

The dynamics behavior and intrinsic mechanism of CO₂ absorption by amino acid ionic liquids

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1. Introduction

The following tables and figures contain the results of the self-diffusion coefficient of anion, cation, and CO₂ at 350K and 400K for all AAILs-CO₂ systems. Meanwhile, the residence time, the radial distribution function of CO₂-anion, and interaction energy between CO₂ and AAILs at 350K and 400K were listed.

Table S1 (I). Self-diffusion coefficients (unit: 10^{-11} m²/s) of the cation/anion and CO₂ in CO₂-AAILs systems at 350K.

D	[P4444] ⁺				[P66614] ⁺			
	[Gly] ⁻	[Pro] ⁻	[Lys] ⁻	[Im] ⁻	[Gly] ⁻	[Pro] ⁻	[Lys] ⁻	[Im] ⁻
Anion	9.92	3.51	4.73	1.65	1.09	4.95	1.02	1.23
Cation	7.40	2.51	6.66	1.44	1.15	4.35	6.27	6.20
CO ₂	10.40	10.14	7.54	6.84	94.35	17.65	62.17	93.53

Table S1 (II). Self-diffusion coefficients (unit: 10^{-10} m²/s) of the cation/anion and CO₂ in CO₂-AAILs systems at 400K.

D	[P4444] ⁺				[P66614] ⁺			
	[Gly] ⁻	[Pro] ⁻	[Lys] ⁻	[Im] ⁻	[Gly] ⁻	[Pro] ⁻	[Lys] ⁻	[Im] ⁻
Anion	6.47	5.26	5.63	11.06	8.34	2.50	1.79	1.36
Cation	8.65	8.21	1.56	7.72	2.01	1.84	2.27	5.89
CO ₂	1.48	23.17	2.19	22.18	20.92	5.25	4.15	9.49

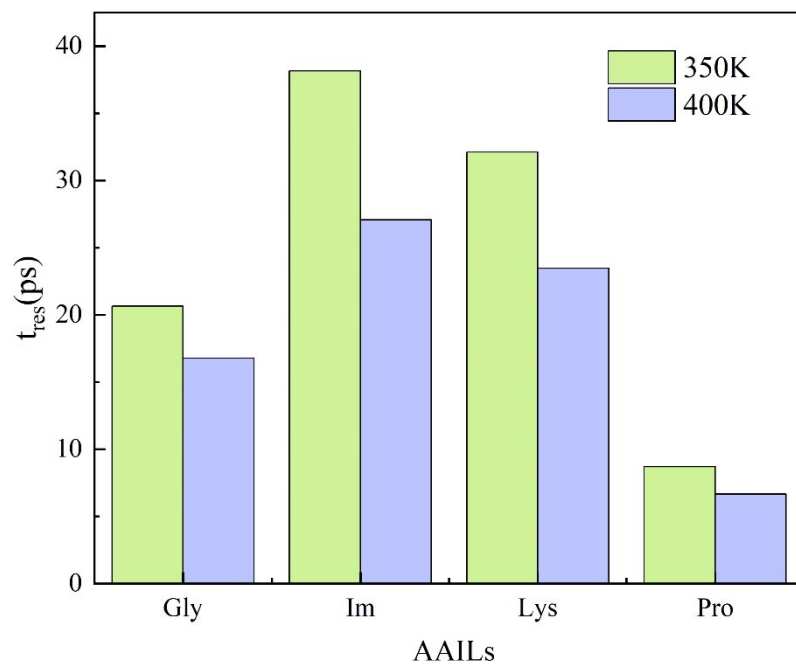


Figure S1. Residence time at 350K and 400K for CO₂-anion in [P4444] [X] ([X]= [Gly]⁻, [Im]⁻, [Lys]⁻, [Pro]⁻).

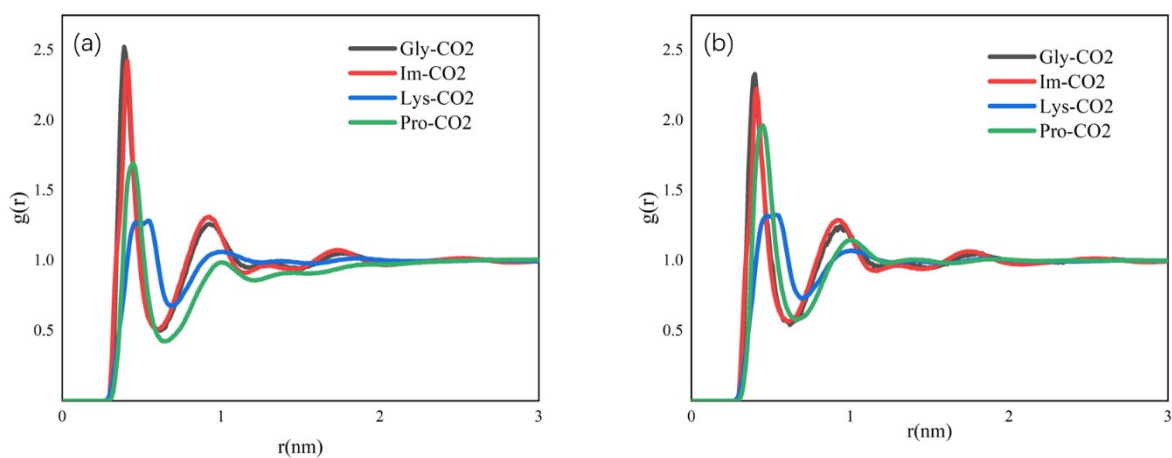


Figure S2. The center of mass radial distribution function for anion-CO₂ in [P4444] [X] ([X]= [Gly]⁻, [Im]⁻, [Lys]⁻, [Pro]⁻) at (a) 350 K, and (b) 400K.

Table S2. Interaction Energy for the four types AAILs-CO₂ systems at 350K and 400K.

AAIL	T(K)	Anion-CO ₂ (Kcal/mol)		Cation-CO ₂ (Kcal/mol)		Interaction Energy of AAIL-CO ₂ (Kcal/mol)
		E _{ele}	E _{vdW}	E _{ele}	E _{vdW}	
[P ₄₄₄₄][Gly]	350	-2.95±0.05	-2.38±0.01	-1.06±0.02	-9.96±0.02	-16.35
	400	-2.47±0.10	-2.56±0.02	-0.95±0.04	-10.32±0.04	-16.30
[P ₄₄₄₄][Im]	350	-2.99±0.04	-2.61±0.01	-1.27±0.02	-9.83±0.02	-16.70
	400	-3.37±0.09	-2.70±0.03	-1.30±0.04	-10.16±0.06	-17.53
[P ₄₄₄₄][Pro]	350	-0.14±0.05	-1.65±0.03	-1.15±0.01	-4.44±0.08	-7.38
	400	-2.01±0.04	-2.65±0.01	-1.04±0.02	-4.82±0.02	-10.52
[P ₄₄₄₄][Lys]	350	-1.77±0.09	-3.07±0.06	-1.03±0.03	-6.69±0.11	-9.42
	400	-2.20±0.05	-2.43±0.01	-0.95±0.02	-6.96±0.02	-12.54