Electronic Supporting Information (ESI)

New Chiral Coordination Polymers Constructed from Well Elaborated Achiral and Chiral Ligands

Yun-Wu Li, Ying Tao, Li-Fu Wang, Tong-Liang Hu, and Xian-He Bu*

Department of Chemistry, and Tianjin Key Lab on Metal and Molecule-based Material Chemistry, Nankai University, Tianjin 300071, China

Contents List

- **1**. Scheme S1: Structures of two ligands: H₂pdtp and H₂cdtp.
- 2. Scheme S2: The route for ligands synthesis.
- **3**. Table S1: The selected bond lengths [Å] and angles [°] of CCPs 1 and 2.
- 4. Fig. S1-2: XRD of CCPs 1 and 2.
- 5. Fig. S3: Twisted conformations of ligands H₂pdtp and their torsion dihedral angles.
- 6. Scheme S3: Two coordination modes of H₂cdtp ligands.

• Corresponding author. E-mail: <u>buxh@nankai.edu.cn</u>. Fax: +86-22-23502458.

1. Scheme S1: Structures of two ligands: H₂pdtp and H₂cdtp.



2. Scheme S2: The route for ligands synthesis.^{S1}



Reference

S1 (a) F. D. Popp, J. Heterocycl. Chem., 1974, 11, 79; (b) W. Ried, S. Aboul-Fetouh, Tetrahedron, 1988, 44, 3399; (c) Z. P. Demko, K. B. Sharpless, Org. Lett., 2001, 3, 4091; (d) Z. P.
Demko, K. B. Sharpless, J. Org. Chem., 2001, 66, 7945; (e) J. R. Li, Y. Tao, Q. Yu, X. H. Bu, H.
Sakamoto, S. Kitagawa, Chem.–Eur. J., 2008, 14, 2771; (f) Y. Tao, J. R. Li, Z. Chang, X. H. Bu, Cryst. Growth Des., 2010, 10, 564; (g) T. L. Hu, Y. Tao, Z. Chang, X. H. Bu, Inorg. Chem., 2011, 50, 10994.

3. **Table S1**: The selected bond lengths [Å] and angles [°] of CCPs **1** and **2**.

1			
Hg(1)-N(3A)	2.268(6)	Hg(1)-N(3)	2.268(6)
Hg(1)-Cl(1)	2.476(2)	Hg(1)-Cl(1A)	2.476(2)
N(3A)-Hg(1)-N(3)	116.7(3)	N(3A)-Hg(1)-Cl(1)	106.32(18)
N(3)-Hg(1)-Cl(1)	101.78(18)	N(3A)-Hg(1)-Cl(1A)	101.78(18)
N(3)-Hg(1)-Cl(1A)	106.32(18)	Cl(1)-Hg(1)-Cl(1A)	124.91(11)
Symmetry transformations used to generate equivalent atoms:			
A: - y + 1, - x + 1, - z + 1/2; B: y, x, - z			
		2	
Zn(1)-N(3)	2.024(5)	Zn(1)-N(17)	2.045(5)
Zn(1)-N(16)	2.059(5)	Zn(1)-N(27A)	2.070(6)
Zn(1)-N(2)	2.583(6)	Zn(3)-N(20B)	2.047(5)
Zn(3)-N(6C)	2.051(5)	Zn(3)-N(23)	2.050(5)
Zn(3)-N(10C)	2.060(5)	Zn(3)-N(22)	2.475(6)
Zn(2)-N(13)	1.979(5)	Zn(2)-N(26)	1.997(5)
Zn(2)-N(30)	2.042(5)	Zn(2)-N(11)	2.509(6)
O(1)-Zn(2)	2.049(6)		
N(3)-Zn(1)-N(17)	151.3(2)	N(3)-Zn(1)-N(16)	106.6(2)
N(17)-Zn(1)-N(16)	91.9(2)	N(3)-Zn(1)-N(2)	69.49(18)
N(17)-Zn(1)-N(2)	92.8(2)	N(16)-Zn(1)-N(2)	80.74(19)
N(23)-Zn(3)-N(10C)	111.7(2)	N(20B)-Zn(3)-N(22)	82.2(2)
N(23)-Zn(3)-N(22)	70.0(2)	N(10C)-Zn(3)-N(22)	178.3(2)
N(13)-Zn(2)-N(26)	114.0(2)	N(13)-Zn(2)-N(30)	108.7(2)
N(26)-Zn(2)-N(30)	89.6(2)	N(13)-Zn(2)-O(1)	115.0(3)
N(26)-Zn(2)-O(1)	127.4(3)	N(30)-Zn(2)-O(1)	92.0(2)
N(13)-Zn(2)-N(11)	72.1(2)	N(26)-Zn(2)-N(11)	99.9(2)
N(30)-Zn(2)-N(11)	169.2(2)	O(1)-Zn(2)-N(11)	78.2(2)

Symmetry transformations used to generate equivalent atoms:

 $A: -x+2, \, y+1/2, \, \text{-} \, z+1/2; \, B: -x+3/2, \, \text{-} \, y+2, \, z+1/2; \, C: -x+5/2, \, \text{-} \, y+2, \, z+1/2$

4. Fig. S1-2: XRD of CCPs 1 and 2.



Fig. S1 XRD of compound 1.



Fig. S2 XRD of compound 2.

5. Fig. S3: Twisted conformations of ligands H₂pdtp and their torsion dihedral

angles.



(b)The distortion angle $\theta_2=63.973(12584)^\circ$

6. Scheme S3: Two coordination modes of H_2 cdtp ligands.

