



STRUCTURAL  
CHEMISTRY

**Volume 74 (2018)**

**Supporting information for article:**

**A new Cd<sup>II</sup> coordination polymer with a self-penetrating architecture induced by the molecular conformation of a rigid bi-thiophene ligand**

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## A new Cd<sup>II</sup> coordination polymer with self-penetrating architecture induced by molecular conformation of rigid bithiophene ligand

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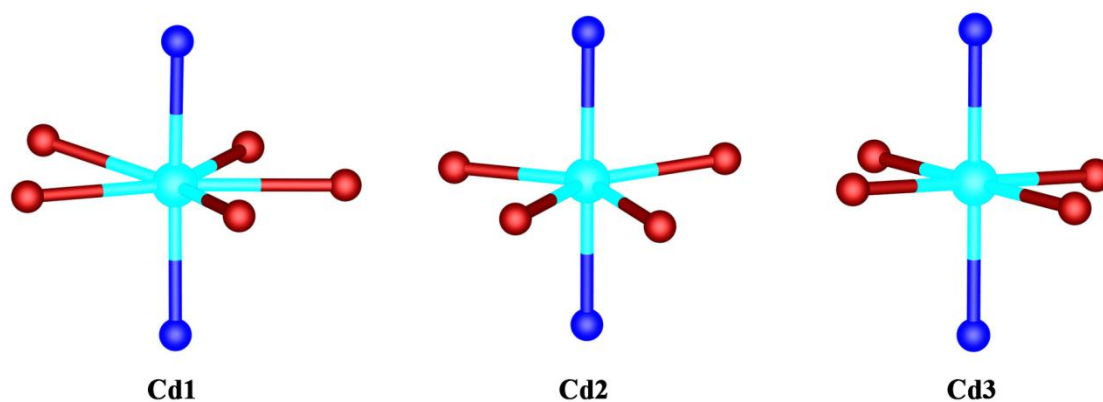
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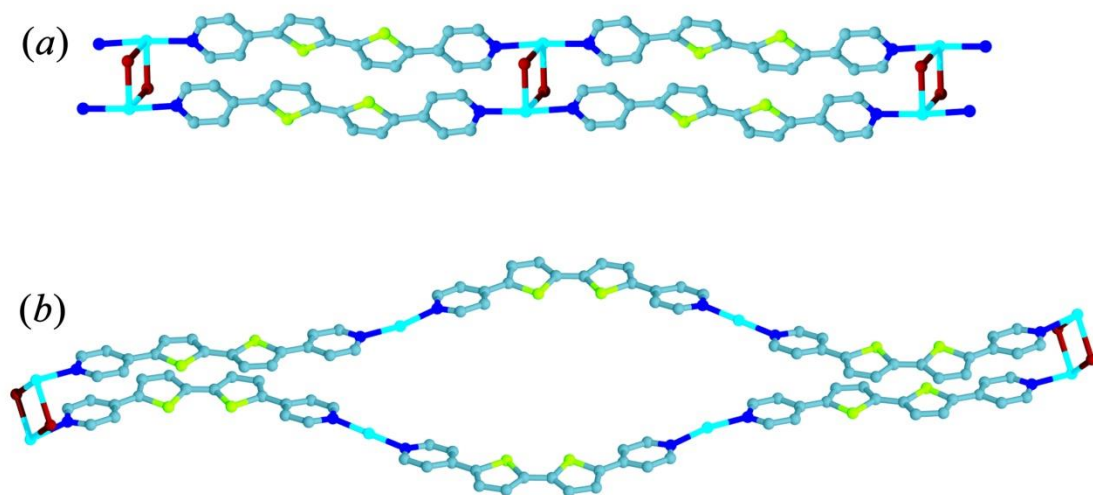
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**Table S1** Energies of HOMO and LUMO as well as the total energies of the *trans*- and *cis*- conformations of bpbp calculated with B3LYP/6-31G(d).

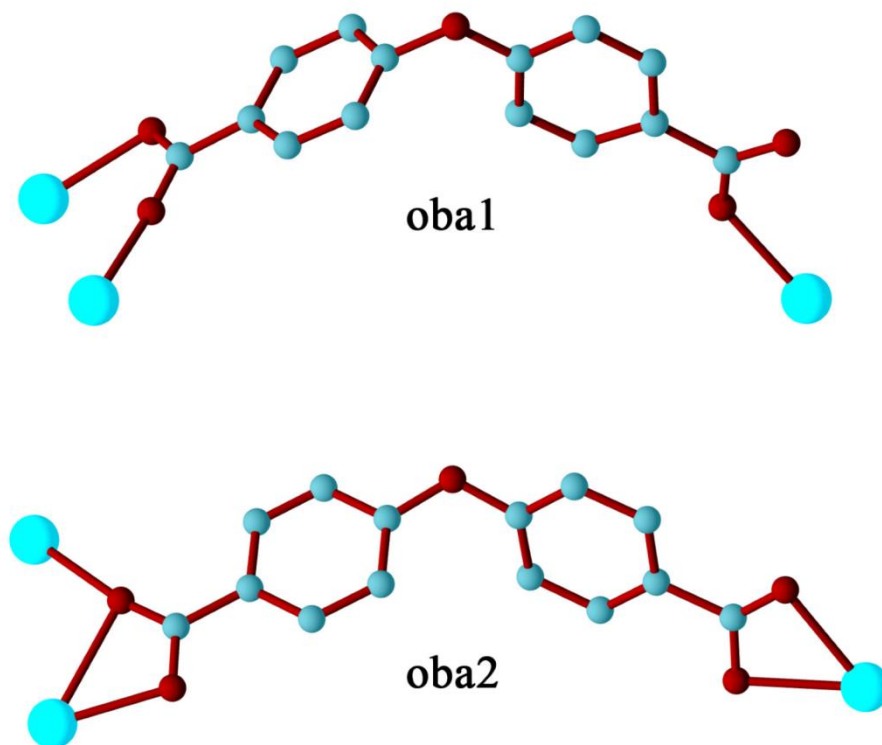
Optimized ligand	HOMO (eV)	LUMO (eV)	Total energy (a. u.)
<i>trans</i> -	-5.634	-2.308	-1599.00928089
<i>cis</i> -	-5.616	-2.279	-1599.00804463



**Figure S1** Coordination geometries of the three unique Cd(II) cations in (I)



**Figure S2** (a) The 1D double chain structure formed by  $\text{Cd}_2(\text{CO}_2)_2$  and *trans*-bpbp ligands. (b) The spindle  $[\text{Cd}_8(\text{cis-bpbp})_4(\text{trans-bpbp})_2]$  ring.



**Figure S3** Two different  $\mu_3\text{-}\eta^1:\eta^2$  coordination modes of oba ligands.