Supporting Information

Superior selective removal of perrhenate/pertechnetate by a MOF-based molecule-trap

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Table S1. Crystallographic parameters for TNU-132 and TNU-132(Re).

	TNU-132	TNU-132(Re)
Chemical formula	$C_{26}H_{18}AgN_4BF_4$	$C_{26}H_{18}Ag_2N_4Re_2O_8$
Formula mass	581.12	1102.58
Crystal system	Monoclinic	Orthorhombic
a/Å	9.4608(3)	21.6514(14)
b/Å	22.8750(5)	10.3653(6)
c/Å	13.4599(3)	24.7561(15)
α/°	90	90
β/°	105.718(2)	90
γ/°	90	90
Unit cell volume/Å^3	2804.01(13)	5555.8(6)
Temperature/K	293(2)	296(2)
Space group	$P2_1/n$	*Pbca*
Z	4	8
Absorption coefficient, μ/mm^{-1}	6.173	10.133
R_{int}	0.0439	0.0757
Final R_1 values ($I > 2\sigma(I)$)	0.0572	0.0378
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1649	0.0879
Final R_1 values (all data)	0.0634	0.0573
Final $wR(F^2)$ values (all data)	0.1735	0.0944
Goodness of fit on F^2	1.035	1.041

Table S2. Selective bond lengths (Å) and angles (°) for TNU-132.

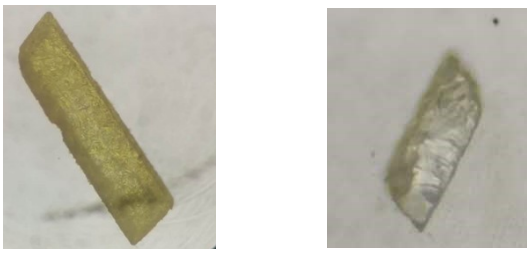
TNU-132			
Ag1–N1	2.282(3)	Ag1–N2A	2.375(3)
Ag1–N3B	2.331(3)	Ag1–N4C	2.432(3)
N2A–Ag1–N4C	87.74(12)	N1–Ag1–N2A	125.80(12)
N1–Ag1–N4C	99.95(12)	N1–Ag1–N3B	120.24(12)
N2A–Ag1–N3B	101.06(12)	N3BAg1–N4C	118.54(12)
Symmetry code: A = 1/2 + *x*, 1/2 – *y*, –1/2 + *z*; B = *x*, *y*, –1 + *z*; C = 2 – *x*, 1 – *y*, 1 – *z*.			
TNU-132(Re)			
Ag1-N3B	2.162(6)	Ag1–N2	2.164(6)
Ag1-O6	2.742(6)	Ag2–N1	2.208(6)
Ag2-O1	2.583(7)	Ag2–N4A	2.180(6)
N3B–Ag1–N2	177.3(3)	O6–Ag1–N2	92.1(2)
N3B–Ag1–O6	89.8(2)	N4A–Ag2–N1	166.2(2)
N4A–Ag2–O1	98.8(2)	O1–Ag2–N1	91.0(2)
Symmetry code: A = 1/2 + *x*, 1/2 – *y*, 2 – *z*; B = *x*, 1/2 – *y*, 1/2 + *z*.			

Table S3. Model parameters and correlation coefficient for Cr(VI) and Re(VII) sorption kinetics by TNU-132.

	k_2 (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
Cr(VI)	0.0013	65.23	0.9994
Re(VII)	0.0021	318.58	0.9998

Table S4. Fitting results of ReO_4^- sorption by TNU-132 based on the Langmuir model.

Samples	**k_2 (g mg^{-1} min^{-1})**	**q_e (mg g^{-1})**	**R^2**
TNU-132	334.38	0.028	0.9998



(a) (b)

Figure S1. Photos of the TNU-132(Cr) crystals (a) and the transparent inner core (b) after taking off the surface layer.

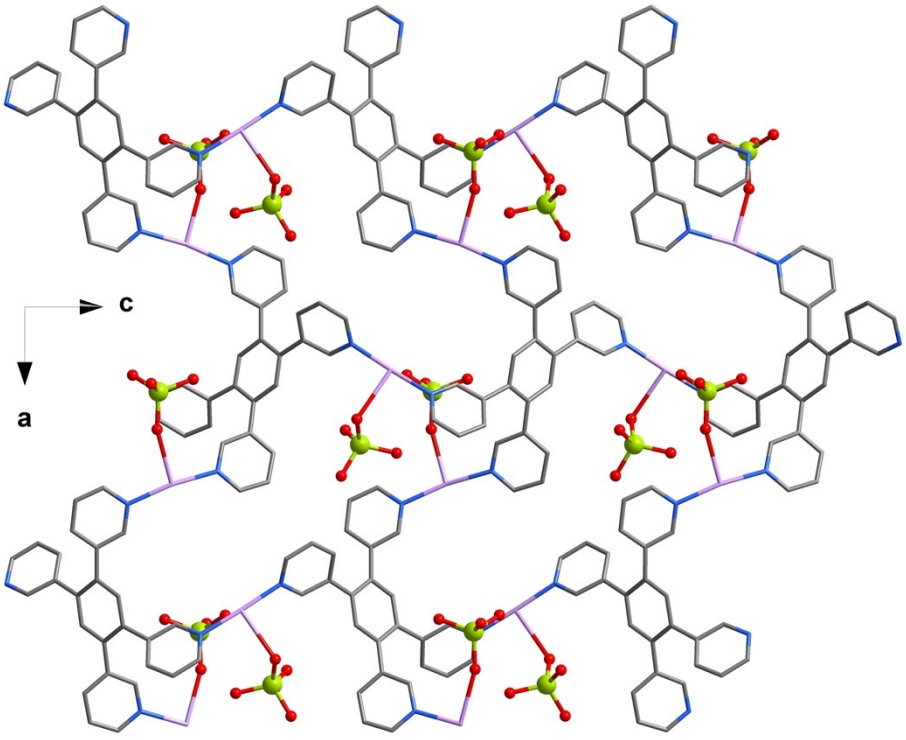


Figure S2. Layered crystallographic structures of TNU-132(Re).