Supporting Information

Functional UiO-66 for highly selective adsorption of N-nitrosodipropylamine: Adsorption performance and mechanisms

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1 Adsorption kinetics

$$q_t = q_e(1 - e^{K_1 t}) \tag{1}$$

$$q_t = \frac{q_e^2 K_2 t}{1 + (q_e K_2 t)} \tag{2}$$

$$q_t = K_3 t^{0.5} + C \tag{3}$$

In the above formula, q_t (μg/g) represents the amount of NDEA adsorbed at t (h) time. q_e (μg/g) represents the amount of NDEA adsorbed at equilibrium. K_1, K_2, K_3 represent the equilibrium constants of pseudo-first-order, pseudo-second-order and intraparticle diffusion model dynamic equations. C represents the characteristic constant of the boundary layer.

2 Adsorption isotherms

$$q_e = \frac{q_m K_L C_e}{1 + K_L C_e} \tag{4}$$

$$q_e = K_F C_e^{\frac{1}{n}} \tag{5}$$

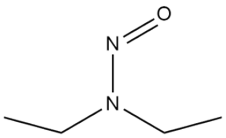
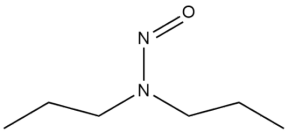
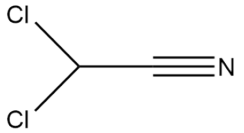
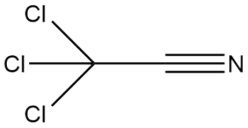
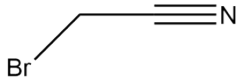
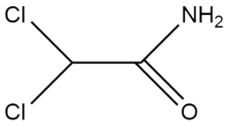
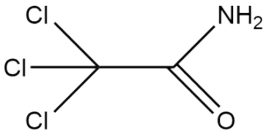
$$q_e = \frac{RT \ln(K_T C_f)}{\beta} \tag{6}$$

In the above formula, q_e (μg/g) represents the amount of adsorption at equilibrium; C_e (μg/ml) represents the remaining NDEA; q_m (μg/g) represents the maximum adsorption capacity of the adsorbent; K_L, K_F and K_T represent the constants of Langmuir, Freundlich and Temkin models, respectively. 1/n value represents adsorption capacity index. β is a constant. R (8.314 J/mol·K) and T (298 K) were the universal gas constant and temperature in Kelvin, respectively.

3 Methods and detection limits

For the capture limit of DNPA by adsorbent materials, a method of quantitative analysis of DNPA by gas chromatography-mass spectrometry (GC-MS) was established by using the pretreatment method of liquid-liquid extraction, and a standard working curve of y=28294x+24456 (R^2=0.996) with the linear range of 0.1-10 μg/mL was obtained. According to the method, the detection limit of DNPA was 0.0123 μg/mL, and the limit of quantification (LOQ) was 0.0409 μg/mL. The recoveries of DNPA spiked samples in tap water ranged from 92.20% to 105.23%.

Table S1 Structural formula of seven kinds of N-DBPs

Compound	Chemical formula	Structural formula
N-nitrosodiethylamine	NDEA	
N-nitrosodipropylamine	NDPA	
Dichloroacetonitrile	DCAN	
Trichloroacetonitrile	TCAN	
Bromoacetonitrile	BAN	
2,2-Dichloroacetamide	DCAcAm	
2,2,2-Trichloroacetamide	TCAcAm	

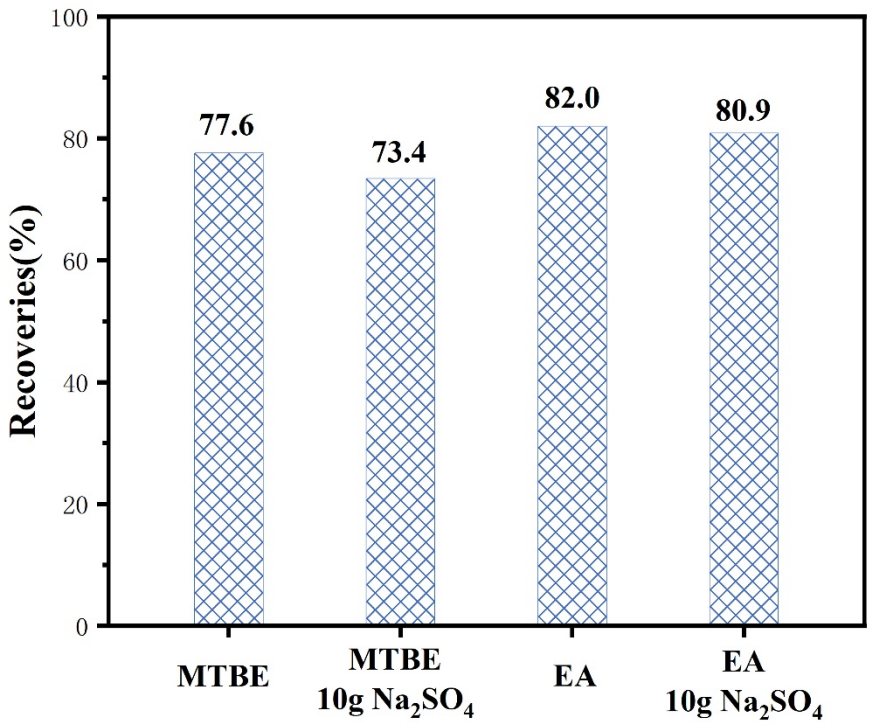


Fig. S1 Recoveries of NDPA at different organic solvents and salt concentrations.

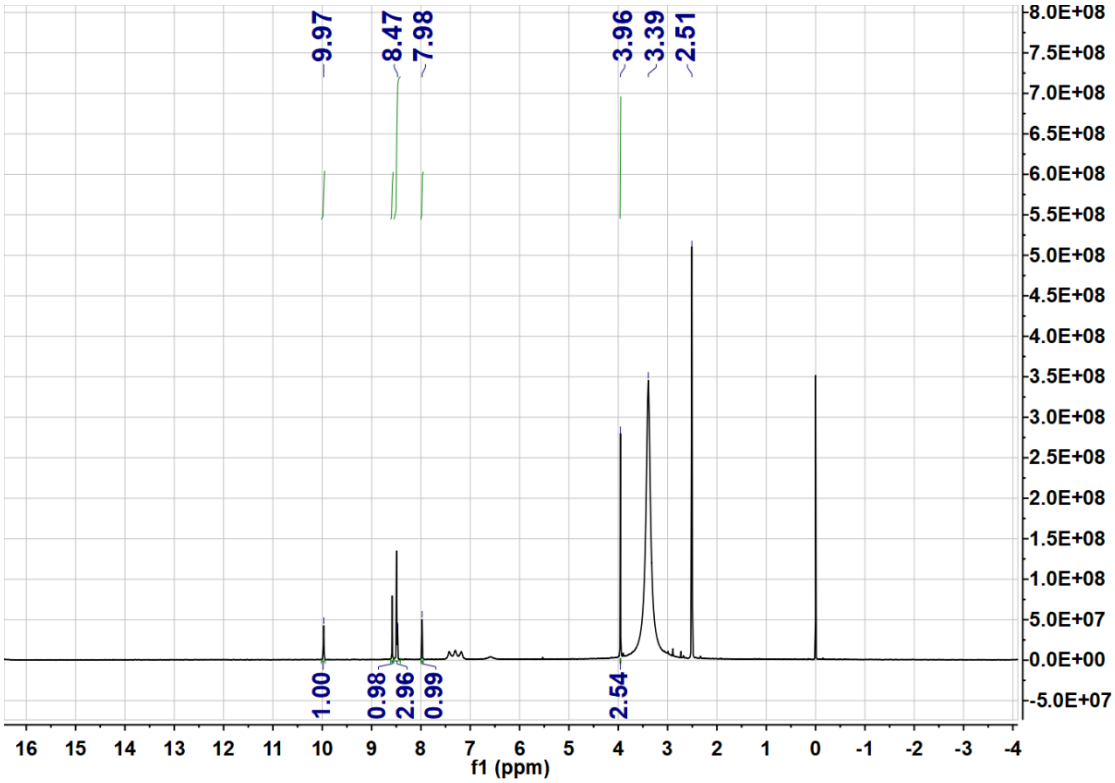


Fig. S2 ^{1}H NMR spectrum of digested (I^{-})Meim-UiO-66 sample in DMSO-d_6 (HF)(r.t).

The ^{1}H NMR spectrum of digested (I^{-})Meim-UiO-66 showed a unique peak at 3.96 attributed to methyl group in Meim-BDC^{+}.

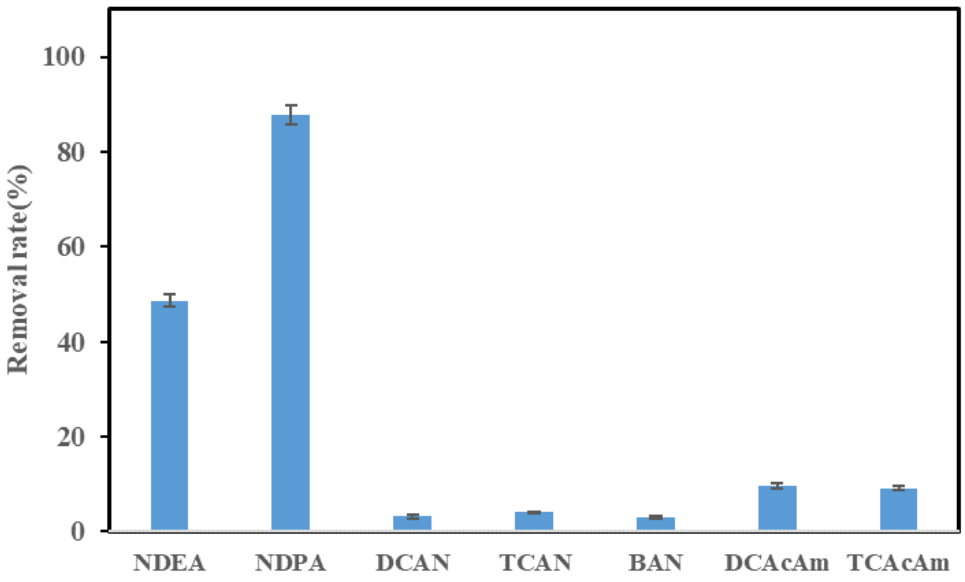


Fig. S3 Removal rate of seven kinds of N-DBPs by UiO-66-NH_2.