Electronic Supplementary Material (ESI) for Nanoscale Advances.

Electronic Supplementary Information

Boosted ability of ZIF-8 for early-stage adsorption and degradation of chemical warfare agent simulants

*Sojin Oh, Sujeong Lee, Gihyun Lee, and Moonhyun Oh**

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea
*Corresponding author.
E-mail: moh@yonsei.ac.kr

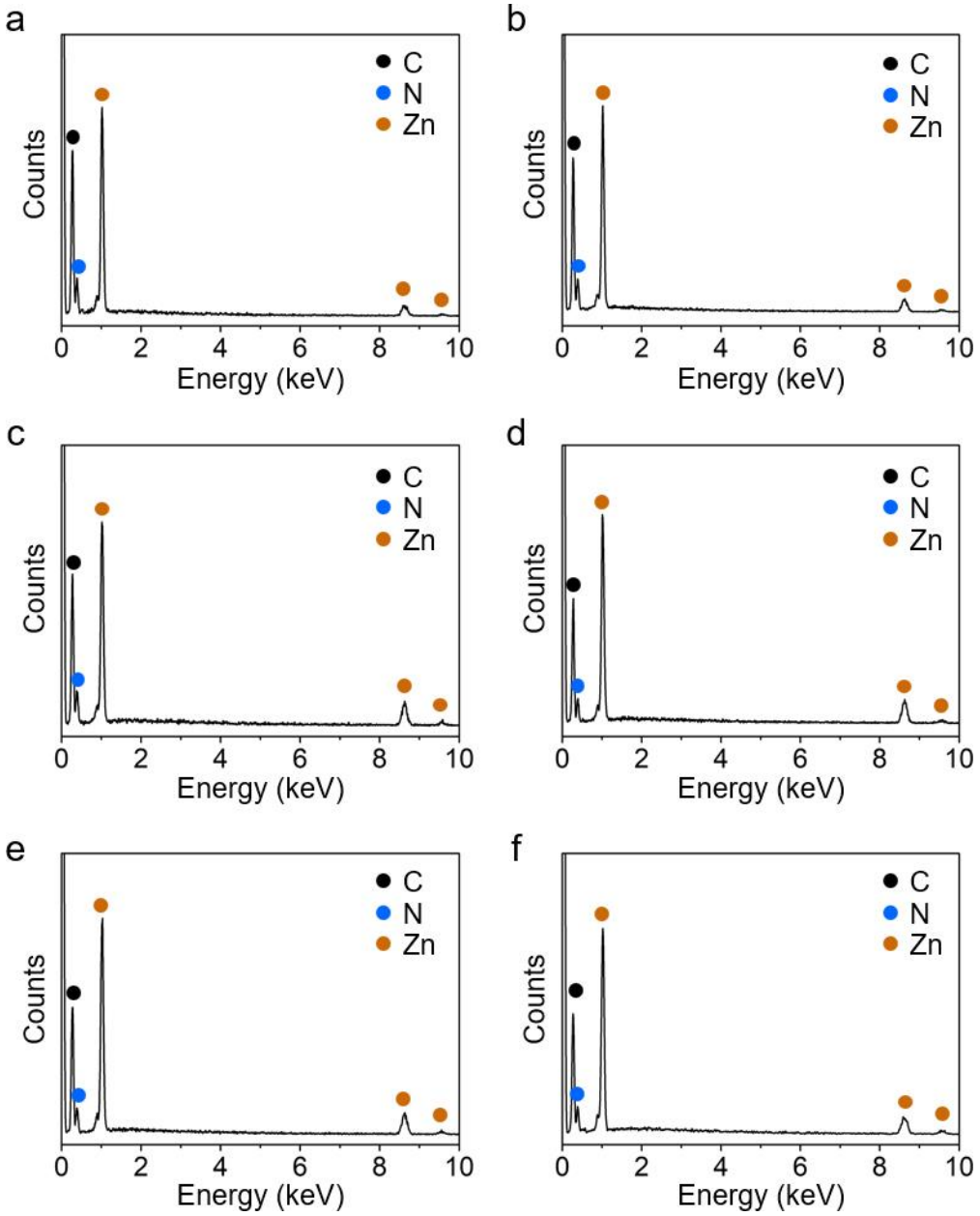

Fig. S1 EDX spectra of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8.

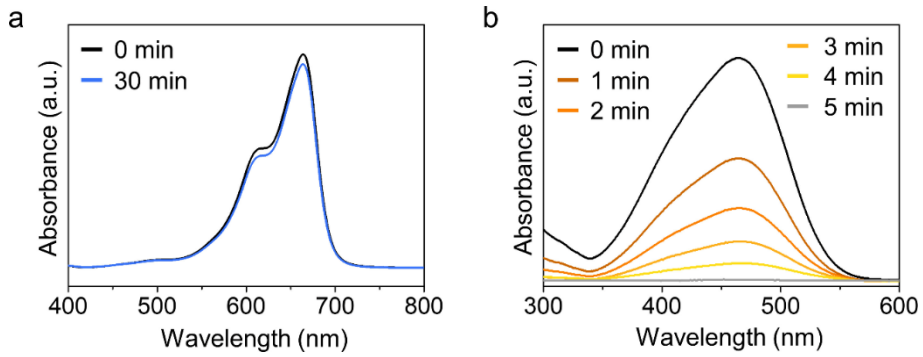

Fig. S2 UV-vis spectra showing the adsorption properties of 550-ZIF-8 for the organic pollutants; (a) positively charged methylene blue and (b) negatively charged methyl orange.

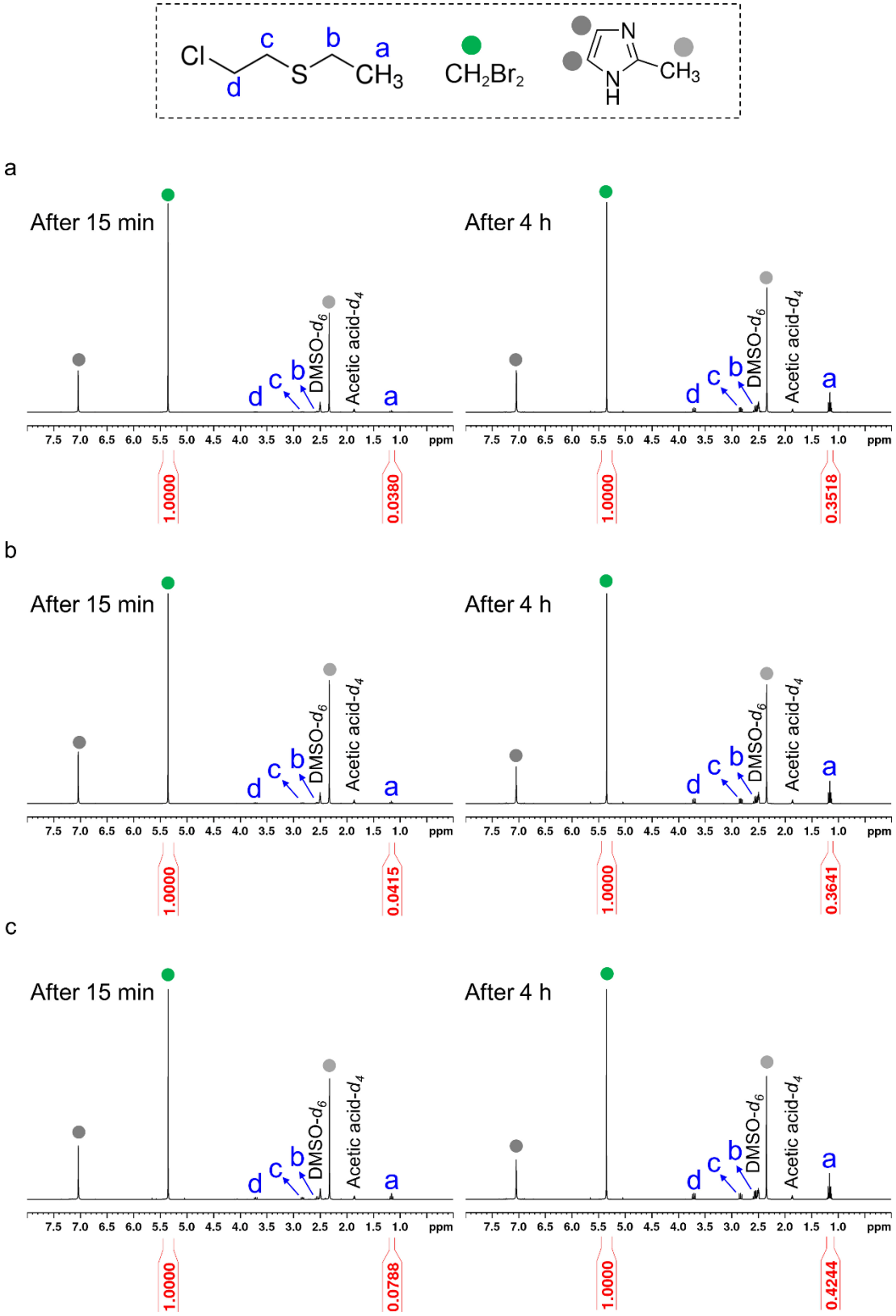

Fig. S3 ^{1}H NMR spectra showing CEES adsorption on ZIF samples after 15 min (left) and 4 h (right); (a) ZIF-8, (b) 450-ZIF-8, and (c) 500-ZIF-8.

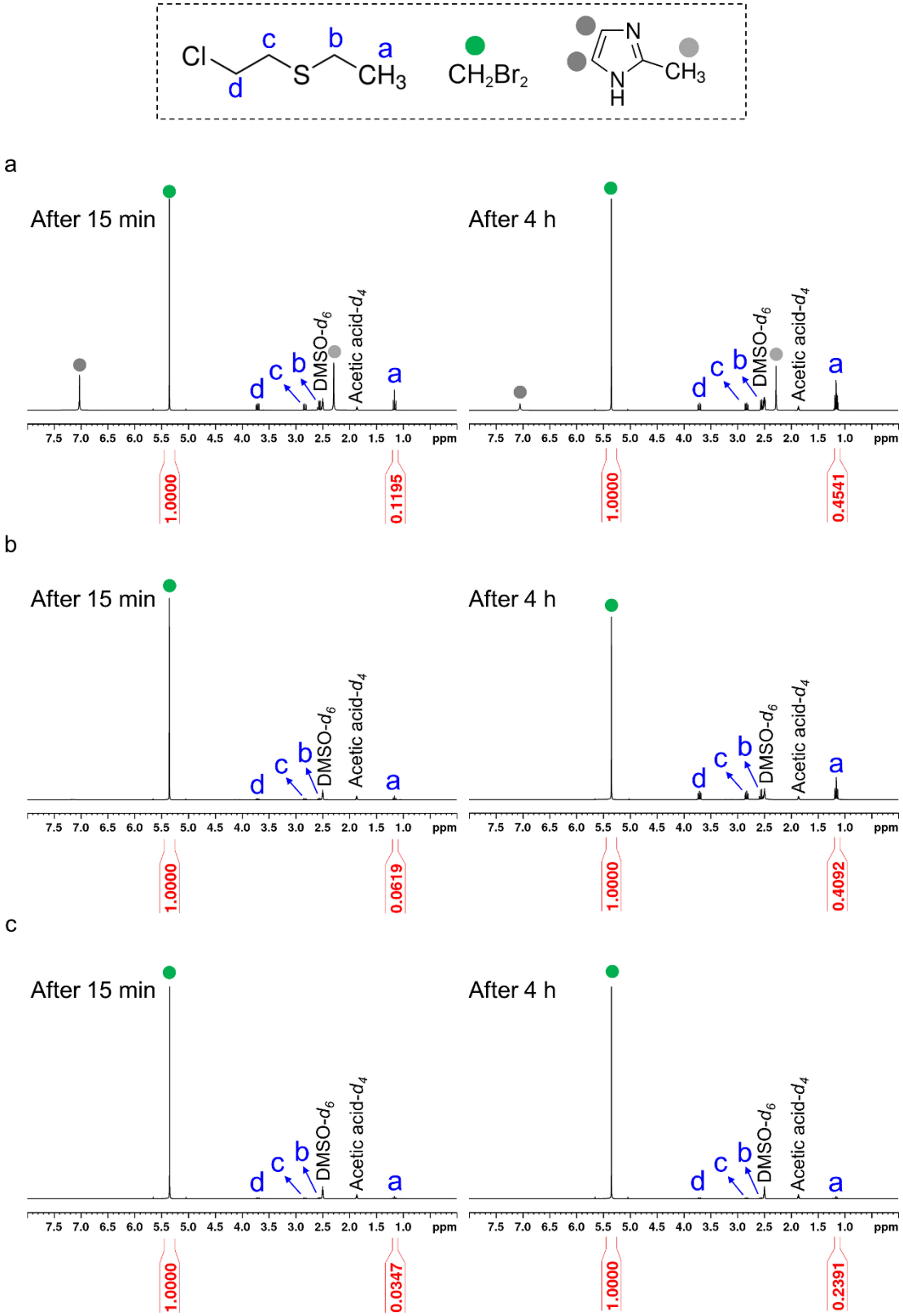

Fig. S4 ^{1}H NMR spectra showing CEES adsorption on ZIF samples after 15 min (left) and 4 h (right); (a) 550-ZIF-8, (b) 570-ZIF-8, and (c) 600-ZIF-8.

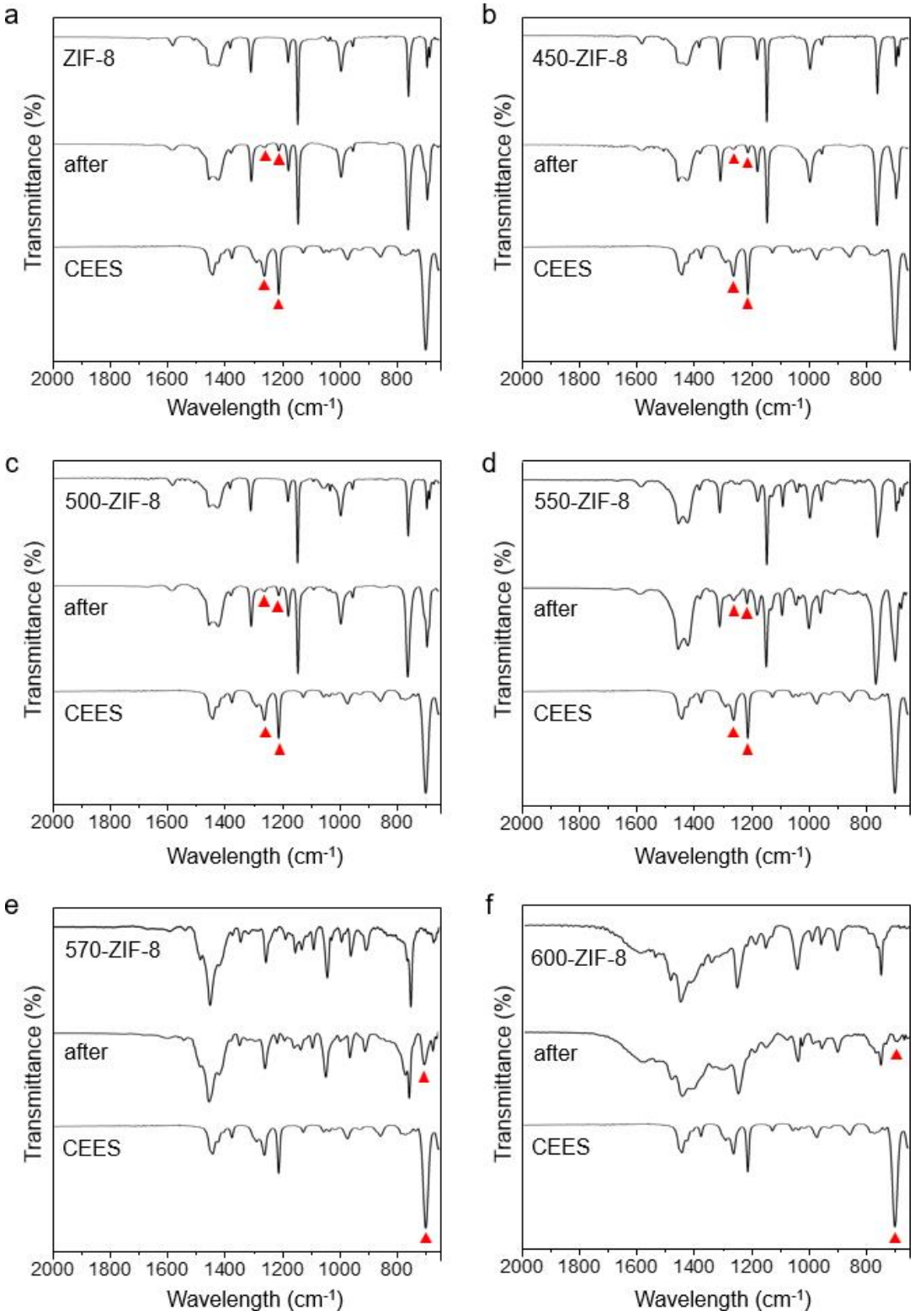

Fig. S5 IR spectra of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 before and after the exposure to CEES vapors.

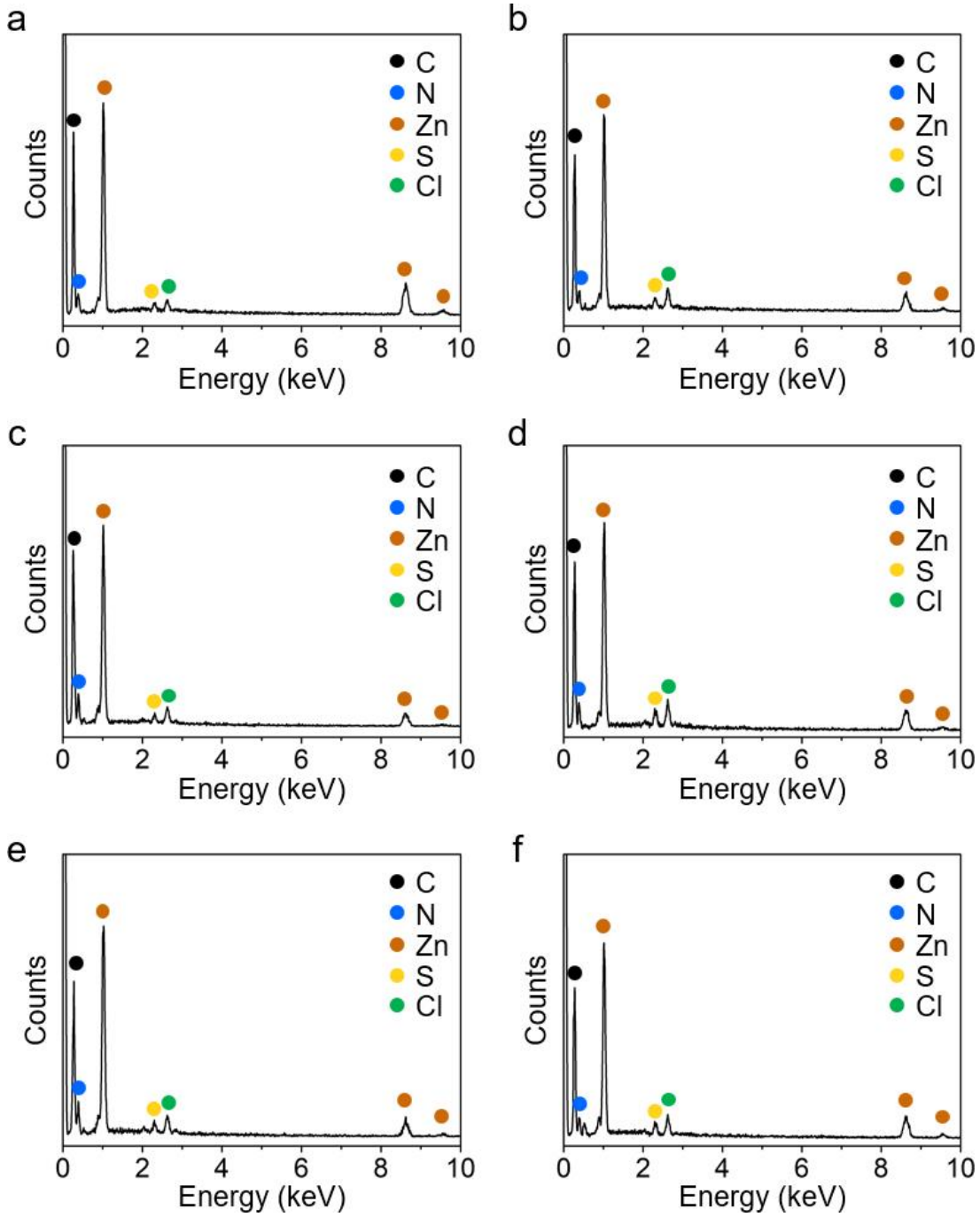

Fig. S6 EDX spectra of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 after adsorption of CEES.

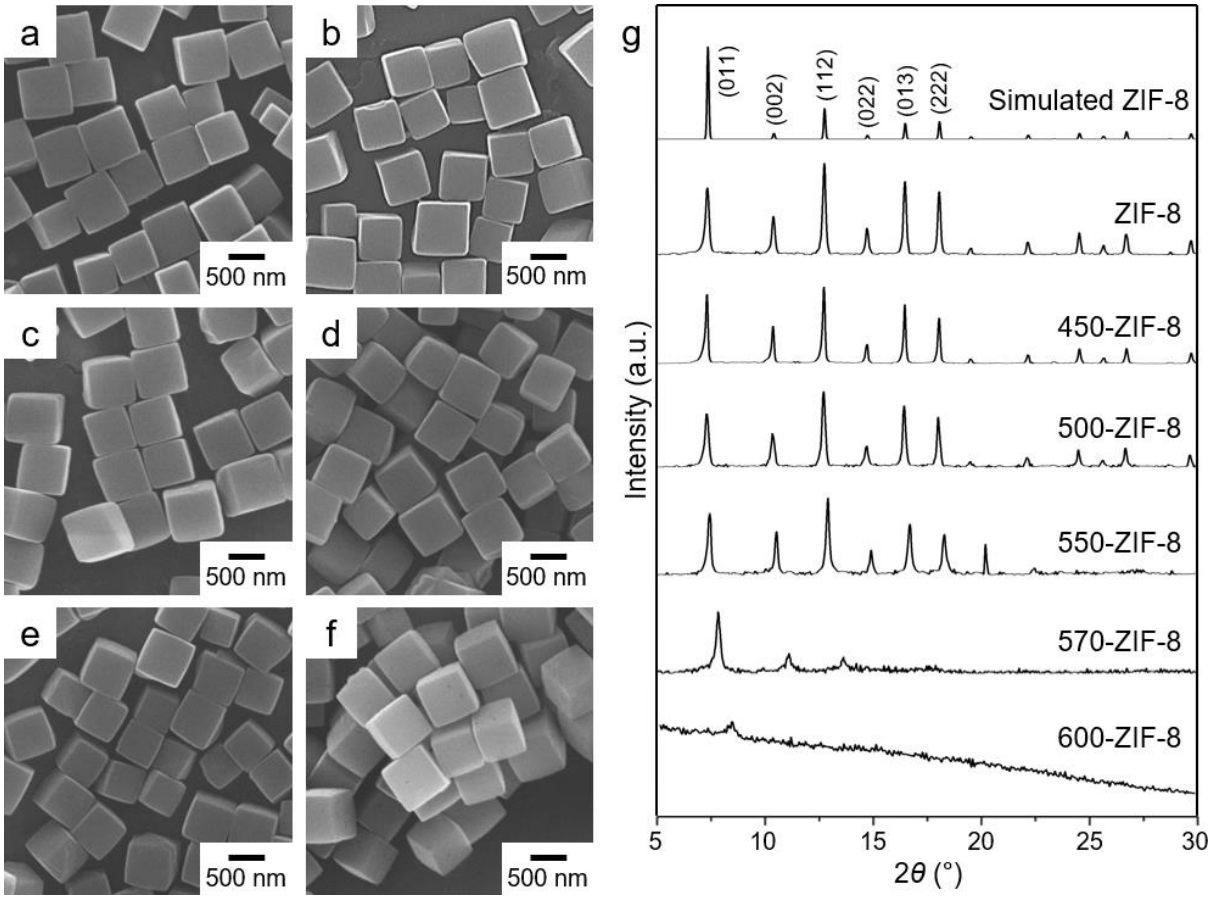

Fig. S7 SEM images of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 after adsorption of CEES. (g) PXRD patterns of ZIF-8 and T-ZIF-8 samples after adsorption of CEES.

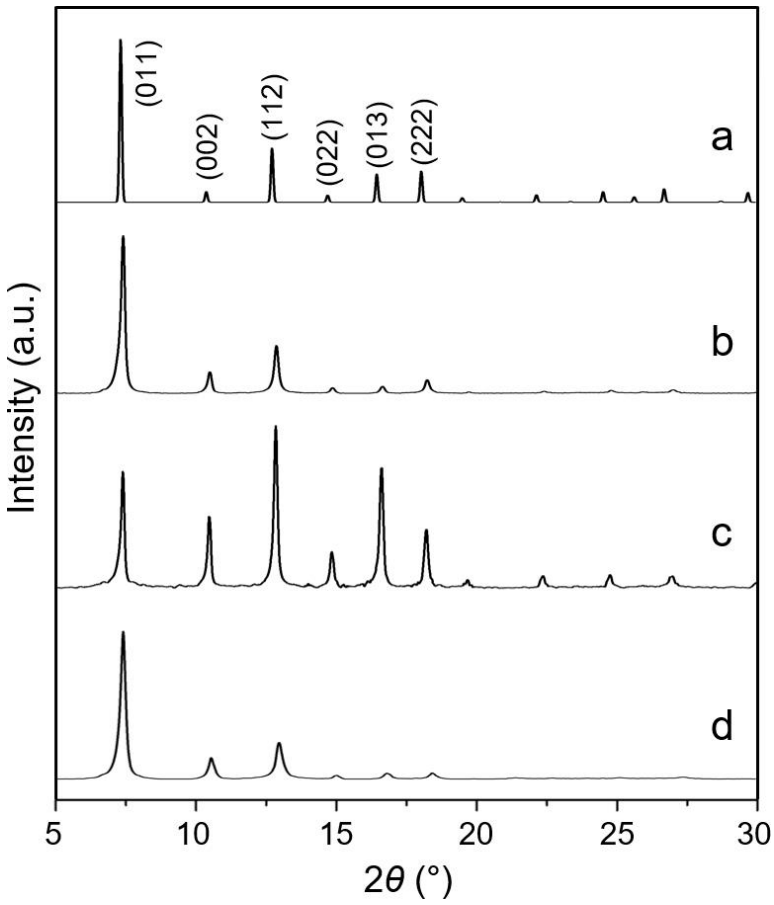

Fig. S8 (a) Simulated PXRD pattern of ZIF-8. (b) PXRD pattern of ZIF-8 before adsorption of CEES. (c) PXRD pattern of ZIF-8 after adsorption of CEES. (d) PXRD pattern of the sample shown in (c) after washing with methanol to remove the adsorbed CEES.

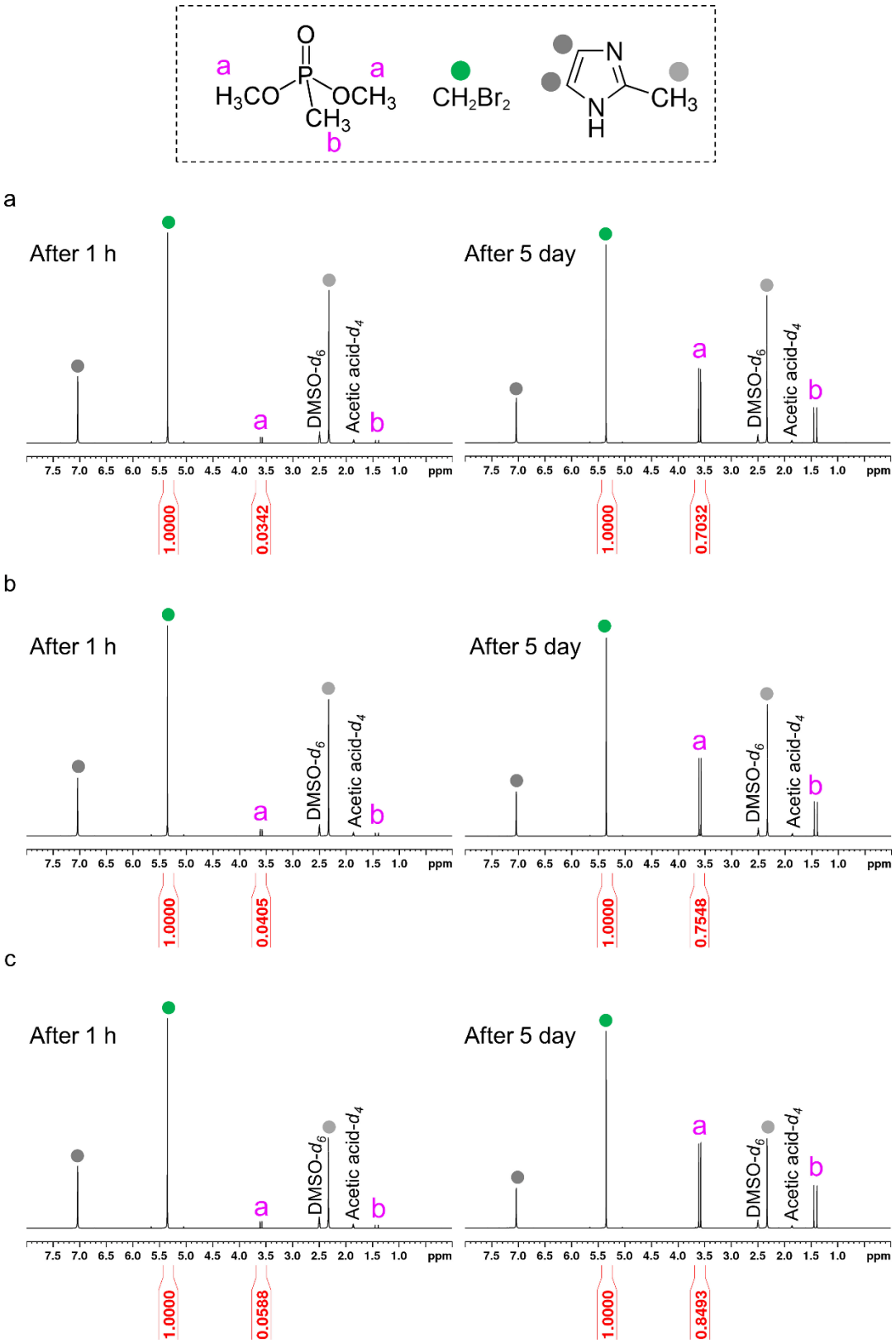

Fig. S9 ^{1}H NMR spectra showing DMMP adsorption on ZIF samples after 1 h (left) and 5 day (right); (a) ZIF-8, (b) 450-ZIF-8, and (c) 500-ZIF-8.

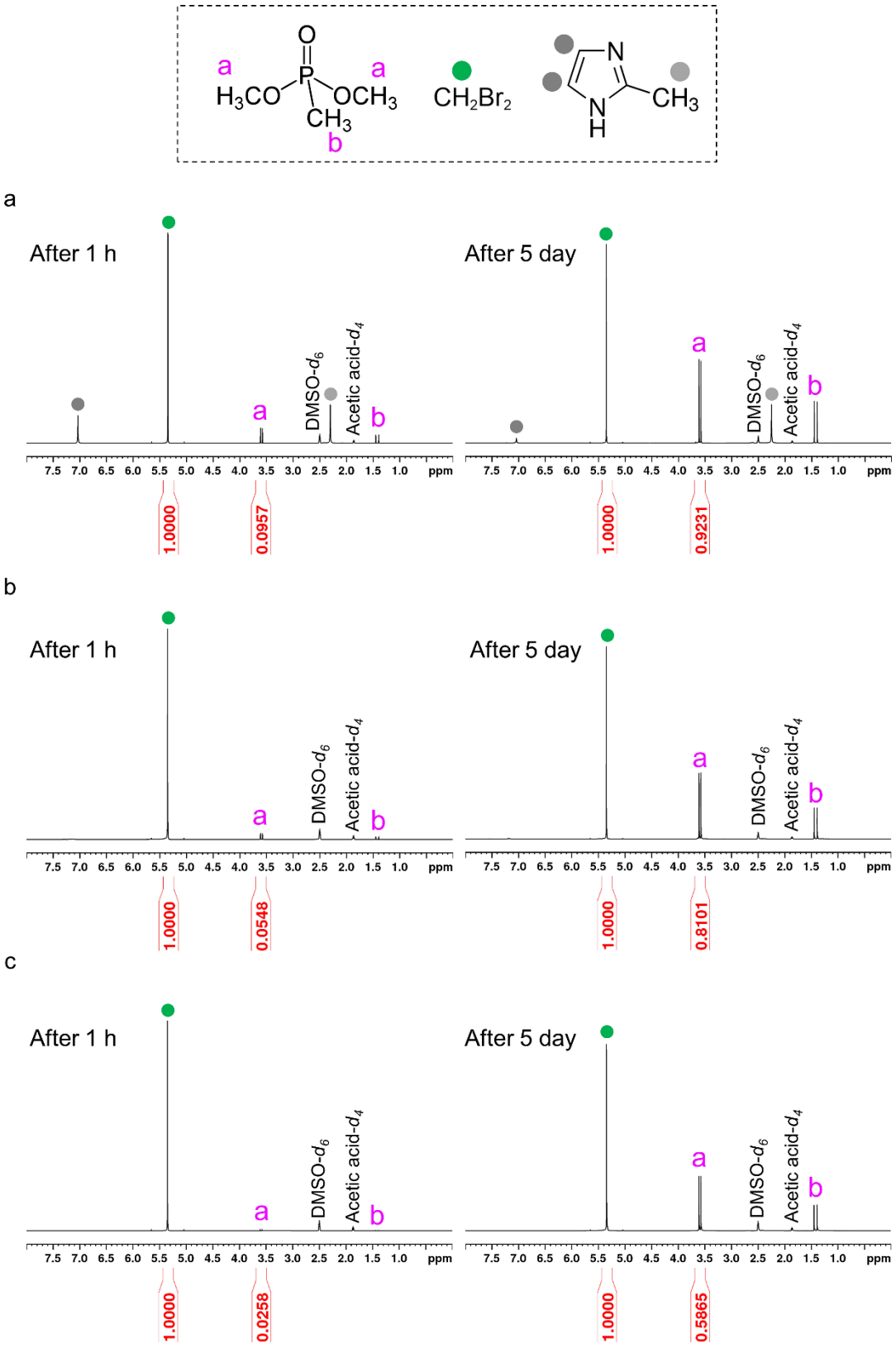

Fig. S10 ^{1}H NMR spectra showing DMMP adsorption on ZIF samples after 1 h (left) and 5 day (right); (a) 550-ZIF-8, (b) 570-ZIF-8, and (c) 600-ZIF-8.

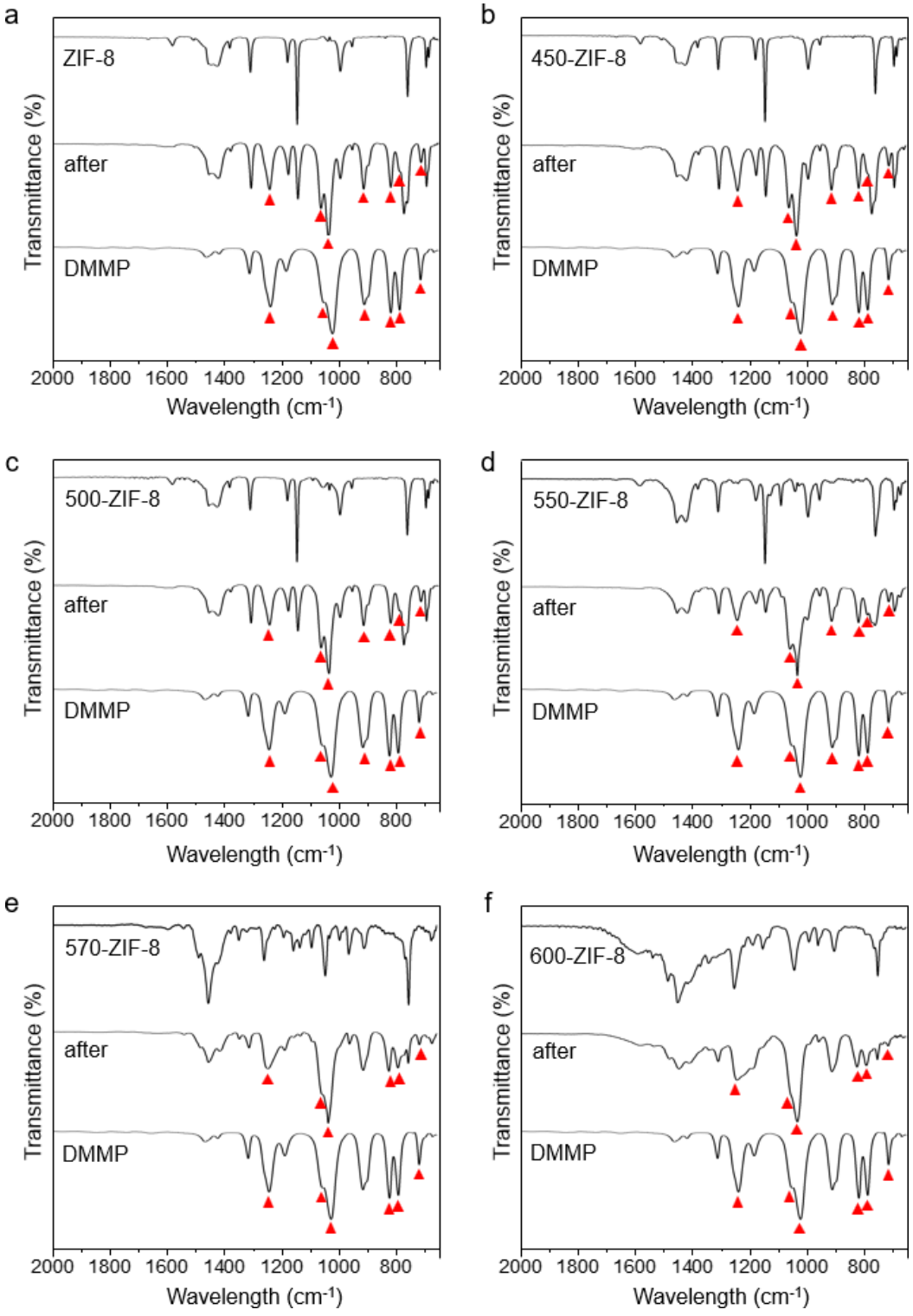

Fig. S11 IR spectra of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 before and after the exposure to DMMP vapors.

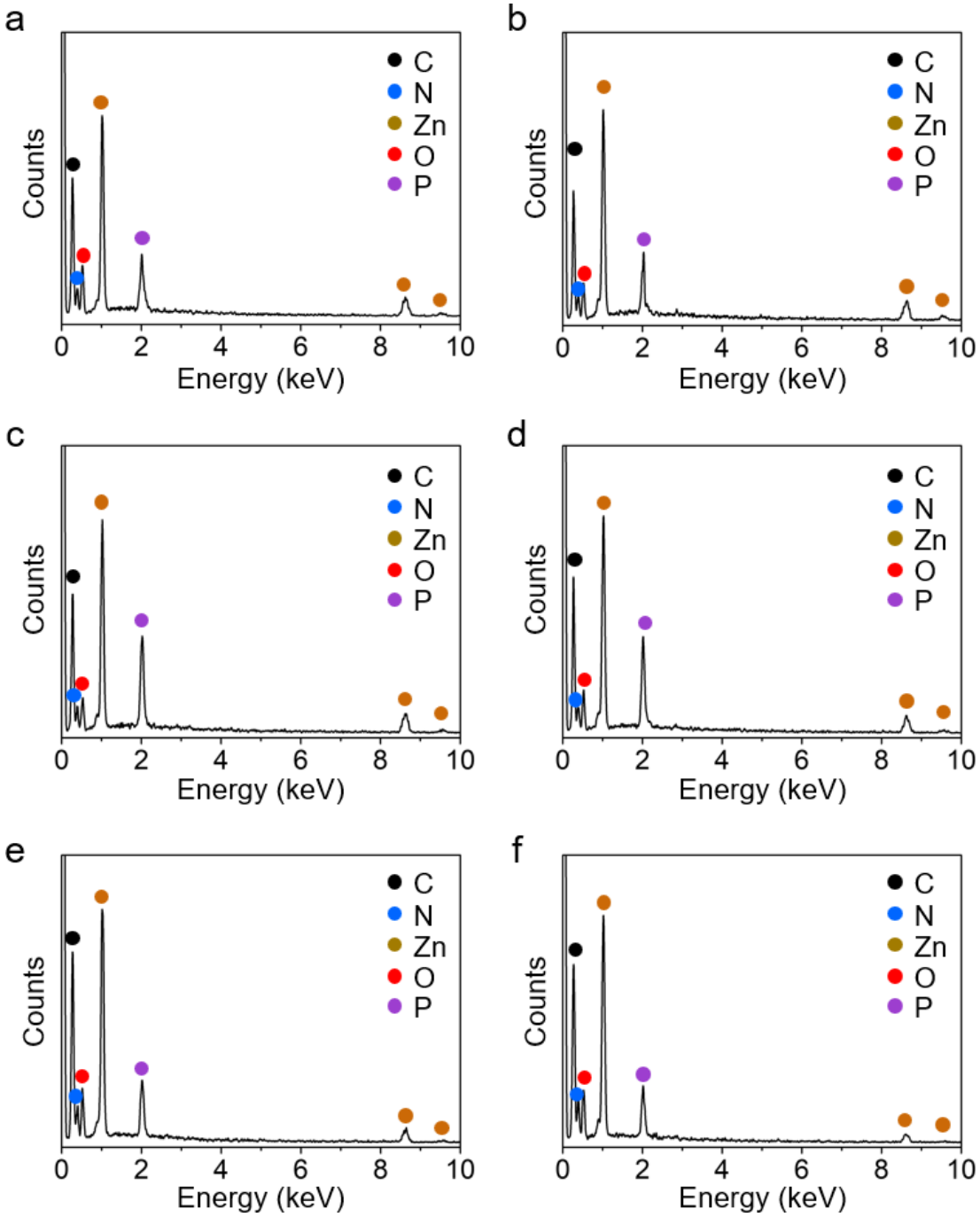

Fig. S12 EDX spectra of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 after adsorption of DMMP.

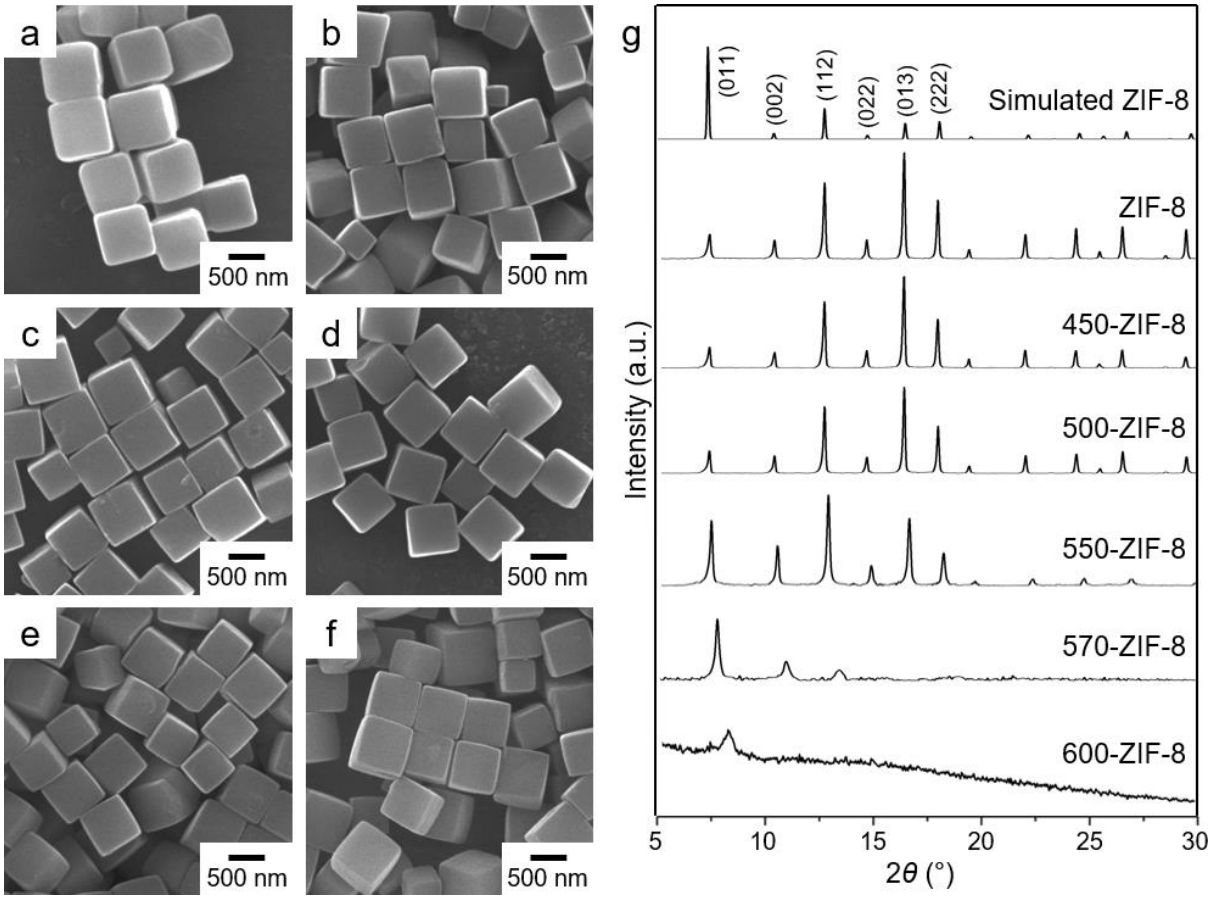

Fig. S13 SEM images of (a) ZIF-8, (b) 450-ZIF-8, (c) 500-ZIF-8, (d) 550-ZIF-8, (e) 570-ZIF-8, and (f) 600-ZIF-8 after adsorption of DMMP. (g) PXRD patterns of ZIF-8 and T-ZIF-8 samples after adsorption of DMMP.

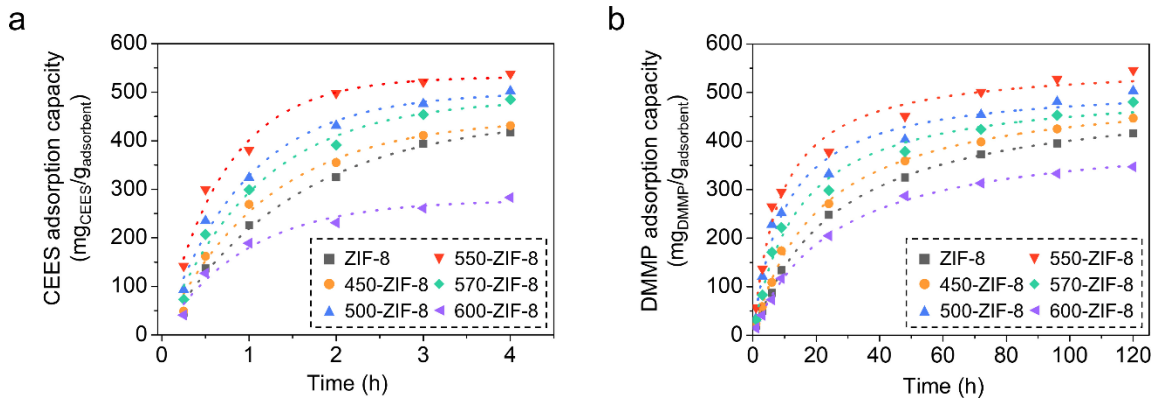

Fig. S14 (a) CEES adsorption kinetic and (b) DMMP adsorption kinetic of ZIF-8 and T-ZIF-8 samples with the pseudo-first order model.

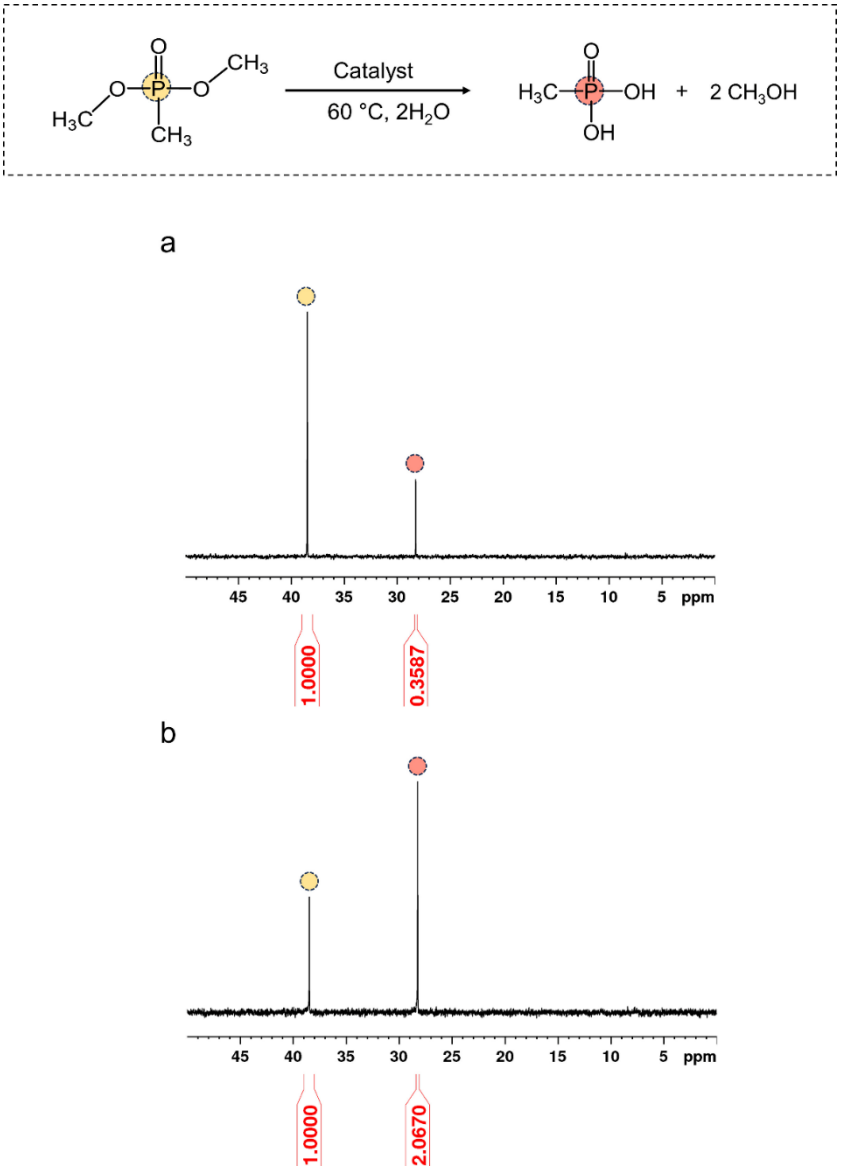

Fig. S15 ^{31}P NMR spectra showing catalytic degradation of DMMP after 72 h; (a) ZIF-8, and (b) 550-ZIF-8.

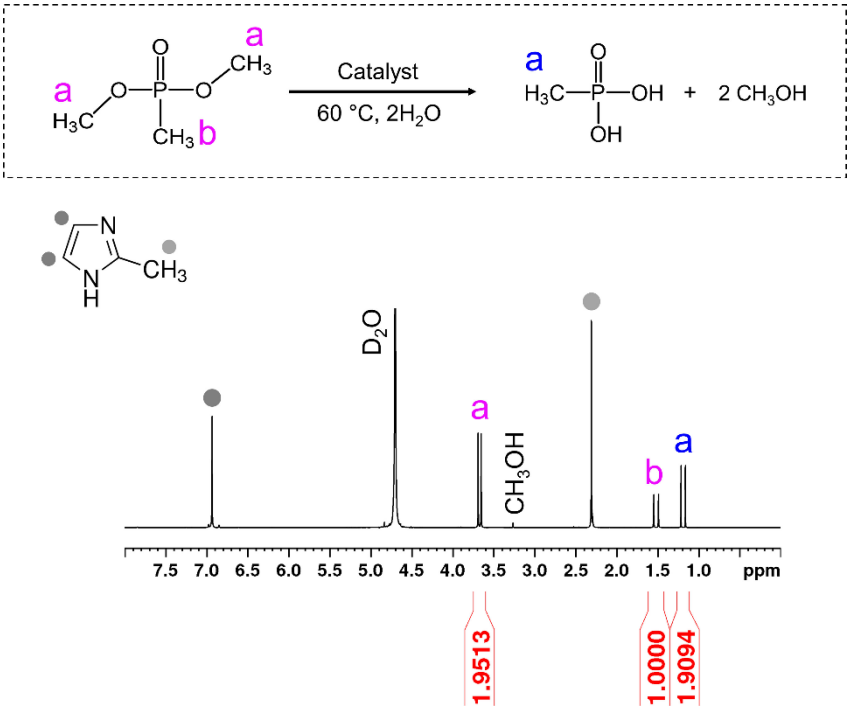

Fig. S16 ^{1}H NMR spectrum showing catalytic degradation of DMMP after 72 h in the presence of 550-ZIF-8.

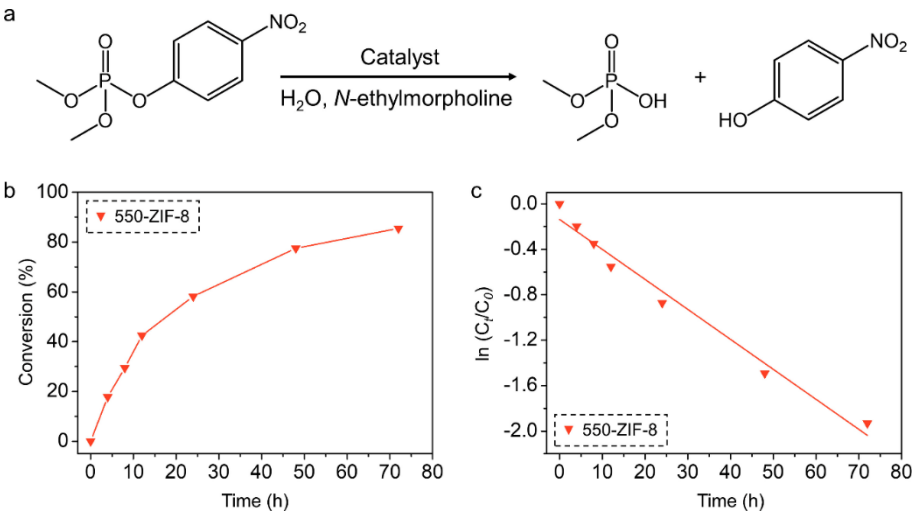

Fig. S17 (a) Hydrolytic decomposition of DMNP to dimethoxy phosphate (DMP). (b) The plot for the conversion of DMNP to DMP with 550-ZIF-8 in varied time points. (c) Linear relationship between $\ln(C_t/C_0)$ and reaction time in the presence of 550-ZIF-8. C_0 and C_t represent the amounts of DMNP at the initial stage and time t, respectively.

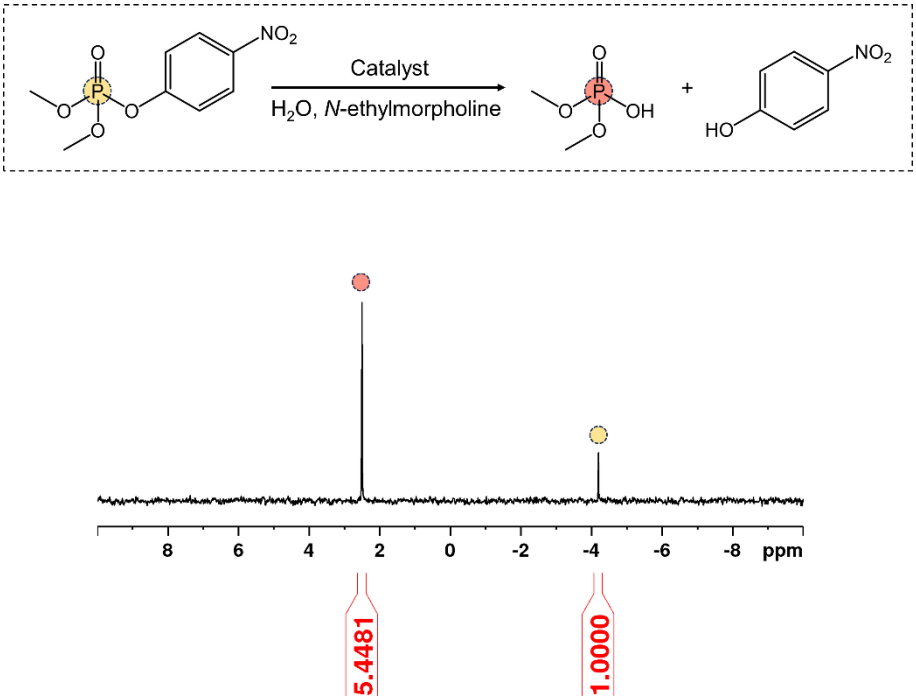

Fig. S18 ^{31}P NMR spectrum showing catalytic degradation of DMNP after 72 h in the presence of 550-ZIF-8.

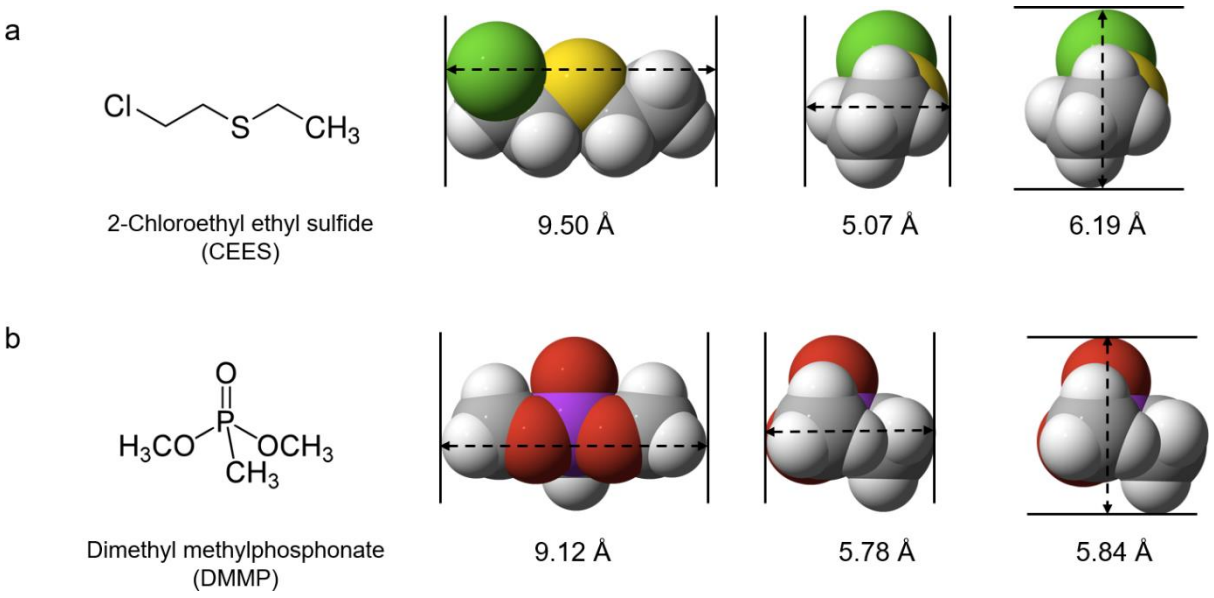

Fig. S19 Structures and van der Waals models of (a) CEES and (b) DMMP; C: gray, S: yellow, Cl: green, H: white, O: red, P: purple.

Table S1 BET surface areas and total pore volumes of ZIF-8 and T-ZIF-8 samples.

	Surface area ($m^2\ g^{-1}$)	Total pore volume ($cm^3\ g^{-1}$)
ZIF-8	1320.1	0.67
450-ZIF-8	1313.4	0.65
500-ZIF-8	1245.2	0.65
550-ZIF-8	1158.7	0.58
570-ZIF-8	913.5	0.44
600-ZIF-8	670.4	0.37

Table S2 Kinetic parameters of the pseudo-first order model for the adsorption of CEES and DMMP on ZIF-8 and T-ZIF-8 samples.

	CEES			DMMP		
	q_e (mg/g)	k (h^{-1})	R^2	q_e (mg/g)	k (h^{-1})	R^2
ZIF-8	446.4	0.6651	0.9910	404.6	0.0389	0.9993
450-ZIF-8	450.5	0.8375	0.9818	426.6	0.0456	0.9974
500-ZIF-8	500.0	1.0672	0.9842	455.0	0.0856	0.9796
550-ZIF-8	531.8	1.4040	0.9820	497.1	0.0986	0.9818
570-ZIF-8	486.7	0.9235	0.9801	439.3	0.0627	0.9877
600-ZIF-8	278.3	1.0377	0.9680	340.2	0.0401	0.9982