Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A Novel 3-fold Interpenetration Metal−Organic Framework with Tunable Luminescence and Selective Adsorption of CO_2 Properties

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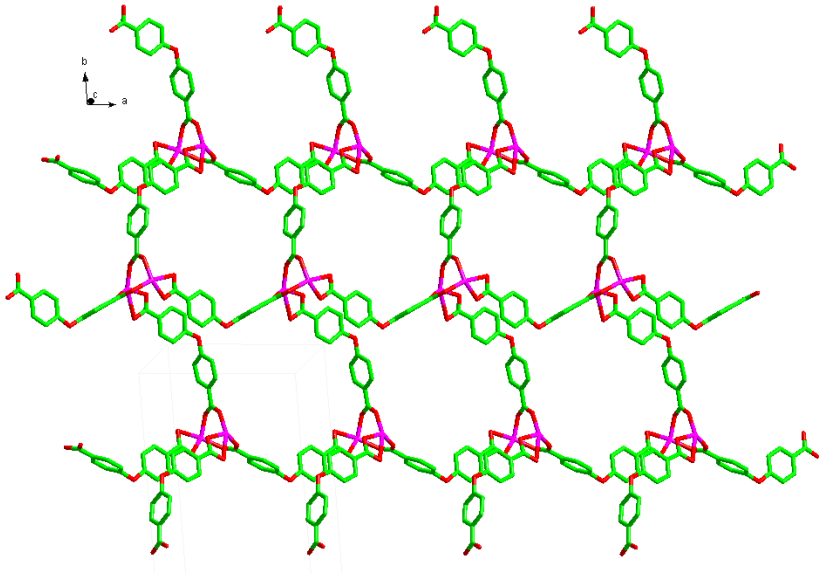

Figure S1. Along *c* axis direction, the two-dimensional layers in polymer **1**.

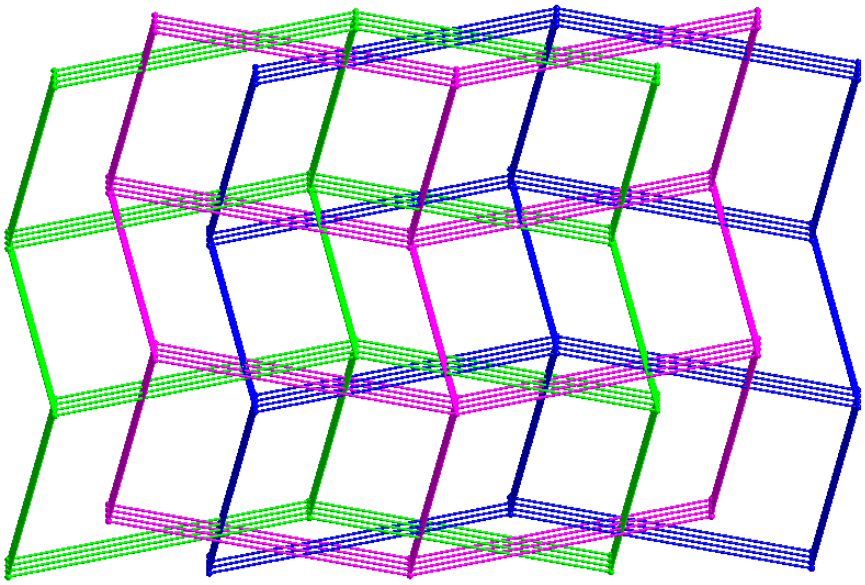

Figure S2. Schematic description of the 6-connected **α-Po** nets.

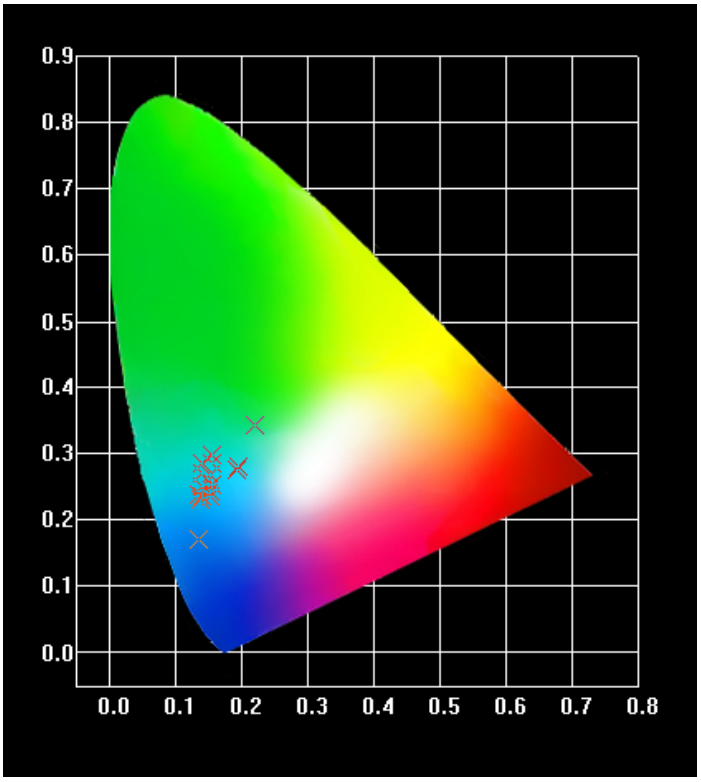

Figure S3. The CIE chromaticity coordinates of the emissions spectrum excited at 285−380 nm.

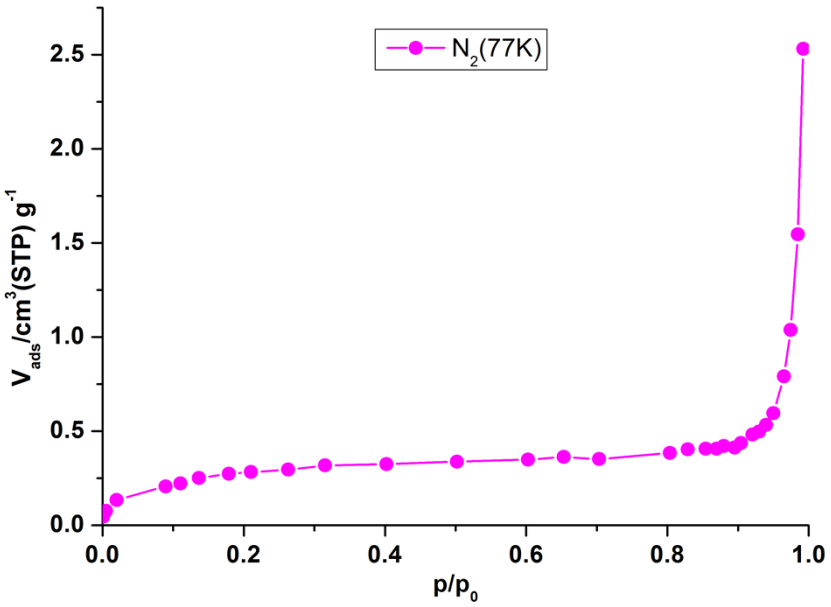

Figure S4. Adsorption isotherms of N_2 at 77 K of **1**.

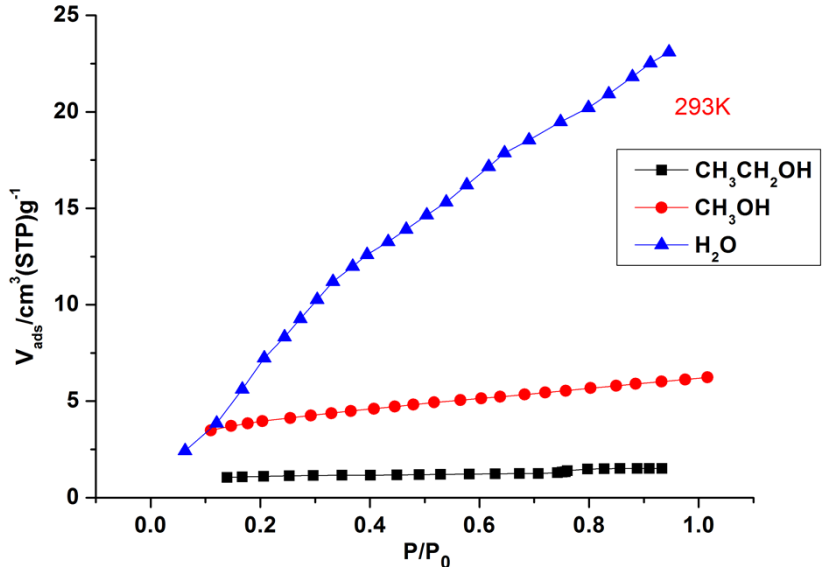

Figure S5. Comparison of vapor adsorption isotherms of **1** for water, ethanol and methanol vapour at 293 K.

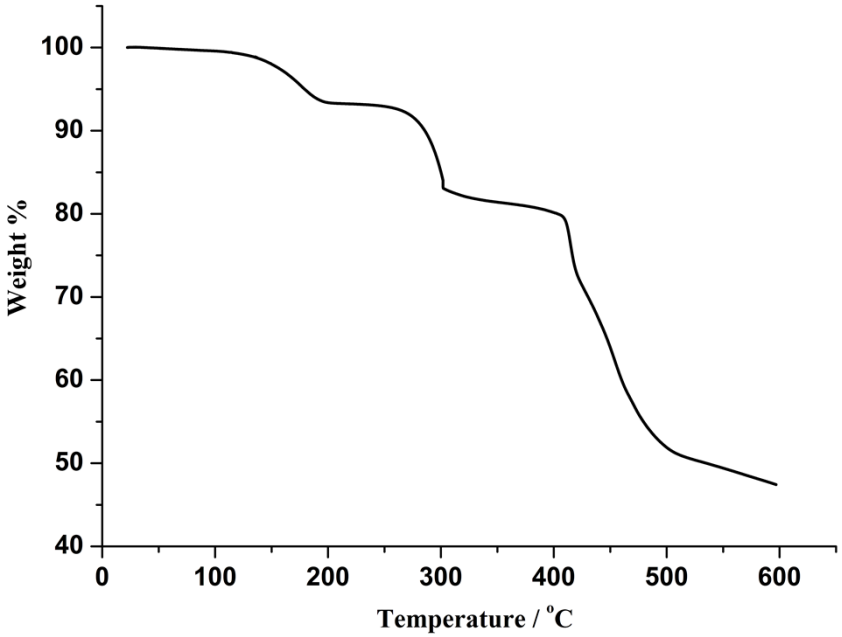

Figure S6. TG curve of as-synthesized 1.

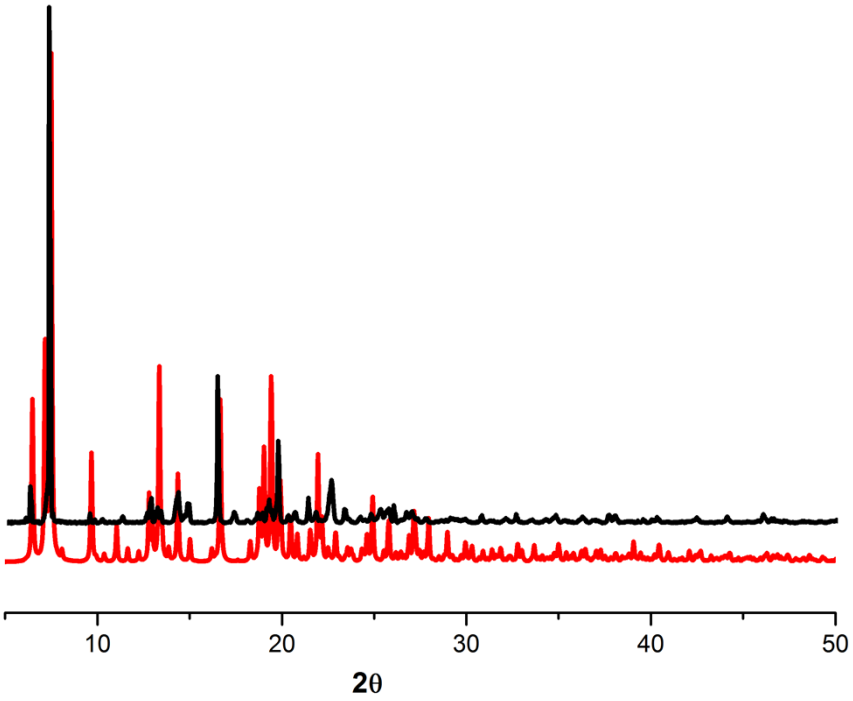

Figure S7. Powder XRD patterns for **1**: (red: simulated one; black: the as-synthesized sample).

Table S1. Crystallographic data for **1**.

	1
Chemical formula	$C_{52}H_{48}N_6O_{16}Zn_2$
M_r	1143.70
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	14.5740 (7), 23.5585 (11), 15.4557 (7)
β (°)	110.801 (3)
V (Å^3)	4960.7 (4)
Z	4
μ (mm^{-1})	1.531
Crystal size (mm)	0.30 × 0.25 × 0.20
T_{min}, T_{max}	0.7441, 0.8179
R_{int}	0.0465
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0474, 0.1262, 1.051
No. of reflections	8734
No. of parameters	623
No. of restraints	20
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.498, −0.391

Table S2 Selected geometric parameters (Å, °)

N1—Zn2	2.026 (3)	O9—Zn2^{iii}	2.475 (2)
N4—Zn1^{i}	2.029 (3)	O10—Zn2^{iii}	1.970 (2)
O1—Zn1	1.991 (3)	Zn1—O4^{iv}	1.931 (2)
O2—Zn2	1.954 (2)	Zn1—N4^{v}	2.029 (3)
O4—Zn1^{ii}	1.931 (2)	Zn2—O10^{vi}	1.970 (2)
O6—Zn1	1.927 (3)	Zn2—O9^{vi}	2.475 (2)
O7—Zn2	1.964 (2)		
O6—Zn1—O4^{iv}	133.60 (12)	O7—Zn2—O10^{vi}	104.17 (10)
O6—Zn1—O1	103.89 (11)	O2—Zn2—N1	100.25 (11)
O4^{iv}—Zn1—O1	103.50 (11)	O7—Zn2—N1	107.27 (11)
O6—Zn1—N4^{v}	105.99 (13)	O10^{vi}—Zn2—N1	102.54 (11)
O4^{iv}—Zn1—N4^{v}	108.43 (12)	O2—Zn2—O9^{vi}	84.89 (10)
O1—Zn1—N4^{v}	94.38 (12)	O7—Zn2—O9^{vi}	156.25 (11)
O2—Zn2—O7	103.74 (11)	O10^{vi}—Zn2—O9^{vi}	57.61 (9)
O2—Zn2—O10^{vi}	136.44 (11)	N1—Zn2—O9^{vi}	92.55 (10)

Symmetry codes: (i) ***x*****−1, −*****y*****+3/2, *****z*****−3/2; (ii) −*****x*****, *****y*****+1/2, −*****z*****+5/2; (iii)** ***x*****+1, *****y*****, *****z*****; (iv) −*****x*****, *****y*****−1/2, −*****z*****+5/2; (v)** ***x*****+1, −*****y*****+3/2, *****z*****+3/2; (vi)** ***x*****−1, *****y*****, *****z*****.**