Asian Journal of Chemistry; Vol. 27, No. 6 (2015), 2339-2340

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2015.17610

NOTE

Synthesis and Characterization of Novel Cadmium Complex

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Received: 15 March 2014; *Accepted*: 16 May 2014; *Published online*: 17 March 2015; AJC-17024

A cadmium complex with m.f. $[CdI_2(imidazole)_2]_n$ (**1**) has been prepared *via* solvothermal reactions and characterized by X-ray single-crystal diffraction. Compound **1** is characterized by a one-dimensional (1-D) infinite chain-like structure. The $[CdI_2(imidazole)_2]_n$ chains stack together *via* van der Waals interactions to construct a three-dimensional (3-D) packing diagram.

Keywords: Cadmium, Crystal, Imidazole, Solvothermal, Iodine.

Coordination polymers are interesting owing to their rich and attractive properties and many building blocks have been used to construct coordination polymers[1-3]. The building units are various, such as N-containing ligands nicotinic acid, isonicotinic acid and imidazole[4-6]. The imidazolate anions can apply monodentate, bidentate or bridging modes to build coordination polymers. Coordination polymers with d^{10} metal are also interesting. Cadmium ion as d^{10} metal ion, has different coordination geometries such as trigonal-bipyramidal, tetrahedral and octahedral. Therefore, cadmium ion is suitable for the build of coordination polymers. Up to date, more and more cadmium-imidazole coordination polymers have been prepared. In this work, we report the synthesis and X-ray crystal structure of a cadmium complex $[CdI_2(imidazole)_2]_n$ (**1**) which is synthesized through solvothermal reactions and features a 1-D infinite chain-like structure.

Synthesis of $[CdI_2(imidazole)_2]_n$ (1): All reactants were commercially available and used without further purification. It was synthesized by mixing CdI_2 (0.5 mmol, 180 mg), imidazole (1 mmol, 68 mg) and 10 mL ethanol in a 23 mL Teflon-lined stainless steel autoclave and heated at 453 K for 7 days, followed by slowly cooled down to room temperature and colorless crystals were collected.

X-ray structure determination: A colorless single crystal with the size of 0.35 mm × 0.26 mm × 0.23 mm was selected for data collection. The X-ray diffraction data was collected on a Rigaku Mercury CCD X-ray diffractometer with MoK$_\alpha$ radiation (λ = 0.71073 Å) at 296 (2) K. A total of 1545 reflections (491 unique) were measured, of which 480 were observed with $I > 2\sigma(I)$. The data reduction and cell refinement of **1** was processed using Crystal Clear software. The structure was solved by direct methods with Siemens SHELXTL™ version 5 package of crystallographic software and refined by full-matrix least-squares fitting on F^2. Hydrogen atoms were generated geometrically and refined isotropically. All non-H atoms were refined with anisotropic displacement parameters.

TABLE-1
CRYSTALLOGRAPHIC DATA OF CADMIUM COMPLEX

Formula	$C_6H_8CdI_2N_4$	$2\theta_{max}$ (°)	50
Formula weight	502.36	Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 11, -5 ≤ l ≤ 5
Color	Colorless	Reflections collected	1545
Crystal size/mm^3	0.35 0.26 0.0.23	Independent, observed reflections (R_{int})	491, 480 (0.0406)
Crystal system	Monoclinic	$D_{Calcd.}$ (g/cm^3)	2.853
Space group	C2/m	μ(mm^{-1})	7.111
a(Å)	14.0512(14)	T (K)	296(2)
b(Å)	9.2864(14)	F(000)	452
c(Å)	4.4815(6)	R1, wR2	0.0312, 0.0805
β(°)	90.006(2)	S	1.013
V(Å^3)	584.77(13)	Largest and mean Δ/σ	0.001, 0
Z	2	Δρ(max, min) (e/Å^3)	1.295, -0.643

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

Cd(1)-N(1)	2.303(3)
Cd(1)-N(1)#1	2.303(3)
Cd(1)-I(1)	3.0933(4)
Cd(1)-I(1)#1	3.0933(4)
Cd(1)-I(1)#2	3.0933(4)
Cd(1)-I(1)#3	3.0933(4)
N(1)-Cd(1)-N(1)#1	180.0
N(1)-Cd(1)-I(1)#2	89.91(6)
N(1)#1-Cd(1)-I(1)#2	90.09(6)
N(1)-Cd(1)-I(1)#3	90.09(6)
N(1)#1-Cd(1)-I(1)#3	89.91(6)
I(1)#2-Cd(1)-I(1)#3	180.0
N(1)-Cd(1)-I(1)	89.91(6)
N(1)#1-Cd(1)-I(1)	90.09(6)
I(1)#2-Cd(1)-I(1)	87.162(14)
I(1)#3-Cd(1)-I(1)	92.838(14)
N(1)-Cd(1)-I(1)#1	90.09(6)
N(1)#1-Cd(1)-I(1)#1	89.91(6)
I(1)#2-Cd(1)-I(1)#1	92.838(13)
I(1)#3-Cd(1)-I(1)#1	87.162(14)
I(1)-Cd(1)-I(1)#1	180.0

Symmetry codes: #1 -x+1, -y+1, -z-2; #2 -x+1, -y+1, -z-3; #3 x, y, z+1

Table-1 gives the summary of the crystallographic data and structural analysis of compound **1**, while Table-2 lists the selected bond lengths and bond angles. The crystal structure and 1-D chain-like structure of complex **1** are depicted in Fig. 1. The results of X-ray diffraction analysis reveal that the crystal structure of **1** consists of a neutral infinite 1-D chain-like structure of $[CdI_2(imidazole)_2]_n$. Complex **1** is crystallized in the space group C2/m of the monoclinic system with two formula units in a cell. All crystallographically independent atoms reside at special positions. The coordination environment of the cadmium ion exhibits an octahedral geometry with two nitrogen atoms from two imidazole ligands and four bridging iodine atoms forming the base square plane. The cadmium ion is exactly located on this plane. The imidazole ring is totally coplanar. The bond length of Cd-N is 2.303 (3) Å, while that of Cd-I is 3.0933 (4) Å. These bond lengths are normal and comparable with those reported[7-9]. Each iodine atom bridges two cadmium ions and every two cadmium ions are interconnected by two μ_2-iodine atoms with the distance between the cadmium ions being of 4.4815 (6) Å. The $[CdI_2(imidazole)_2]_n$ chains stack together through van der Waals interactions to form a 3-D packing diagram (Fig. 2).

Conclusion

A cadmium complex $[CdI_2(imidazole)_2]_n$ (**1**) is prepared through solvothermal reactions. This complex was structurally characterized using X-ray single-crystal diffraction. It is characteristic of a 1-D infinite chain-like structure. The complex $[CdI_2(imidazole)_2]_n$ chains stack together *via* can der Waals interactions to complete a 3-D packing diagram.

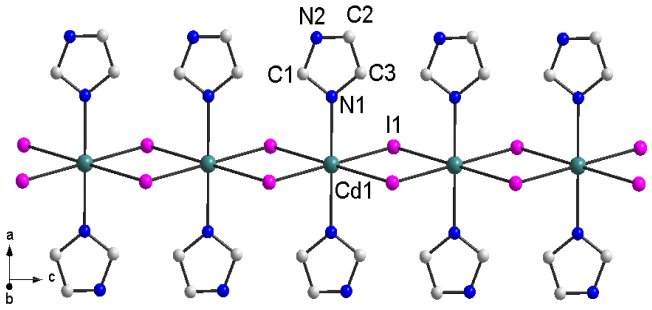

Fig. 1. ORTEP drawing of compound **1** with the hydrogen atoms been omitted for clarity

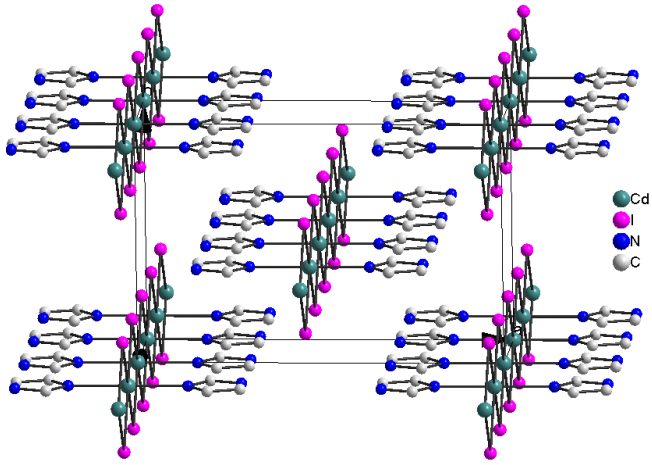

Fig. 2. Crystal packing diagram of compound **1**

ACKNOWLEDGEMENTS

The authors thank for the financial support from NSF of China (21361013), NSF of Jiangxi Province (20132BAB203010, 20114BAB203028), the open foundation (No. 20130014) of the State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences and the Science and Technology Project of Jiangxi Provincial Department of Education (GJJ13555).

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