Supporting Information

Direct CO_2 Capture from Air via Crystallization with a Tri-chelating Iminoguanidine Ligand

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Summary

11 Figures, 1 Table, 7 pages including cover.

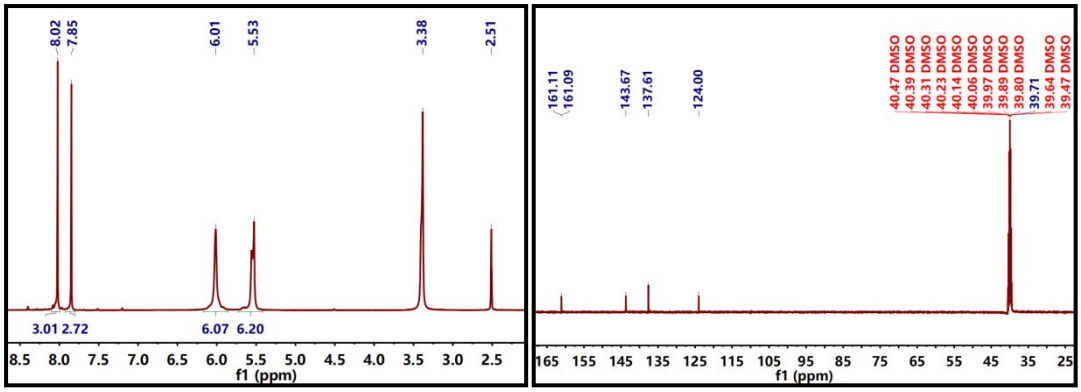

Figure S1. ^{1}H-NMR (left) and ^{13}C-NMR (right) pattern of BTIG.

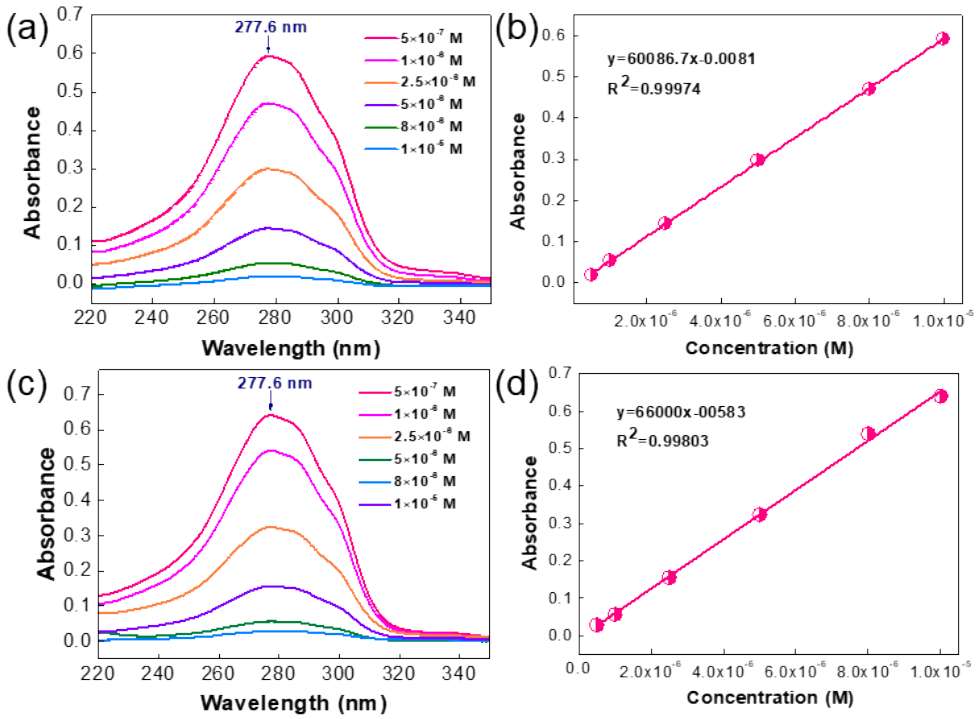

Figure S2. Standard solubility curve of BTIG and BTIG·3HCl. UV spectra of standard BTIG (a) and BTIG·3HCl (c) aqueous solutions of different concentrations. Absorbance at 277.6 nm versus concentration plots of BTIG (b) and BTIG·3HCl (d).

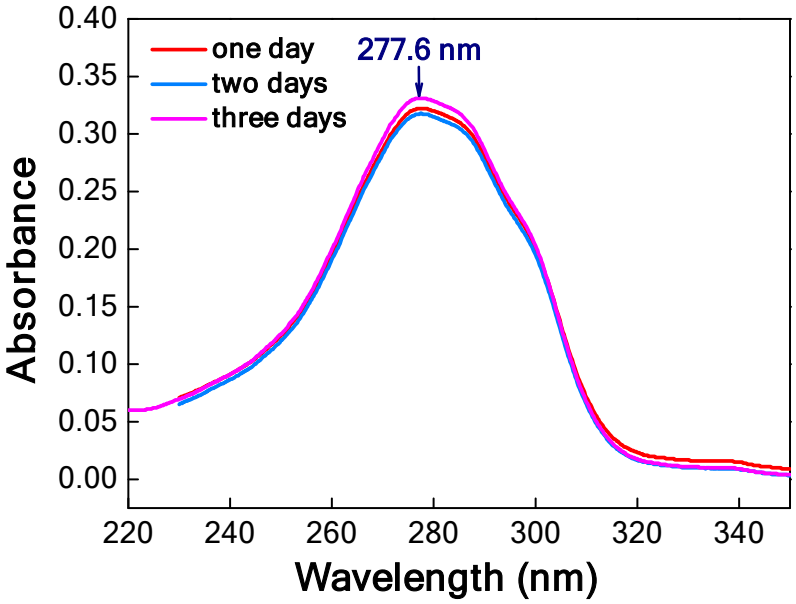

Figure S3. UV spectra of supernatant after shaking excess BTIG in 10 mL water for 1, 2, 3 days at 25 ℃.

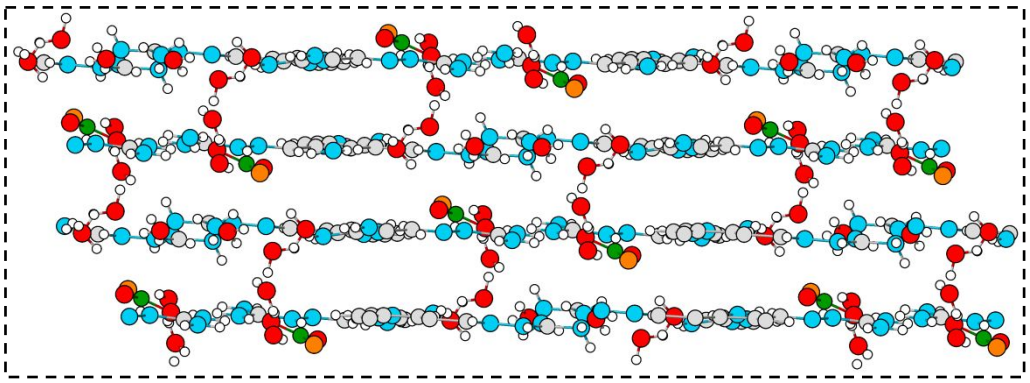

Figure S4. Stacks of the hydrogen bonds networks in BTIG crystal.

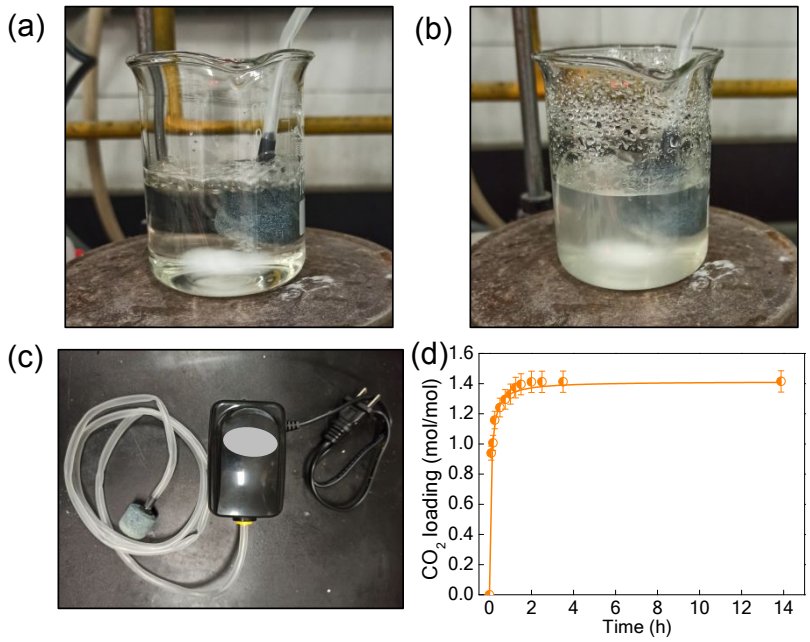

Figure S5. (a) Experimental device of CO_2 capture from air with the assist of air pump, (b) CO_2 is saturated in the solution and precipitates out in the form of BTIG-CO_2 salts, (c) picture of the air pump, and (d) sorption kinetics of bubbling process.

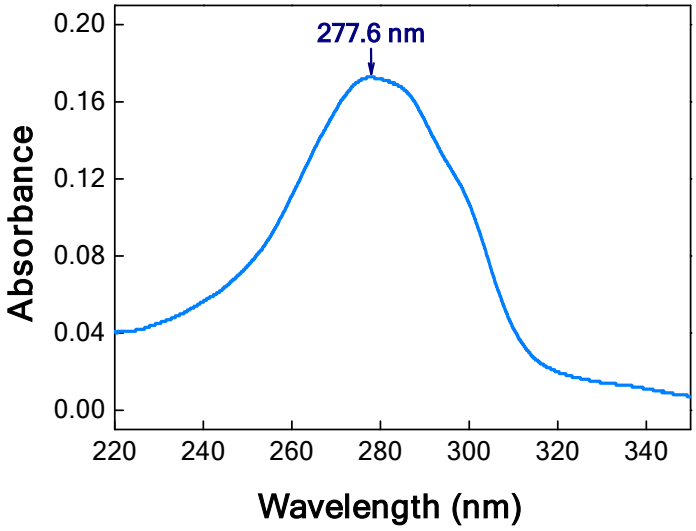

Figure S6. UV spectrum of residual liquid from simulated flue gas capture experiment.

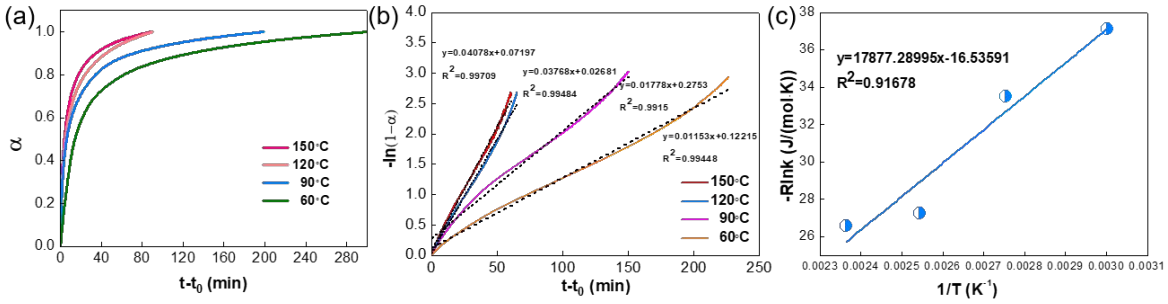

Figure S7. Kinetic analysis of BTIG-CO_2 decomposition. (a) Conversion fraction (α) of decomposition versus time ($t-t_0$) plots. (b) Fitting plots of equation 1 corresponding to Avrami-Erofeev model at measured temperatures, the slopes represent rate constant. (c) Arrhenius plot.

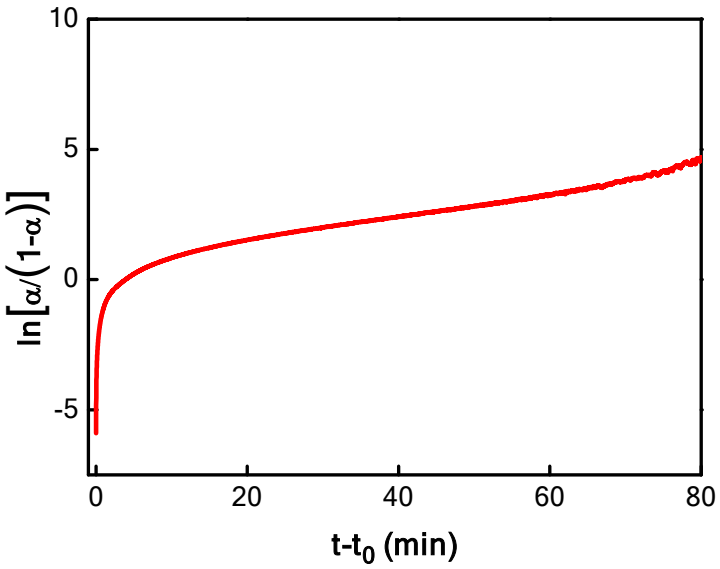

Figure S8. Fitting curves of kinetics data to Prout-Tompkins model.

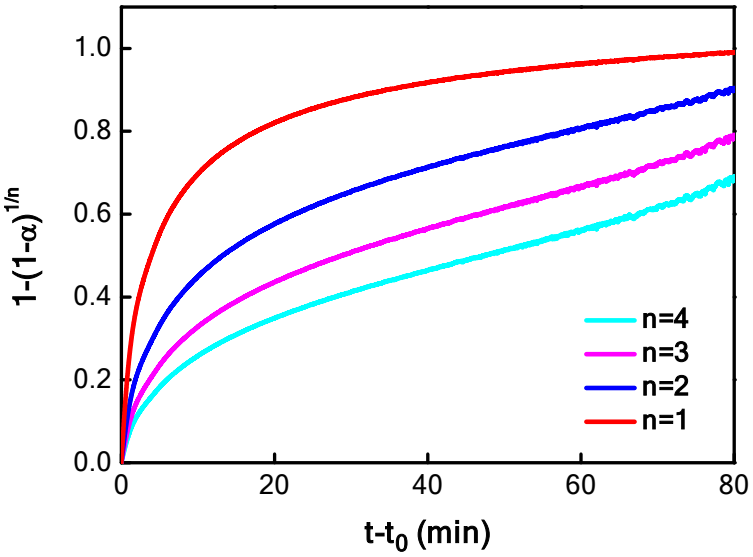

Figure S9. Fitting curves of kinetics data to Geometrical phase boundary model.

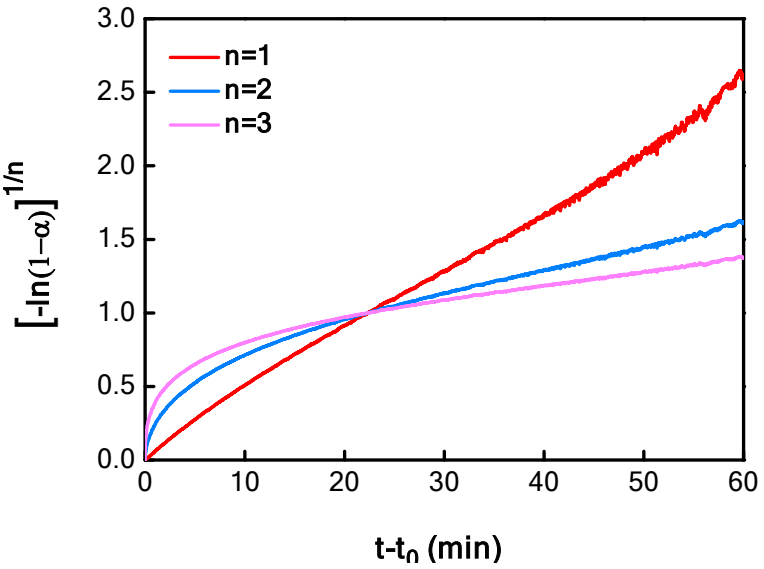

Figure S10. Fitting curve of kinetics data to Avrami-Erofeev model.

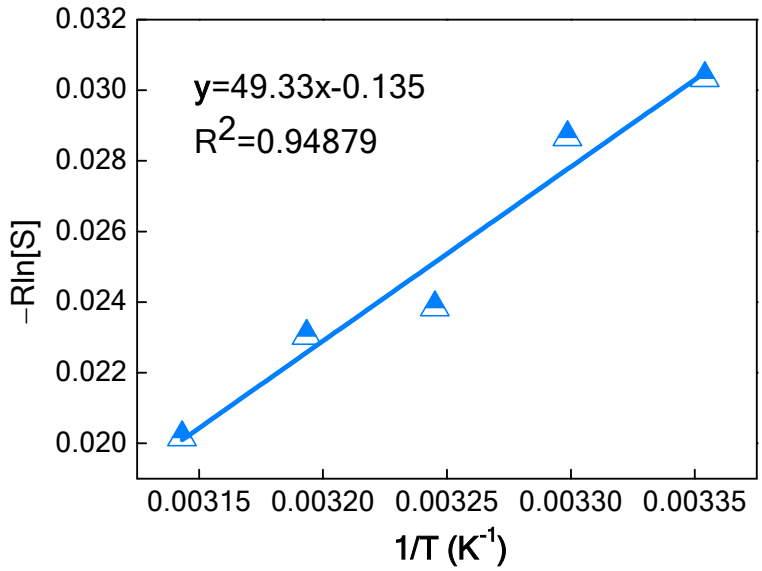

Figure S11. Van't Hoff plot fitting of BTIG dissolution step.

Table S1. pH and solubility data of BTIG and BTIG-CO_2 at different temperature.

Temperature (℃)	pH of BTIG-CO_2 saturated solution	Concentration of BTIG saturated solution (M)	K_{sp} of BTIG-CO_2
25	8.33	0.0260	1.94×10^{-23}
30	8.45	0.0318	1.19×10^{-22}
35	8.55	0.0568	5.42×10^{-22}
40	8.7	0.0626	4.29×10^{-21}
45	8.8	0.0884	3.44×10^{-20}