Electronic Supplementary Material (ESI) for CrystEngComm.

Synthesis, crystal structure and luminescence studies of zinc(II) and cadmium(II) complexes with 6-(1H-tetrazol-5-yl)-2-naphthoic acid

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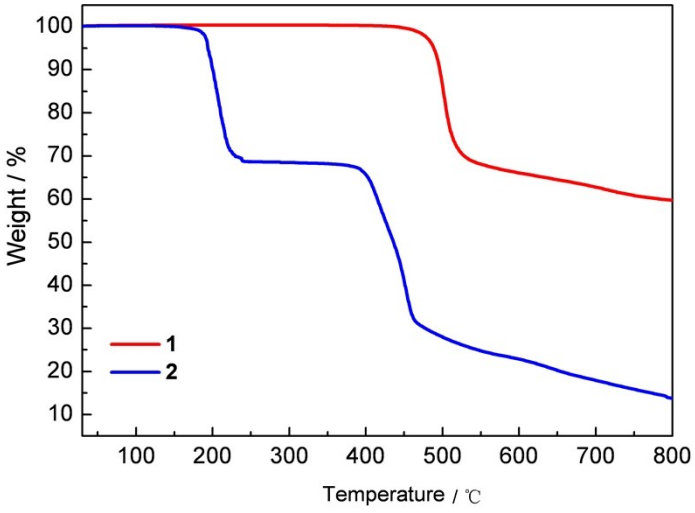

Figure S1. TGA curve of 1 and 2

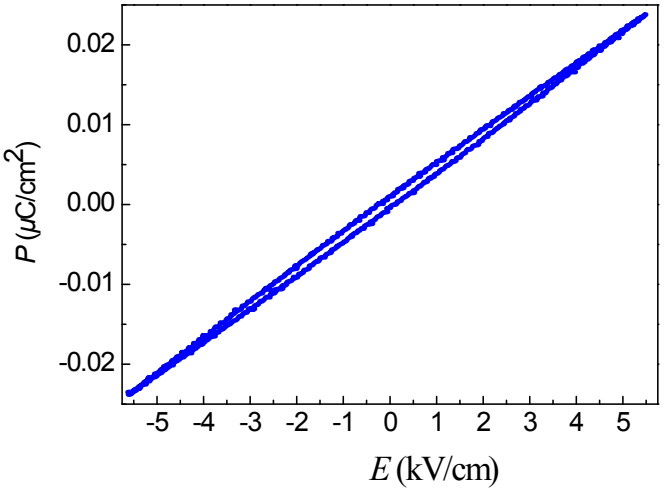

Figure S2. Electric hysteresis loop of **1**, observed for a powdered sample in the form of a pellet at room temperature.

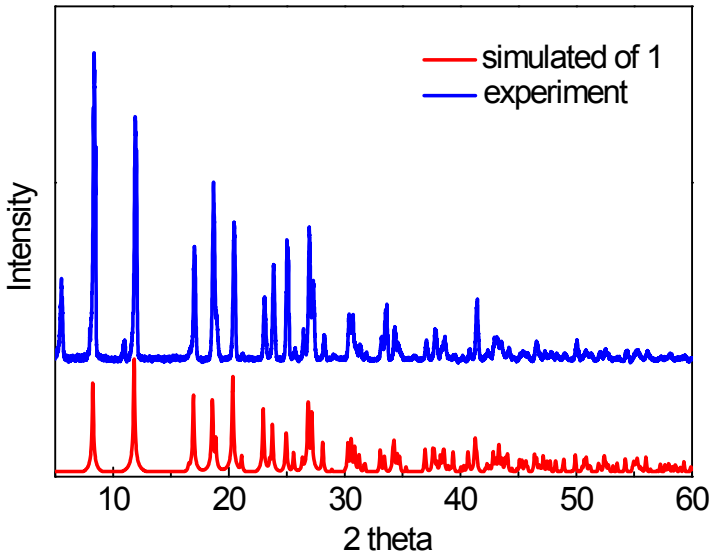

Figure S3. XRD pattern of 1

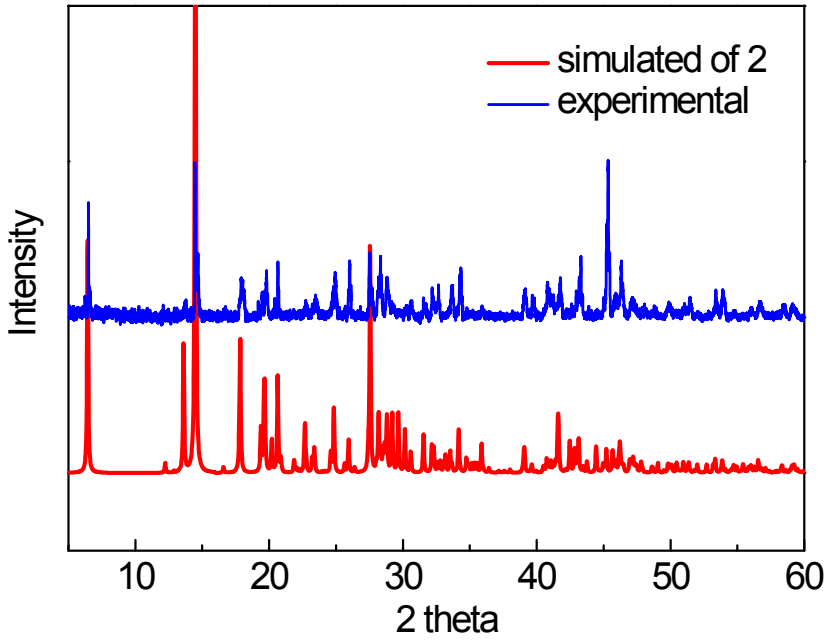

Figure S4. XRD pattern of 2

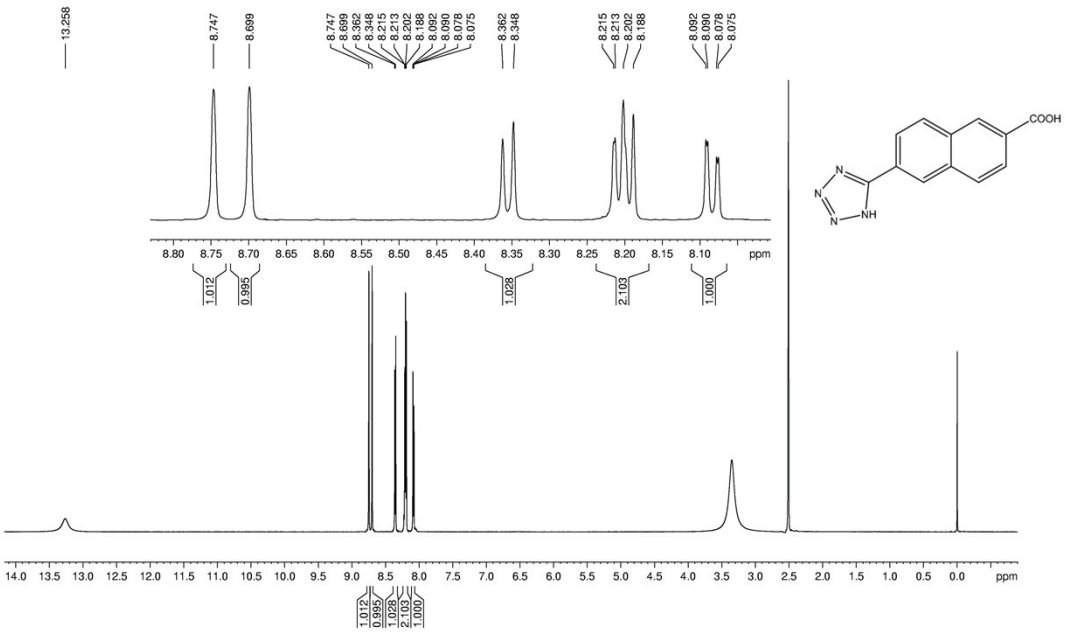

Figure S5. HNMR spectra of free ligand

Table S1 Comparison of Coordination-bond length (unit: Å) between Experimental and Theory

Name	Exp.	The.	Name	Exp.	The.
Compound 1					
Zn-O1	1.951	1.996	Zn-O1	1.968	2.011
Zn-N1	1.978	2.004	Zn-N2	1.993	2.017

The dihedral angles between the naphthyl group and the tetrazolyl group				29.6°	30.2°
Compound 2					
Cd-O1	2.336	2.232	Cd-O2	2.286	2.429
Cd-O3	2.361	2.478	Cd-N1	2.357	2.398
Cd-N2	2.368	2.451	Cd-N3	2.323	2.341
The dihedral angles between the naphthyl group and the tetrazolyl group				87.6°	88.55°

Computational Details

Geometry optimization and electronic structure calculations were carried out using the VASP program [3-4]. Projector-augmented wave (PAW) [5] method, featuring the accuracy of augmented plane-wave methods as well as the efficiency of the pseudopotential approach, was explicitly used. Generalized gradient approximation (GGA) of Perdew Burke Ernzerhof (PBE)[6] was used to describe Exchange-correlation effects. Furthermore, long dispersion interaction was corrected by one non-local correlation vdW-DF [7] based on opt88 functional. The 3d and 4s electrons of Zn and Cd, 2s and 2p electrons of C, N and O, and 1s electrons of H were explicitly treated as valence electrons. The electron wave function is expanded in plane waves up to a cutoff energy of 450 eV. For the Brillouin zone integration, we use the K-points grid of 4×2×2 for 1 (Zn) and 4×8×4 for 2 (Cd). And both cutoff energy and K-point grid was verified to be enough to exactly calculate the energy of Brillouin zone. The optimization convergence in Hellmann-Feynman force was set to 2.0× 10−2 eV/Å, and the SCF energy convergence was set to 1.0×10−6. Band structure and Partial Density of State (PDOS) were also identified. Moreover, frontier molecular orbits analysis at Gamma point was also plot by using DMol3 program [8-9] with the exchange-correction functional of GGA-PBE[6] and DNP basic set[9].

Reference

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