Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Dual hydrogen-bond donor groups-containing Zn-MOF for the highly effective coupling of CO_2 and epoxides under mild and solvent-free conditions

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X-ray Crystallography

Table S1 Crystal data and structure refinement for $Zn_3(L)_3(H_2L)$

Empirical formula	$C_{32}H_{20}N_4O_{16}Zn_3$
Formula weight	912.63
Temperature/K	302.93
Crystal system	monoclinic
Space group	*C2/c*
a/Å	33.5352(13)
b/Å	9.8226(4)
c/Å	18.0794(7)
Volume/Å3	5949.1(4)
Z	4
*ρ*calcg/cm3	1.019
μ/mm-1	1.248
F(000)	1832.0
Reflections collected	43220
Independent reflections	5401 [R_{int} = 0.0611, R_{sigma} = 0.0341]
Data/restraints/parameters	5401/0/272
Goodness-of-fit on F2	1.118
Final *R* indexes [I>=2*σ* (I)]	R_1 = 0.0404, wR_2 = 0.1340
Final *R* indexes [all data]	R_1 = 0.0537, wR_2 = 0.1414

Table S2 The selected bond lengths (Å) and angles (deg) of $Zn_3(L)_3(H_2L)$

Zn1- O1	1.956(3)	O1- Zn1- $O3^{i}$	108.58(14)
Zn1- $O3^{i}$	1.978(3)	O1- Zn1- O8	111.53(11)
Zn1- O5	1.941(3)	$O3^{i}$- Zn1- O8	97.01(12)
Zn1- O8	2.016(3)	O5- Zn1- O1	98.55(16)
Zn2- $O2^{ii}$	2.048(3)	O5- Zn1- $O3^{i}$	103.75(14)
Zn2- $O2^{iii}$	2.048(3)	O5- Zn1- O8	135.48(16)
Zn2- O4	2.033(2)	$O2^{ii}$- Zn2- $O2^{iii}$	180.0
Zn2- $O4^{iv}$	2.033(2)	$O2^{iii}$- Zn2- $O8^{iii}$	90.17(10)
Zn2- $O8^{iii}$	2.263(2)	$O2^{iii}$- Zn2- $O8^{ii}$	89.83(10)
Zn2- $O8^{ii}$	2.263(2)	O4- Zn2- $O2^{iii}$	93.88(11)
		O4- Zn2- $O2^{ii}$	86.12(11)
		$O4^{iv}$- Zn2- $O2^{ii}$	93.88(11)
		$O4^{iv}$- Zn2- $O2^{iii}$	86.12(11)
$O4^{iv}$- Zn2- $O8^{ii}$	89.36(10)	$O4^{iv}$- Zn2- O4	180.0
O4- Zn2- $O8^{ii}$	90.64(10)	$O4^{iv}$- Zn2- $O8^{iii}$	90.64(10)
$O8^{iii}$- Zn2- $O8^{ii}$	180.0	O4- Zn2- $O8^{iii}$	89.36(10)

Symmetry codes: (i) x, -y, -0.5+z; (ii) 0.5-x, -0.5+y, 1.5-z; (iii) x, -y, 0.5+z; (iv) 0.5-x, -0.5-y, 2-z

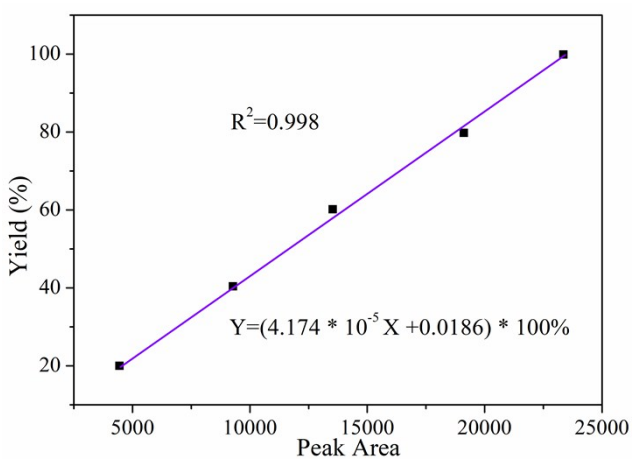

Fig. S1 Calibration curve of PC yield based on GC results

In the GC chromatograms of product PC, the special retention time of PC is 2.8-3.2 min. So the yield could be calculated by the calibration curve of PC yield (Fig. S1) with the peak area in the range of time.

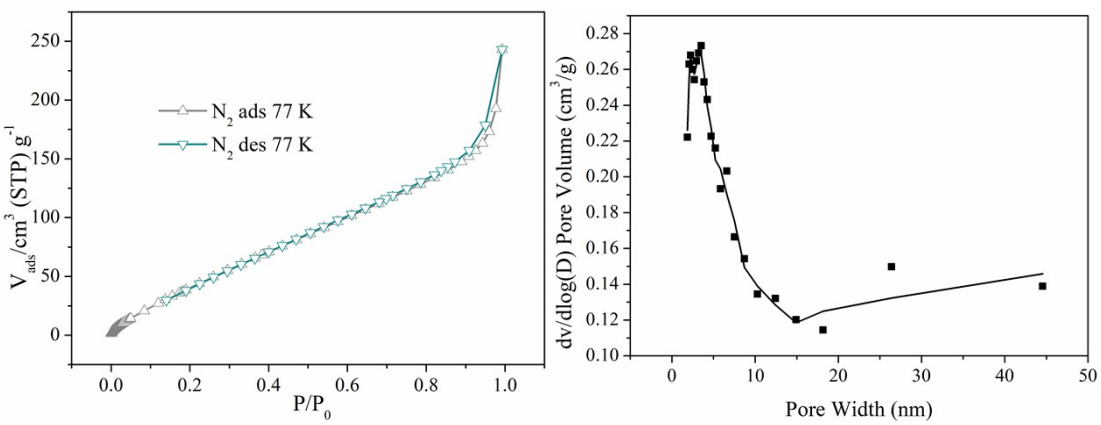

Fig. S2 N_2 adsorption−desorption isotherm of $Zn_3(L)_3(H_2L)$ and the pore size distribution calculated from desorption isotherm