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.

	States	Hole	Electron
L-1	S_3 329 nm f = 0.69	- A A A A A A A A A A A A A A A A A A A	·Xanita and a state of the stat
		49%	49%
		AND THE PARTY AN	
		38%	38%
L-2	S_3 332 nm f = 0.51	-toppediate of the other	A Contraction of the second
		43%	43%
		AND ALL ALL ALL ALL ALL ALL ALL ALL ALL AL	A Contraction of the second se
		36%	36%
		AND STORES	A Contraction of the second se
		18%	18%
Ir-1	S_{10} 343 nm f = 0.95	4.99 0 J 50 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	
		70%	70%
		JOB COLORA TARA	JOB BACK
		23%	23%
	S_{11} 336 nm f = 0.69	225 C C C C C C C C C C C C C C C C C C	Same and the second
		68%	68%
		339 SUSSER	and the second s
		24%	24%
	S_{19} 311 nm f = 0.16	An advertising the second	- Andrew Contraction
		74%	74%
		and the state of t	and the second
		14%	14%
Ir-2	S_9 342 nm f = 1.80	the state of the s	AND - AND
		37%	37%

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.

	South - And - And -	and the second second
	30%	30%
	and the same	the state of the s
S ₁₁ 337 nm	74%	74%
f = 1.19	A and the second second	ALTER AND A
	16%	16%
	ALAR - AMAL	A HAR - A BANK
S ₂₀ 301 nm	64%	64%
f = 0.18	the state of the s	A A A A A A A A A A A A A A A A A A A
	15%	15%

	Emission energy	Electron	Hole
L-1	414 nm	-the design of the second seco	A CARLES CONTRACTOR
		87%	87%
		Statuto-Statuto	Are the to the state of
		12%	12%
L-2	440 nm	togate and the state	404
		61%	61%
		-the war war and the state of t	
		10%	10%

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



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. $\lambda_{ex} = 355 \text{ nm}, A_{355} = 0.4$ in a 1-cm cuvette.