

**Supporting Information**

**for**

**Conformation Control of Flexible 1,4-phenylenediacetate Ligand in  
Coordination Complexes: A Rigidity-Modulated Strategy**

**Tian-Fu Liu<sup>a,b</sup>, Jian Lü<sup>a</sup>, Lin-Xi Shi<sup>a</sup>, Zhen-Gang Guo<sup>a</sup>, Rong Cao \*<sup>a</sup>**

<sup>a</sup> State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fujian, Fuzhou, 350002, P. R. China. Fax: +86-591-8379 6710; Tel: +86-591-8379 6710; E-mail: rcao@fjirsm.ac.cn

<sup>b</sup> Graduate School, Chinese Academy of Sciences, Beijing, 100039, P. R. China

**Figure S1** ORTEP drawing of the basic building block in complex **1a** showing the coordination environment around the zinc atoms with thermal ellipsoids at 30% probability. symmetry code: A (-x,-y+3,-z+1), B (x,y-1,z), C (x,-y+3/2,z-1/2).

**Figure S2** ORTEP drawing of the basic building block in complex **1b** showing the coordination environment around the manganese atom with thermal ellipsoids at 30% probability. symmetry code: A (1-x,-y,2-z), B (1-x,y-1/2,2-z), C (x, 1/2-y,z+1/2), D (2-x,y-1/2,5/2-z), E (2-x,1-y,2-z), F (x-1, 1/2-y,z-1/2), G (x-1,y-1,z)

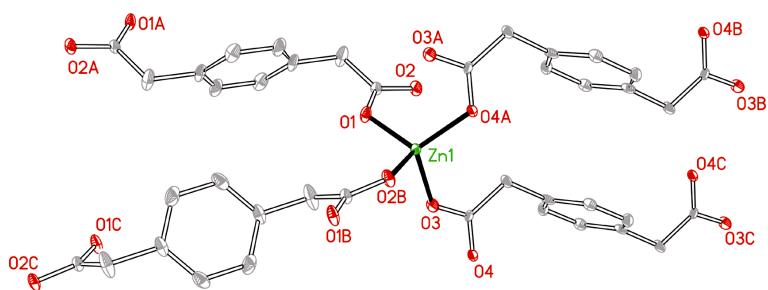
**Figure S3** ORTEP drawing of the basic building block in complex **2b** showing the coordination environment around the zinc atom with thermal ellipsoids at 30% probability. symmetry code: A (x,2/3-y,1-z), B (x,y-1,z).

**Figure S4** ORTEP drawing of the basic building block in complex **2a** showing the coordination environment around the cobalt atom with thermal ellipsoids at 30% probability. symmetry code: A (x,y-1y,z-1), B (-x,1-y,1-z).

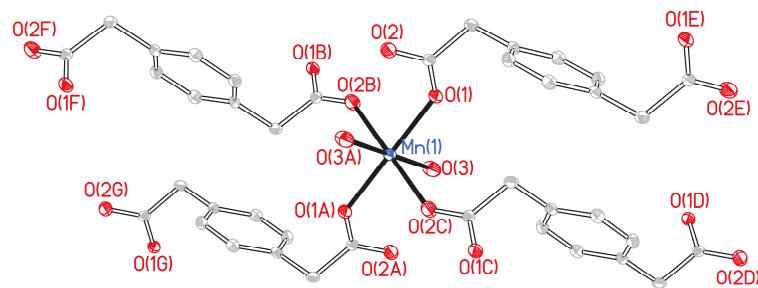
**Figure S5** ORTEP drawing of the basic building block in complex **2c** showing the coordination environment around the cadmium atom with thermal ellipsoids at 30% probability. symmetry code: A (-x,1-y,1-z), B (x,y-1y,z-1).

**Figure S6** (a) Polyhedral presentation of the individual 1-D chains built by zinc ions and *cis*-pda<sup>2-</sup> ligands; (b) Polyhedral presentation of the 2-D coordination net in complex **2a** (*cis*-pda<sup>2-</sup> and 4,4'-bpy ligands are shown in different shades); (c) Packing diagram of complex **2a**.

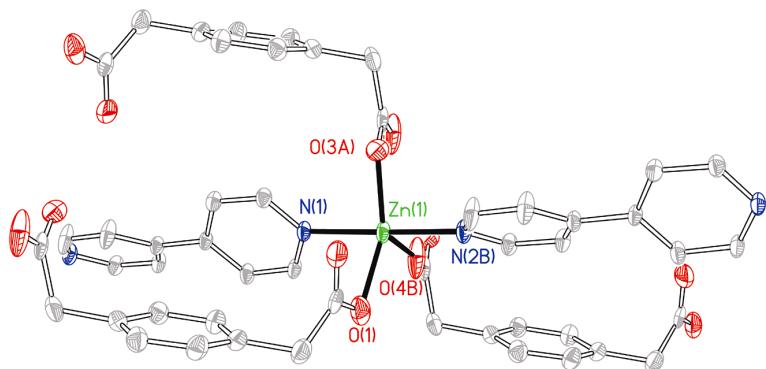
**Figure S7** Solid-state excitation spectra of **1a**, **2a**, **2c**, **4,4'-bipy** and **H<sub>2</sub>pda** at room temperature.



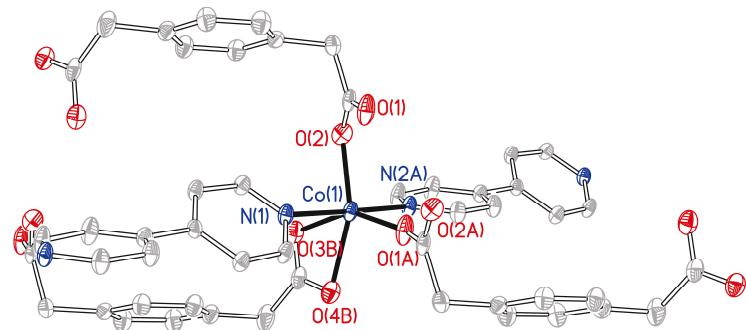
**Figure S1**



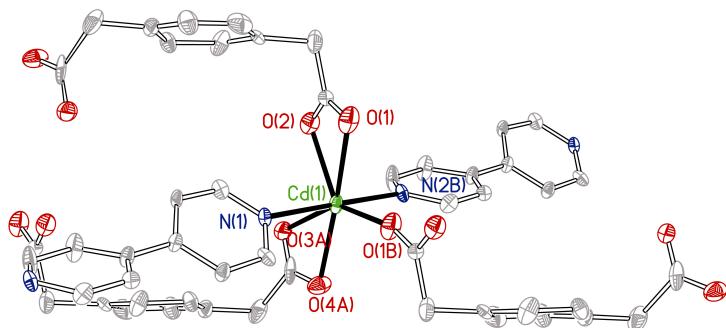
**Figure S2**



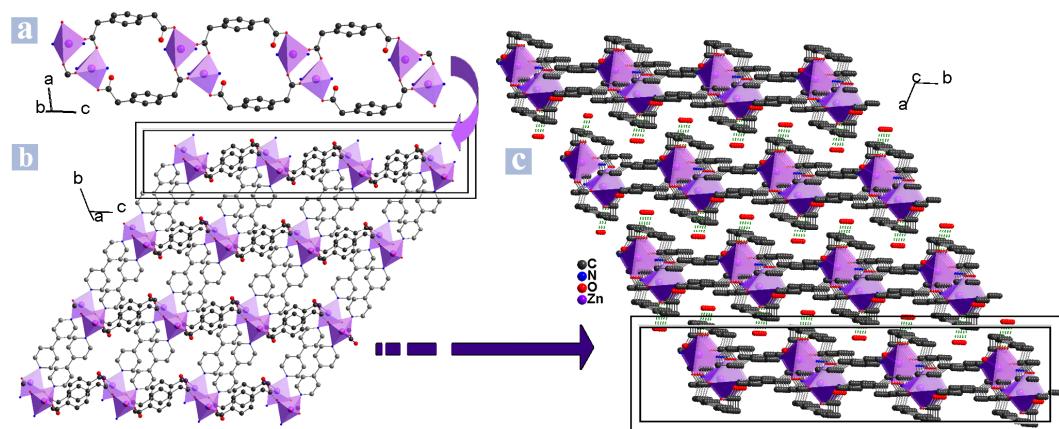
**Figure S3**



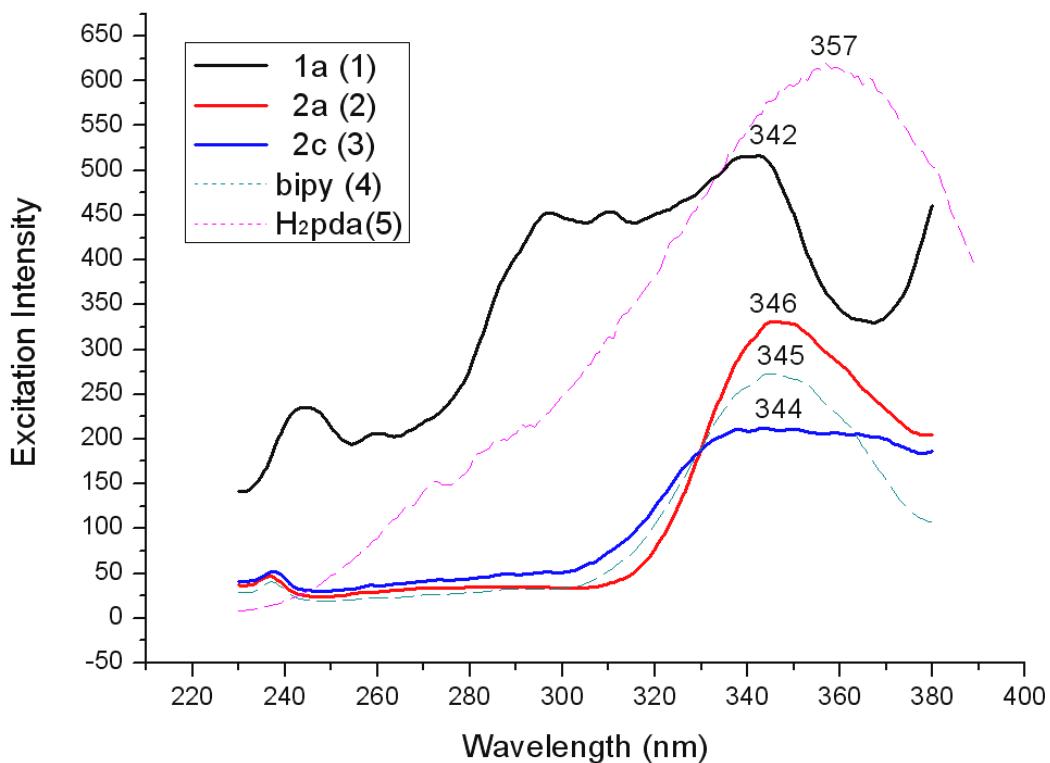
**Figure S4**



**Figure S5**



**Figure S6**



**Figure S7**