

Unraveling the Mechanism of CO₂ Capture and Separation by Porous Liquids

Jie Yin ^a, Wendi Fu ^a, Jinrui Zhang ^a, Hongshun Ran ^a, Naixia Lv ^b, Yanhong Chao ^a

Hongping Li ^{a*}, Wenshuai Zhu ^{a*}, Hui Liu ^{a*}, Huaming Li ^a

[^a] Institute for Energy Research, School of Chemistry and Chemical Engineering,
Jiangsu University, Zhenjiang, 212013, P. R. China

[^b] College of Biology and Chemistry, Xingyi Normal University for Nationalities,
Xingyi, 562400, P. R. China

***Corresponding author:**

E-mail: hongpingli@ujs.edu.cn (H. P. Li); zhuws@ujs.edu.cn (W. S. Zhu);

lh7544@ujs.edu.cn (H. Liu)

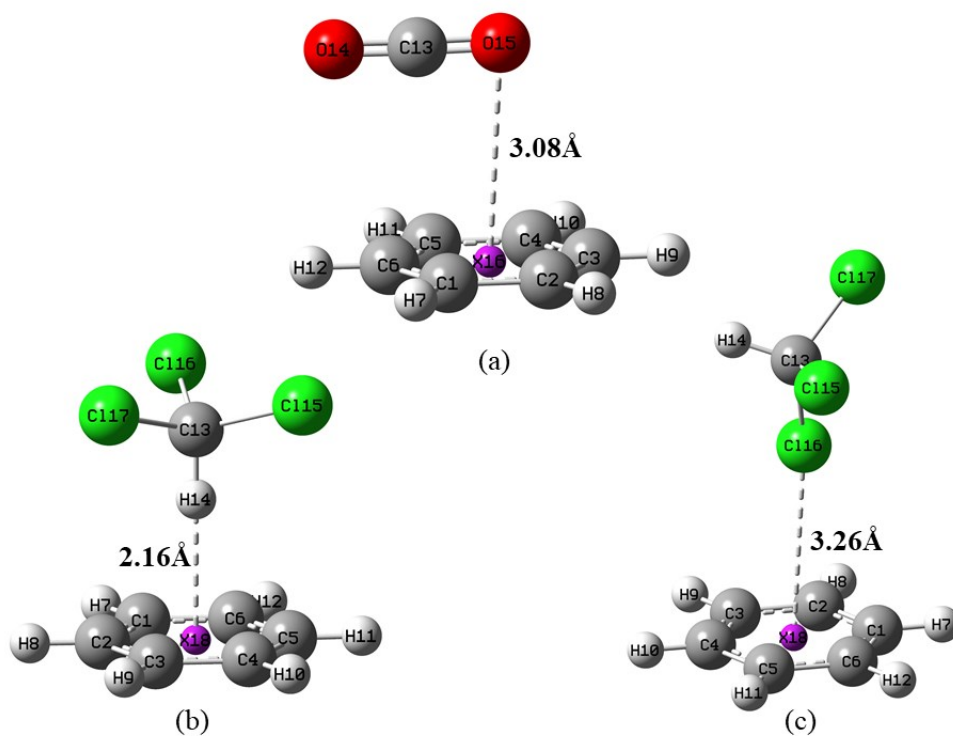


Figure S1 Parameters of interaction between complexes. (a) π - π , between CO₂ and benzene ring ($\Delta E=-2.7$ kcal/mol); (b) C-H $\cdots\pi$, between CHCl₃ and benzene ring ($\Delta E=-6.7$ kcal/mol); (c) Cl $\cdots\pi$, between CHCl₃ and benzene ring ($\Delta E=-2.5$ kcal/mol).

Table S1 Structure parameters after absorption in Cage 3⁰13⁶

□	CO ₂		CHCl ₃	
	Interacting type	Distance	Interacting type	Distance
COM-a	π - π_1	3.24 Å	□	
	π - π_2	3.51 Å		
	π - π_3	5.01 Å		
COM-b	π - π_1	3.28 Å	Cl148···H65-C60	2.74 Å
	π - π_2	3.46 Å	Cl147···H42-C41	2.72 Å
	π - π_3	4.67 Å	Cl147···H37-C33	2.87 Å
COM-c	π - π_1	3.23 Å	Cl147···H23-C22	2.93 Å
	π - π_2	3.52 Å	Cl··· π	3.36 Å
	π - π_3	5.00 Å		
COM-d	O152···H93-C91	2.70 Å	□ C-H··· π	2.28 Å
COM-e	O152···H71-C70	2.72 Å	C-H··· π	2.63 Å
	O151···H146-C145	2.60 Å		
	C150···Cl147	3.21 Å		
	C150···Cl149	3.21 Å		
COM-f	π - π	3.10 Å	C-H··· π	2.25 Å

Table S2 Structure parameters after absorption in Cage 3⁶13⁰

	CO ₂		CHCl ₃	
	Interacting type	Distance	Interacting type	Distance
ABS-a	O176···H24-C21	2.69 Å		
	π - π	3.79 Å		
ABS-b	O176···H162-C155	2.56 Å	Cl171···H22-C17	2.64 Å
	O175···H39-C34	2.71 Å		
	π - π	3.25 Å		
ABS-c	π - π_3	4.54 Å	Cl··· π	3.28 Å
ABS-d			□ C-H··· π	2.42 Å
			Cl173···H162-C155	2.77 Å
			Cl173···H56-C53	2.73 Å
ABS-e	O175···H170-C169	2.34 Å	C-H··· π	2.83 Å
	O175···H39-C34	2.56 Å		
	O176···H23-C19	2.69 Å		
ABS-f	π - π	3.07 Å	C-H··· π	2.48 Å

Table S3 Structure parameters after absorption in Cage 3³13³

	CO ₂		CHCl ₃	
	Interacting type	Distance	Interacting type	Distance
SYS-a	π - π_1	3.46 Å		
	π - π_2	3.11 Å		
	π - π_3	4.39 Å		
SYS-b	π - π_1	3.40 Å	Cl159···H9-C6	2.63 Å
	π - π_2	3.11 Å	Cl159···H154-C144	2.78 Å
	π - π_3	4.37 Å	Cl160···H118-C108	2.88 Å
			Cl161···H23-C19	2.80 Å
SYS-c	π - π_1	3.12 Å	Cl··· π	3.28 Å
	π - π_2	3.27 Å		
	π - π_3	4.86 Å		
SYS-d			C-H··· π_1	3.81 Å
			C-H··· π_2	3.67 Å
			C-H··· π_3	3.95 Å
SYS-e	O163···H158-C162	2.19 Å	C-H··· π_1	3.45 Å
	O164···H118-C108	2.68 Å	C-H··· π_2	4.00 Å
	C162···N120	2.93 Å	C-H··· π_3	4.06 Å
	C162···N138	3.25 Å		
SYS-f	O163···H131-C124	2.71 Å	C-H··· π	2.40 Å
	π - π	3.10 Å		