

ESI

Grafting alkylamine in UiO-66 by charge-assisted coordination

bond for carbon dioxide capture from high-humidity flue gas

Lu-Jian Li, Pei-Qin Liao, Chun-Ting He, Yong-Sheng Wei, Hao-Long Zhou,
Jiao-Min Lin, Xu-Yu Li, and Jie-Peng Zhang*

MOE Key Laboratory of Bioinorganic & Synthetic Chemistry, School of Chemistry &
Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China

Email: zhangjp7@mail.sysu.edu.cn

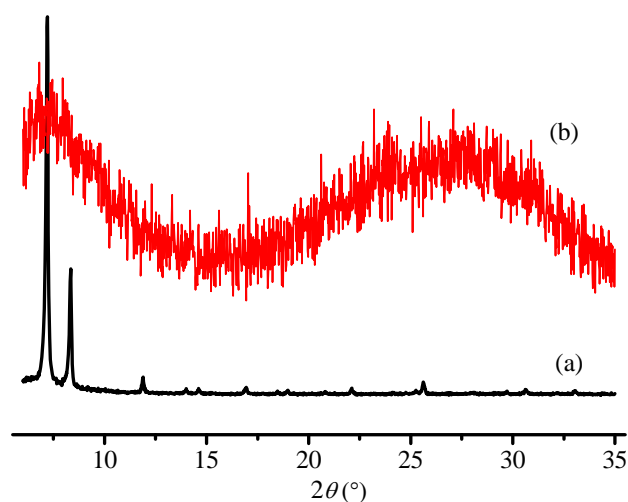


Fig. S1 PXRD of (a) UiO-66 and (b) UiO-66 soaked in pure ethanolamine solvent.

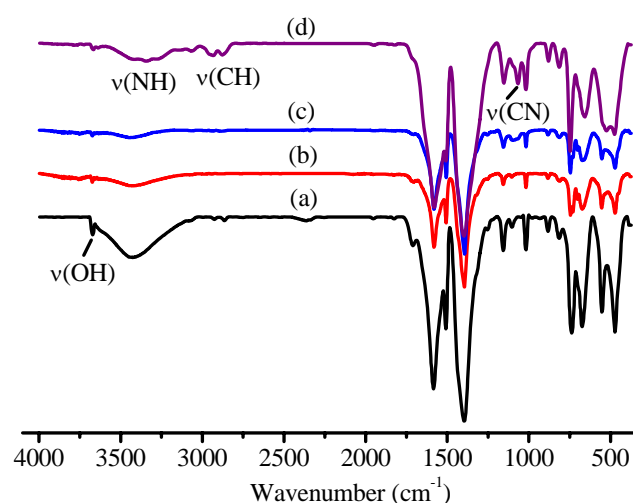


Fig. S2 IR spectra of (a) UiO-66, (b) UiO-66 soaked in diluted ethanolamine solution at room temperature, (c) UiO-66 soaked in diluted ethanolamine solution at 120 °C and (d) UiO-66-EA.

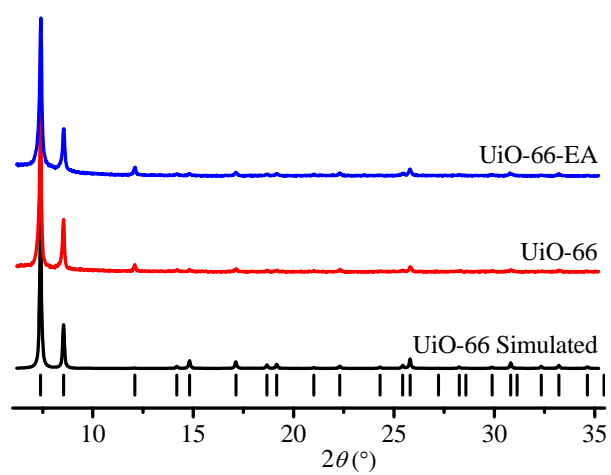


Fig. S3 PXRD of UiO-66 and UiO-66-EA.

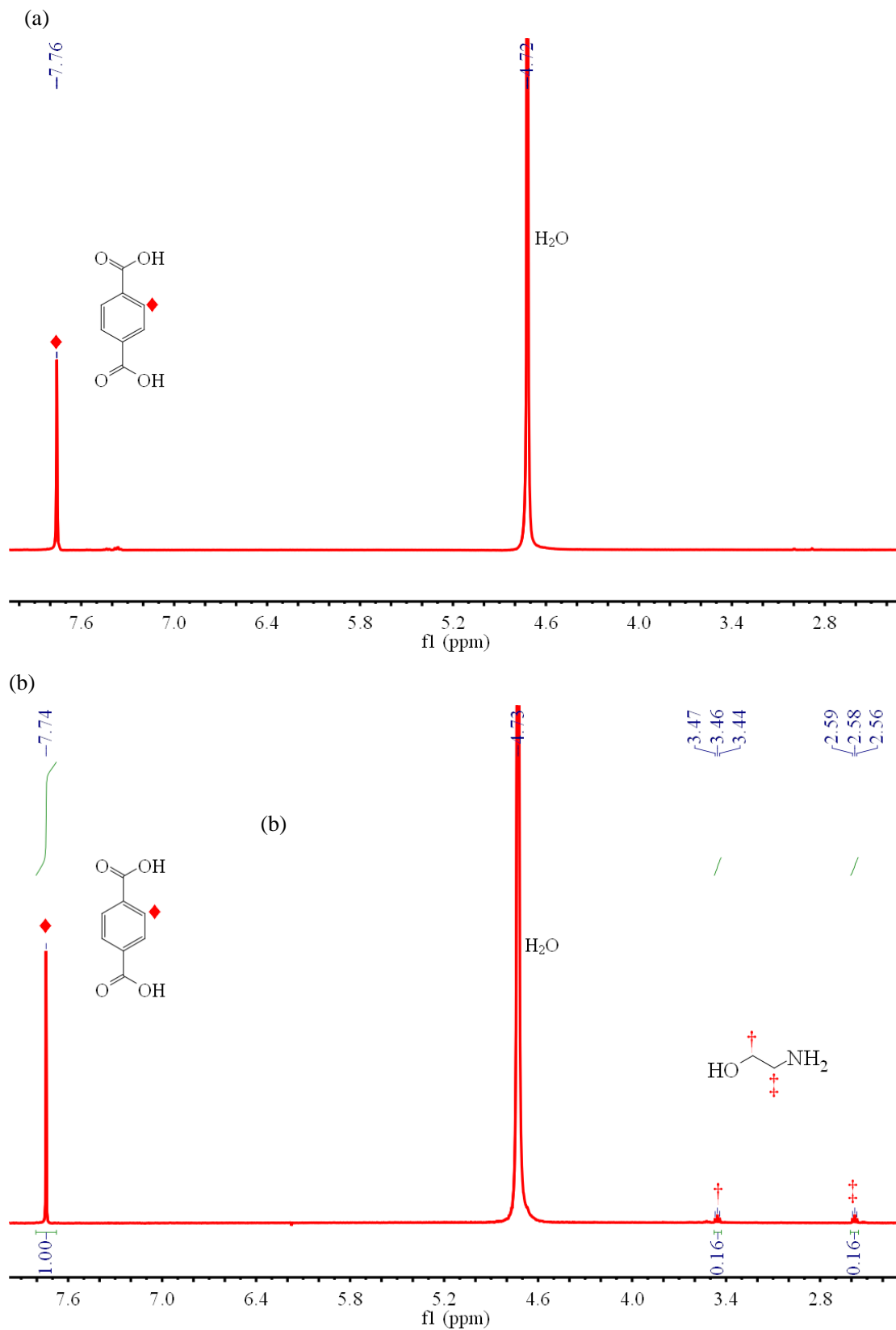


Fig. S4 ^1H NMR of UiO-66 (a) and UiO-66-EA (b).

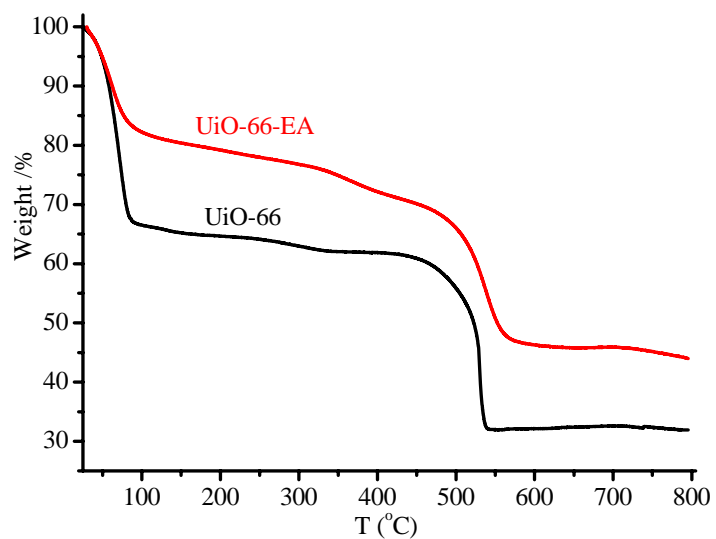


Fig. S5 TG curves of UiO-66 and UiO-66-EA.

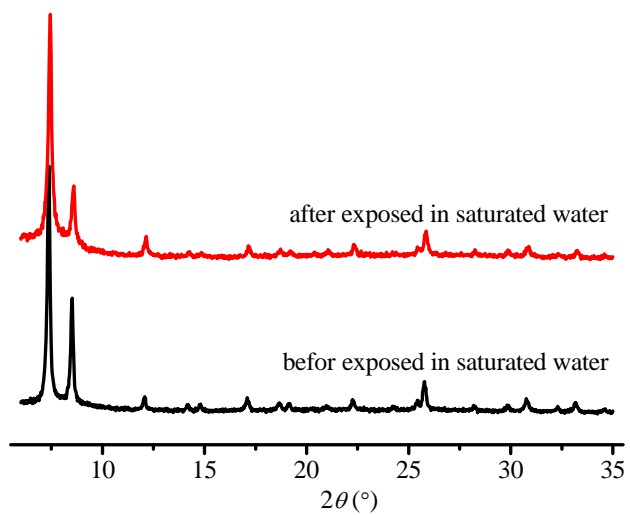


Fig. S6 PXRD of UiO-66-EA before and after exposed in saturated water vapor for three days.

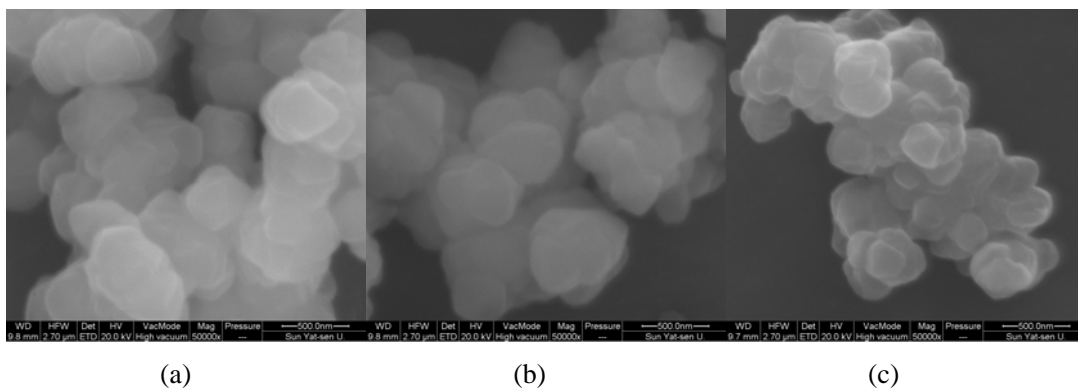


Fig. S7 SEM images of (a) UiO-66, (b) UiO-66-EA before exposed in water vapor, and (c) UiO-66-EA after exposed in water vapor.

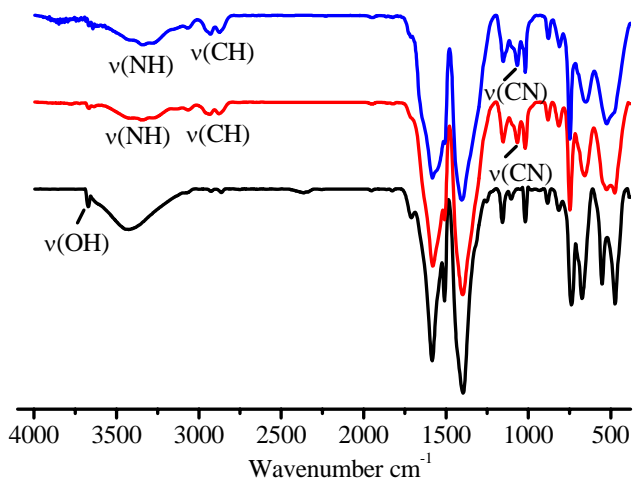


Fig. S8 IR spectra of UiO-66-EA before and after exposed in water vapor for three days: UiO-66 (black), UiO-66-EA before exposed in water vapor (red), UiO-66-EA after exposed in water vapor (blue).

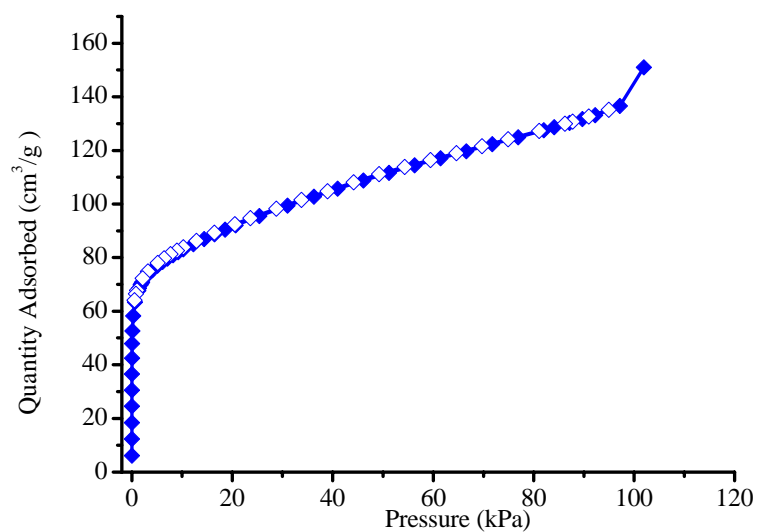


Fig. S9 Nitrogen adsorption isotherm of UiO-66-EA at 77 K.

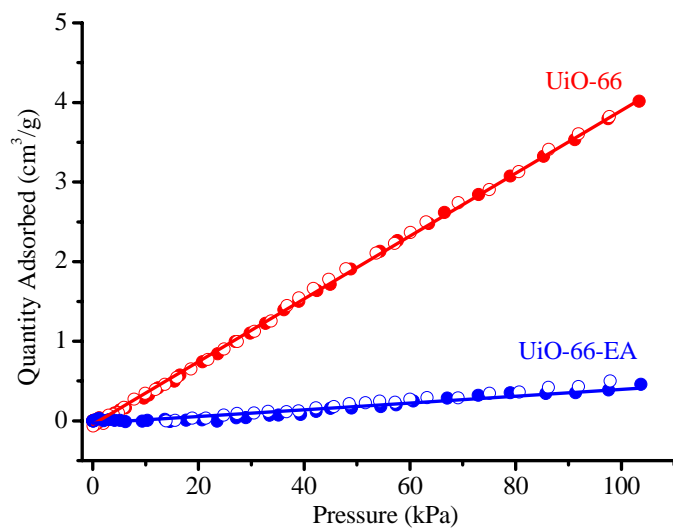


Fig. S10 Nitrogen adsorption (solid) and desorption (open) isotherms and linear fitting of the adsorption isotherms (lines) of UiO-66 and UiO-66-EA at 298 K. To read accurate uptake values from the fluctuating isotherms (due to the low nitrogen uptakes), linear fitting lines of the nitrogen adsorption isotherms (with corrections of the intercepts) were used, which gave N_2 uptakes of 3.0 and $0.32 \text{ cm}^3/\text{g}$ at 0.75 atm for UiO-66 and UiO-66-EA, respectively.

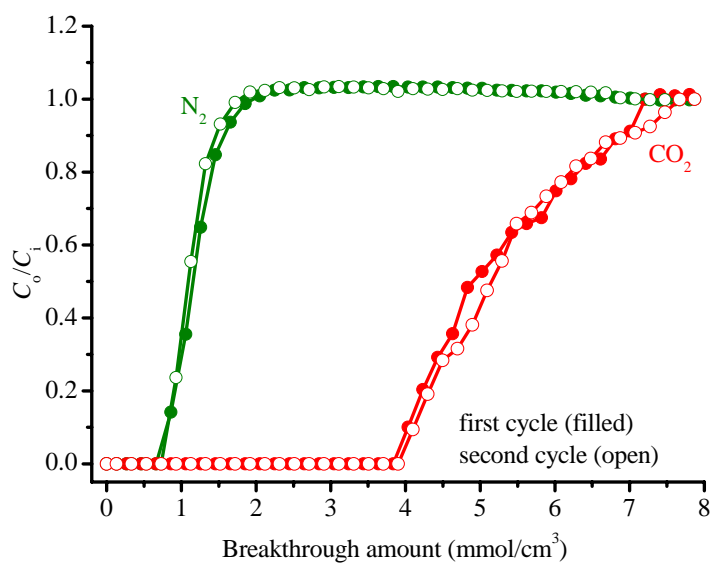


Fig. S11 Repeated breakthrough curves of a UiO-66-EA column for 10:90 CO₂/N₂ (v/v) mixture with 82% relative humidity at 313 K and 1 atm.

Table S1 Comparison of the CO₂ capture properties of UiO-66 derivatives.

Compound (common name)	CO ₂ uptake (cm ³ /g) at 298 K		Q_{st} (kJ/mol)	CO ₂ /N ₂ selectivity (298 K)	Ref
	1 bar	0.15 bar			
UiO-66-NH ₂	69	26.4	29	32	48
UiO-66-(COOH) ₂	34 (303K)	/	35	56 (303K)	52, 53
UiO-66-SO ₃ Li-0.15	73.5	20.8	25.4	39.7	49
UiO-66-SO ₃ H-1	15.2	4.5	50.8	31.4	49
UiO-66-SO ₃ Na-1	13.4	5.2	36.8	83.6	49
UiO-66	46	9.5	30	16	This work
UiO-66-EA	38	23.5	66	365	This work