Electronic Supplementary Information for:

Induction of Trimeric $[Mg_3(OH)(CO_2)_6]$ in a Porous Framework by a Desymmetrized Tritopic Ligand

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Materials and Methods:

$Mg(NO_3)_3 \cdot 6H_2O$ and N,N-Dimethylacetamide (DMA) were purchased from Aldrich Chemical Co. and used as received without further purification. Organic ligand pyridine-3,5-bis(phenyl-4-carboxylic acid) (H_2PBPC) was purchased from Jinan Henghua Sci. & Tec. Co. Ltd. (China) and used as received.

Thermogravimetric analysis (TGA) was carried out under nitrogen atmosphere on a TA Instruments SDT Q500 thermal analyzer. Powder X-ray diffraction (XRD) data were collected on a Bruker D8 Advance powder diffractionmeter with CuKα radiation (40kV, 40 mA). The simulated powder pattern was calculated using single-crystal X-ray diffraction data and processed by the free Mercury 2.3 program provided by the Cambridge Crystallographic Data Centre. The sorption isotherms for N_2 and H_2 were measured by using a Micromeritics ASAP 2020 surface-area and pore-size analyzer.

Single-crystal X-ray analysis of CPF-3 was performed on a Bruker Smart APEX II CCD area diffractometer with nitrogen-flow temperature controller using graphite-monochromated MoKα radiation (λ = 0.71073 Å), operating in the ω and φ scan mode with a scan width of 0.5°. Raw data collection and refinement were done using SMART at 150K for obtaining good diffraction data. Data reduction was performed using SAINT+ and corrected for Lorentz and polarization effects. The SADABS program [1] was used for absorption correction. The structure was solved by direct methods and the structure refinements were based on $|F2|$ with anisotropic displacement using SHELX-97 [2]. All non-hydrogen atoms in the framework were refined with anisotropic displacement parameters. All hydrogen atoms in the organic ligands were placed in calculated positions. The large volume fractions of disordered cations or solvents in the lattice pores could not be modelled in terms of atomic sites and were treated using the SQUEEZE routine [3] in the PLATON software package [4]. Crystal data as well as details of data collection and refinement for CPF-3 are summarized in Table S1.

[1] G. M. Sheldrick, *SADABS*, *Program for Empirical Absorption Correction of Area Detector Data*; University of Göttingen, 1996.
[2] G. M. Sheldrick, *SHELXL-97, Program for Crystal Structure Solution and Refinement*; University of Göttingen, 1997.
[3] P. v.d. Sluis and A.L. Spek, *Acta Crystallogr., Sect. A*, 1990, 46, 194.
[4] A.L. Spek, *J. Appl. Crystallogr*., 2003, 36, 7

Table S1. Crystal data and structure refinement for CPF-3 **(**SQUEEZE).

Empirical formula	$C_{57}H_{33}N_3O_{13}Mg_3$
Formula weight	1040.79
Temperature (K)	150(2)
Crystal system, Space group	Rhombohedral *R*-3*c*
Unit cell dimensions	*a* = 19.4789(3) Å□ *b* = 19.4789(3) Å *c* = 45.5070(12) Å *V* = 14953.3(5) Å^3
Z, Density(cal.)	6, 0.693 g/cm^3
Absorption coefficient	0.066 mm^{-1}
F(000)	3216
Crystal Size (mm)	0.40 × 0.40 × 0.40
Theta range for data collection	1.50 to 25.02
Limiting indices	-14 <= h <= 21, -23 <= k <= 13, -54 <= l <= 54
Reflections collected / unique	16968 / 2948 [R(int) = 0.0450]
Observed Reflection	2108 (I >2σ(I))
Data Completeness measured	0.998
Refinement Method	Full-matrix least-squares on F^2
Parameter/Restraints/Data(obs.)	2948 / 4 / 118
Goodness-of-fit	1.123
Final R indices (I >2σ(I))	R1 = 0.0771, wR2 = 0.2336
R indices (all)	R1 = 0.0951, wR2 = 0.2446
Largest difference peak	1.032 and -0.641 e·A^{-3}

[a] $R1 = \sum(|F_o| - |F_c|) / \sum|F_o|$, $wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$.

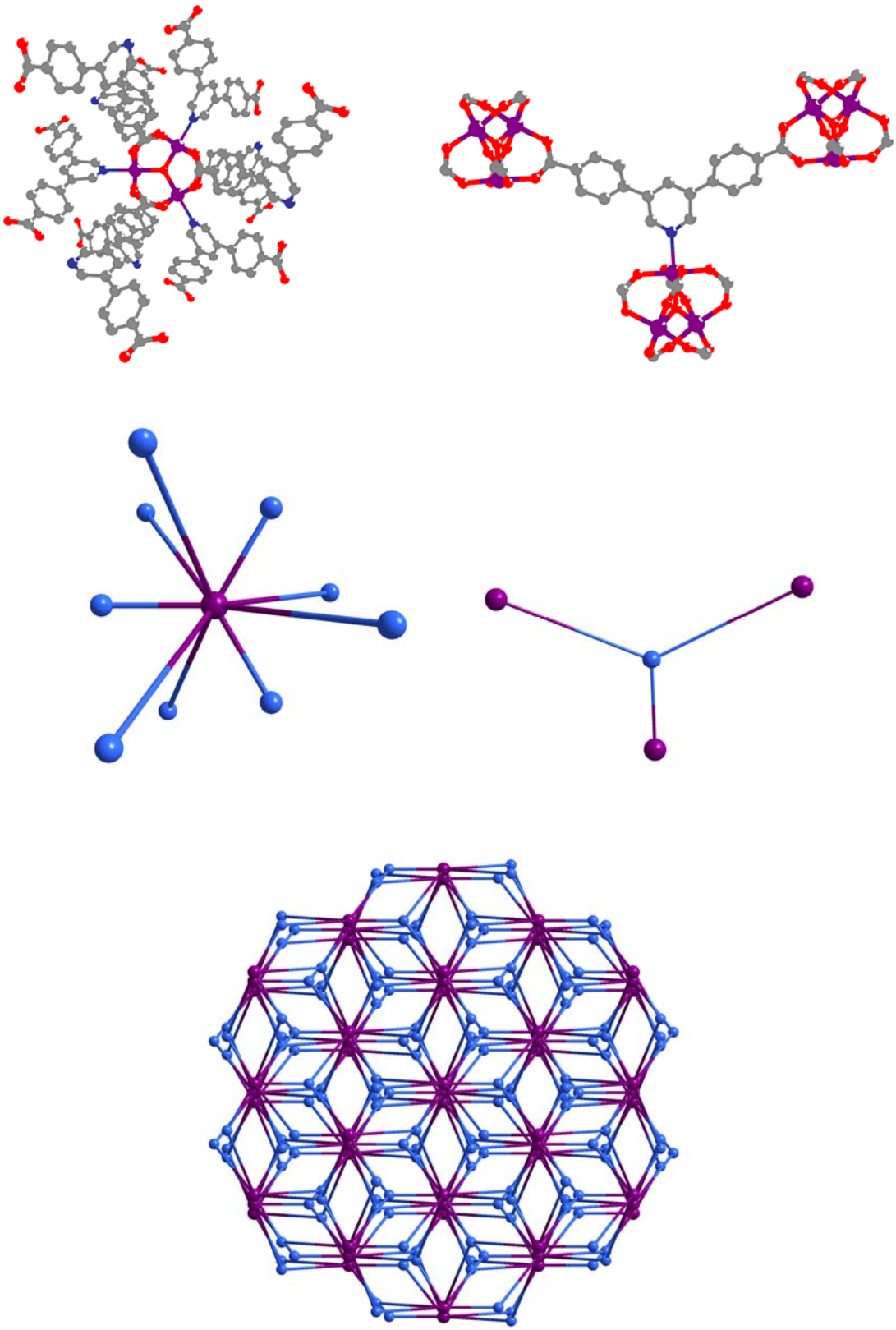

Fig. S1 The (3,9)-connected topology analysis for CPF-3.

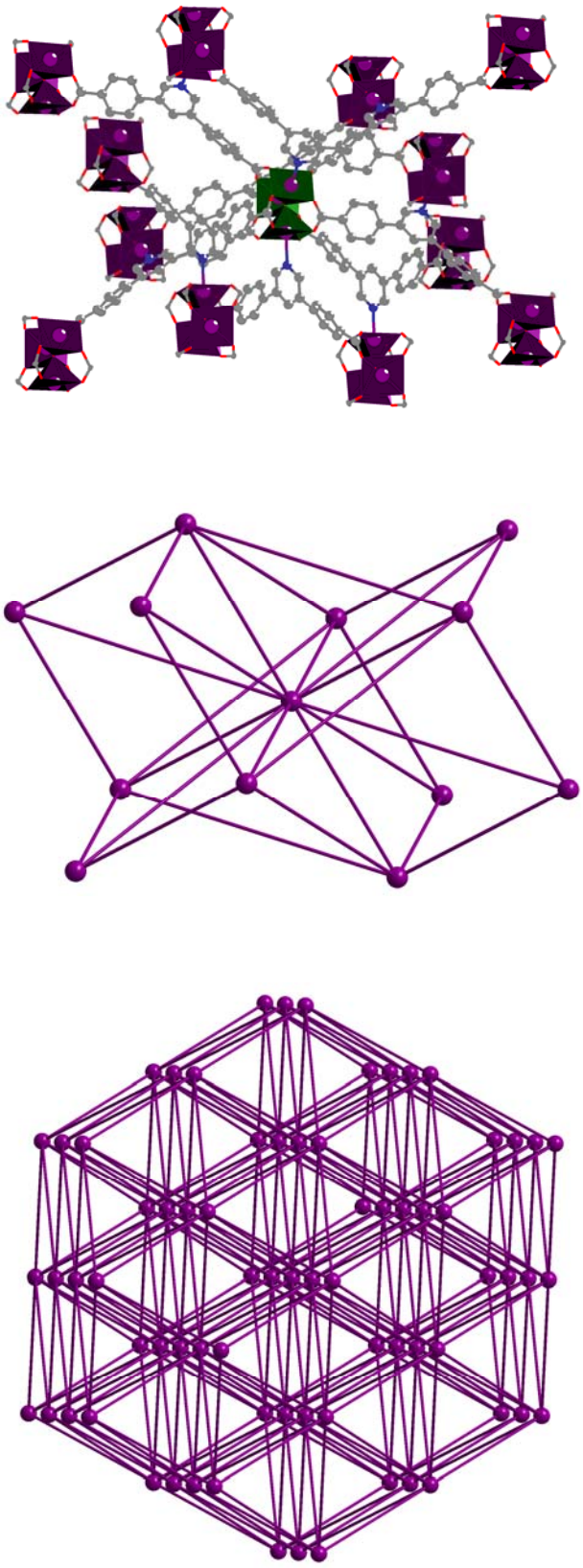

Fig. S2 The 12-connected topology analysis for CPF-3.

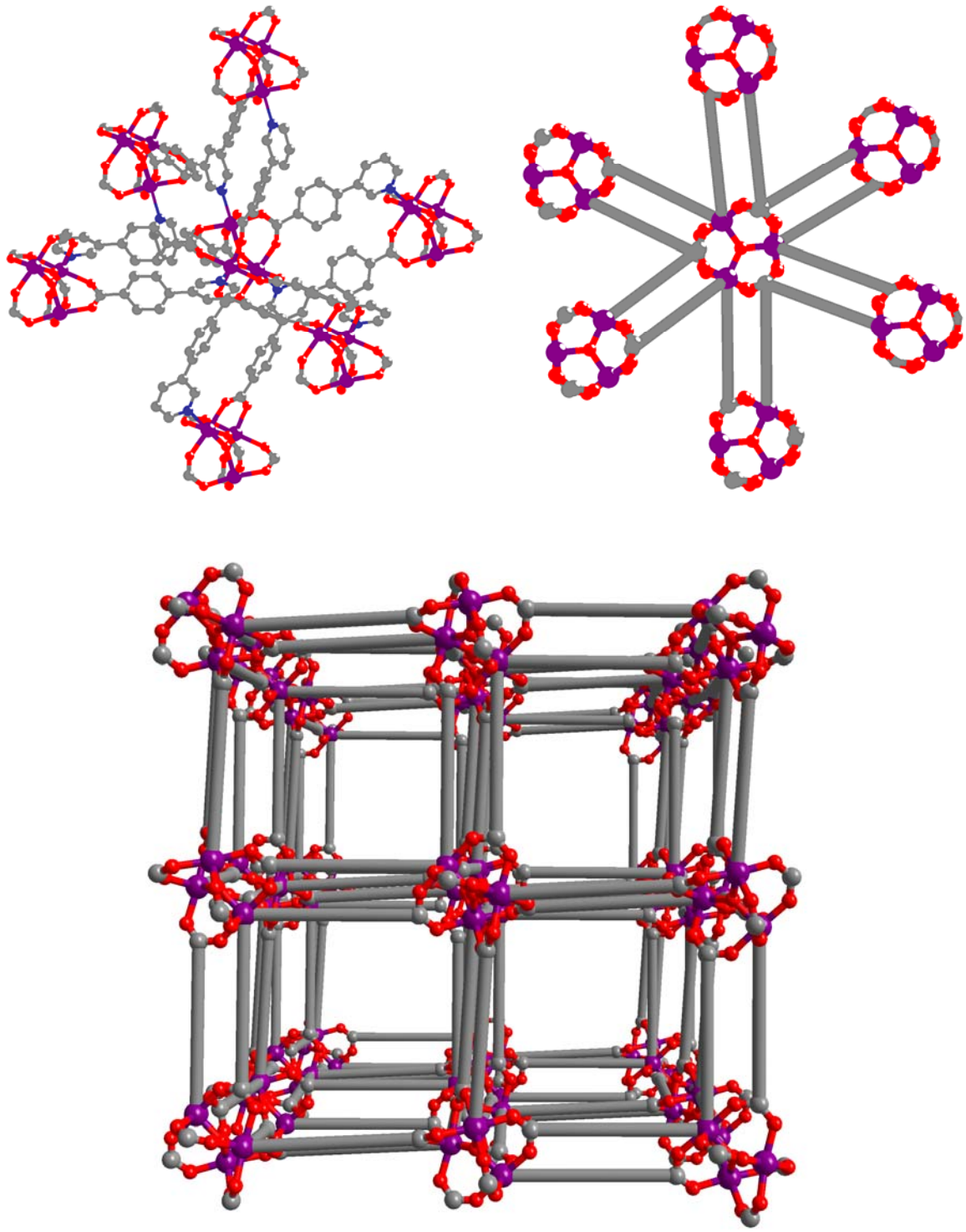

Fig. S3 The 6-connected *a*-Po net for CPF-3 with double linkers.

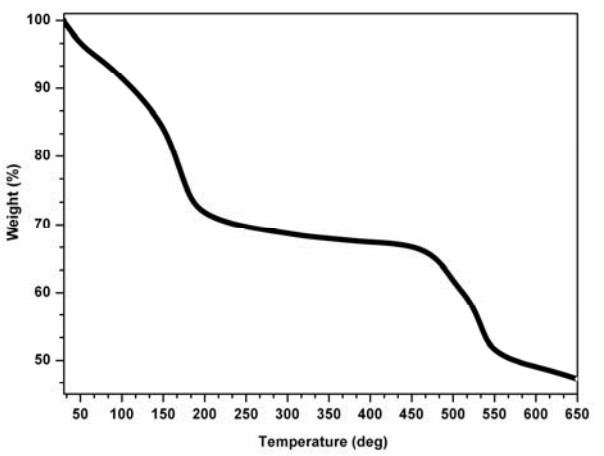

Fig. S4. TGA curve for CPF-3.

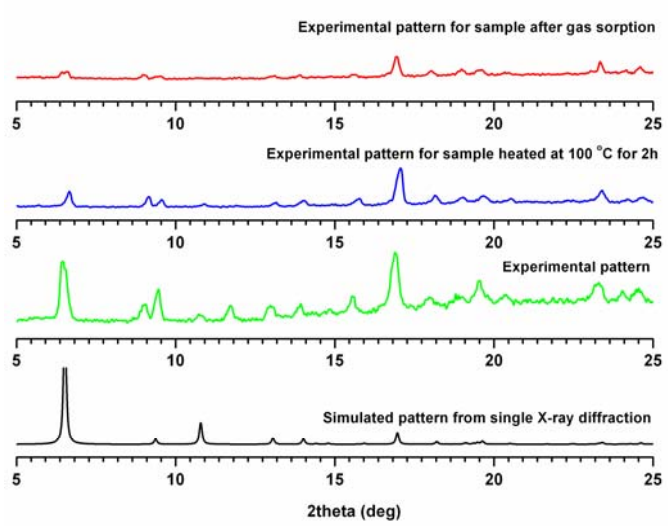

Fig. S5. XRPD patterns for CPF-3.

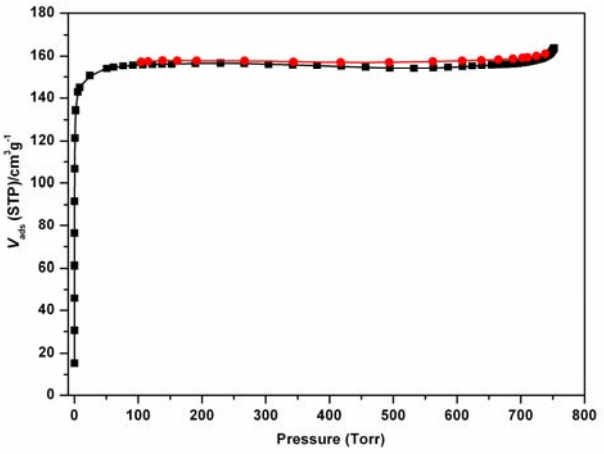

Fig. S6 N_2 adsorption (black) and desorption (red) isotherms at 77 K for CPF-3.

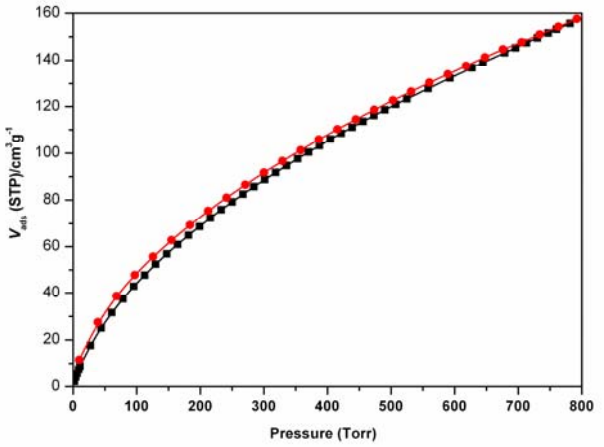

Fig. S7 H_2 adsorption (black) and desorption (red) isotherms at 77 K for CPF-3.

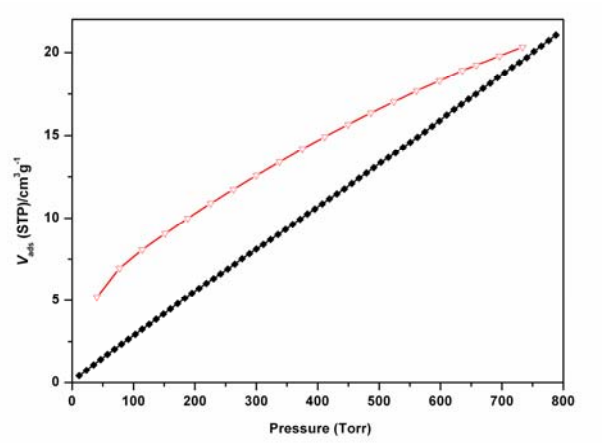

Fig. S8 CO_2 adsorption (black) and desorption (red) isotherms at 298 K for CPF-3.

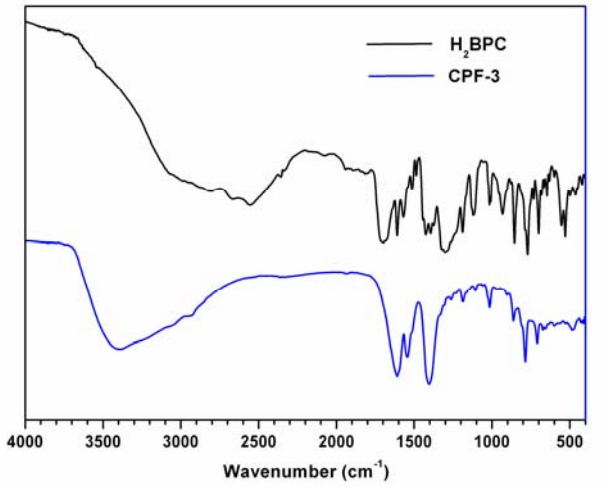

Fig. S9. FT-IR spectra for CPF-3 and H_2BPC.