Electronic Supplementary Material (ESI) for Dalton Transactions.

Selective Th(IV) capture from a new metal-organic framework with O^- groups

Supporting information

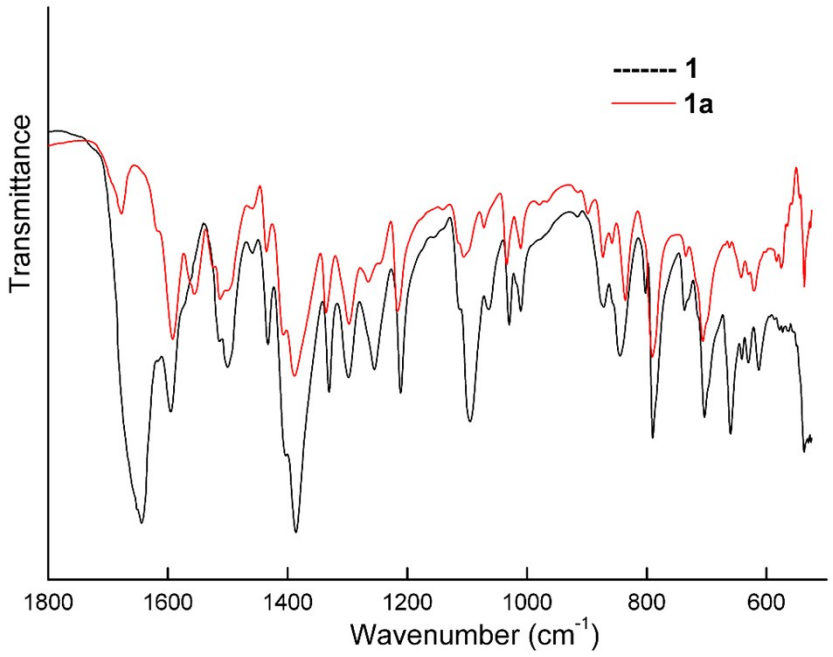

Figure S1. IR spectrum of compound **1** and **1a**.

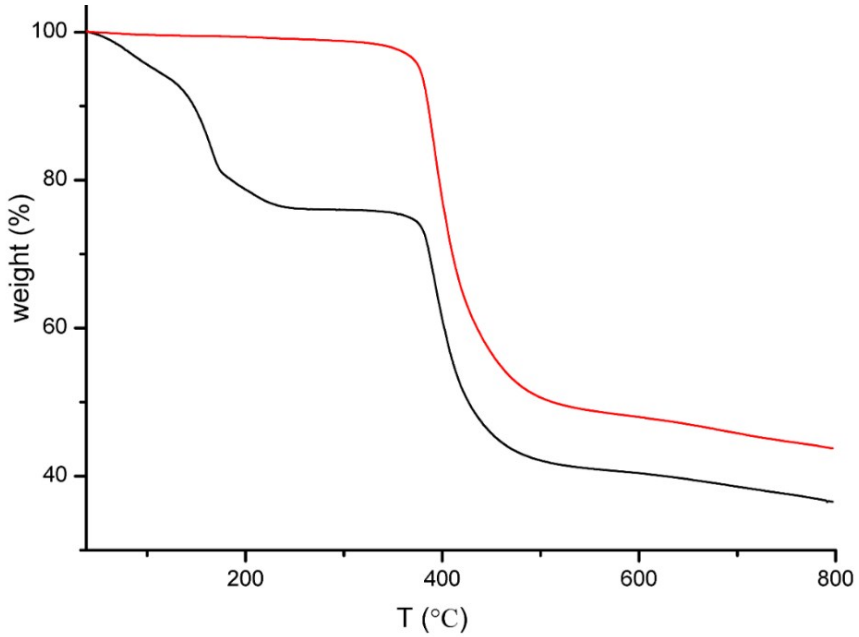

Figure S2. TGA curves for compound **1** (black line) and corresponding activated samples (red line).

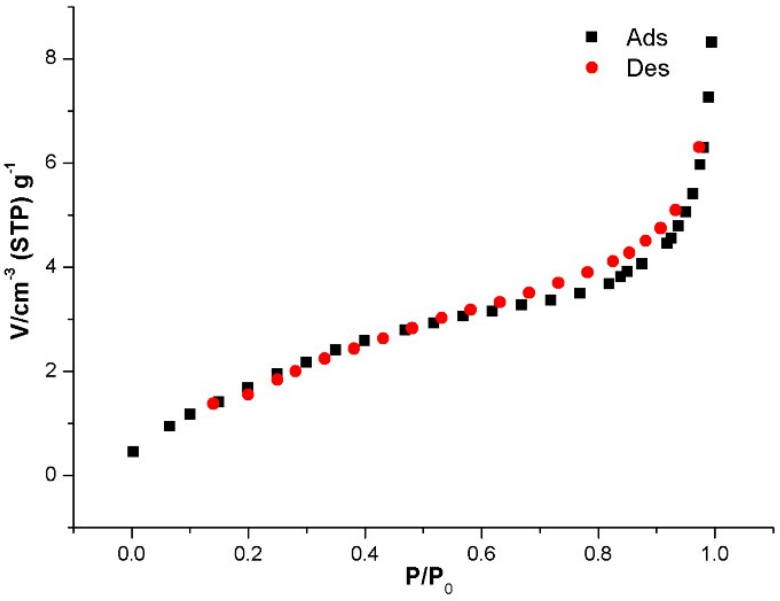

Figure S3. The N_2 adsorption isotherms of **1a** at 77K.

The pseudo-first-order and pseudo-second-order fits were conducted according to the following equation:

$$\log(q_e - q_t) = \log q_e - (\frac{k_1}{2.303})t$$

$$\frac{t}{q} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$$

where q_e and q_t stands for the adsorption capacities at equilibrium and at time t, k_1 and k_2 represents the rate constant of pseudo-first-order and pseudo-second-order model.

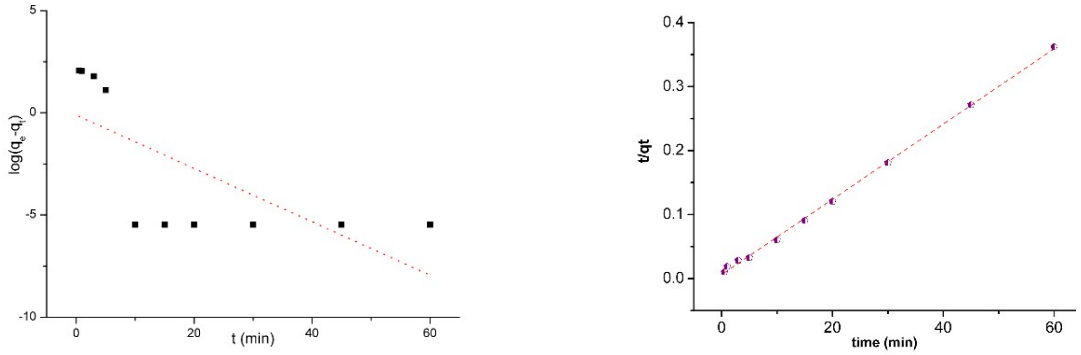

Figure S4. Linear fitting for a pseudo-first-order model (left) and a pseudo-second-order model (right)

Table S1 Pseudo-first-order and pseudo-second-order fits parameter.

Experiment	Pseudo-first-order model			Pseudo-second-order model		
qe (mg g-1)	q_e (mg g^{-1})	k_1 (min^{-1})	R^2	q_e (*mg g-1*)	k_2 (*g mg-1 h-1*)	R^2
165.60	0.77	0.30	0.44	170.06	0.34	0.99

The linear equation of the Langmuir isotherm model is expressed as followed:

$$\frac{c_e}{q_e} = \frac{1}{q_m k_L} + \frac{c_e}{q_m}$$

where q_m is the maximum adsorption of the absorbent and k_L is the Langmuir constant (L mg^{-1}). The values of q_m and k_L can be calculated from c_e/q_e versus c_e plot.

The linear equation of Freundlich model can be express by:

$$\log qe = \log k_F + \frac{1}{n} \log c_e$$

where k_F and n are the Freundlich constants related to the adsorption capacity and intensity.

Table S2 Isotherm parameters of Langmuir and Freundlich models for the adsorption of Th(IV) by **1a**.

Experiment	Langmuir			Freundlich		
q_m (mg g^{-1})	q_m (mg g-1)	k_1 (L mg^{-1})	R^2	k_F (mg g^{-1})	n	R^2
165.60	167.5	10.0	0.98	158.48	8.43	0.59

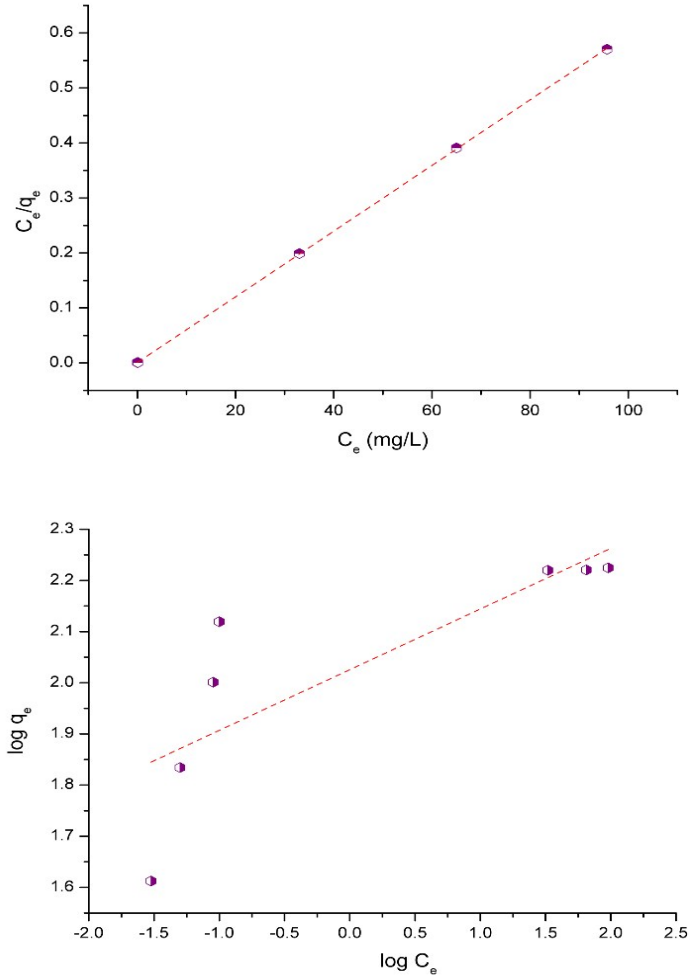

Figure S5. Linear fitting for the Langmuir model (top) and Freundlich model (down).

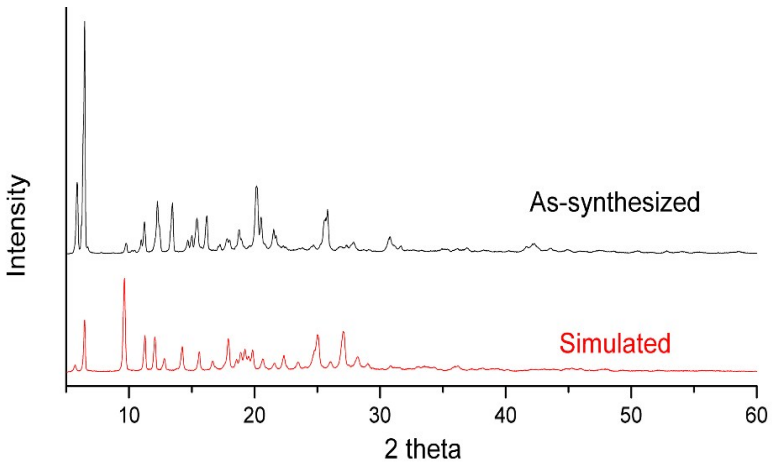

Figure S6. PXRD for synthesized **1** and its simulated pattern.

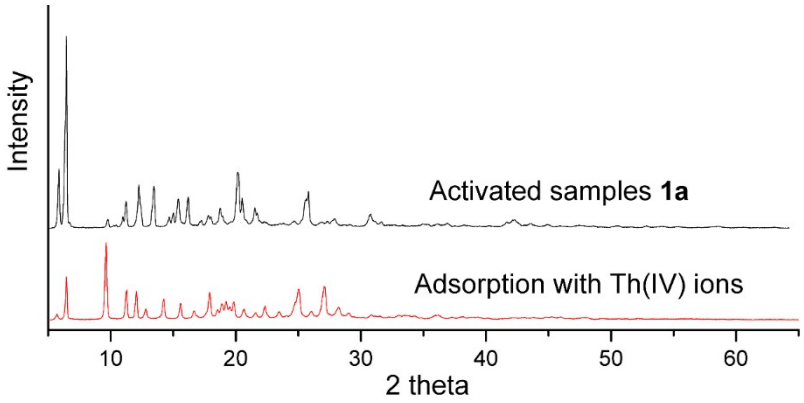

Figure S7. PXRD for the activated sample **1a** and after Th(IV) adsorptions with initial concentration of 100 ppm.

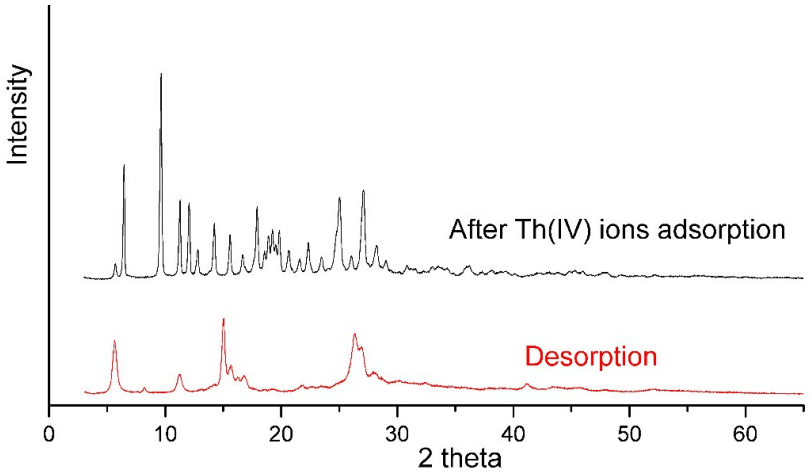

Figure S8. PXRD for samples with adsorption of Th(IV) ions and desorption.