

Supporting Information

Heteroleptic tris-cyclometalated iridium(III) complexes supported by *o*-carboranyl-pyridine ligand

Hye Jin Bae,^a Hyungjun Kim,^a Kang Mun Lee,^a Taewon Kim,^b Maengsun Eo,^a Yoon Sup Lee,^a
Youngkyu Do*^a and Min Hyung Lee*^b

^a *Department of Chemistry, KAIST, Daejeon 305–701 and* ^b *Department of Chemistry and EHSRC, University of Ulsan, Ulsan 680–749, Republic of Korea*

Contents

1. Experimental	S2
2. Photophysical Measurements	S7
3. Cyclic Voltammetry	S9
4. Computational Details	S10

1. Experimental

General Considerations. All operations were performed under an inert nitrogen atmosphere using standard Schlenk and glove box techniques. Anhydrous grade solvents (Aldrich) were dried by passing through an activated alumina column and stored over activated molecular sieves (5Å). Spectrophotometric-grade tetrahydrofuran was used as received from Aldrich. Commercial reagents were used without any further purification after purchasing from Aldrich (2-phenylpyridine (*ppy*), 2,4-difluorophenylboronic acid, 2-bromopyridine, Na₂CO₃, 2-ethoxyethanol, tetrakis(triphenylphosphine)palladium(0), ethynyl(trimethyl)silane, copper(I) iodide, diethyl sulfide, triethylamine, K₂CO₃, bis(triphenylphosphine)palladium(II) dichloride, *n*-BuLi (1.6 M in hexane)), Strem (iridium(III) chloride hydrate), and KatChem (B₁₀H₁₄, decaborane). 1-(2'-Pyridyl)-*ortho*-carborane (*CBpyH*),¹ [(*ppy*)₂Ir(μ-Cl)₂Ir(*ppy*)₂] and [(*dfppy*)₂Ir(μ-Cl)₂Ir(*dfppy*)₂] (*ppy* = 2-phenylpyridinato-C²,N, *dfppy* = 2-(4,6-difluorophenyl)pyridinato-C²,N)² were analogously synthesized according to the reported procedures. Deuterated solvents from Cambridge Isotope Laboratories were used. NMR spectra of compounds were recorded on a Bruker Avance 400 spectrometer (400.13 MHz for ¹H, 100.62 MHz for ¹³C, 128.38 MHz for ¹¹B) at ambient temperature. Chemical shifts are given in ppm, and are referenced against external Me₄Si (¹H, ¹³C) and BF₃·Et₂O (¹¹B). Elemental analyses were performed on an EA1110 (Fisons Instruments) by the Environmental Analysis Laboratory at KAIST.

Synthesis of (*ppy*)₂Ir(*CBpy*) (1). *n*-BuLi (1.6 M in *n*-hexane, 0.34 mL, 0.55 mmol) was added to a solution of *CBpyH* (110 mg, 0.5 mmol) in THF (10 mL) at -78 °C. The mixture was stirred at -78 °C for 1 h and then allowed to warm to room temperature. After stirring for 2 h, the resulting solution was added slowly to the slurry of [(*ppy*)₂Ir(μ-Cl)₂Ir(*ppy*)₂] (268 mg, 0.25 mmol) in THF (15 mL) at 0 °C. The reaction mixture was stirred for 8 h at room temperature. After removal of the solvent under vacuum, the residue was purified by column chromatography on silica (eluent: *n*-hexane/CH₂Cl₂ = 1:1), which gave **1** (150 mg, 42%) as yellow powder. Single crystals of **1** suitable for X-ray diffraction study were obtained by slow diffusion of *n*-hexane into a THF solution of **1**. ¹H NMR (DMSO-*d*₆): δ 9.34 (d, *J* = 5.7 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 1H), 8.11 (d, *J* = 8.1 Hz, 1H), 7.93-7.86 (m, 4H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 6.3 Hz, 1H), 7.36 (t, *J* = 6.6 Hz, 1H), 7.30 (d, *J* = 4.6 Hz, 1H), 7.16 (t, *J* = 6.6 Hz, 1H), 6.96 (t, *J* = 7.6 Hz, 2H), 6.82-6.75 (m, 2H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.38 (d, *J* = 7.7 Hz, 1H), 5.90 (d, *J* = 7.7 Hz, 1H), 2.80-0.50 (br, 10H, CB-BH). ¹³C NMR (DMSO-*d*₆): δ 170.74, 168.69, 164.02, 161.14, 153.08, 151.93, 150.73, 149.18, 146.16, 144.64, 140.54, 139.83, 139.04, 133.05, 131.04, 130.26, 130.10, 128.05, 126.35, 125.62, 125.58, 124.15, 123.77, 123.22, 121.95, 120.92, 120.59, 85.78 (CB-C), 79.18 (CB-C). ¹¹B NMR (DMSO-*d*₆): δ 1.6 (br s, 3B), -2.7 (br s, 7B). Anal. Calcd for C₂₉H₃₀IrB₁₀N₃: C, 48.32; H, 4.19; N, 5.83. Found: C, 47.97; H, 4.49; N, 5.43.

Synthesis of (*dfppy*)₂Ir(*CBpy*) (2). A procedure analogous to that for **1** was employed with *n*-BuLi (1.6 M in *n*-hexane, 0.34 mL, 0.55 mmol), *CBpyH* (110 mg, 0.5 mmol), and [(*dfppy*)₂Ir(μ-Cl)₂Ir(*dfppy*)₂] (304 mg, 0.25 mmol) to afford **2** as a pale yellow solid (160 mg, 40%). Single crystals of **2** suitable for X-ray diffraction study were obtained by slow diffusion of *n*-hexane into a THF solution of **2**. ¹H NMR (THF-*d*₈): δ 9.59 (d, *J* = 6.3 Hz, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 7.98-7.89 (m, 3H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.55-7.52 (m, 2H), 7.36-7.32 (m, 1H), 7.12-7.01 (m, 2H),

6.65–6.59 (m, 1H), 6.53–6.47 (m, 1H), 5.97(dd, $J = 9.7, 2.3$ Hz, 1H), 5.51 (dd, $J = 8.8, 2.3$ Hz, 1H), 3.00–1.00 (br, 10H, CB-BH). ^{13}C NMR (THF- d_8): δ 169.34, 167.38, 165.78, 165.06, 164.06, 163.26, 162.53, 162.26, 161.47, 160.80, 153.83, 153.09, 151.83, 150.52, 139.83, 139.13, 129.59, 128.36, 127.25, 125.49, 124.00, 123.14, 123.13, 115.00, 112.24, 99.20, 97.67, 84.75 (CB-C), 75.43 (CB-C). ^{11}B NMR (THF- d_8): δ 2.8, 1.5 (br s, 3B), $-1.7, -4.5$ (br s, 7B). Anal. Calcd for $\text{C}_{29}\text{H}_{26}\text{F}_4\text{IrB}_{10}\text{N}_3$: C, 43.93; H, 3.31; N, 5.30. Found: C, 43.41; H, 3.40; N, 4.77.

X-ray Crystallography. A specimen of suitable size and quality was coated with Paratone oil and mounted onto a glass capillary. The crystallographic measurement was performed using a Bruker Apex II-CCD area detector diffractometer, with graphite-monochromated MoK α radiation ($\lambda = 0.71073$ Å). The hemisphere of reflection data were collected as ω scan frames with $0.3^\circ/\text{frame}$ and an exposure time of 10 s/frame. Cell parameters were determined and refined by SMART program.³ Data reduction was performed using SAINT software.⁴ The data were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using the SADABS program.⁵ The structure was solved by direct methods and all nonhydrogen atoms were subjected to anisotropic refinement by full-matrix least-squares on F^2 by using the SHELXTL/PC package.⁶ Hydrogen atoms were placed at their geometrically calculated positions and refined riding on the corresponding carbon atoms with isotropic thermal parameters. The detailed crystallographic data and selected bond lengths and angles are given in Table S1 and S2, respectively.

-
1. Coult, R.; Fox, M. A.; Gill, W. R.; Herbertson, P. L.; MacBride, J. A. H.; Wade, K. *J. Organomet. Chem.* **1993**, *462*, 19-29.
 2. Sprouse, S.; King, K. A.; Spellane, P. J.; Watts, R. J. *J. Am. Chem. Soc.* **1984**, *106*, 6647-6653.
 3. SMART, version 5.0, Data collection software, Bruker AXS, Inc., Madison, WI, **1998**.
 4. SAINT, version 5.0, Data integration software, Bruker AXS Inc., Madison, WI, **1998**.
 5. Sheldrick, G. M. SADABS, Program for absorption correction with the Bruker SMART system, Universitat Göttingen, Germany, **1996**.
 6. Sheldrick, G. M. SHELXL-93: Program for the refinement of crystal structures; Universitat Göttingen: Germany, **1993**.

Table S1. Crystallographic data and parameters for **1** and **2**

	1	2
formula	C ₂₉ H ₃₀ B ₁₀ IrN ₃	C ₂₉ H ₂₆ B ₁₀ F ₄ IrN ₃
formula weight	720.86	792.83
crystal system	Orthorhombic	Monoclinic
space group	<i>Pna</i> 2 ₁	<i>C</i> 2/ <i>c</i>
<i>a</i> (Å)	31.951(3)	36.952(3)
<i>b</i> (Å)	10.1535(8)	10.8814(8)
<i>c</i> (Å)	10.6068(8)	15.9920(12)
α (°)	90	90
β (°)	90	108.927(3)
γ (°)	90	90
<i>V</i> (Å ³)	3441.0(5)	6082.6(8)
<i>Z</i>	4	8
ρ_{calc} (g cm ⁻³)	1.391	1.732
μ (mm ⁻¹)	3.903	4.443
<i>F</i> (000)	1408	3072
<i>T</i> (K)	296	296
scan mode	<i>multi</i>	<i>multi</i>
<i>hkl</i> range	-38 → +38, -12 → +11, -12 → +12	-46 → +38, -13 → +13, -19 → +20
Flack parameter	0.053(17)	-
measd reflns	39805	42593
unique reflns [<i>R</i> _{int}]	6438 [0.0810]	6325 [0.0689]
reflns used for refinement	6438	6325
refined parameters	388	424
R1 ^a (<i>I</i> > 2σ(<i>I</i>))	0.0521	0.0589
wR2 ^b all data	0.1357	0.2022
GOF on <i>F</i> ²	1.028	1.033
ρ_{fin} (max/min) (e Å ⁻³)	2.242, -1.007	3.265, -2.081

^a R1 = $\sum ||F_o| - |F_c|| / \sum |F_o|$. ^b wR2 = $\{[\sum w(F_o^2 - F_c^2)^2] / [\sum w(F_o^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (deg) for **1** and **2**

	1	2
Lengths		
Ir–C(1)	2.175(11)	2.178(10)
Ir–C(8)	2.055(13)	2.036(11)
Ir–C(19)	2.030(8)	2.000(11)
Ir–N(1)	2.227(8)	2.191(9)
Ir–N(2)	2.098(10)	2.070(9)
Ir–N(3)	2.039(10)	2.035(9)
C(1)–C(2)	1.703(15)	1.667(14)
C(2)–C(3)	1.512(15)	1.492(15)
Angles		
C(1)–Ir–N(1)	78.6(3)	78.5(3)
C(1)–Ir–C(19)	95.7(4)	95.0(4)
C(8)–Ir–N(1)	92.3(4)	94.8(3)
C(8)–Ir–C(19)	93.5(4)	91.7(4)
C(1)–Ir–N(2)	99.0(4)	101.7(4)
C(8)–Ir–N(2)	80.4(5)	79.1(4)
C(19)–Ir–N(2)	92.1(3)	92.7(4)
N(1)–Ir–N(2)	93.6(4)	91.4(4)
C(1)–Ir–N(3)	93.2(4)	89.8(4)
C(8)–Ir–N(3)	88.6(5)	90.1(4)
C(19)–Ir–N(3)	80.2(3)	80.9(4)
N(1)–Ir–N(3)	95.1(4)	96.0(4)
N(2)–Ir–N(3)	166.2(4)	167.4(4)

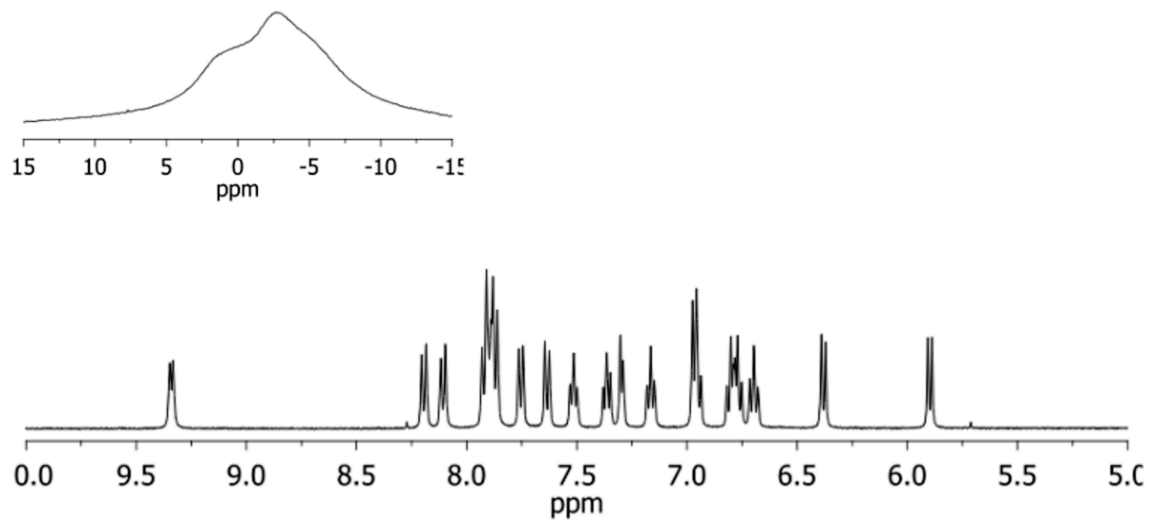


Figure S1. ¹¹B (top) and ¹H (bottom) NMR spectra of **1** in DMSO-*d*₆.

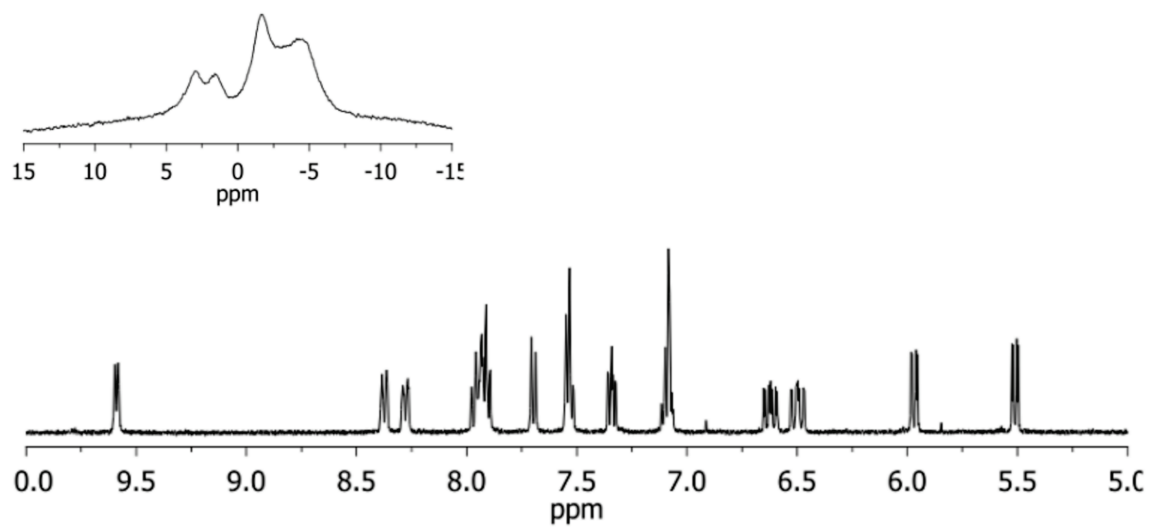


Figure S2. ¹¹B (top) and ¹H (bottom) NMR spectra of **2** in THF-*d*₈.

2. Photophysical Measurements

UV–vis absorption and PL spectra were recorded on a Jasco V-530 and a Spex Fluorog-3 Luminescence spectrophotometer, respectively. Solution PL experiments were performed in degassed THF solution with a 1-cm quartz cuvette (2.0×10^{-5} M for **1** and **2**). Low-temperature PL measurements were carried out with 5-mm diameter quartz tubes that were placed in a quartz walled Dewar flask filled with liquid nitrogen (77 K). Absolute PL quantum efficiency (PLQY, Φ_{em}) was measured by an integrating sphere method in film state with IESP-150B (Optel) quantum efficiency measurement equipment. The film was obtained from spin casting of a THF solution of PMMA containing **1** or **2** (5 wt%). Emission lifetimes were measured using a time-correlated single-photon counting (TCSPC) spectrometer (FLS920, EDINBURGH Instruments) equipped with a EPL-375 picosecond pulsed semiconductor diode laser as an excitation source and a microchannel plate photomultiplier tube (MCP-PMT, 200–850 nm) as a detector at 298 K.

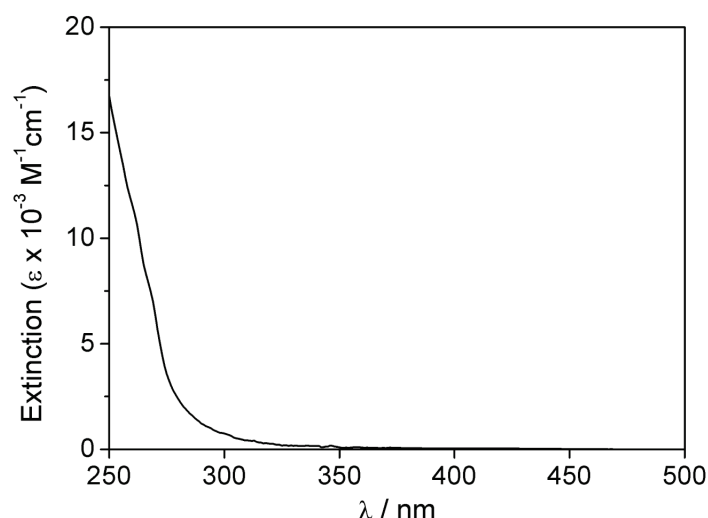


Figure S3. UV–vis absorption spectrum of *CBpyH* (2×10^{-5} M in THF).

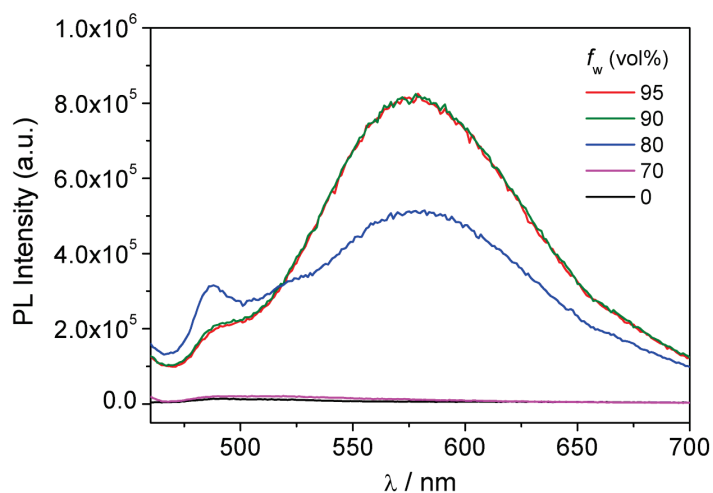


Figure S4. PL spectra of **1** ($\lambda_{\text{ex}} = 395$ nm) in water-THF mixtures with different water fractions.

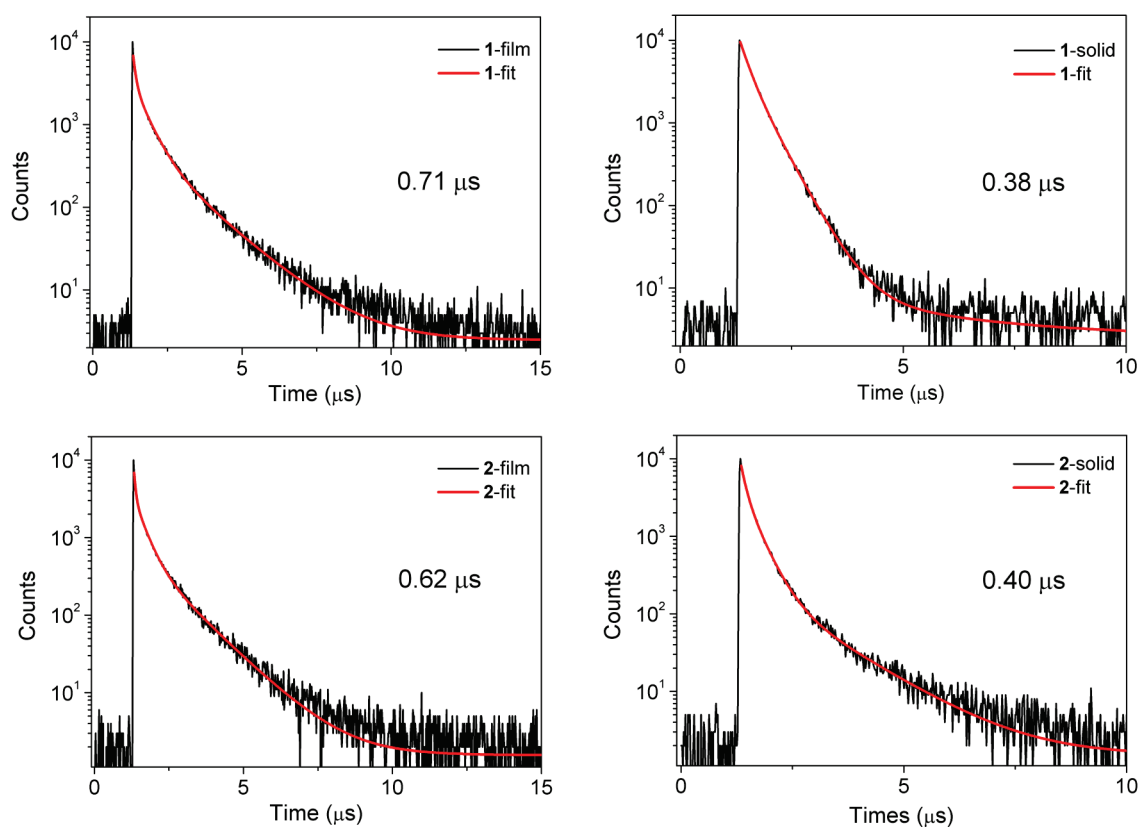


Figure S5. Emission decay curves of **1** and **2** in film (5 wt% in PMMA) and solid state at room temperature (black line). The red-line corresponds to the fitting curve for the experimental data.

3. Cyclic Voltammetry

Cyclic voltammetry measurements were carried out for **1** and **2** (5×10^{-4} M) with a three-electrode cell configuration consisting of platinum working and counter electrodes and a Ag/AgNO₃ (0.01 M in CH₃CN) reference electrode at room temperature. Tetra-*n*-butylammonium hexafluorophosphate (0.1 M) was used as the supporting electrolyte. The redox potentials were recorded at a scan rate of 100 mV/s and are reported with reference to the ferrocene/ferrocenium (Fc/Fc⁺) redox couple. The measurements were performed using an AUTOLAB/PGSTAT12 system.

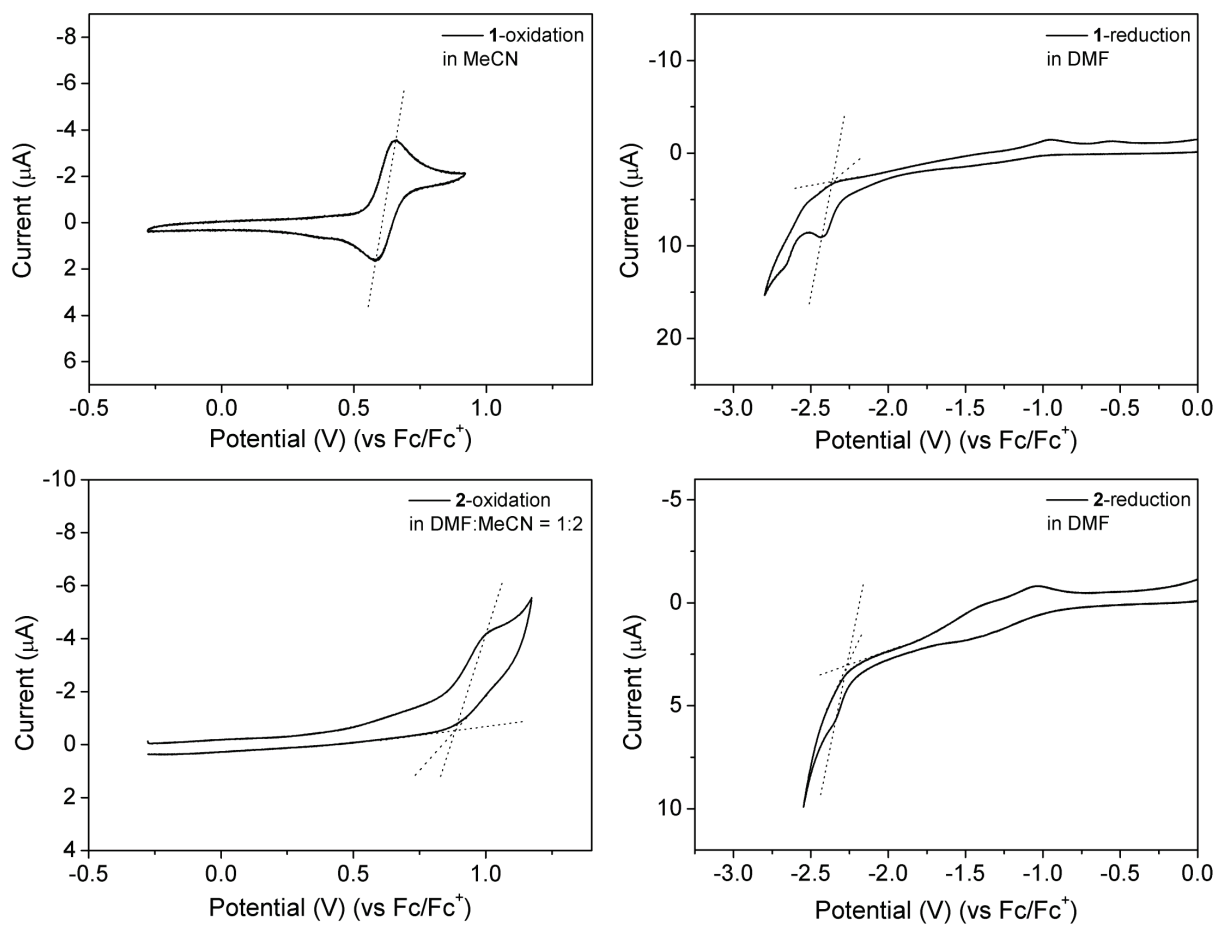


Figure S6. Cyclic voltammograms of **1** and **2** (5×10^{-4} M, scan rate = 100 mV/s).

4. Computational Details

The geometries of the ground (S_0) and lowest-lying triplet excited (T_1) states of **1** were optimized using the density functional theory (DFT) method. The electronic transition energies including electron correlation effects were computed by the time dependent density functional theory (TD-DFT)¹ method using the hybrid B3LYP functional (TD-B3LYP).² To include the solvation effect of THF, the polarizable continuum model (PCM) was used in the calculations. The 6-31G(d) basis set³ was used for all atoms except for the iridium atom which was treated with LANL2DZ effective core potentials (ECPs) and corresponding basis sets.⁴ All calculations described here were carried out using the GAUSSIAN 09 program.⁵

1. Runge, E.; Gross, E. K. U. *Phys. Rev. Lett.* **1984**, *52*, 997-1000.

2. Yanai, T.; Tew, D. P.; Handy, N. C. *Chem. Phys. Lett.* **2004**, *393*, 51-57.

3. Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654-3665; Hariharan, P. C.; Pople, J. A. *Theoret. Chim. Acta.* **1973**, *28*, 213-222; Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257-2261.

4. Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270-283.

5. Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., *Gaussian 09, Revision A.02*. Gaussian, Inc.: Wallingford CT, 2009.

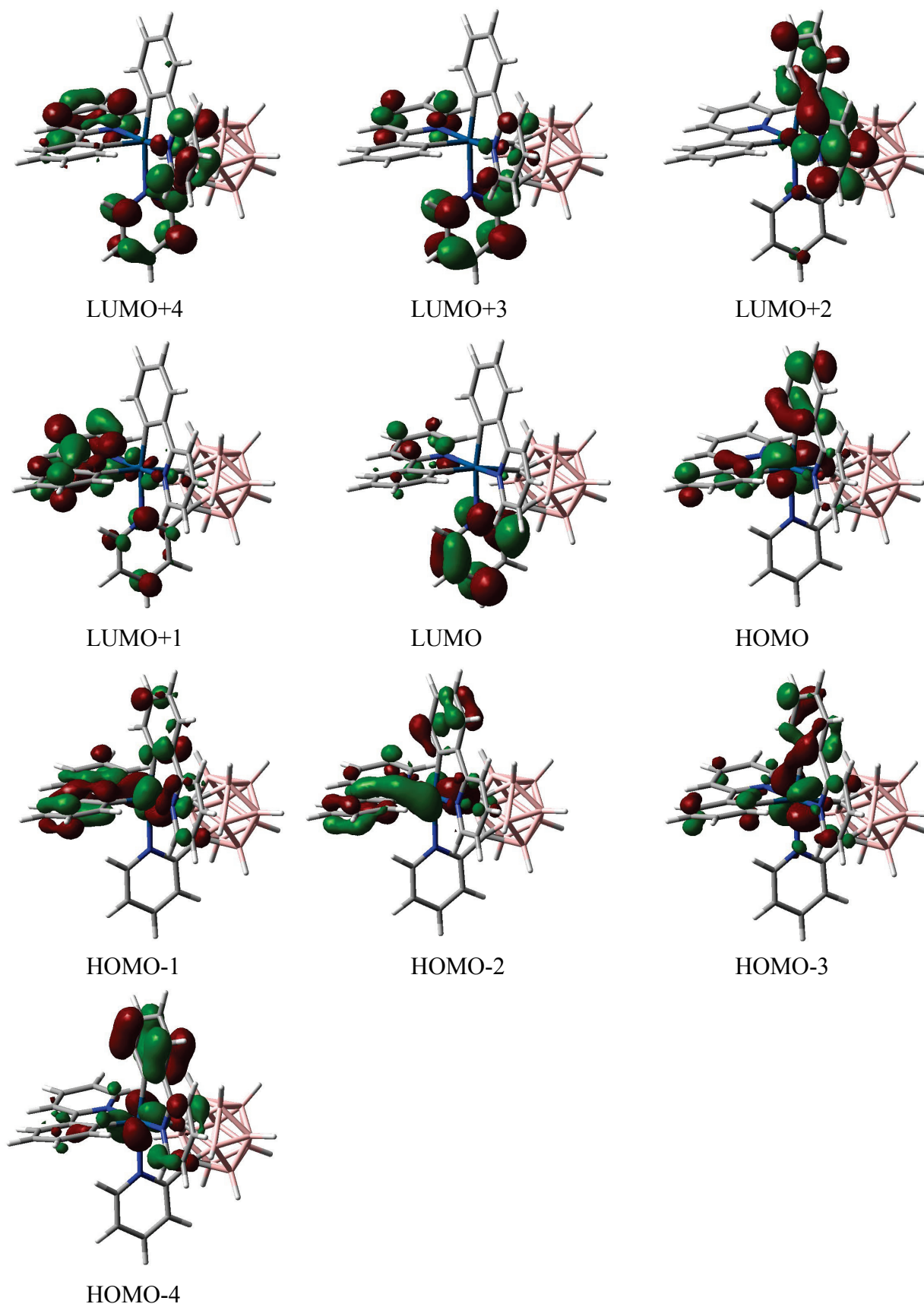


Figure S7. Molecular orbitals of **1** from B3LYP calculations (Isovalue = 0.04) at their lowest singlet ground state (S_0) optimized geometries.

Table S3. Molecular orbital distributions (in %) of **1** at their lowest singlet ground state (S_0) optimized geometries.

molecular orbital	Ir	Ph1	Py1	Ph2	Py2	Py in CBpy	Carborane
LUMO+4	3.06	4.14	26.29	4.75	24.44	28.68	8.64
LUMO+3	3.24	1.62	13.68	2.71	15.15	52.01	11.59
LUMO+2	4.45	21.11	58.61	2.57	1.55	6.05	5.67
LUMO+1	5.01	1.99	5.56	17.90	47.57	17.46	4.52
LUMO	2.94	1.01	3.04	4.16	13.63	62.90	12.32
HOMO	45.77	24.35	4.53	17.08	2.75	1.19	4.33
HOMO-1	42.07	13.12	10.93	17.55	12.37	1.41	2.55
HOMO-2	39.69	11.40	6.09	24.28	8.41	0.57	9.55
HOMO-3	50.29	19.21	9.24	10.09	5.88	4.11	1.19
HOMO-4	41.43	26.68	12.71	8.87	4.42	1.06	4.82

Table S4. Molecular orbital energies (in eV) of **1** from B3LYP calculations at their lowest singlet ground state (S_0) optimized geometries.

MO	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4
Energy	-6.39	-6.28	-6.16	-6.01	-5.32	-1.63	-1.57	-1.48	-1.15	-0.94

Table S5. Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{\text{calc.}}$) for **1** from TD-B3LYP calculations using the B3LYP geometries at their lowest singlet state (S_0) fully optimized geometries.

state	$\lambda_{\text{calc.}}$ (/nm)	$f_{\text{calc.}}$	major contribution
1	410.4	0.0374	HOMO \rightarrow LUMO(77.55%) HOMO \rightarrow LUMO+1(16.83%)
2	406.19	0.0029	HOMO \rightarrow LUMO+1(80.66%) HOMO \rightarrow LUMO(17.79%)
3	396.54	0.0348	HOMO \rightarrow LUMO+2(93.32%)
4	350.81	0.0052	HOMO \rightarrow LUMO+3(94.35%)
5	339.21	0.0312	HOMO-1 \rightarrow LUMO(45.88%) HOMO-1 \rightarrow LUMO+1(33.49%)
6	334.73	0.0491	HOMO-1 \rightarrow LUMO+1(35.92%) HOMO-1 \rightarrow LUMO(33.89%) HOMO-2 \rightarrow LUMO+1(10.16%)
7	332.37	0.0071	HOMO \rightarrow LUMO+4(84.81%)
8	329.86	0.0009	HOMO \rightarrow LUMO+5(82.43%)
9	326.43	0.0235	HOMO-2 \rightarrow LUMO(32.04%) HOMO-2 \rightarrow LUMO+1(31.91%)
10	325.03	0.0095	HOMO-1 \rightarrow LUMO+2(48.09%) HOMO-2 \rightarrow LUMO(17.41%) HOMO-3 \rightarrow LUMO+2(10.14%)

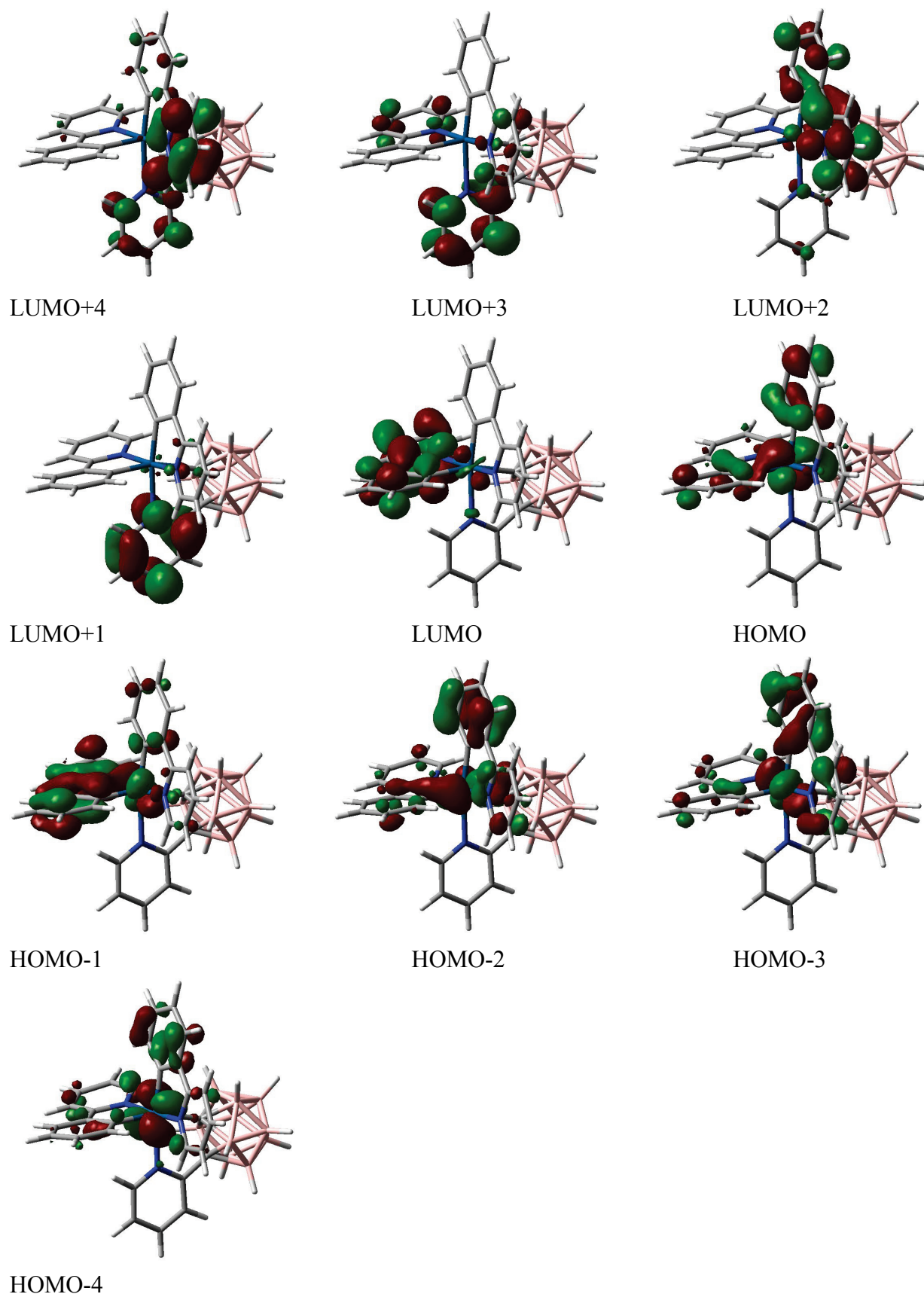


Figure S8. The selected frontier orbitals of **1** from B3LYP calculations (Isovalue = 0.04 a.u.) at their lowest triplet excited state (T_1) optimized geometries.

Table S6. Molecular orbital distributions (in %) of **1** at their lowest triplet excited state (T_1) optimized geometries.

molecular orbital	Ir	Ph1	Py1	Ph2	Py2	Py in CBpy	Carborane
LUMO+4	3.09	7.31	53.26	2.05	4.39	22.20	7.69
LUMO+3	3.32	2.00	13.05	2.31	11.87	55.81	11.65
LUMO+2	4.43	19.96	59.19	2.05	1.14	6.52	6.70
LUMO+1	2.50	1.60	5.94	0.27	0.43	74.54	14.71
LUMO	6.41	1.56	0.93	27.54	57.83	3.78	1.96
HOMO	41.69	21.11	3.76	21.19	4.05	0.96	7.23
HOMO-1	32.84	9.79	5.92	25.78	20.90	1.31	3.45
HOMO-2	41.78	19.57	12.64	12.89	6.18	0.22	6.73
HOMO-3	41.16	24.48	15.09	8.85	6.09	1.63	2.69
HOMO-4	60.78	13.08	5.89	8.14	7.36	2.03	2.72

Table S7. Molecular orbital energies (in eV) of **1** from B3LYP calculations at their lowest triplet excited state (T_1) optimized geometries.

MO	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4
Energy	-6.42	-6.33	-6.22	-5.94	-5.10	-1.88	-1.56	-1.46	-1.10	-0.94

Table S8. Computed phosphorescence emission wavelengths (λ_{calc} , in nm) and oscillator strengths (f_{calc}) for **1** from TD-B3LYP calculations using the B3LYP geometries.

state	λ_{calc} (/nm)	f_{calc}	major contribution
1	476.0	0	HOMO \rightarrow LUMO(80.01%) HOMO-1 \rightarrow LUMO(13.74%)

Table S9. Cartesian coordinates of **1** from B3LYP calculation (in Å).

S ₀			T ₁				
	X	Y	Z		X	Y	Z
C	-1.54994	3.995565	-2.6276	C	1.509605	4.088689	2.546428
C	-1.08825	4.066909	-1.32075	C	1.054831	4.140083	1.231759
C	-1.72753	2.739572	-3.22015	C	1.699062	2.847956	3.166689
C	-0.22804	4.016936	1.604742	C	0.210441	4.036447	-1.70063
C	0.109574	3.876827	2.941473	C	-0.1259	3.863484	-3.03621
C	-0.79595	2.890299	-0.60818	C	0.776718	2.955531	0.536833
C	1.78428	0.103731	-0.60999	C	-1.79159	0.107364	0.535193
C	-0.35719	2.886258	0.780142	C	0.346636	2.922694	-0.85894
C	2.695749	-0.92284	0.357366	C	-2.67419	-1.01287	-0.32616
C	-1.43478	1.570239	-2.51877	C	1.424258	1.664375	2.484572
C	-0.94645	1.606403	-1.20123	C	0.941385	1.684211	1.161707
C	0.314301	2.593418	3.458377	C	-0.32204	2.569934	-3.52541
C	0.200847	1.512348	2.599628	C	-0.198	1.505119	-2.64408
C	1.88721	-1.69183	1.35852	C	-1.85012	-1.8682	-1.24172
C	-0.48498	-1.7216	-2.56866	C	0.484982	-1.56602	2.649572
C	2.500208	-2.58405	2.2424	C	-2.43941	-2.8805	-2.00392
C	-0.99609	-2.68841	-3.42367	C	0.982144	-2.51366	3.523485
C	1.719498	-3.31277	3.134181	C	-1.63716	-3.67621	-2.81668
C	-2.27745	-0.26362	0.672168	C	2.215709	-0.32168	-0.7315
C	-2.16994	-3.34783	-3.05857	C	2.129141	-3.26717	3.143884
C	-2.95631	0.388792	1.71794	C	2.85279	0.250621	-1.84951
C	-2.26867	-1.96139	-1.07426	C	2.239171	-1.94397	1.101691
C	-0.20406	-2.22255	2.21776	C	0.247429	-2.40155	-2.0733
C	0.337409	-3.13271	3.118443	C	-0.26504	-3.43686	-2.84878
C	-2.93843	-1.37762	0.088104	C	2.894396	-1.41584	-0.03601
C	-2.80928	-2.96993	-1.88665	C	2.744333	-2.96248	1.954436
C	-4.19569	-0.05417	2.183613	C	4.094211	-0.18913	-2.2982
C	-4.18091	-1.83352	0.564897	C	4.171045	-1.84488	-0.50875
C	-4.80886	-1.17708	1.616657	C	4.74288	-1.25243	-1.61332
H	4.675006	1.444387	-2.81038	H	-4.69716	1.674954	2.545053
H	5.017629	2.098815	0.176732	H	-5.00393	2.007199	-0.4993
H	6.260502	-0.46668	-0.98582	H	-6.25782	-0.42524	0.913474
H	2.26725	2.498768	-1.16227	H	-2.27296	2.549832	0.829058
H	4.271711	-1.5966	-3.05364	H	-4.29865	-1.32361	3.115195
H	-1.77339	4.903513	-3.18039	H	1.720604	5.008687	3.083922
H	-0.95403	5.040854	-0.85745	H	0.918805	5.106985	0.755574

H	1.834557	0.288982	-3.10855	H	-1.85555	0.55999	2.998707
H	4.742045	-0.55717	1.752395	H	-4.70521	-0.80274	-1.77916
H	-0.41072	5.000251	1.187854	H	0.384784	5.03012	-1.30526
H	-2.09733	2.673148	-4.241	H	2.063731	2.806157	4.189897
H	0.20415	4.752177	3.577481	H	-0.22623	4.724265	-3.69077
H	2.451535	1.223536	1.589	H	-2.41262	0.983873	-1.77541
H	4.299063	-2.77131	-0.18452	H	-4.28469	-2.79554	0.386354
H	-1.58773	0.619084	-3.01731	H	1.583281	0.718189	2.987685
H	1.731259	-2.2961	-1.4438	H	-1.73121	-2.18557	1.627687
H	0.410905	-1.17786	-2.82347	H	-0.37664	-0.97398	2.922658
H	0.567536	2.43006	4.500187	H	-0.57441	2.383971	-4.56351
H	3.576862	-2.69838	2.216311	H	-3.50989	-3.03474	-1.94754
H	0.361817	0.499629	2.945163	H	-0.34912	0.482879	-2.96654
H	-0.47599	-2.91111	-4.34884	H	0.488038	-2.66871	4.476107
H	-2.51399	1.261516	2.189368	H	2.379207	1.073303	-2.37589
H	2.184215	-4.0106	3.824537	H	-2.07916	-4.47074	-3.41085
H	-2.59351	-4.12393	-3.68966	H	2.523688	-4.04361	3.791959
H	-1.27112	-2.04023	2.171655	H	1.304397	-2.16241	-2.07605
H	-0.31701	-3.68044	3.788447	H	0.403736	-4.03354	-3.46026
H	-3.74921	-3.43005	-1.60618	H	3.648938	-3.48411	1.658855
H	-4.68886	0.478159	2.994286	H	4.571616	0.278274	-3.15445
H	-4.66659	-2.6971	0.117622	H	4.704205	-2.63983	0.004651
H	-5.76935	-1.52733	1.984332	H	5.711984	-1.60093	-1.96355
B	4.16285	0.799688	-1.95215	B	-4.17545	0.942082	1.767336
B	4.370065	1.18519	-0.22378	B	-4.36203	1.142031	0.004458
B	5.084961	-0.30631	-0.89994	B	-5.08171	-0.27187	0.826158
B	2.785701	1.442888	-1.01338	B	-2.79108	1.483852	0.783584
B	3.938569	-0.9646	-2.10238	B	-3.95163	-0.79629	2.107579
B	2.528024	0.129242	-2.15754	B	-2.54301	0.29922	2.067093
B	4.280171	-0.33643	0.680348	B	-4.25814	-0.46754	-0.73123
B	2.872294	0.749868	0.595692	B	-2.85528	0.624194	-0.74515
B	4.019772	-1.6534	-0.47188	B	-4.00819	-1.65402	0.558691
B	2.448192	-1.37707	-1.25377	B	-2.44813	-1.29853	1.331506
N	-0.10758	1.64305	1.293844	N	0.115091	1.669259	-1.34606
N	-1.06651	-1.38935	-1.39936	N	1.020204	-1.3092	1.436436
N	0.544041	-1.50641	1.354838	N	-0.52072	-1.62703	-1.28545
Ir	-0.37418	0.068615	-0.03222	Ir	0.409781	0.12482	0.04751