[Electronic Supplementary Information]

Electronic absorption spectroscopy of imidazolium-based ionic liquids studied by far-ultraviolet spectroscopy and quantum chemical calculation

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Table S1 Calculated oscillator strength (*f*), wavelength (λ), main initial state, and main final state in the 150-300 nm wavelength region for (a) $[C_2mim]^+$, (b) $[C_4mim]^+$, and (c) $[C_8mim]^+$ based on TD–CAM–B3LYP.

(a) $[C_2mim]^+$

Transition number	Oscillator strength (*f*)	Wavelength (λ)	Initial state	Final state
1	0.1115	194.05 nm	HOMO	LUMO
2	0.0004	175.11 nm	HOMO–1	LUMO
3	0.0139	161.51 nm	HOMO	LUMO+1
4	0.6783	155.34 nm	HOMO–1	LUMO
5	0.1043	150.28 nm	HOMO–1	LUMO+1

(b) $[C_4mim]^+$

Transition number	Oscillator strength (*f*)	Wavelength (λ)	Initial state	Final state
1	0.1038	193.80 nm	HOMO	LUMO
2	0.0023	176.30 nm	HOMO	LUMO+1
3	0.0243	161.79 nm	HOMO	LUMO+1
4	0.4244	159.37 nm	HOMO–1	LUMO
5	0.0276	156.13 nm	HOMO–2	LUMO
6	0.1452	153.30 nm	HOMO–3	LUMO
7	0.0975	152.16 nm	HOMO–1	LUMO+1

(c) $[C_8mim]^+$

Transition number	Oscillator strength (*f*)	Wavelength (λ)	Initial state	Final state
1	0.1015	193.75 nm	HOMO–3	LUMO+1
2	0.0200	179.20 nm	HOMO–6	LUMO+1
3	0.0339	171.85 nm	HOMO–3	LUMO+2
4	0.0001	166.01 nm	HOMO	LUMO+1
5	0.0100	162.77 nm	HOMO–1	LUMO+1
6	0.0060	162.07 nm	HOMO–2	LUMO+1
7	0.0131	161.88 nm	HOMO–3	LUMO+2
8	0.1109	157.39 nm	HOMO–6	LUMO+2
9	0.0300	156.52 nm	HOMO–6	LUMO+3
10	0.0308	155.63 nm	HOMO–4	LUMO+1
11	0.4254	155.32 nm	HOMO–3	LUMO+1
12	0.0172	152.94 nm	HOMO–5	LUMO+2
13	0.0106	152.11 nm	HOMO	LUMO+2

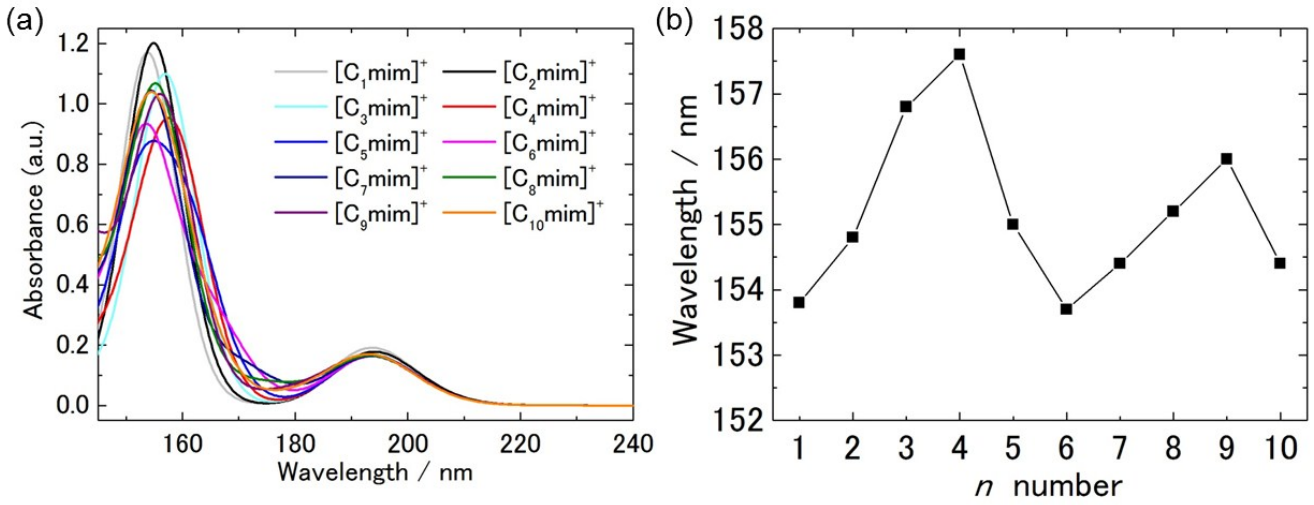

Fig. S1 (a) Calculated spectra of $[C_n\text{mim}]^+$ (n = 1–10) and (b) their peak wavelengths in the 150-160 nm region against the number of n.

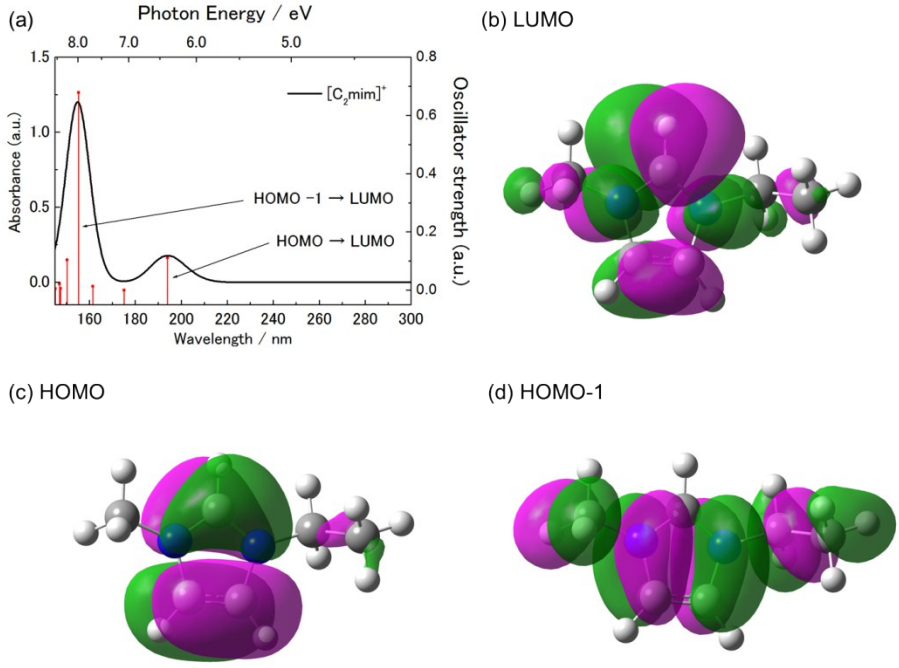

Fig. S2 (a) A calculated spectrum of [C_2mim] and (b–d) molecular orbitals of (b) LUMO, (c) HOMO, and (d) HOMO–1.

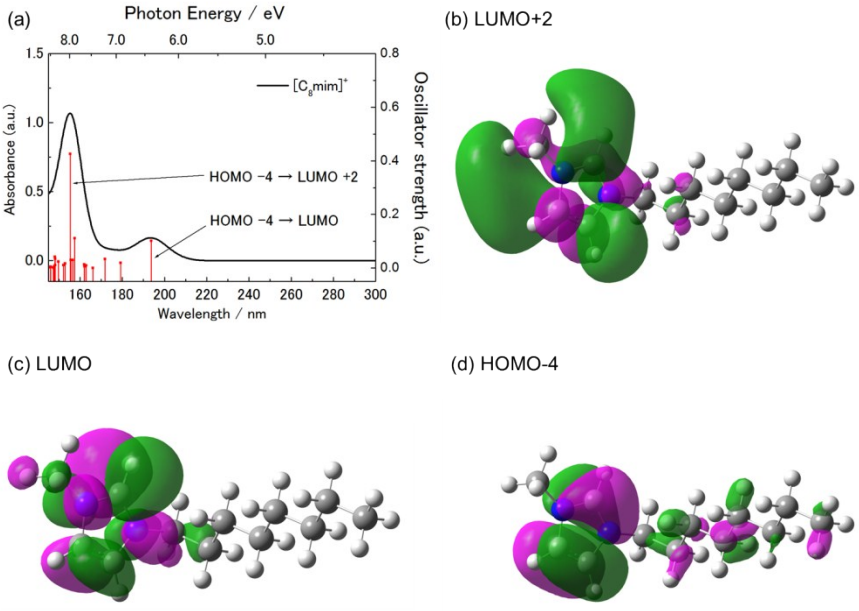

Fig. S3 (a) A calculated spectrum of [C_8mim] and (b–d) molecular orbitals of (b) LUMO+2, (c) LUMO, and (d) LUMO–4.

Table S2 Calculated assignments and wavelengths of the main transitions around (a) 190 and (b) 160 nm for $[C_n\text{mim}]^+$ (n = 1–10)

(a)

n number	Initial state	Final state	Wavelength
1	HOMO	LUMO	192.65
2	HOMO	LUMO	193.61
3	HOMO	LUMO	194.05
4	HOMO	LUMO	193.68
5	HOMO–3	LUMO	193.80
6	HOMO–2	LUMO	193.70
7	HOMO–3	LUMO	193.80
8	HOMO–3	LUMO	193.71
9	HOMO–5	LUMO	193.80
10	HOMO–6	LUMO	193.67

(b)

n number	Initial state	Final state	Wavelength
1	HOMO–1	LUMO	154.32
2	HOMO–1	LUMO	155.34
3	HOMO–1	LUMO	157.33
4	HOMO–1	LUMO	159.37
5	HOMO–4	LUMO	151.37
6	HOMO–6	LUMO	153.01
7	HOMO	LUMO+1	155.70
8	HOMO–3	LUMO+1	155.32
9	HOMO–7	LUMO	155.90
10	HOMO–12	LUMO	154.42

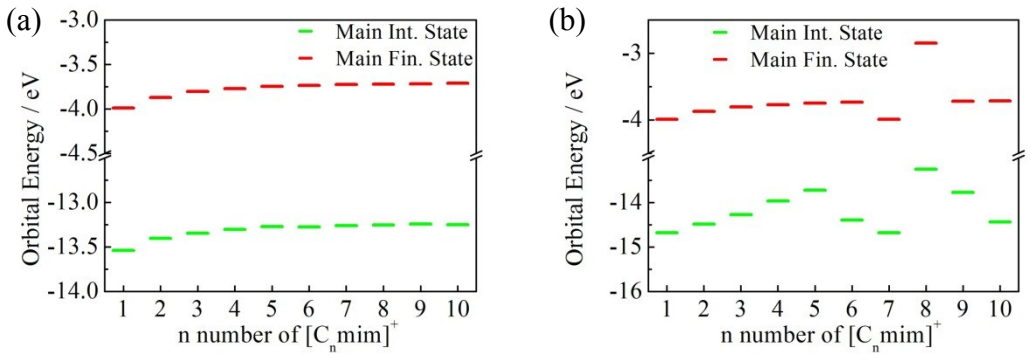

Fig. S4 Calculated orbital energies of main initial states (green) and final states (red) of the peak around (a) 190 and (b) 160 nm for $[C_n\text{mim}]^+$ (n = 1–10).