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Supplementary Materials

Deep NIR-I Emissive Iridium(III) Complex Bearing D-A Ligand: Synthesis, Photophysical Properties and DFT/TDDFT Computation

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Table S1. The frontier orbital energy for complex **4**.

Spin State	Orbital	Energy (eV) (Calculated)
Singlet state	LUMO+5	−0.8547
	LUMO+4	−1.3739
	LUMO+3	−1.3872
	LUMO+2	−2.1481
	LUMO+1	−2.5426
	LUMO	−2.5845
	HOMO	−5.3057
	HOMO-1	−5.8311
	HOMO-2	−6.0224
	HOMO-3	−6.3375
	HOMO-4	−6.3400
	HOMO-5	−6.6431
Triple state	LUMO+1	−2.5655
	LUMO	−2.6545
	HOMO	−5.1713
	HOMO-1	−5.7337

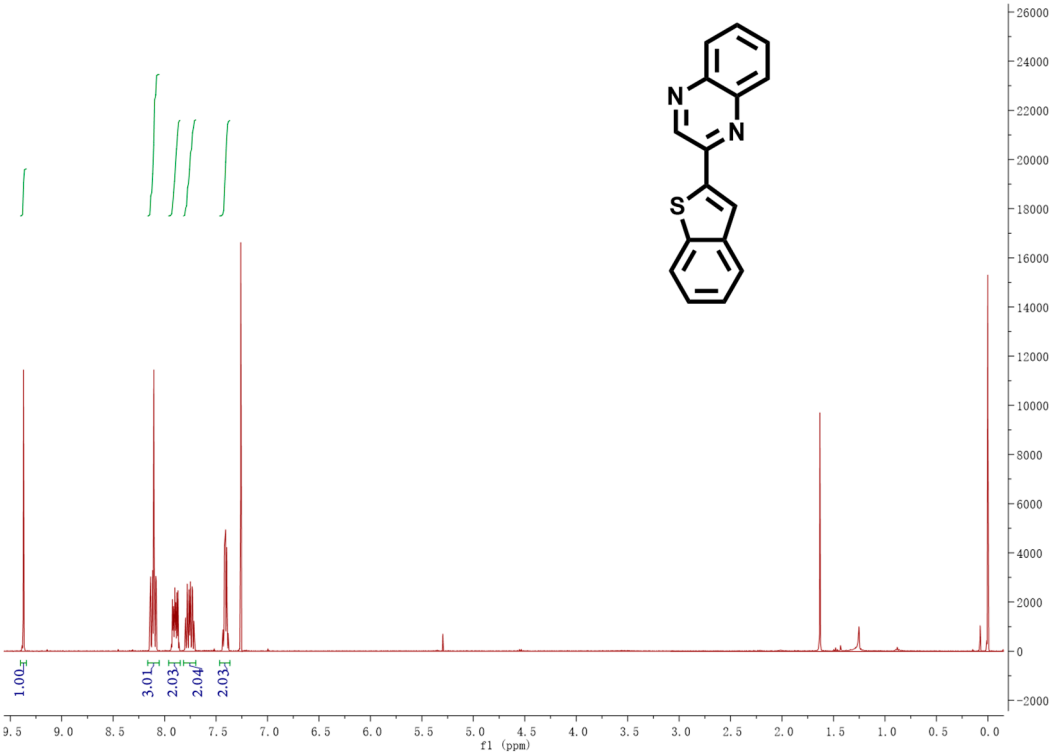

Figure S1. ^{1}H NMR spectrum of ligand **1**.

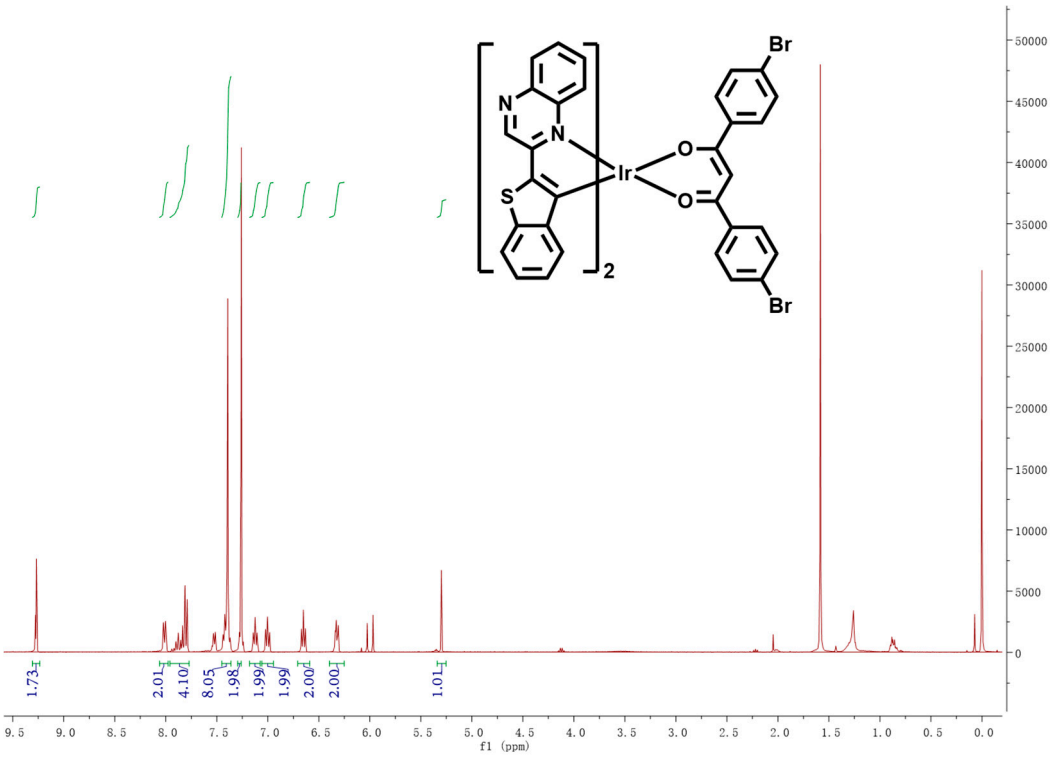

Figure S2. ^{1}H NMR spectrum of complex **4.**

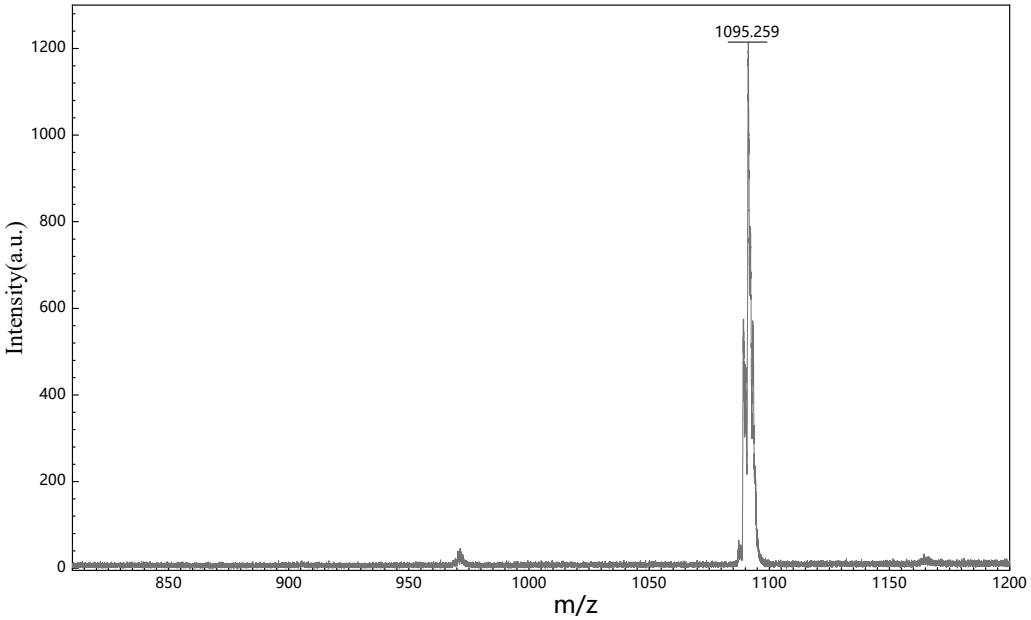

Figure S3. MALDI-TOF spectrum of complex **4**.

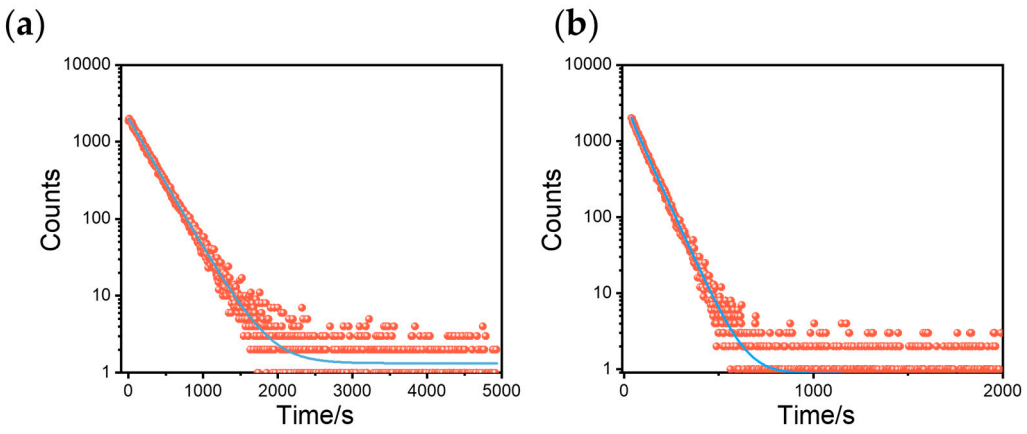

Figure S4. Transient photoluminescence decay spectra of complex **4** in (**a**) CH_2Cl_2 and (**b**) CH_3OH/H_2O.

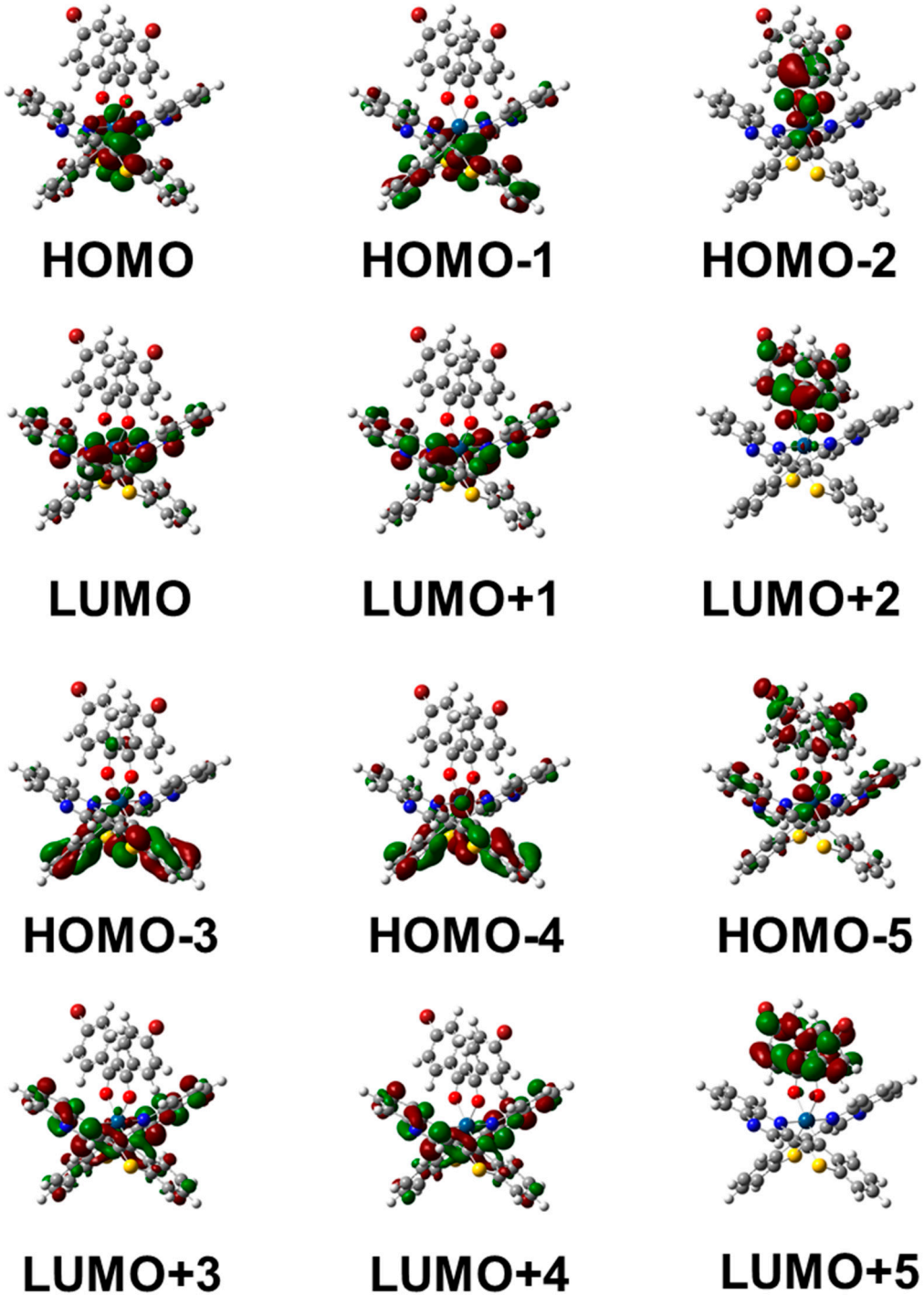

Figure S5. Isodensity plots of ground state frontier orbitals of complex **4.**

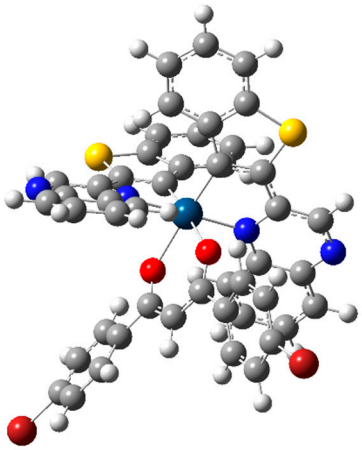

Figure S6. The excited state geometry structure of complex **4**.

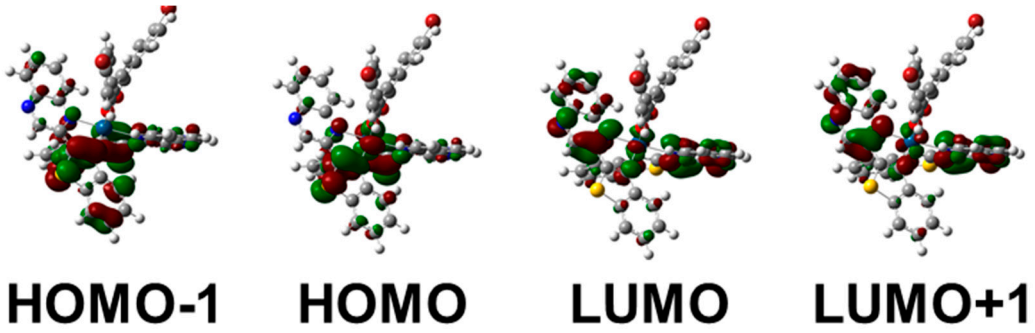

Figure S7. Isodensity plots of excited state frontier orbitals of complex **4.**