ³)	2.506
Space group	C2/c	μ (mm ⁻¹)	14.014
a (Å)	17.678(3)	T (K)	296(2)
b (Å)	9.4405(16)	F(000)	784
c (Å)	7.2560(12)	R1, wR2	0.0635, 0.1066
β (°)	110.589(8)	S	1.033
V (Å ³)	1133.6(3)	Largest and Mean $\Delta\sigma$	0.001, 0
Z	4	$\Delta\rho$ (max, min) (e/Å ³)	1.078, -1.180

 TABLE-2
 SELECTED BOND LENGTHS (Å) AND BOND ANGLES (°) of **1**

Hg(1)-N(1)	2.367(3)	N(1)#1-Hg(1)-Cl(1)	160.94(8)
Hg(1)-N(1)#1	2.367(3)	Cl(1)#1-Hg(1)-Cl(1)	102.60(4)
Hg(1)-Cl(1)	2.5912(8)	N(1)-Hg(1)-Cl(1)#2	96.24(11)
Hg(1)-Cl(1)#1	2.5912(8)	N(1)#1-Hg(1)-Cl(1)#2	84.08(11)
Hg(1)-Cl(1)#2	2.8133(10)	Cl(1)#1-Hg(1)-Cl(1)#2	94.44(3)
Hg(1)-Cl(1)#3	2.8133(10)	Cl(1)-Hg(1)-Cl(1)#2	85.32(3)
-	-	N(1)-Hg(1)-Cl(1)#3	84.08(11)
N(1)-Hg(1)-N(1)#1	71.54(17)	N(1)#1-Hg(1)-Cl(1)#3	96.24(11)
N(1)-Hg(1)-Cl(1)#1	160.94(8)	Cl(1)#1-Hg(1)-Cl(1)#3	85.32(3)
N(1)#1-Hg(1)-Cl(1)#1	93.98(8)	Cl(1)-Hg(1)-Cl(1)#3	94.44(3)
N(1)-Hg(1)-Cl(1)	93.98(8)	Cl(1)#2-Hg(1)-Cl(1)#3	179.61(3)

Symmetry transformations used to generate equivalent atoms: #1 -x-1, y, -z-1/2; #2 -x-1, -y+3, -z-1; #3 x, -y+3, z+1/2

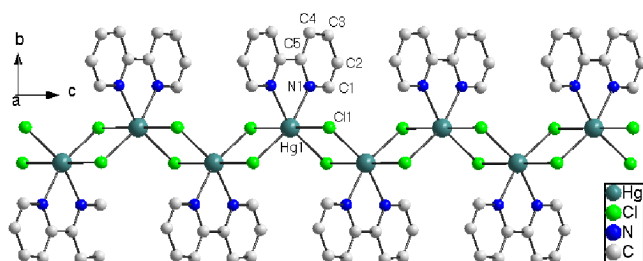


Fig. 1. Molecular and 1-D chain-like structure of compound **1** with the hydrogen atoms been omitted for clarity

bond length is 2.8133(10) Å. The bond lengths of Hg-N and Hg-Cl in the coordination polyhedron are all in the normal range and comparable with those found in other compounds¹⁵⁻¹⁸. The adjacent mercury ions are interconnected by two μ_2 -chlorine atoms to construct 1-D chain-like structure (Fig. 1). The 2,2'-bipy acts as a bidentate ligand to chelate one mercury ion. The dihedral angle between two pyridyl rings in one 2,2'-bipy molecule is 4.830(1)°. The distance between two mercury ions is 3.9772(6) Å. The 1-D chains stack together through van der Waals interaction to complete a 3-D packing diagram (Fig. 2).

Conclusion

A mercury chloride bipyridine compound $[HgCl_2(2,2'$ -bipy)]_n (**1**) is prepared through hydrothermal reaction and structurally characterized by single-crystal X-ray diffraction. Compound **1** features a 1-D infinite chain-like structure with the mercury ion displaying a slightly distorted octahedral

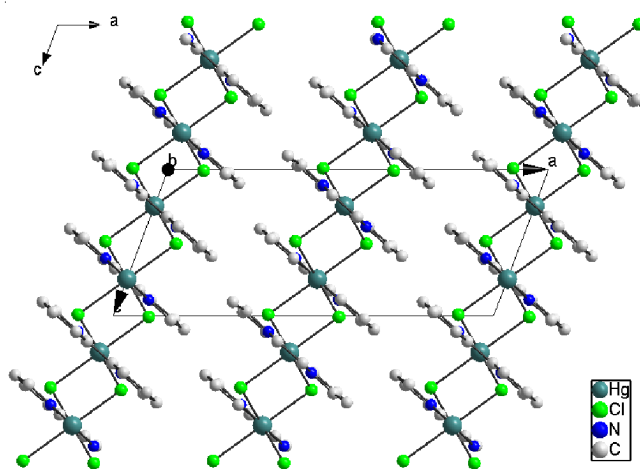


Fig. 2. Crystal packing diagram of compound **1** viewed down along b axis

geometry. The 1-D chains pile up together through van der Waals interaction to form a 3-D packing motif.

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