

Electronic supplementary information

Light-Modulated Aggregation Behavior of Some Unsubstituted Cinnamate-Based Ionic Liquids in Aqueous Solutions

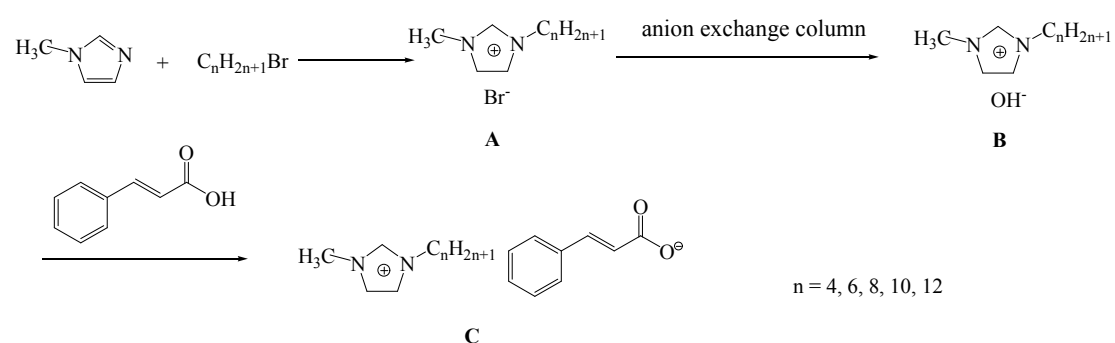
Jie Yang,^{a,c} Huiyong Wang,^{ab} Jianji Wang,^{*ab} Xiaojia Guo^{ab} and Yue Zhang^{ab}

^a Henan Key Laboratory of Green Chemical Media and Reactions, School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 453007, P. R. China

^b Collaborative Innovation Center of Henan Province for Green Manufacturing of Fine Chemicals, Key Laboratory of Green Chemical Media and Reactions, Ministry of Education, Henan Normal University, Xinxiang, Henan 453007, P. R. China

^c School of Basic Medicine, Xinxiang Medical University, Xinxiang, Henan 453007, P. R. China

Synthesis and characteristics of [C_nmim][CA](n = 4, 6, 8, 10, 12) ionic liquids



Scheme S1. Synthetic route of the photo-responsive ionic liquids

1-dodecyl-3-methylimidazolium ortho-methoxycinnate ([C₁₂mim][CA]):

¹H NMR ((DMSO-d₆): δ = 9.79 (1H, s), 7.84 (1H, s), 7.76 (1H, s), 7.43(2H, d), 7.30 (2H, t), 7.22 (1H, t), 7.03 (1H, d), 6.35 (1H, d), 4.17 (2H, t), 3.88 (3H, s), 1.76 (2H, m), 1.19 (2H, m), 0.84 (3H, t) ppm.

¹³C NMR: δ = 169.7, 137.9, 137.6, 134.6, 132.2, 129.0, 128.0, 127.2, 124.0, 122.7, 49.1, 36.1, 31.8, 30.0, 29.5, 29.5, 29.4, 29.3, 29.2, 28.9, 26.0, 22.6, 14.4 ppm.

HRMS: calcd for [C₁₆H₃₁N₂]⁺: 251.2482; found: 251.2476; calcd for [C₁₀H₉O₃]⁻: 147.0441; found: 147.0442

1-decyl-3-methylimidazolium cinnate ([C₁₀mim][CA]):

¹H NMR ((DMSO-d₆): δ = 9.87 (1H, s), 7.86 (1H, s), 7.78 (1H, s), 7.44 (2H, d), 7.30 (2H, t), 7.22

(1H, t), 7.06 (1H, d), 6.38 (1H, d), 4.17 (2H, t), 3.88 (3H, s), 1.74 (2H, m), 1.19 (2H, m), 0.82 (3H, t) ppm.

¹³C NMR: δ = 170.0, 138.0, 137.5, 135.0, 131.7, 129.0, 128.1, 127.2, 124.0, 122.7, 49.1, 36.0, 31.8, 30.0, 29.4, 29.3, 29.2, 28.9, 26.0, 22.6, 14.4 ppm.

HRMS: calcd for [C₁₄H₂₇N₂]⁺: 223.2169; found: 223.2151; calcd for [C₁₀H₉O₃]⁻: 147.0441; found: 147.0449.

1-octyl-3-methylimidazolium cinnate ([C₈mim][CA]):

¹H NMR ((DMSO-d₆): δ = 9.41 (1H, s), 7.77 (1H, s), 7.70 (1H, s), 7.45 (2H, d), 7.31 (2H, t), 7.23 (1H, t), 7.08 (1H, d), 6.39 (1H, d), 4.14 (2H, t), 3.84 (3H, s), 1.74 (2H, m), 1.20 (2H, m), 0.82 (3H, t) ppm.

¹³C NMR: δ = 171.8, 139.9, 139.3, 136.8, 133.7, 130.8, 129.9, 129.0, 125.8, 124.6, 50.9, 37.9, 33.5, 31.9, 30.8, 31.0, 27.9, 24.4, 16.2 ppm.

HRMS: calcd for [C₁₂H₂₃N₂]⁺: 195.1856; found: 195.1843; calcd for [C₁₀H₉O₃]⁻: 147.0441; found: 147.0448.

1-hexyl-3-methylimidazolium cinnate ([C₆mim][CA]):

¹H NMR ((DMSO-d₆): δ = 9.81 (1H, s), 7.85 (1H, s), 7.77 (1H, s), 7.44 (2H, d), 7.31 (2H, t), 7.23 (1H, t), 7.04 (1H, d), 6.37 (1H, d), 4.17 (2H, t), 3.88 (3H, s), 1.75 (2H, m), 1.22 (2H, m), 0.81 (3H, t) ppm.

¹³C NMR: δ = 170.0, 137.9, 137.5, 134.9, 131.9, 129.0, 128.1, 127.2, 124.0, 122.7, 49.1, 36.1, 31.0, 29.9, 25.7, 22.4, 14.3 ppm.

HRMS (*m/z*): calcd for [C₁₀H₁₉N₂]⁺: 167.1543; found: 167.1553; calcd for [C₁₀H₉O₃]⁻: 147.0441; found: 147.0454.

1-butyl-3-methylimidazolium cinnate ([C₄mim][CA]):

¹H NMR ((DMSO-d₆): δ = 9.84 (1H, s), 7.85 (1H, s), 7.78 (1H, s), 7.44 (2H, d), 7.31 (2H, t), 7.23 (1H, t), 7.04 (1H, d), 6.37 (1H, d), 4.18 (2H, t), 3.88 (3H, s), 1.74 (2H, m), 1.23 (2H, m), 0.86 (3H, t) ppm.

¹³C NMR: δ = 172.0, 140.2, 139.7, 136.9, 134.3, 131.2, 130.3, 129.4, 126.2, 124.9, 51.0, 38.3, 34.1, 21.5, 15.95 ppm.

HRMS (*m/z*): calcd for [C₈H₁₅N₂]⁺: 139.1230; found: 139.1239; calcd for [C₁₀H₉O₃]⁻: 147.0441; found: 147.0449.

Table S1. Bromide content in [C_nmim][CA] ionic liquids

IL	[Br ⁻]/mol.kg ⁻¹
[C ₄ mim][CA]	0.0010
[C ₆ mim][CA]	0.0079
[C ₈ mim][CA]	0.0073
[C ₁₀ mim][CA]	0.0070
[C ₁₂ mim][CA]	<0.00002

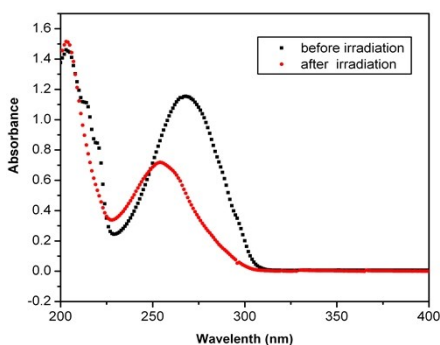
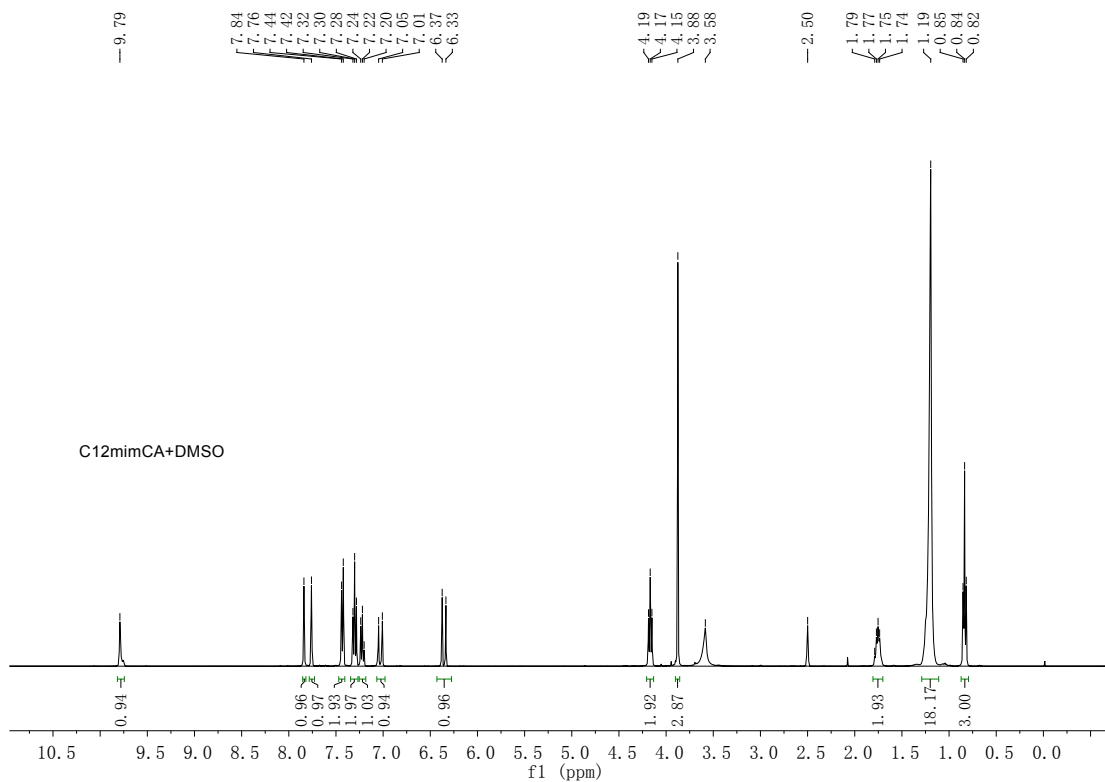
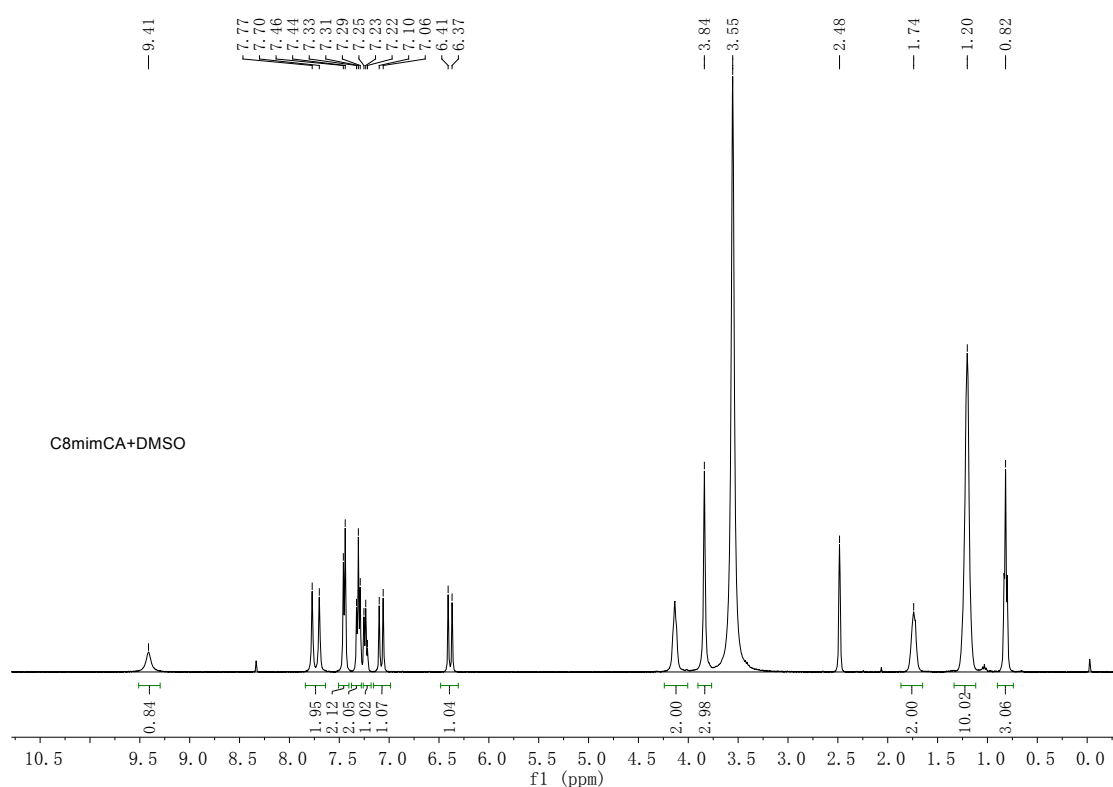
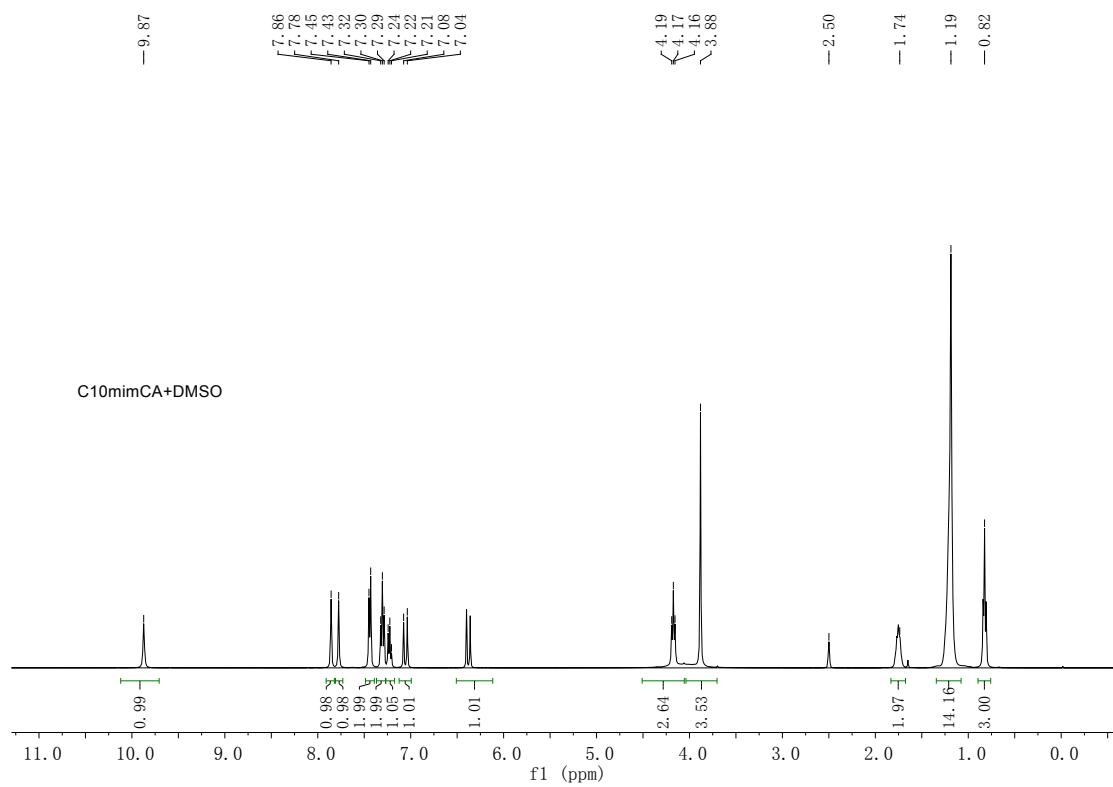
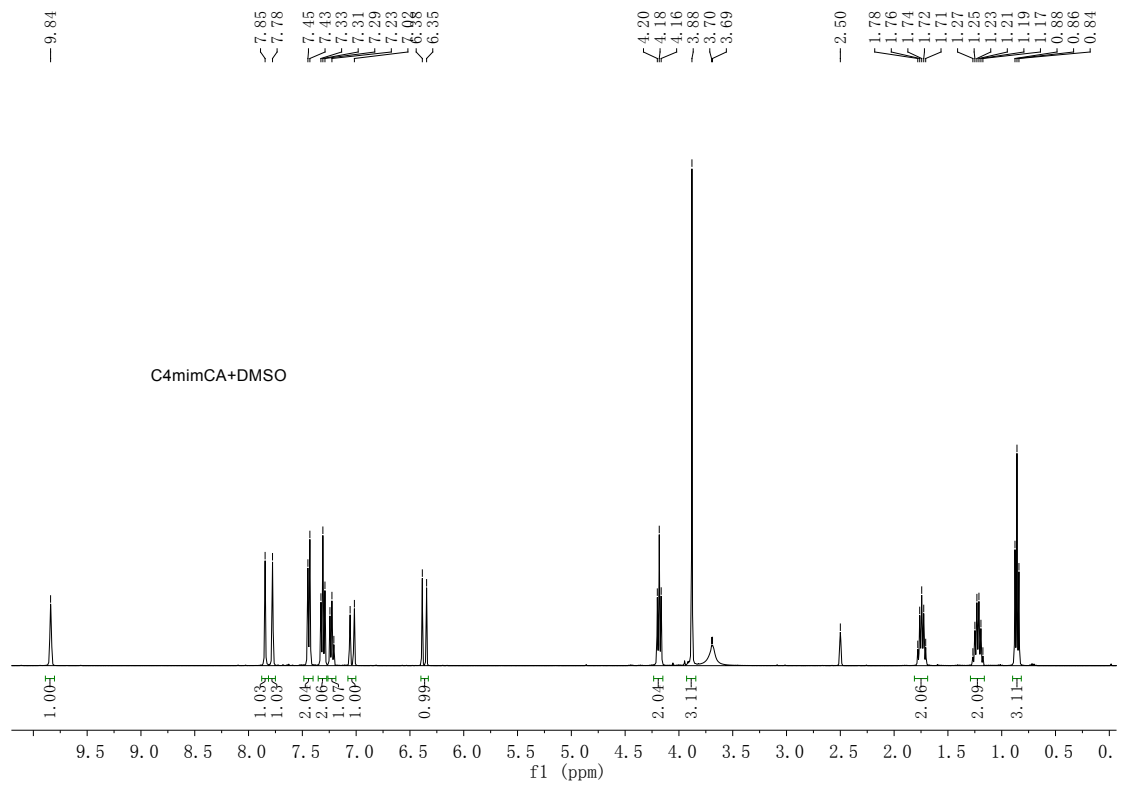
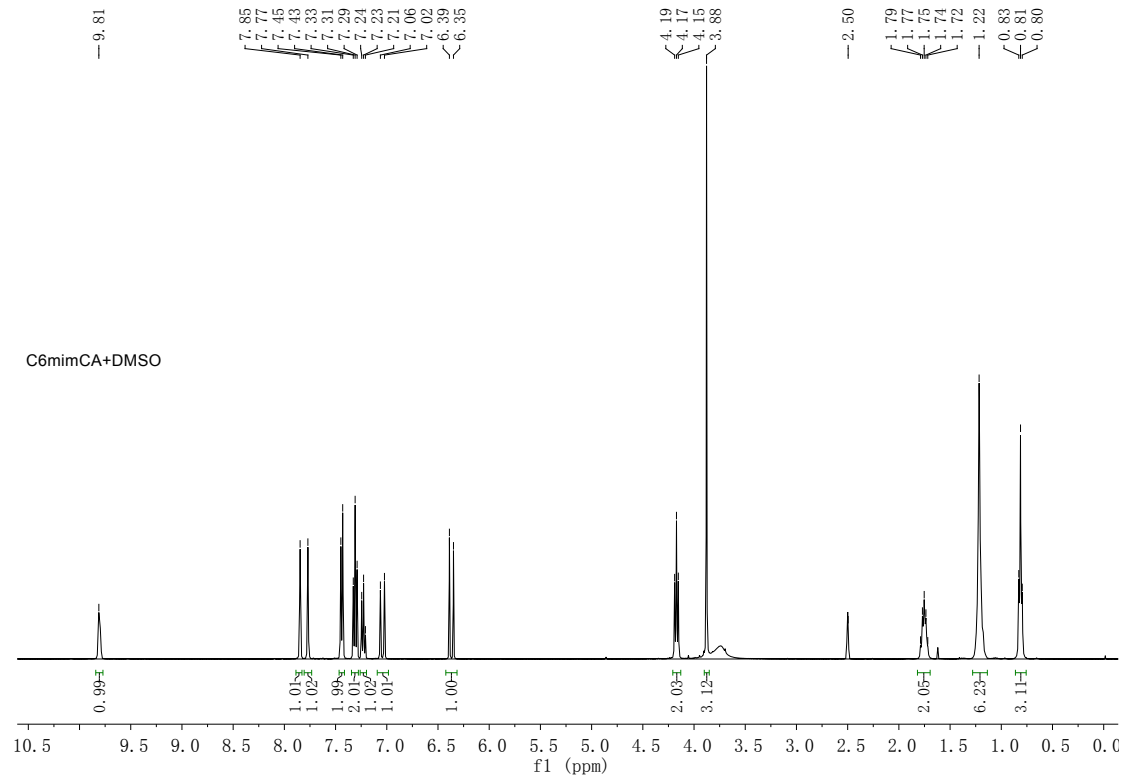


Fig. S1 UV-vis spectra of aqueous trans- cinnamic acid (H[CA])
at the concentration of 1 mM before and after irradiation

¹H -NMR spectra for [C_nmim][CA] ionic liquids:







^{13}C -NMR spectra for $[\text{C}_n\text{mim}][\text{CA}]$ ionic liquids:

