Electronic Supplementary Material (ESI) for CrystEngComm.

A Porous Lanthanide Metal-Organic Framework Based on a Flexible Cyclotriphosphazene -Functionalized Hexacarboxylate Exhibiting Selective Gas Adsorption

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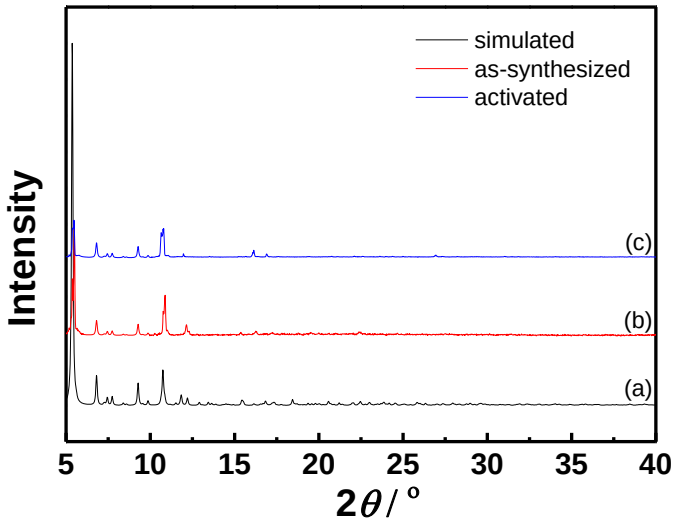


Fig. S1 PXRD patterns of **ZJNU-61**(Ho): (a) simulated; (b) as-synthesized; and (c) activated at 333 K.

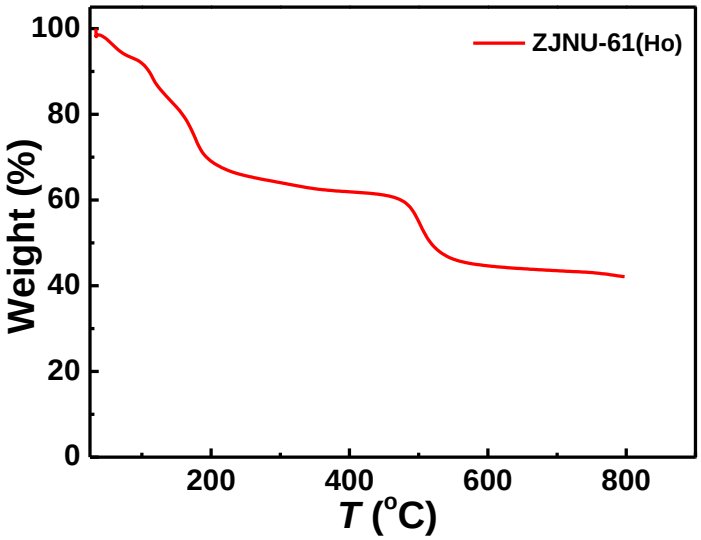


Fig. S2 TGA curve of the as-synthesized **ZJNU-61**(Ho) under nitrogen atmosphere with a heating rate of 5 K min^{-1}

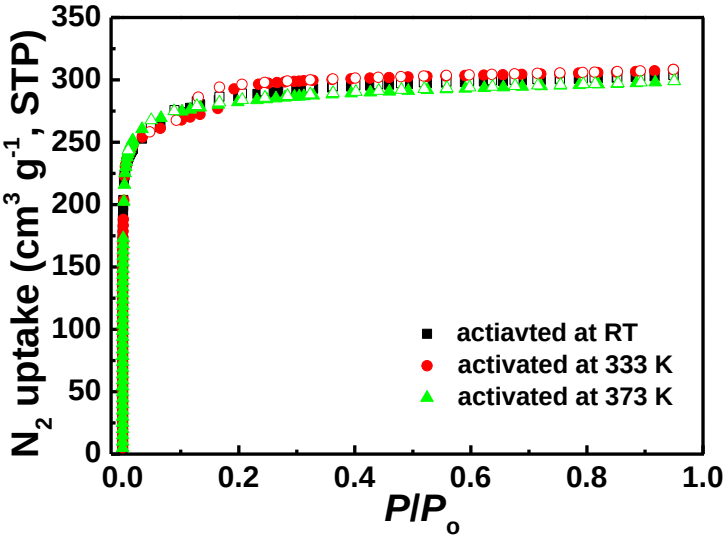
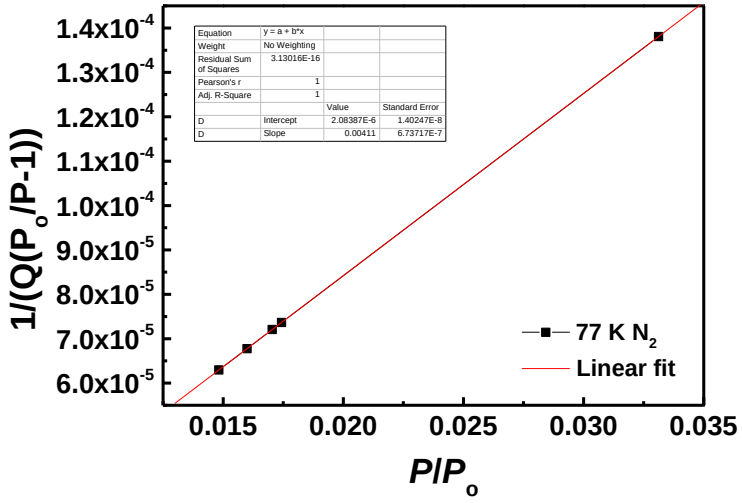


Fig. S3 N_2 adsorption-desorption isotherms at 77 K of **ZJNU-60(Ho)** activated at room temperature, 333 K and 373 K, respectively.



$S_{BET} = 1/(2.08387 \times 10^{-6} + 0.00411)/22414 \times 6.023 \times 10^{23} \times 0.162 \times 10^{-18} = 1058.6\ m^2\ g^{-1}$

Fig. S4 BET plot. Only the range below $P/P_o = 0.035$ satisfies the first consistency criterion for applying the BET theory.

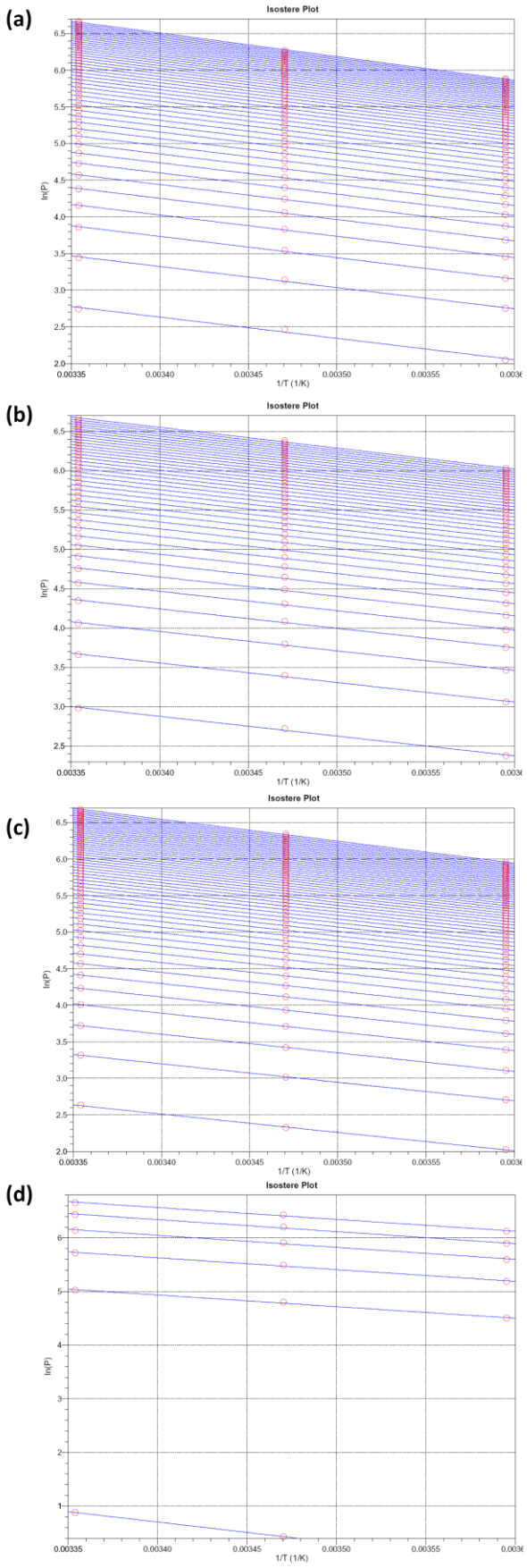


Fig. S5 Van't Hoff isochores for C_2H_2 (a), C_2H_4 (b), C_2H_6 (c) and CH_4 (d) adsorption.

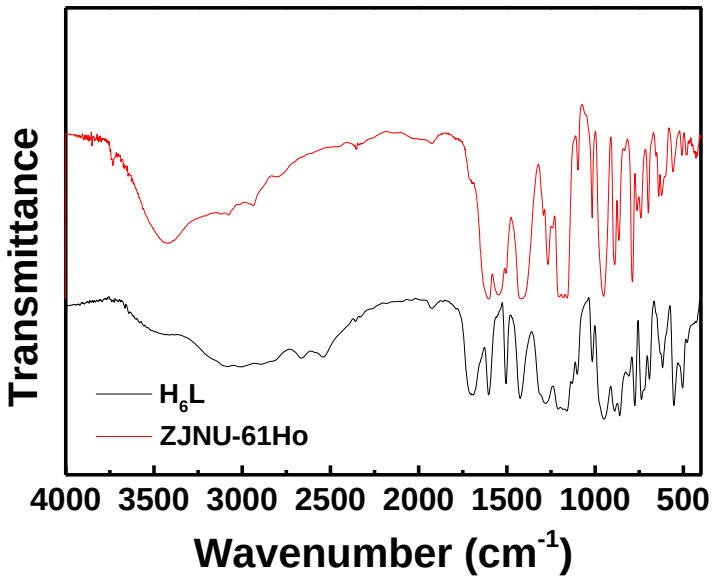
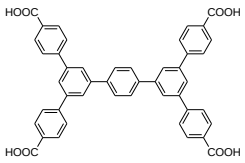
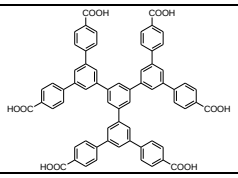
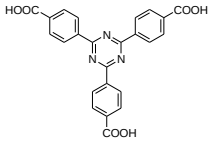
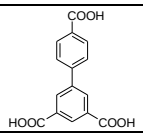
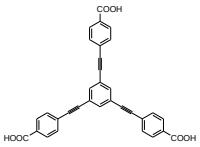
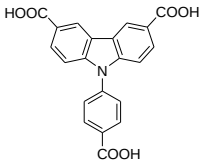
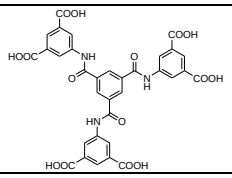
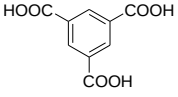
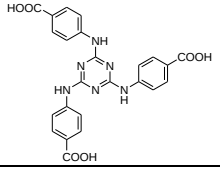
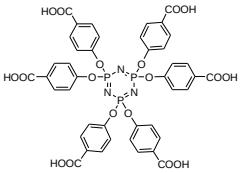
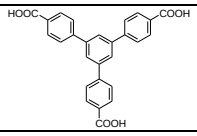
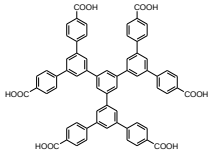
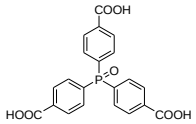
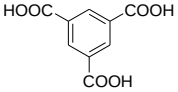
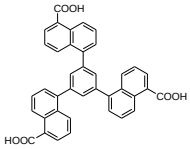
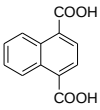
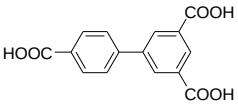
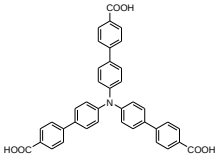
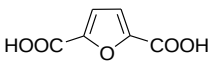
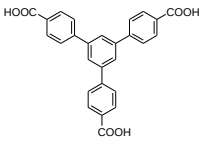
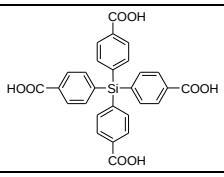


Fig. S6 FTIR spectra of the organic ligand H_6L and the as-synthesized **ZJNU-61**(Ho).

Table S1 BET surface areas of the reported Ln-MOFs.

Ln-MOFs	Ligands	BET (Langmuir) (m^2 g^{-1})	*Ref.*
Y-ftw-MOF-2		3690 (3740)	*1*
UTSA-62		2190	2
Tb-TATB		1783 (3855)	3
Y-BPT		1608	4
SUMOF-7III		1489 (1814)	5
Y-L		1435	4
NJU-Bai11		1152 (1293)	6
Y-BTC		1080	7
La-TATAB		1074 (1295)	8

ZJNU-61(Ho)		1058.6	*This work*
MIL-103 Tb-BTB		1000	9
UTSA-61		770	10
Y-TPO		692.0 (1011.2)	11
Dy-BTC		655	
UTSA-30		592 (604)	12
Y-NDC		546	13
Yb-BPT		515.6	14
FIR-8		457.1 (633.8)	15
$Gd(FDA)_{1.5}$		438 (726)	16
Ce-BTB		294	17
Nd-L		153 (201)	18

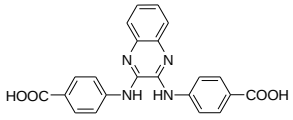
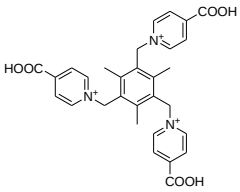
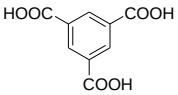
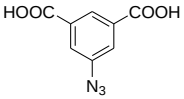
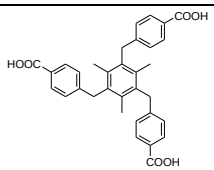
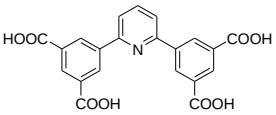
Er-DADQ		136.78	19
La-TTTPC		54 (104)	20
Tb-BTC (MOF-76)		(334)	21
SGR-Gd-110		NA	22
Yb-L		NA	23
Eu-L		NA	24

Table S2 Crystallographic Data and Structure Refinement Details for **ZJNU-61**(Ho).

MOF	**ZJNU-61(Ho)**
Empirical formula	C_{168} H_{241} Ho_4 N_{27} O_{59} P_6
Formula weight	4428.40
Temperature (K)	193(2) K
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 15.8769(5) Å b = 23.5103(8) Å c = 23.1577(8) Å α = 90^o β = 101.226(2) γ = 90^o
Volume (Å^3)	8478.7(5)
Z	2
D_c (g cm^{-3})	1.735
μ (mm^{-1})	2.005
F(000)	4536
Crystal size (mm)	0.280 ×0.250 ×0.100
θ range for data collection (^{o})	1.434 to 27.546
Limiting indices	-20 ≤ h ≤ 20 -30 ≤ k ≤ 30 -30 ≤ l ≤ 28
Reflections collected / unique	168354 / 38907 [$R_{(int)}$ = 0.0568]
Completeness to θ = 25.242	99.9%
Refinement method	Full-matrix least-squares on F^2
Max. and min. transmission	0.822 and 0.584

Data / restraints / parameters	38907 / 13 / 1193
GOF	1.006
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0561$ $wR_2 = 0.1462$
R indices (all data)	$R_1 = 0.0614$ $wR_2 = 0.1525$
Absolute structure parameter	0.045(11)
Largest diff. peak and hole ($e \cdot Å^{-3}$)	2.693 and -2.719
CCDC	1471569

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