Impacts of Extending the π-Conjugation of the 2,2′-Biquinoline Ligand on the Photophysics and Reverse Saturable Absorption of Heteroleptic Cationic Iridium(III) Complexes

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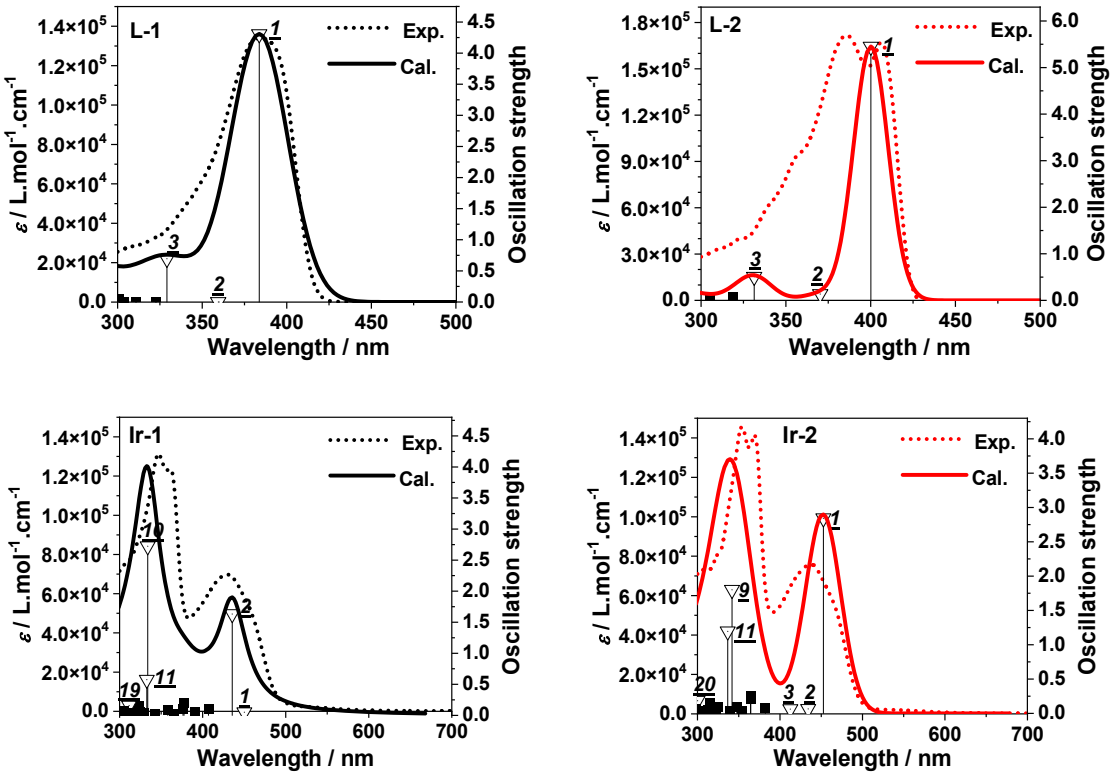


Fig. S1. Comparison of the experimental and calculated absorption spectra for **L-1**, **L-2**, **Ir-1** and **Ir-2** in toluene. Calculations were performed with linear response TDDFT with PBE1 functional and LANL2DZ/6-31G* basis sets. Vertical lines indicate the oscillation strength of the optical transitions.

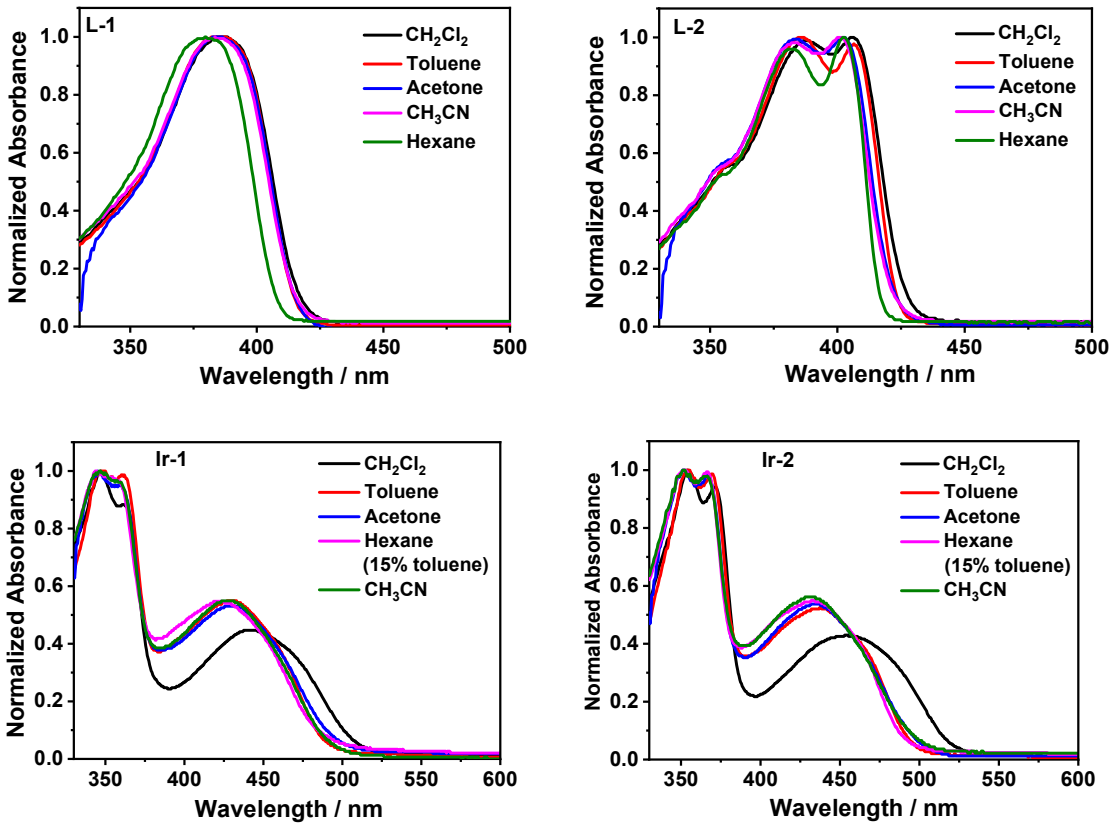
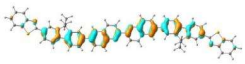
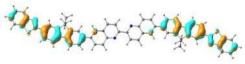
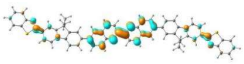
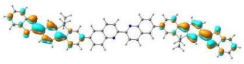
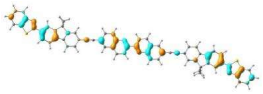
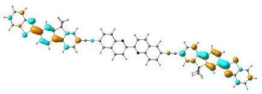
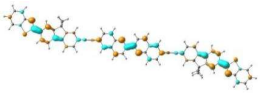
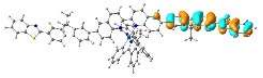
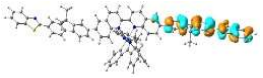
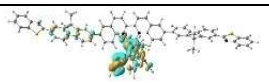


Figure S2. Normalized UV-vis absorption spectra of **L-1**, **L-2**, **Ir-1**, and **Ir-2** in different solvents.

Table S1. Natural transition orbitals (NTOs) representing the main transitions contributing to the high-energy absorption bands of **L-1**, **L-2**, **Ir-1**, and **Ir-2** in toluene.

	States	Hole	Electron
L-1	S_3 329 nm $f = 0.69$	 49%  38%	 49%  38%
L-2	S_3 332 nm $f = 0.51$	 43%  36%  18%	 43%  36%  18%
Ir-1	S_{10} 343 nm $f = 0.95$	 70%  23%	 70%  23%
	S_{11} 336 nm $f = 0.69$	 68%  24%	 68%  24%
	S_{19} 311 nm $f = 0.16$	 74%  14%	 74%  14%
Ir-2	S_9 342 nm $f = 1.80$	 37%	 37%

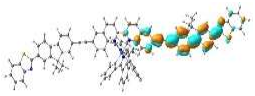
		
	30%	30%
S_{11} 337 nm $f = 1.19$		
	74%	74%
		
	16%	16%
S_{20} 301 nm $f = 0.18$		
	64%	64%
		
	15%	15%

Table S2. NTOs representing the fluorescence emitting states for **L-1** and **L-2** in toluene.

	Emission energy	Electron	Hole
L-1	414 nm	 87%  12%	 87%  12%
L-2	440 nm	 61%  10%	 61%  10%

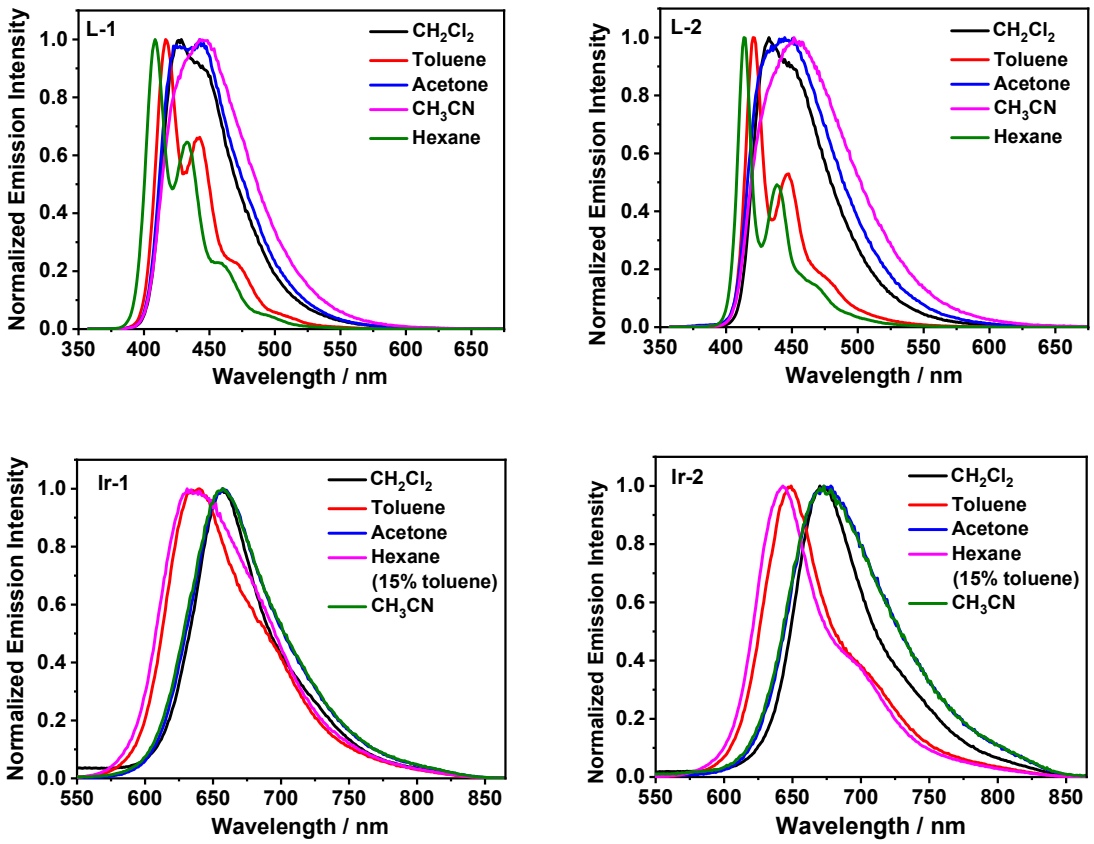


Figure S3. Normalized emission spectra of **L-1**, **L-2**, **Ir-1**, and **Ir-2** in different solvents at room temperature.

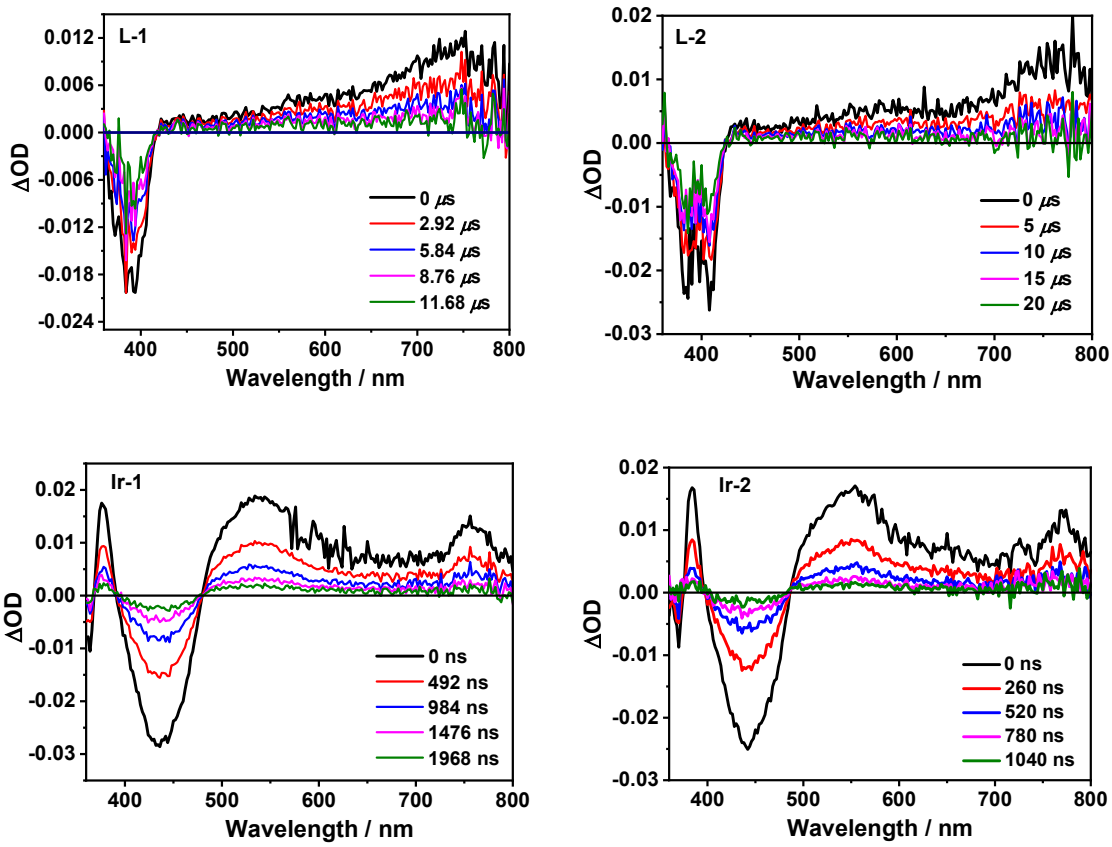


Figure S4. Nanosecond time-resolved TA spectra of **L-1**, **L-2**, **Ir-1**, and **Ir-2** in toluene. λ_{ex} = 355 nm, A_{355} = 0.4 in a 1-cm cuvette.