Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Inclusion Complexes of Organic Salts with β-Cyclodextrin as Organocatalysts for CO_2 Cycloaddition with Epoxides

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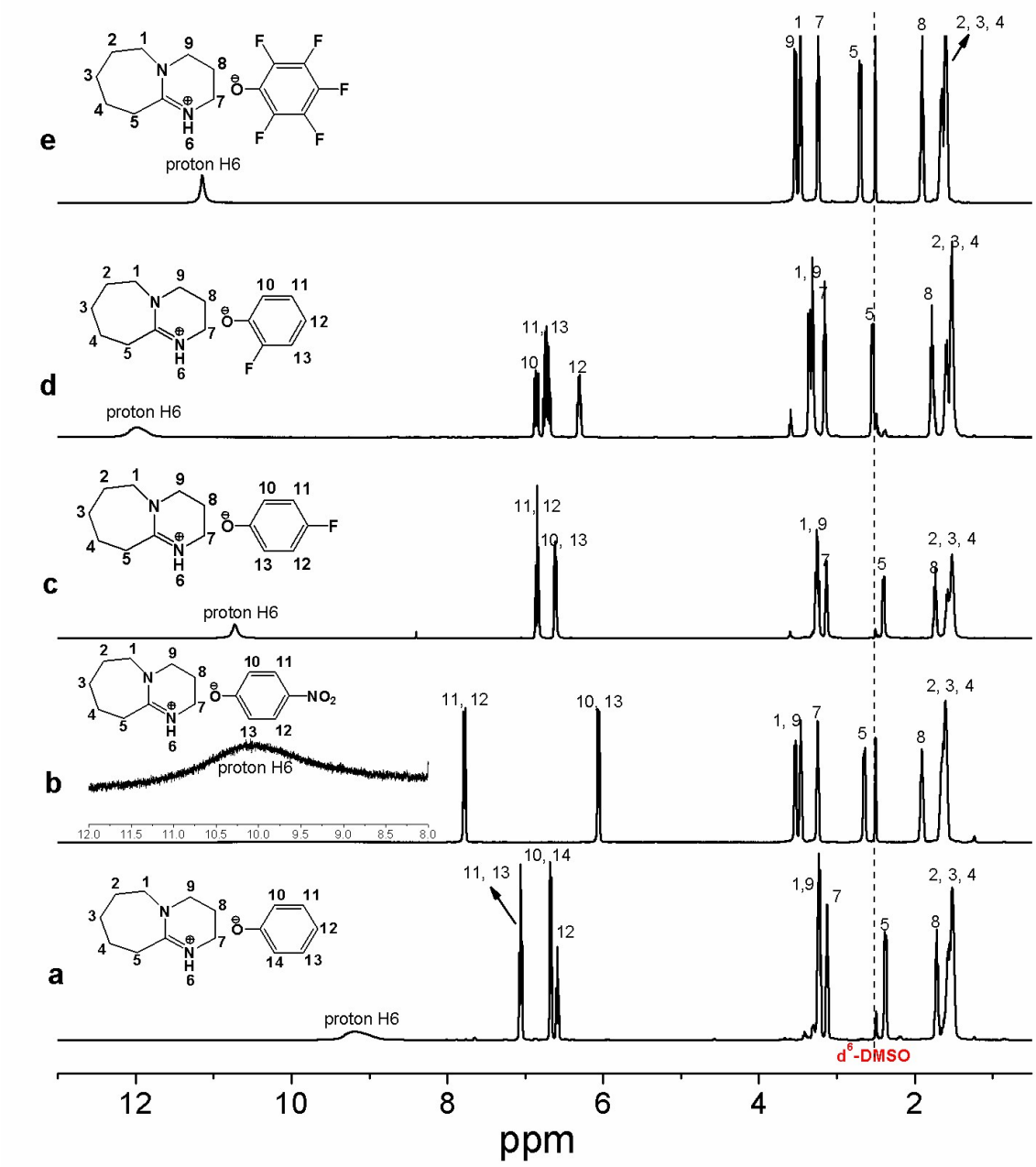


Fig. S1 ^{1}H NMR spectra of (a) [DBUH][PhO]; (b) [DBUH][*p*-NO_2-PhO]; (c) [DBUH][*p*-FPhO]; (d) [DBUH][*o*-FPhO]; (e) [DBUH][PFPhO].

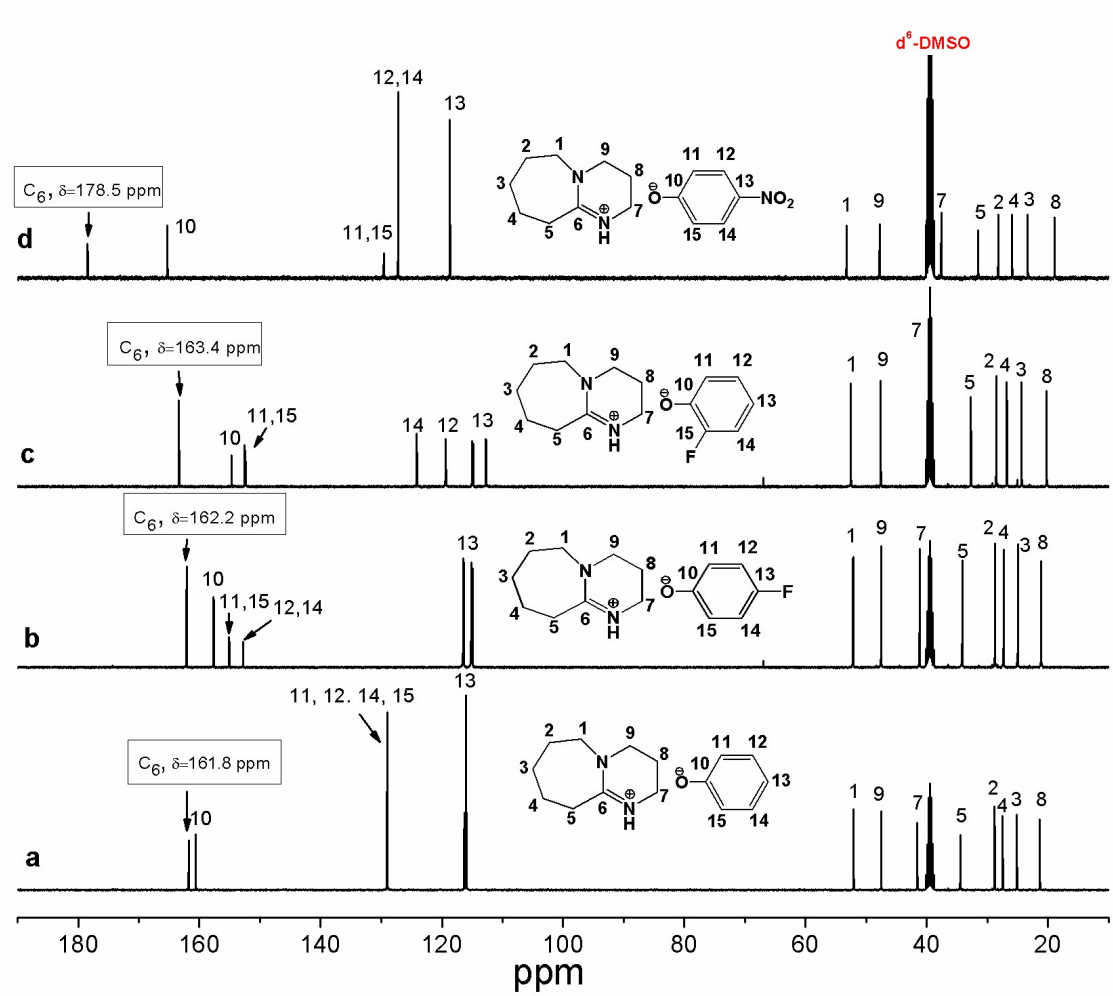


Fig. S2 ^{13}C NMR spectra of (a) [DBUH][PhO]; (b) [DBUH][*p*-FPhO]; (c) [DBUH][*o*-FPhO]; (d) [DBUH][*p*-NO_2-PhO].

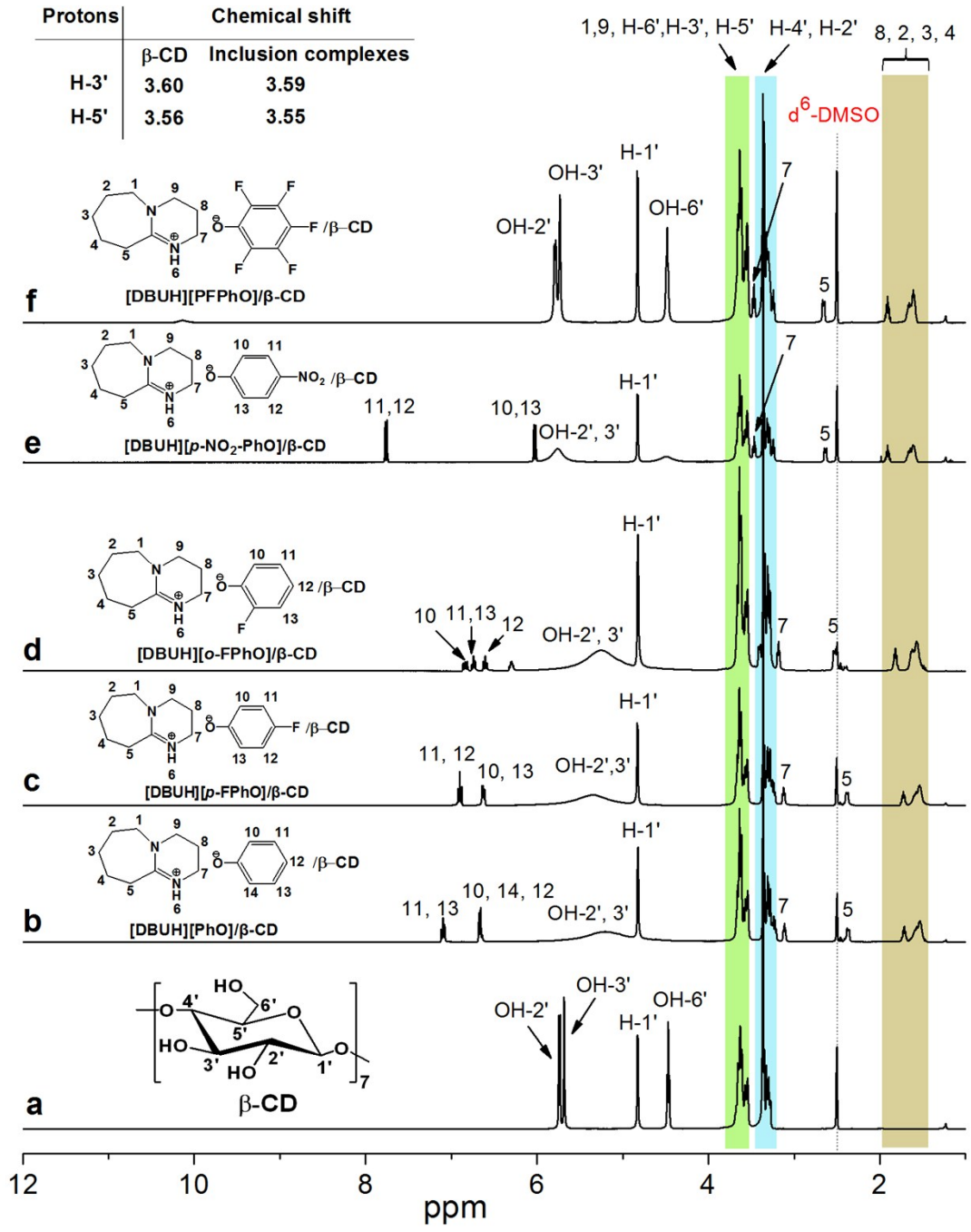


Fig. S3 ^{1}H NMR spectra of (a) β-CD; (b) [DBUH][PhO]/β-CD; (c) [DBUH][*p*-FPhO]/β-CD; (d) [DBUH][*o*-FPhO]/β-CD; (e) [DBUH][*p*-NO_2-PhO]/β-CD; (f) [DBUH][PFPhO]/β-CD.

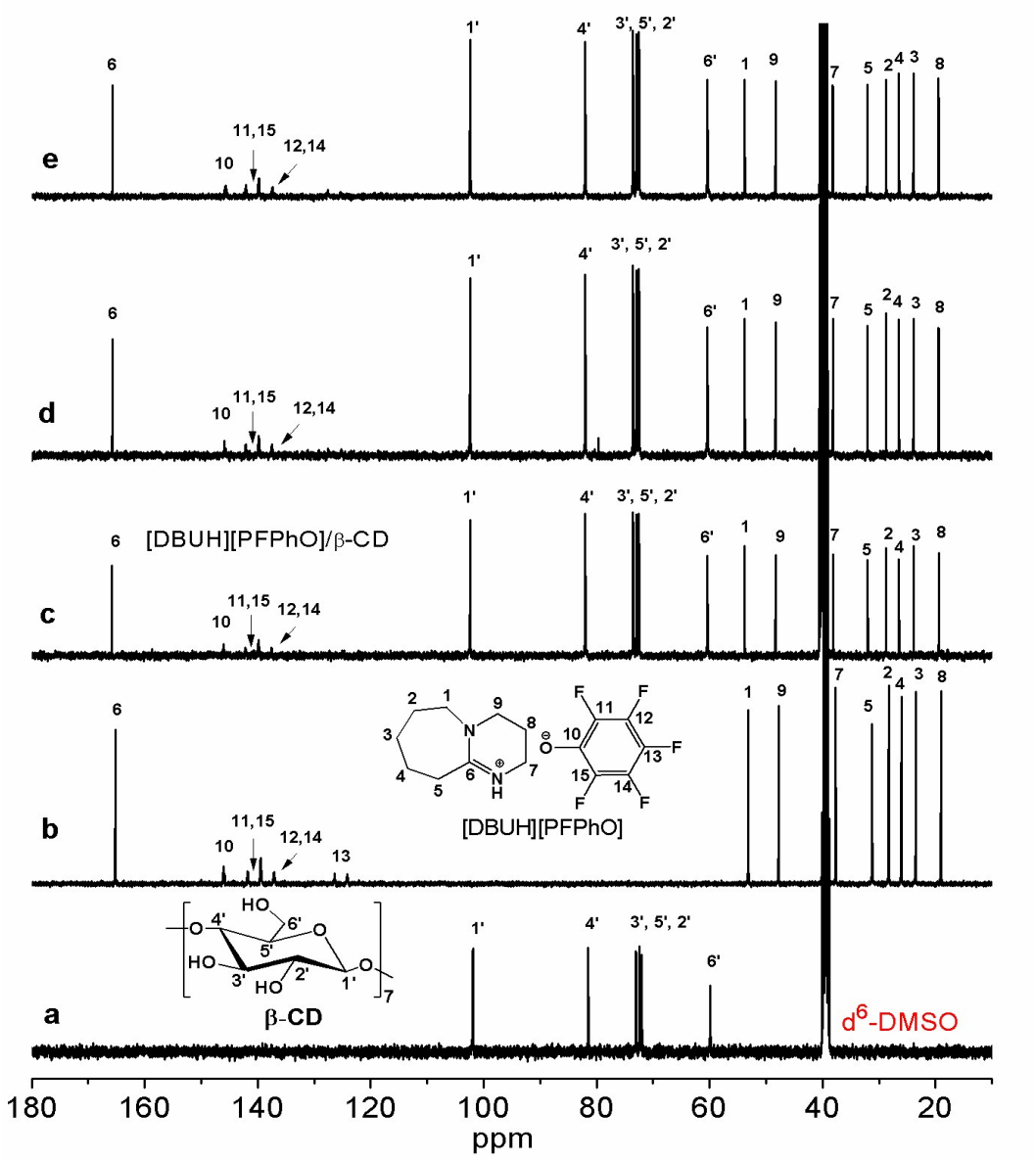


Fig. S4 ^{13}C NMR spectra of (a) β-CD; (b) [DBUH][PFPhO]; (c) [DBUH][PFPhO]/β-CD (0.054 mmol/mL in d^6-DMSO); (d) [DBUH][PFPhO]/β-CD (0.108 mmol/mL in d^6-DMSO); (e) [DBUH][PFPhO]/β-CD (0.134 mmol/mL in d^6-DMSO).

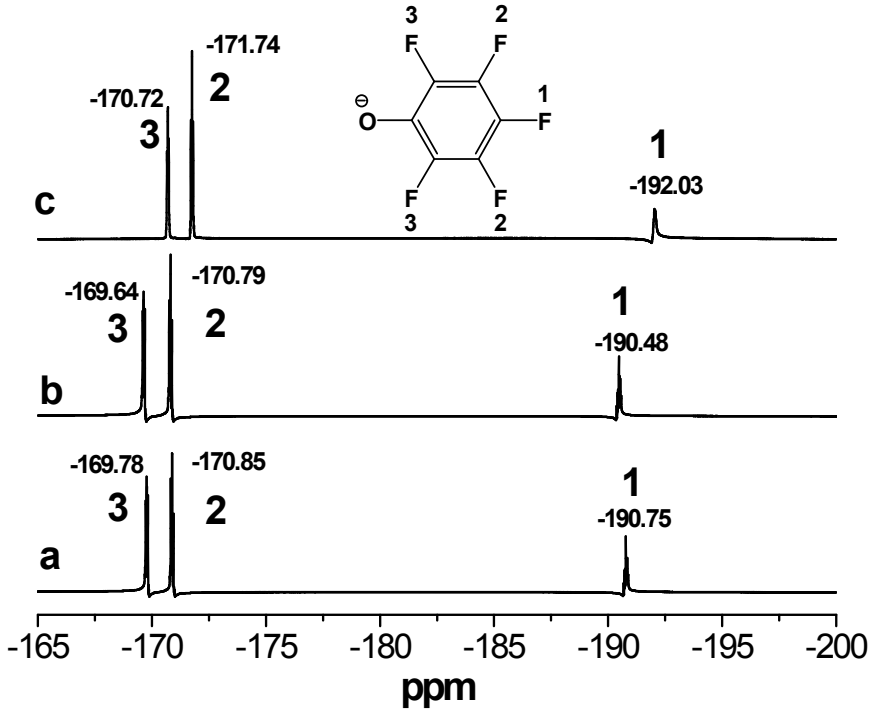


Fig. S5 The ^{19}F NMR spectra (500 MHz) of the [DBUH][PFPhO]/β-CD (a) 0.108 mmol/mL in d^6-DMSO; (b) 0.134 mmol/mL in d^6-DMSO; (c) 0.108 mmol/mL in d^6-DMSO at 70 ^{0}C.

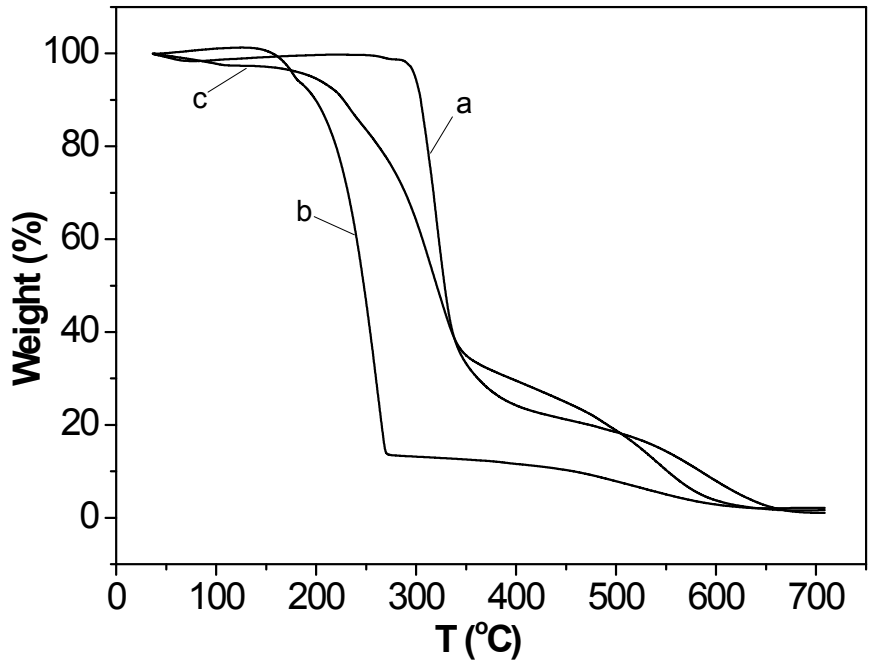


Fig. S6 The thermal gravity analysis of (a) β-CD; (b) [DBUH][PFPhO]; (c) [DBUH][PFPhO]/β-CD.

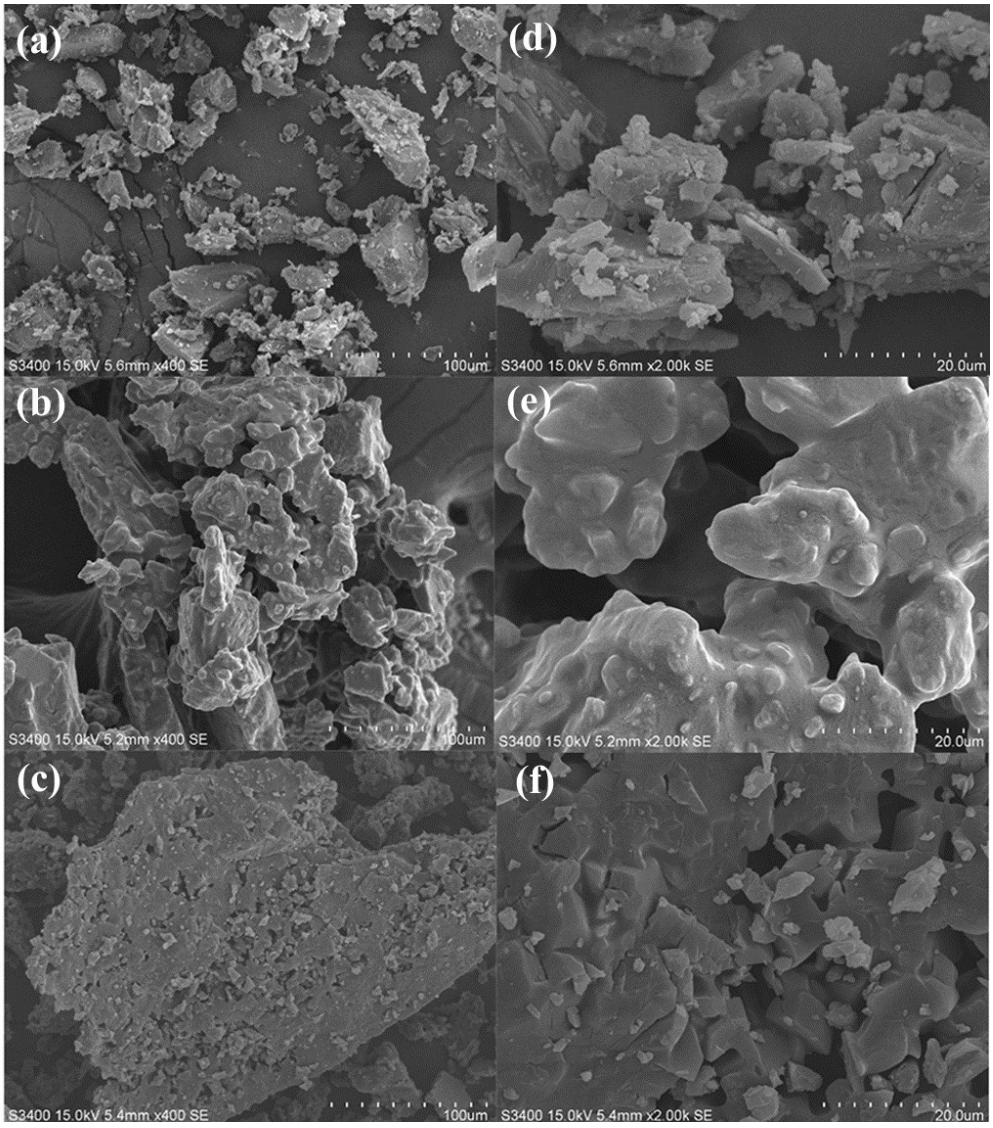


Fig. S7 The SEM images of β-CD (a, d); [DBUH][PFPhO] (b, c); [DBUH][PFPhO]/β-CD (e, f).

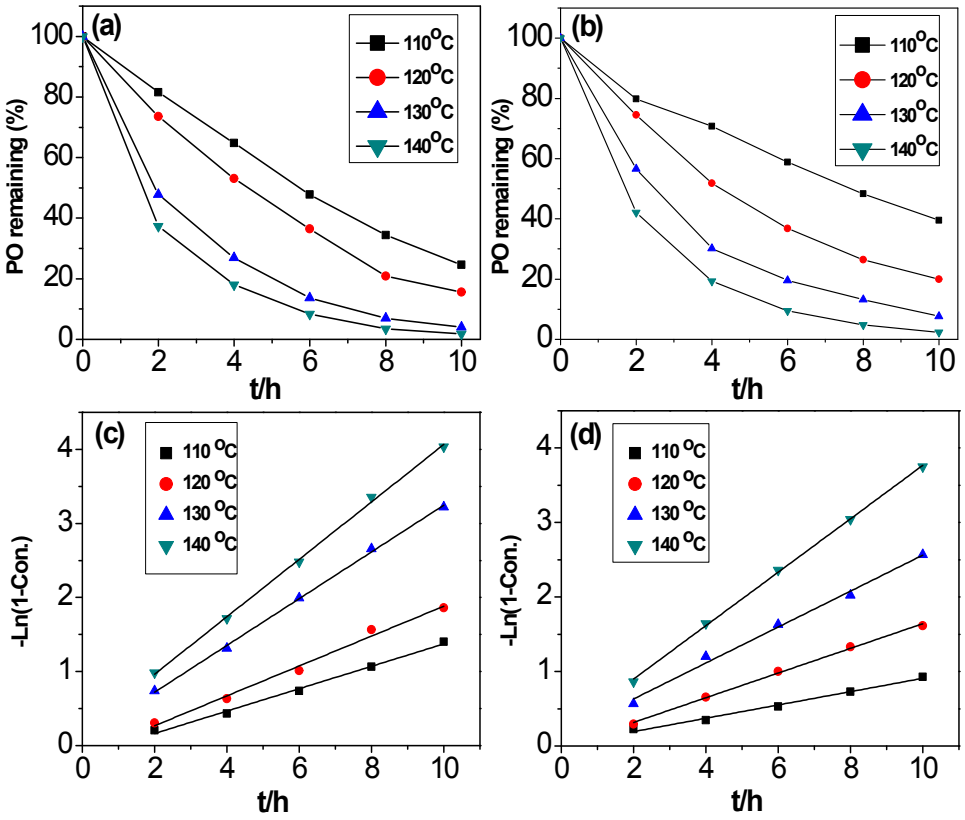


Fig. S8 Relationship of PO remaining with reaction time at different temperature over cayalyst: (a) **[**DBUH][PFPhO]/β-CD; (b) [DBUH][PFPhO]; and relationship of -Ln(1-Con.) with reaction time at different temperature over cayalyst: (c) **[**DBUH][PFPhO]/β-CD; (d) [DBUH][PFPhO].

Table S1. The pKa value of phenol and other derivatives

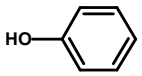
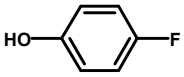
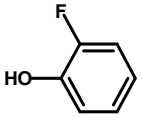
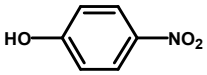
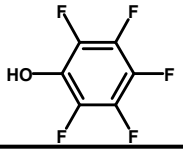
Entry	Anion part	pKa
1		9.94
2		9.81
3		8.71
4		7.15
5		5.50

Table S2. The effect of amount of [DBUH][PFPhO]/β-CD on the catalyst activity. [a]

Entry	The amount of catalyst [b]	Con.%	Sel.%
1	1.0 mmol%	89.9	99.3
2	1.5 mmol%	98.7	98.2
3	2.0 mmol%	79.9	97.9

[a] Reaction conditions: PO 0.7 mL (10 mmol), 130 ^{o}C, 3 MPa, 10 h; [b] The amount of catalyst was based on that of [DBUH][PFPhO].

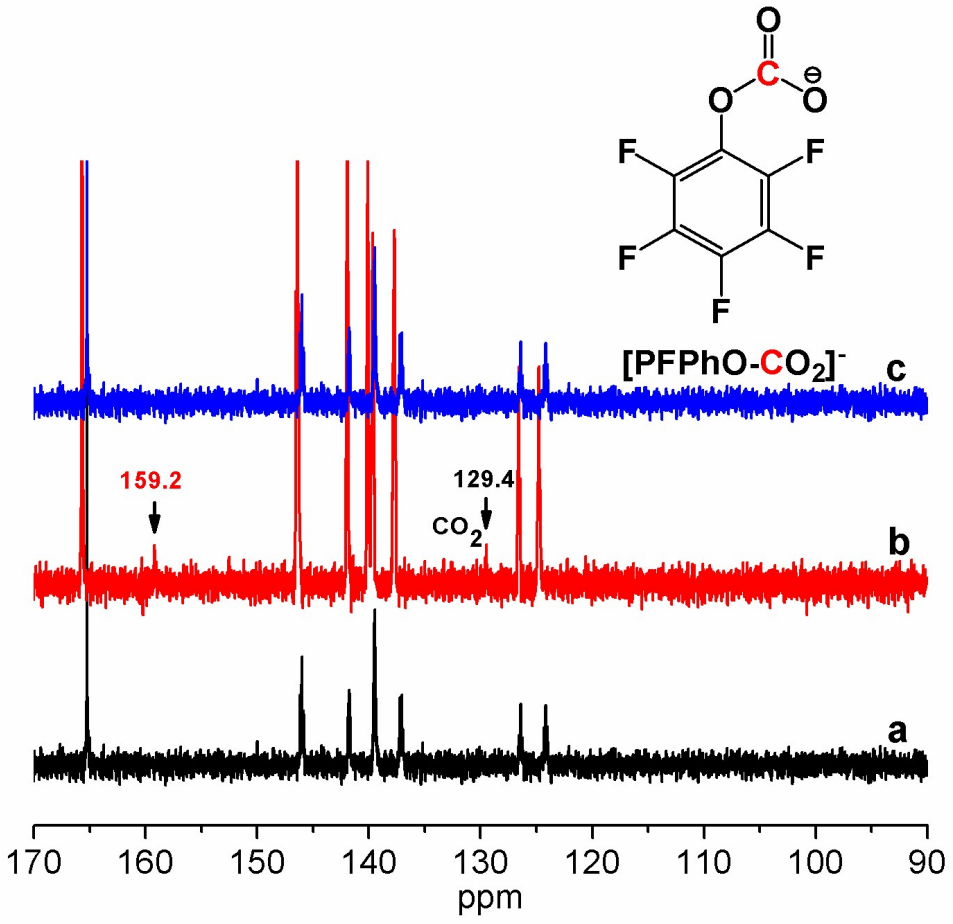
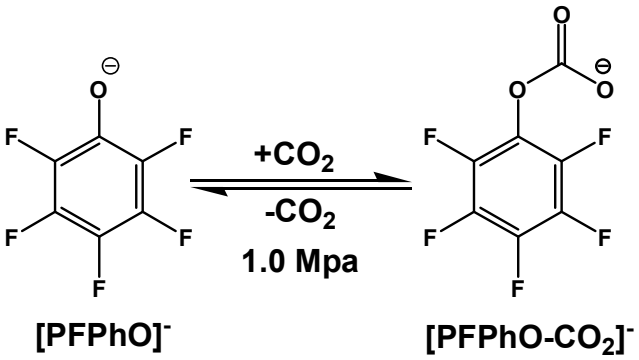


Fig. S9 ^{13}C NMR spectra of (a) Fresh [DBUH][PFPhO]; (b) [DBUH][PFPhO] after the absorption of CO_2; (c) [DBUH][PFPhO] after removing the CO_2 by vacuuming.



Scheme S1 The plausible mechanism of CO_2 absorption by $[PFPhO]^-$.