Ling-Chuan Li, Xiao-Li Zhou*, Yan-Li Liu and Li-Ping Wang

Crystal structure of *catena*-poly[di-μ$_2$-chlorido-1, 10-phenanthroline-κ^2*N*,*N*′-cadmium(II)], $C_{12}H_8Cl_2CdN_2$

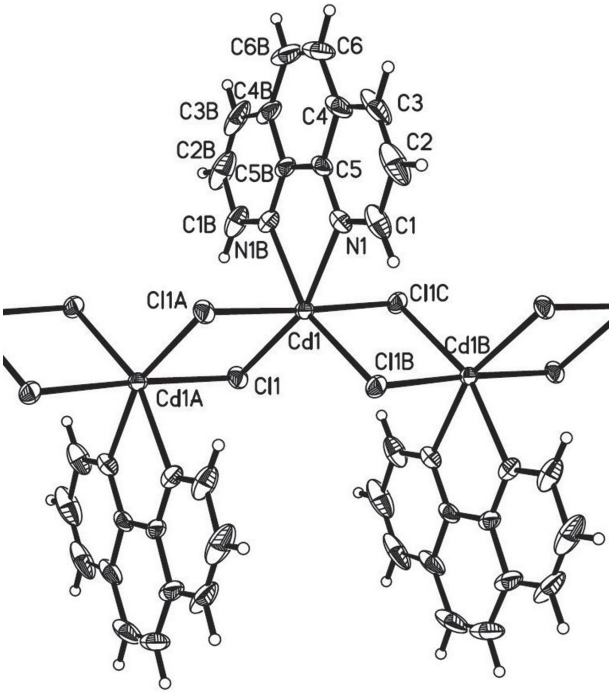

Figure 1: View of the title complex, showing the labeling of the 30% probability ellipsolids. H atoms have been omitted for clarity.

https://doi.org/10.1515/ncrs-2020-0019
Received January 7, 2020; accepted February 26, 2020; available online April 9, 2020

Abstract

$C_{12}H_8Cl_2CdN_2$, monoclinic, $C2/c$ (no. 15), $a = 16.969(5)$ Å, $b = 10.515(3)$ Å, $c = 7.238(2)$ Å, $\beta = 110.710(10)°$, $V = 1208.0(6)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0245$, $wR_{ref}(F^2) = 0.0806$, $T = 298(2)$ K.

***Corresponding author: Xiao-Li Zhou,** Dean's Office, Zhengzhou Institute of Technology, Zhengzhou 450044, P.R. China, e-mail: zhenggongchem@163.com. https://orcid.org/0000-0001-8424-8932
Ling-Chuan Li: School of Civil Engineering, Zhengzhou Institute of Technology, Zhengzhou 450044, P.R. China
Yan-Li Liu and Li-Ping Wang: School of Chemical and Food Engineering, Zhengzhou Institute of Technology, Zhengzhou 450044, P.R. China

CCDC no.: 1986402

A part of the title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.21 × 0.19 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.22 mm^{-1}
Diffractometer, scan mode:	Bruker D8 VENTURE PHOTON, φ and ω
θ_{max}, completeness:	27.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	16070, 1402, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1303
$N(param)_{refined}$:	79
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.92906(2)	0.7500	0.03231(17)
Cl1	0.59574(5)	1.07724(6)	1.01183(11)	0.0398(2)
N1	0.42417(14)	0.7464(2)	0.5998(3)	0.0387(5)
C1	0.3488(2)	0.7473(4)	0.4548(5)	0.0596(9)
H1	0.3252	0.8245	0.3999	0.071*
C2	0.3055(3)	0.6359(6)	0.3849(7)	0.0855(17)
H2	0.2522	0.6397	0.2874	0.103*
C3	0.3381(4)	0.5245(5)	0.4533(7)	0.092(2)
H3	0.3079	0.4505	0.4045	0.110*
C4	0.4185(3)	0.5176(3)	0.6004(6)	0.0685(13)
C5	0.4588(2)	0.6342(2)	0.6722(4)	0.0427(7)
C6	0.4623(4)	0.4025(3)	0.6815(8)	0.106(3)
H6	0.4364	0.3250	0.6353	0.128*

Source of material

A *N*,*N*-dimethylformamide (DMF) solution (3 mL) of 1,10-phenanthroline (0.0360 g, 0.2 mmol) was placed into the bottom of the tube as a lower layer, and then a pure methanol solvent (7 mL) was added slowly along the tube wall into the tube as a middle layer, finally, a methanol solution (3 mL) of $CdCl_2$

(0.0366 g, 0.2 mmol) was also put cautiously along the tube wall into the tube as a upper layer. The resulting three-layer solution was not mixed and was left at room temperature. After three weeks, quality colorless crystals of the title polymer were obtained from the solution and dried in air.

Experimental details

H atoms were generated geometrically and refined as riding atoms with C—H = 0.93 Å and $U_{iso}(H) = 1.2$ times $U_{eq}(C)$ for aromatic H atoms.

Comment

As is well known, 1,10-phenanthroline, a rigid ligand with a six-element heterocyclic structure containing nitrogen, has a three-ring conjugated planar structure, so that the electron density of nitrogen atoms on the aromatic ring is strengthened [4, 5]. So phenanthroline complexes may be luminous material with good luminous properties. When it is coordinated with metal ions, as a bidentate chelating ligand, novel and stable metal organic complexes with potential and superior optical functions can be formed [6–10].

Single crystal X-ray diffraction analysis reveals that the title structure contain a 1-D polymer. As is shown in the figure, The Cd atom is six-coordinated by two imidazole N atoms of one 1,10-phenanthroline ligand and four bridging chloride ions in a distorted octahedral geometry. The two bond lengths of Cd—N are 2.353(2) Å, the four bond lengths of Cd—Cl are 2.5457(9) and 2.7561(10) Å, respectively. The bond angles around the Cd atom vary from 70.57(12)° (N1—Cd1—N1) to 177.25(3)° (Cl1—Cd1—Cl1). In the crystal, the adjacent molecules are stacked through the aromatic π–π interactions (the average interplanar distance between phenanthroline rings is 3.62 Å) and intermolecular interactions to form a three-dimensional supramolecular network.

Acknowledgements: We gratefully acknowledge the financial support from Scientific and Technological Project of Henan Province (no. 152102210016), National Project Incubation Fund of Zhengzhou Institute of Engineering and Technology (GJJKTPY2018K1) for financial support and thank Professor XiangRu Meng of Zhengzhou University for her help.

References

1. Bruker. APEX3 and SAINT. Bruker AXS Inc., Madison, WI, USA (2016).
2. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. Acta Crystallogr. **C71** (2015) 3–8.
4. Richter, F.; Smith, G. F.: Derivatives of 1,10-phenanthroline. J. Am. Chem. Soc. **66** (1944) 396–398.
5. Guérin, J.; Aronica, C.; Boeuf, G.; Chauvin, J.; Moreau, J.; Lemercier, G.: Optical properties of new 5-(4-phenylethynyl)-substituted-1,10-phenanthroline derivatives. J. Lumin. **131** (2011) 2668–2673.
6. Chen, Z.; Zhang, S.; Zhang, S.; Sun, Q.; Xiao, Y.; Wang, K.: Cadmium-based coordination polymers from 1D to 3D: Synthesis, Structures, and Photoluminescent and Electrochemiluminescent Properties. ChemPlusChem **84** (2019) 190–202.
7. Wu, Z.-F.; Tan, B.; Deng, Z.-H.; Xie, Z.-L.; Fu, J.-J.; Shen, N.-N.; Huang, X.-Y.: Dual-emission luminescence of magnesium coordination polymers based on mixed organic ligands. Chem. Eur. J. **22** (2015) 1334–1339.
8. Fazal, A.; Al-Dawsari, A.; El Ali, B.; Ouahab, L.; Fettouhi, M.: Bimetallic bis(diphenylphosphino)acetylene bridged copper(I) complexes with 1,10-phenanthroline derivatives: synthesis, crystal structure, and spectroscopic characterization. J. Coord. Chem. **67** (2014) 2357–2364.
9. Guo, L.; Deng, J.; Zhang, L.; Xiu, Q.; Wen, G.; Zhong, C.: Synthesis and applications of 3,6-carbazole-based conjugated side-chaincopolymers containing complexes of 1,10-phenanthroline with Zn(II), Cd(II) and Ni(II) for dye-sensitized solar cells. Dyes Pigments **92** (2012) 1062–1068.
10. Carballo, R.; Covelo, B.; Fernández-Hermida, N.; Lago, A. B.; Vázquez López, E. M.: Non-covalent interactions in a nickel(II) complex with benzilate and 1,10-phenanthroline. J. Chem. Crystallogr. **41** (2011) 1949–1954.