Electronic Supplementary Material (ESI) for CrystEngComm

Variable Crystal Structures Based on 4,4'-(diethynylanthracene-9,10-diyl) dibenzoic Acid: From 0D Dimer to 3D Net Framework

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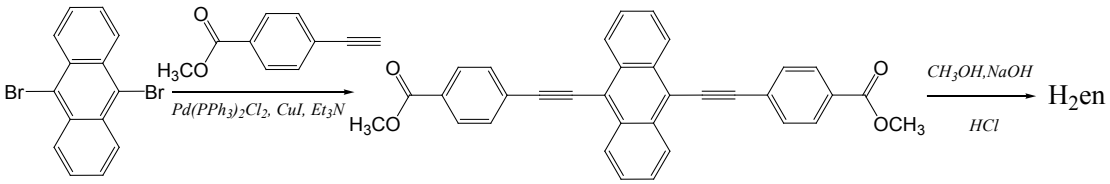
The synthesis of H2L:



A mixture of 9,10-dibromoanthracene (1.2 g, 3.2 mmol) and freshly distilled THF (30 mL) was degassed with dry Ar for 20 min. Bis(triphenylphosphine)palladium dichloride (45 mg) and copper iodide (25 mg) were added and the mixture stirred at room temperature for 15 min. A solution of methyl 4-ethynylbenzoate (1.03 g, 6.4 mmol) in anhydrous THF (10 mL) was then added dropwise and mixture stirred overnight at 80 ℃. Upon completion, volatile materials were removed under reduced pressure, and the residue added to water (100 mL), which was extracted with CH_2Cl_2. The organic phase was washed with water and then brine, and dried over Na_2SO_4. The CH_2Cl_2 was removed under reduced pressure to afford the yellow solid product (1.8 g, 80%). 3 g of yellow product was mixed with 50 mL CH_3OH solution with saturated KOH and 20 mL of THF, and the mixture refluxed for 12 h. After the hydrolysis was complete, THF and CH_3OH were removed under reduced pressure. The remained product were dissolved in 250 mL aqua, and then acidified to pH 2 -3 with concentrated aqueous HCl, and the precipitate was separated by filtration and washed successively with water to yield yellow H_2L (2.6 g, yield 81%).

Table S1. Crystallographic Data and Structure Refinement for **1 - 3**

	compound1	compound2	compound3
Chemical formula	$C_{70}H_{66}Co_2N_2O_{20}$	$C_{70}H_{60}Cd_2N_2O_{17}$	$C_{54}H_{46}EuO_{12}N_2$
Formula Mass	1373.16	1426.07	1066.93
Crystal system	Monoclinic	Orthorhombic	Triclinic
a/Å	24.117(5)	18.4701(16)	9.9355(10)
b/Å	7.1088(14)	44.767(5)	12.1661(13)
c/Å	19.077(4)	7.2462(8)	23.473(3)
α/°	90.00	90.00	75.392(2)
β/°	112.94(3)	90.00	80.660(2)
γ/°	90.00	90.00	79.549(2)
Unit cell volume/Å^3	3012.1(10)	5991.5(11)	2679.7(5)
Space group	$P2_1/c$	*Pnma*	$P\bar{1}$
No. of formula units per unit cell, *Z*	2	4	2
Final R_1 values ($I > 2\sigma(I)$)	0.0847	0.1115	0.0511
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1764	0.2230	0.1077
Final R_1 values (all data)	0.1658	0.1873	0.0672
Final $wR(F^2)$ values (all data)	0.2243	0.2737	0.1132

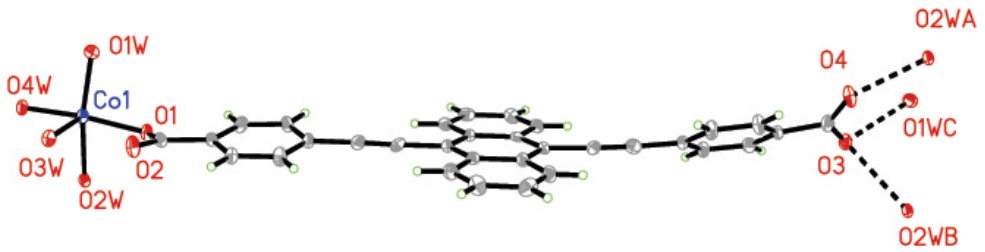


Figure S1 The perspective view of the hydrogen bonds of the deprotonated carboxyl.

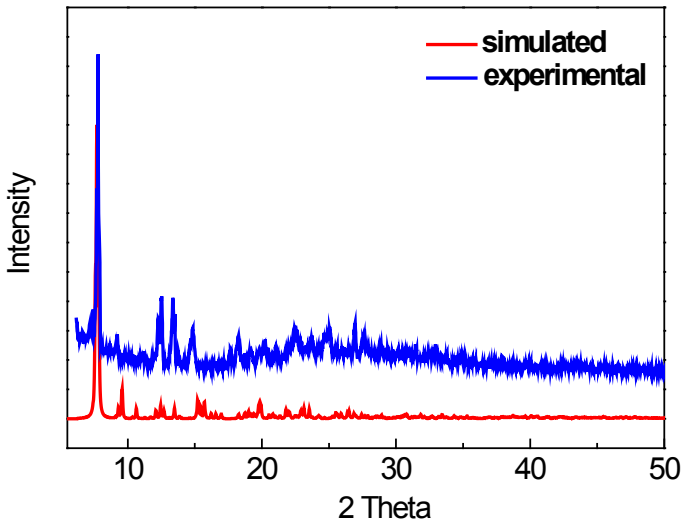


Fig.S2 XRD pattern of **3**.The blue lines represents the spectra of sample after

gas-sorption measurement.

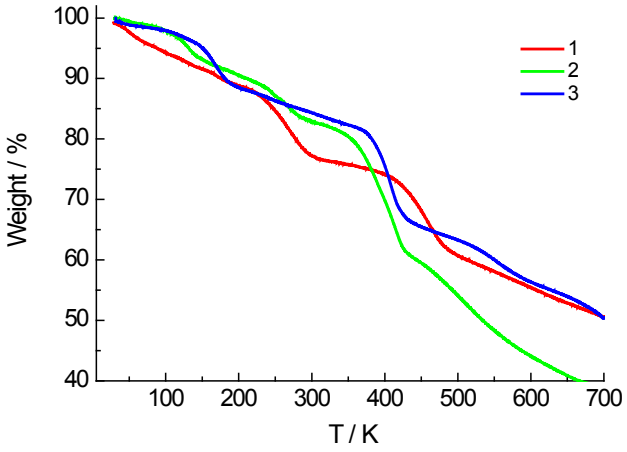
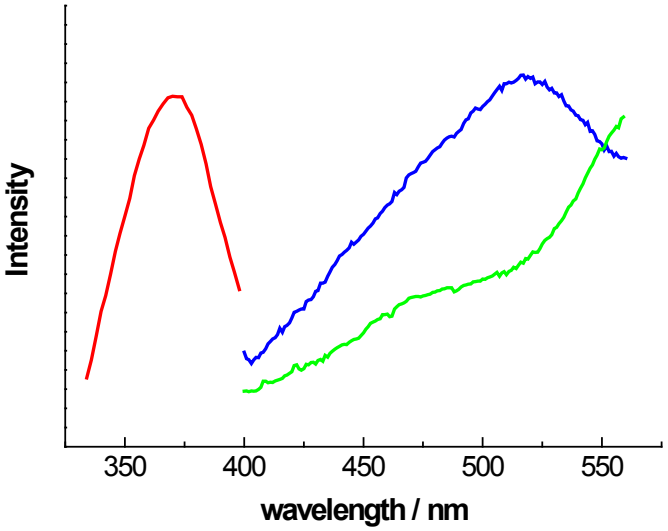
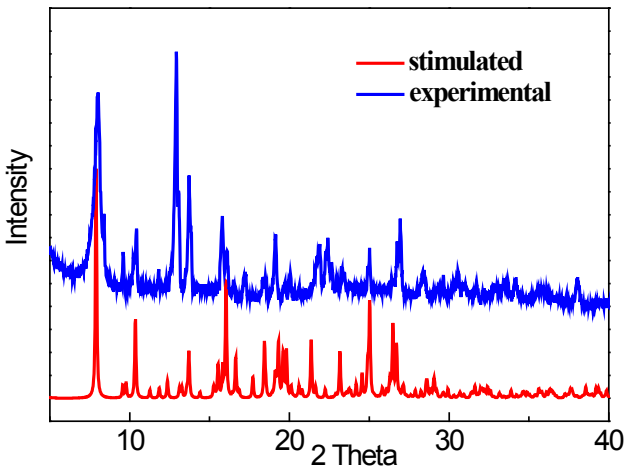


Figure S3 TGA curve of 1-3



Figures S4 The solid-state excitation spectra of the CPs **1**- **3** at room temperature.



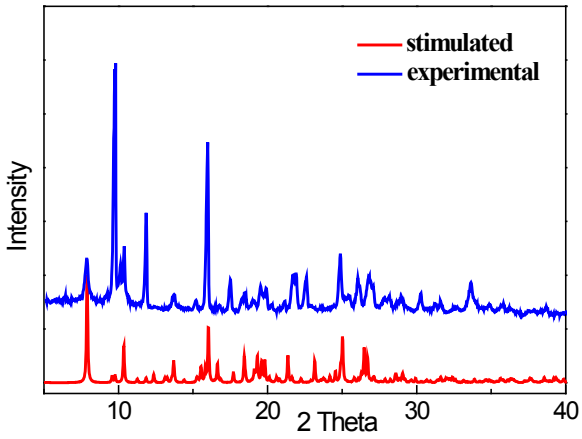


Fig.S5 XRD pattern of **1-2**. The difference between the two peaks might be caused by the impurities in the samples.

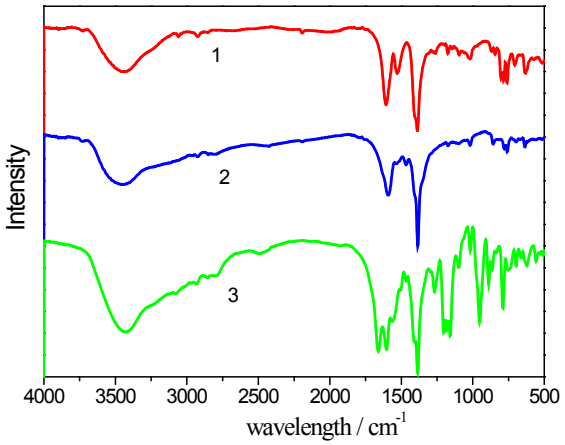


Figure S6 IR spectra of 1 -3