Electronic Supplementary Information for:

Tuning the Luminescence Lifetimes of Ruthenium (II) Polypyridine Complexes and Its Application in Luminescent Oxygen Sensing

Shaomin Ji,[a] Wanhua Wu,[a] Wenting Wu,[a] Peng Song,[b] Keli Han,[b] Zhonggang Wang,[c] Shasha Liu,[b]

Huimin Guo [d] and Jianzhang Zhao*[a]

[a] *State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, P.O. Box 40, 158 Zhongshan Road, Dalian 116012, P. R. China.*

[b] *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, P. R. China.*

[c] *Department of Polymer Science and Materials, School of Chemical Engineering, Dalian University of Technology, P.O. Box 40, 158 Zhongshan Road, Dalian 116012, P. R. China.*

[d] *Department of Chemistry, School of Chemical Engineering, Dalian University of Technology, P.O. Box 40, 158 Zhongshan Road, Dalian 116012;* ≠

E-mail: zhaojzh@dlut.edu.cn

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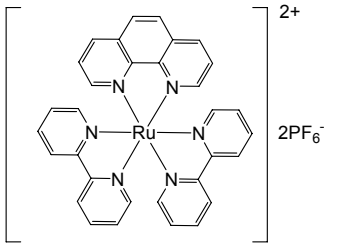

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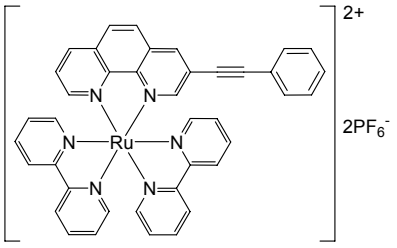

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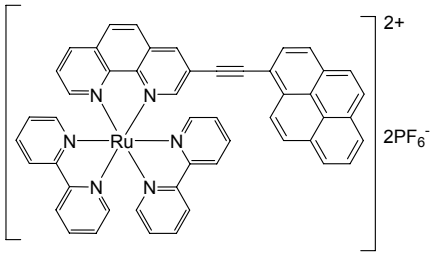

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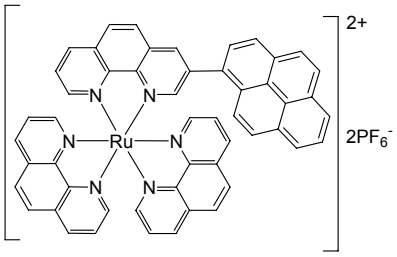

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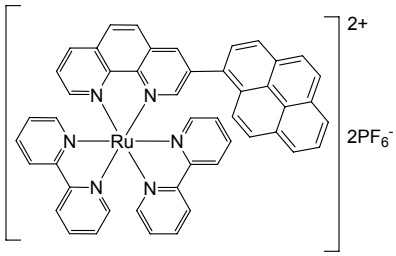

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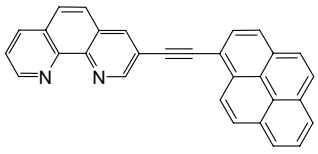
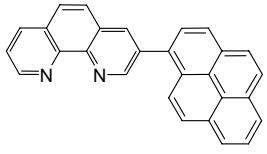


ligand of complex 3



ligand of complex 5

Complex 1 $[(bpy)_2Ru(1,10\text{-phenanthroline})]^{2+}(PF_6)_2$

Complex 2 $[(bpy)_2Ru(3\text{-phenylethynyl-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$

Complex 3 $[(bpy)_2Ru(3\text{-ethynylpyrenyl-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$

Complex 4 $[(1,10\text{-phenanthroline})_2Ru(3\text{-pyrenyl-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$

Complex 5 $[(bpy)_2Ru(3\text{-pyrenyl-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$

Experimental Section

General

The chemicals for synthesis were A.R. grade and were used as received.

The ground state structure of complexes were optimized using density functional theory (DFT)[1] with B3LYP functional and 6-31G(d)/ LanL2DZ basis set. The excited state related calculations were carried out with the Time dependent density functional theory (TD-DFT) with the optimized structure of the ground state (DFT 6-31G(d)/ LanL2DZ) There are no imaginary frequencies in frequency analysis of all calculated structures, therefore each calculated structure express an energy minimum. All these calculations were performed with Gaussian 03.[2]

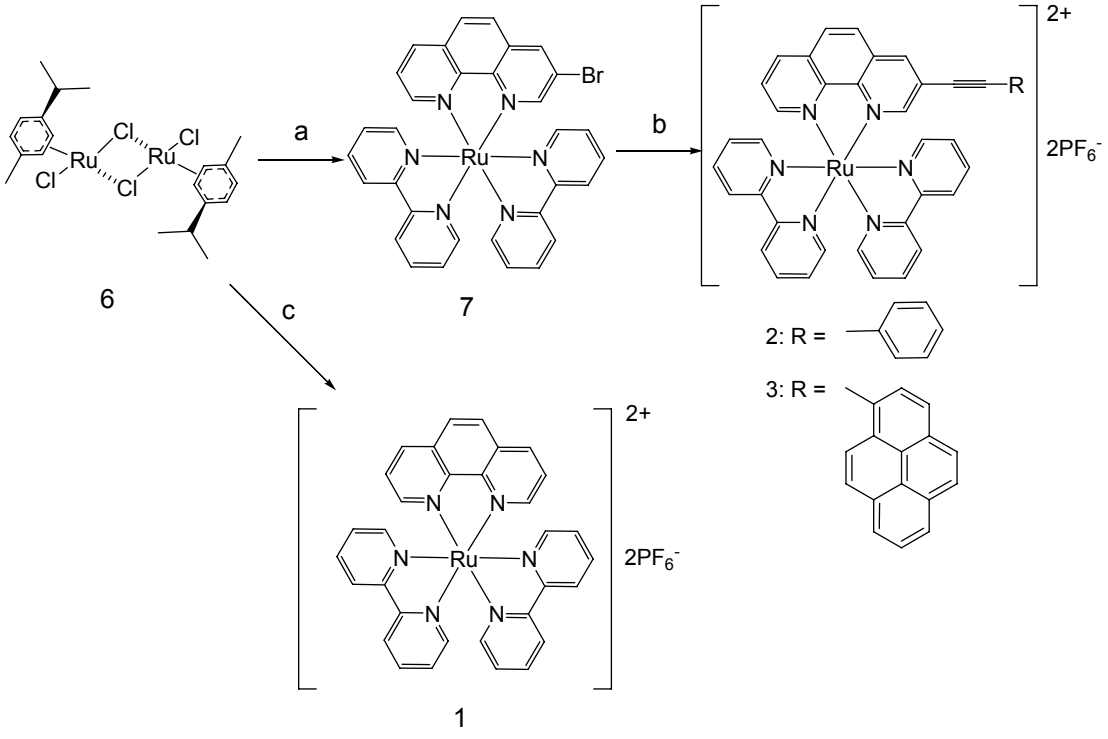
Reference:

1. Hohenberg P, Kohn W. *Phys. Rev.* 1964; **136**: B864.

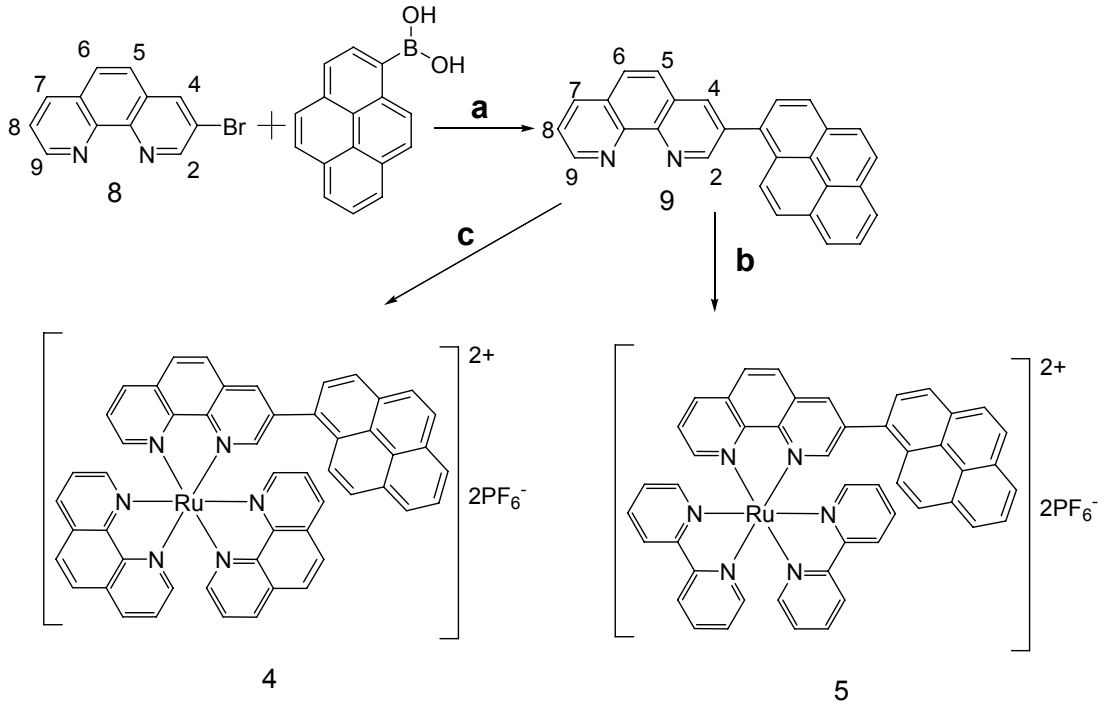
2. M. J. Frisch, et al. Gaussian 03, Revision D. 01, Gaussian,Inc., Wallingford CT, 2004

Synthesis :

Scheme S1. Syntheses of $[(bpy)_2Ru(1,10\text{-phenanthroline})]^{2+}(PF_6)_2$ and **2**, **3**. a: 3-bromo-1,10-phenanthroline, EtOH, r.t. 2 h, 2,2'-bipyridine, H_2O,100 ºC, 22 h; b: phenylethynyl or ethynylpyrene, $Pd(PPh_3)_2Cl_2$, DMF, NEt_3, CuI, Ar, r.t., 24 h; c: phenanthroline, EtOH, r.t. 2 h, 2,2'-bipyridine, H_2O, 100 ºC, 22 h.



Scheme S2. Syntheses of **4**, **5**. a: $Pd(PPh_3)_4$, sat. $Ba(OH)_2$, toluene-ethanol-water(3/1/4), Ar, 100 ºC, 48 h; b: **6**, 2,2'-bipyridine, EtOH, r.t. 2 h, 100 ºC, 24 h ; c **6**, 1,10-phenanthroline, EtOH, r.t. 2 h, 100 ºC, 24 h.



$[(bpy)_2Ru(1,10\text{-phenanthroline})]^{2+}(PF_6)_2$ (1) was synthesized as reported previously. [*Synthetic Metals* **2004**, *145*, 259-264.] ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) = 8.87-8.81 (m, 6H), 8.45-8.44 (d, 2H, *J* = 4.8 Hz), 8.41 (s, 2H), 8.28-8.24 (t, 2H, *J* = 8.0 Hz), 8.19-8.13 (m, 4H), 7.95-7.89 (m, 4H), 7.66-7.62 (t, 2H, *J* = 6.0 Hz), 7.41-7.37 (t, 2H, *J* = 6.4 Hz). ESI-HRMS [$(M\text{-}PF_6)^+$], calcd, *m*/*z* = 739.0753; found *m*/*z* = 739.0469; [$(M\text{-}2PF_6)^{2+}/2$], calcd, *m*/*z* = 297.0553; found *m*/*z* = 297.0457.

3-bromo-1,10-phenanthroline (8) was synthesized as reported previously. **[***Tetrahedron Lett.,* **1995,** *36***,** 3489-3490**]** Pale brown solid was obtained in 41% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 9.22–9.21 (d, $1H_9$, *J* = 4.0 Hz), 9.20–9.19 (d, $1H_2$, *J* =2.0 Hz), 8.42–8.41 (d, $1H_4$, *J* =2.0 Hz), 8.28–8.27 (d, $1H_7$, *J* =8.0 Hz), 7.86–7.84 (d, $1H_5$, *J* =8.8 Hz), 7.74–7.72 (d, $1H_6$, *J* =8.8 Hz), 7.70–7.67 (m, $1H_8$). ESI-HRMS [$(M+H)^+$], calcd, *m*/*z* = 258.9871; found *m*/*z* = 258.9217.

$[(bpy)_2Ru(3\text{-bromo-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$ (7) A solution of $[RuCl_2(cymene)]_2$ (153.1 mg, 0.25 mmol) and 3-bromo-1,10-phenanthroline (130 mg, 0.5 mmol) in ethanol (5 mL) was stirred for 2h. The reaction was monitored by TLC. Then 10mL water and 2,2'-bipyridine (158.7 mg, 1.0 mmol) was added to the solution, which was then refluxed for an additional 20h. After cooling, the solution was concentrated under reduced pressure and treated with a saturated aqueous solution of NH_4PF_6, which gave a red precipitate. The solid was washed with water and dried. Dark red solid was obtained in 95.0 % yield. ^{1}H NMR (400 MHz, acetone-d_6) δ (ppm) = 9.07 (d, 1H, *J* = 1.6 Hz) , 8.86–8.80 (m, 5H), 8.48–8.44 (m, 3H), 8.37–8.35 (d, 1H, *J* =9.2 Hz), 8.28–8.24 (t, 2H, *J* =8.0 Hz), 8.21–8.11 (m, 4H), 8.06–8.04 (d, 1H, *J* = 5.2 Hz), 7.97–7.93 (q, 1H, *J* = 3.2 Hz), 7.87–7.86 (d, 1H, *J* =5.6 Hz), 7.65–7.58 (m, 2H), 7.41–7.37 (m, 2H). HRMS(ES): m/z 336.9673 [$(M\text{-}2PF_6)^{2+}/2$]. calcd, *m*/*z* = 336.0105; found *m*/*z* = 335.9709.

$[(bpy)_2Ru(3\text{-phenylethynyl-}1,10\text{-phenanthroline})]^{2+}(PF_6)_2$ (2). 2 was synthesized as reported previously. [*J. Am. Chem. Soc.* **2002**, *124*, 3749-3762] Red solid was obtained in 49.0 % yield. Mp 175.9–177.5 °C. ^{1}H NMR (400

MHz, acetone-d_6) δ (ppm) = 8.96 (d, 1H, *J* = 1.2 Hz), 8.80–8.86 (q, 5H, *J* = 8.0 Hz), 8.55 (d, 1H, *J* = 1.6 Hz), 8.45–8.46 (d, 1H, *J* = 4.0 Hz), 8.44 (s, 1H), 8.23–8.28 (t, 2H, *J* = 6.8 Hz), 8.21–8.22 (d, 1H, *J* = 5.6 Hz), 8.13–8.18 (m, 3H), 8.07–8.08 (d,1H, *J* = 5.6 Hz), 7.93–7.96 (q, 1H, *J* = 3.2 Hz), 7.88–7.90 (d, 1H, *J* = 5.6 Hz), 7.62–7.66 (m, 3H), 7.45–7.52 (m, 5H), 7.39–7.43 (t, 2H, *J* = 3.2 Hz). ESI–HRMS [$(M\text{-}2PF_6)^{2+}/2$], calcd, *m*/*z* = 347.07; found *m*/*z* = 346.80.

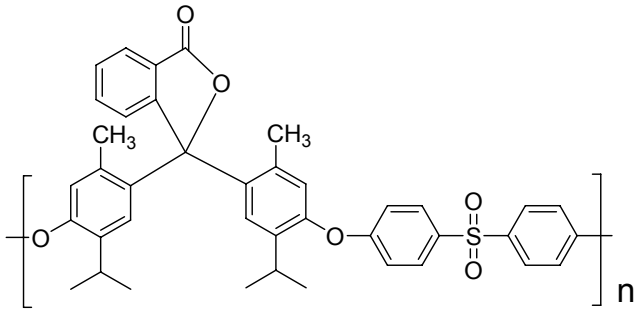
[$(bpy)_2$Ru(3-ethynylpyrene-1,10-phenanthroline)]$^{2+}(PF_6)_2$ （3） Complex **7** (100 mg, 0.1 mmol), $Pd(PPh_3)_2Cl_2$ (35.0 mg, 0.05 mmol), and CuI (9.8 mg, 0.05 mmol) were combined in 5 mL of anhydrous DMF and 2 mL $HN(i\text{-}Pr)_2$. The mixture was purged with nitrogen, and stirred 1 h at room temperature. Ethynylpyrene (46.0 mg, 0.2 mmol) was added and the color of solution was changed to dark. Then the solution was stirred 24 h at room temperature. At the end of the reaction, the mixture was filtered and the filtrate was concentrated under reduced pressure. The crude product was then subjected to column chromatography (silica gel. Eluted with acetonitrile : water : saturated aqueous $NaNO_3$ =100:9:1, V/V) and treated with a saturated aqueous solution of NH_4PF_6, which gave a red precipitate. The solid was washed with water and dried. Dark red solid was obtained in 36% yield. Mp >300 °C ^{1}H NMR (400 MHz, acetone-d_6) δ (ppm) = 9.16 (d, 1H, *J* = 1.2 Hz), 8.91–8.93 (d, 1H, *J* = 8.0 Hz), 8.82–8.88 (q, 4H, *J* = 8.4 Hz), 8.69 (d, 1H, *J* = 1.6 Hz), 8.49–8.50 (d, 1H, *J* = 4.0 Hz), 8.46–8.48 (d, 3H, *J* = 8.0 Hz), 8.35–8.44 (m, 4H), 8.25–8.32 (m, 4H), 8.14–8.23 (m, 7H), 7.94–7.98 (t, 2H, *J* = 8.0 Hz), 7.73–7.76 (t, 1H, *J* = 6.4 Hz), 7.64–7.68 (t, 1H, *J* = 6.0 Hz), 7.42–7.46 (q, 2H, *J* = 4.8 Hz). ^{13}C NMR (100 MHz, acetone-d_6): δ 158.3, 158.2, 158.0, 157.8, 154.7, 153.6, 153.0, 152.9, 152.7, 152.6, 148.2, 147.1, 139.2, 138.8, 138.7, 137.7, 133.0, 132.7, 132.2, 131.9, 131.5, 131.2, 130.4, 129.9, 129.8, 129.7, 128.6, 128.5, 128.4, 128.3, 127.8, 127.5, 127.2, 127.0, 126.9, 125.5, 125.2, 125.1, 124.9, 124.8, 124.5, 123.1, 116.0, 95.3, 91.0. ESI-HRMS: [$(M\text{-}PF_6)^+$] calcd, m/z = 963.1379; found, 963.1351m/z; [$(M\text{-}2PF_6)^{2+}/2$] calcd, *m*/*z* = 409.0866, found *m*/*z* = 409.0851.

3-Pyrenyl-1,10-phenanthroline (9) 3-Bromo-1,10-phenanthroline (191 mg, 0.74 mmol) and 1-pyrene boronic acid (200 mg, 0.81 mmol) were dissolved in 30 mL toluene and 10mL ethanol. The yellow solution was degassed with Ar for 30min. A saturated aqueous solution of $Ba(OH)_2$ (40 mL) was added, and the biphasic mixture was degassed an additional 30min. $Pd(PPh_3)_4$ (34.7 mg, 0.03 mmol) was added and the reaction mixture refluxed with vigorous stirring under Ar for 2 days. The color of the solution changed from yellow to green. Once cool, the layers were separated and the aqueous layer was extracted with toluene (3×20 mL) and the combined organic extracts were washed with water (3×20 mL). The organic fractions were dried over $MgSO_4$, filtered, and rotary evaporated to a brown oily residue. The oil was triturated with petroleum ether , and the mixture gave an olive drab precipitate. The olive drab product was obtained in 82 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 9.50–9.49 (d, $1H_2$, *J* = 2.0 Hz), 9.28–9.27 (d, $1H_9$, *J* = 3.6 Hz), 8.51–8.50 (d, $1H_4$, *J* = 2.0 Hz), 8.37–8.31 (m, $2H_{(7,pyrene)}$), 8.26–8.15 (m, $5H_{(pyrene)}$), 8.13–8.04 (m, $3H_{(pyrene)}$), 7.94–7.92(d, $1H_6$, *J* = 8.0Hz), 7.91–7.89 (q, $1H_5$, *J* = 8.0Hz), 7.72–7.68 (m, $1H_8$). ESI-HRMS [$(2M+H)^+$], calcd, *m*/*z* = 761.2704; found *m*/*z* = 761.4384. [$(M+H)^+$], calcd, *m*/*z* = 381.1392; found *m*/*z* = 381.2060.

Preparation the oxygen sensing film:

The polymer used for the fabrication of the O_2 sensing film is cardo poly(aryl ether ketone), IMPES-C (MW: 261477; Scheme S3). 10.0 mg of IMPES-C polymer was dissolved in 0.5 mL chloroform, then 0.2 mL of complex Ru(II) solution in acetonitrile (1.0×10^{-3} mol dm^{-3}) was added into the solution. After thorough mixing, about 0.3 mL of the solution was coated on a silica glass disk (diameter: 1.6 cm). The solvent was evaporated at r.t. and a transparent film was obtained. The thickness of the film of complex **3** was estimated as 19 μm, by the weight of the film (4.6 mg) and the density of the polymer (1.172 g cm^{-3}). The thickness of the film of complex **1**, **2**, **4**, **and 5** were estimated with the same method as 18 μm, 13 μm, 18 μm and 13 μm, respectively.

Scheme S3. Structure of polymer IMPES-C.



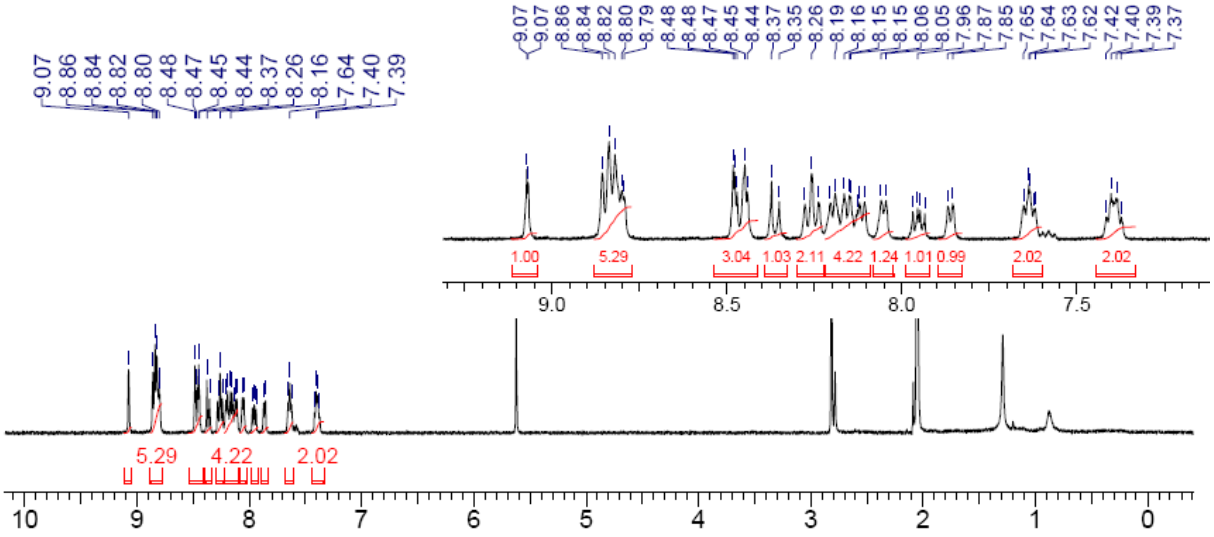


Figure S1. ^{1}H NMR of **7** ($CDCl_3$, 400 MHz)

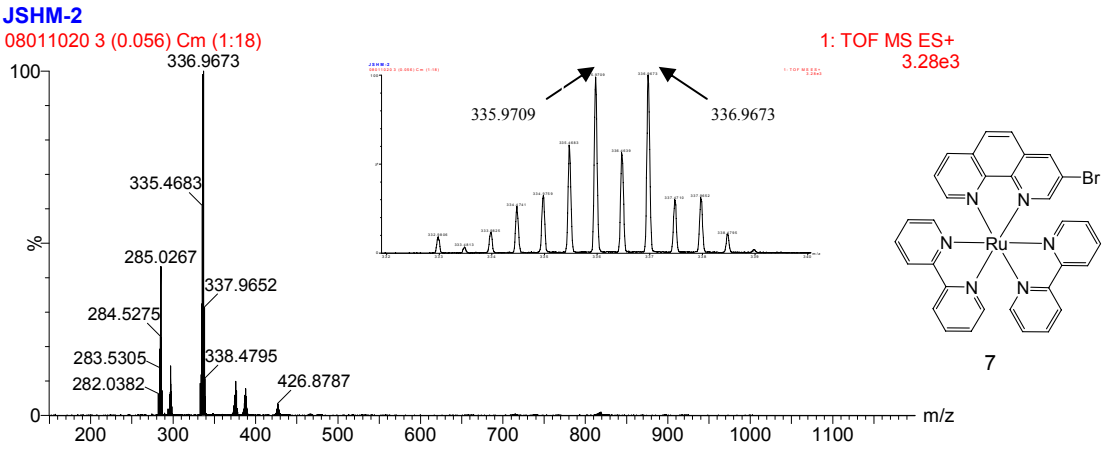


Figure S2. TOF MS (ESI) of **7.**

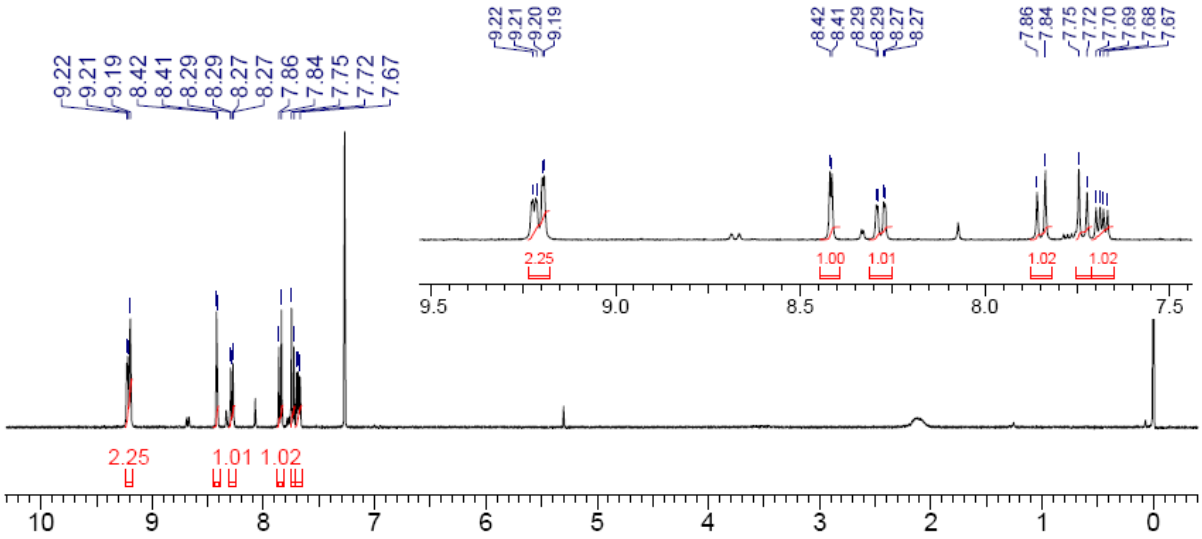


Figure S3. ^{1}H NMR of **8** ($CDCl_3$, 400 MHz)

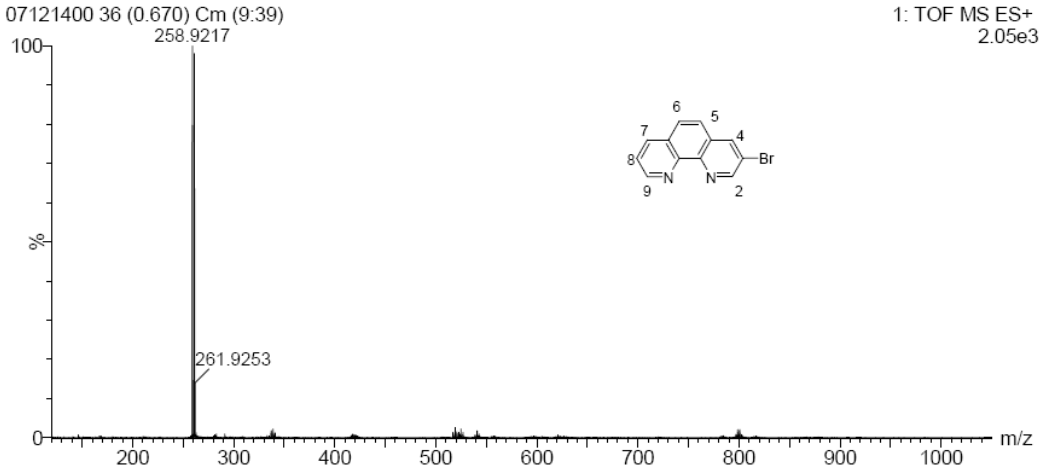


Figure S4. TOF ESI MS of **8.**

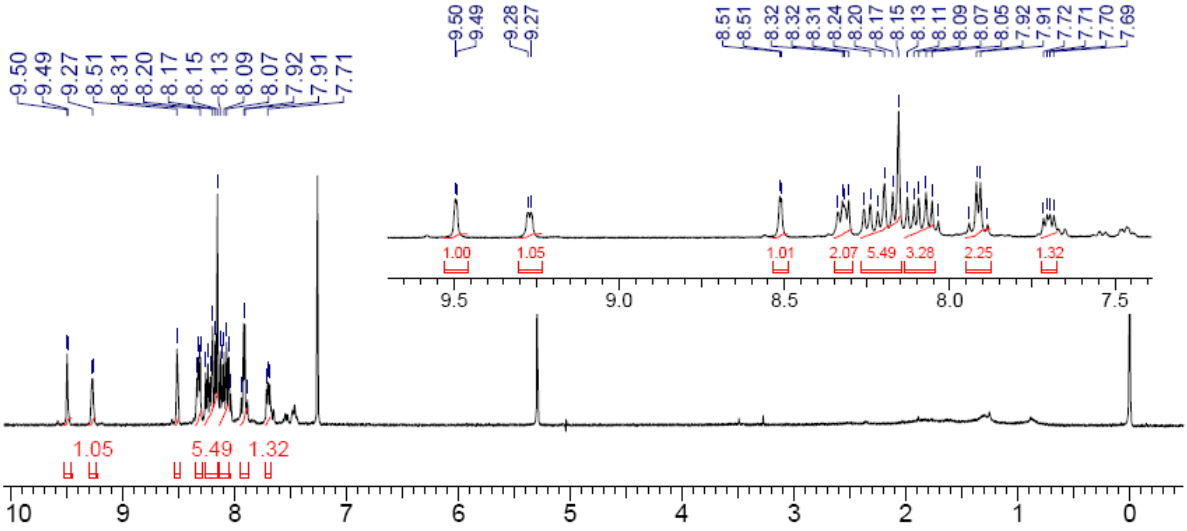


Figure S5. ^{1}H NMR of **9** ($CDCl_3$, 400 MHz).

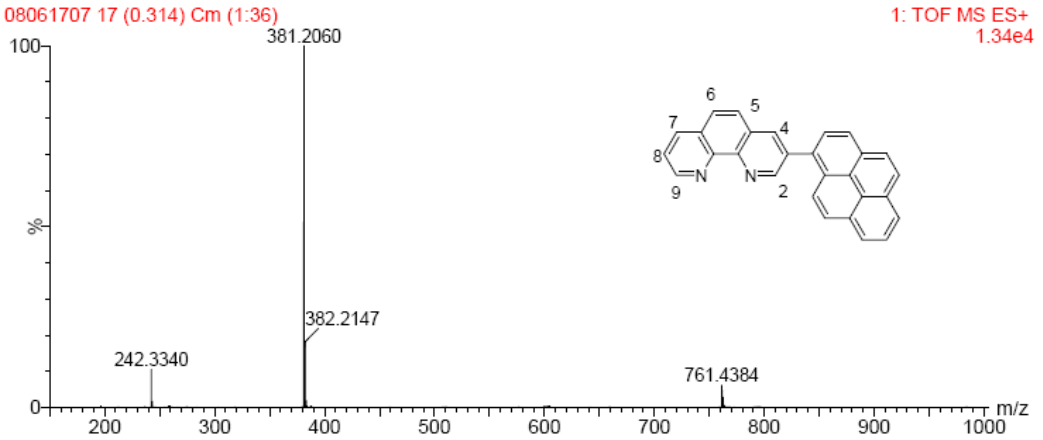


Figure S6. TOF ESI MS of **9.**

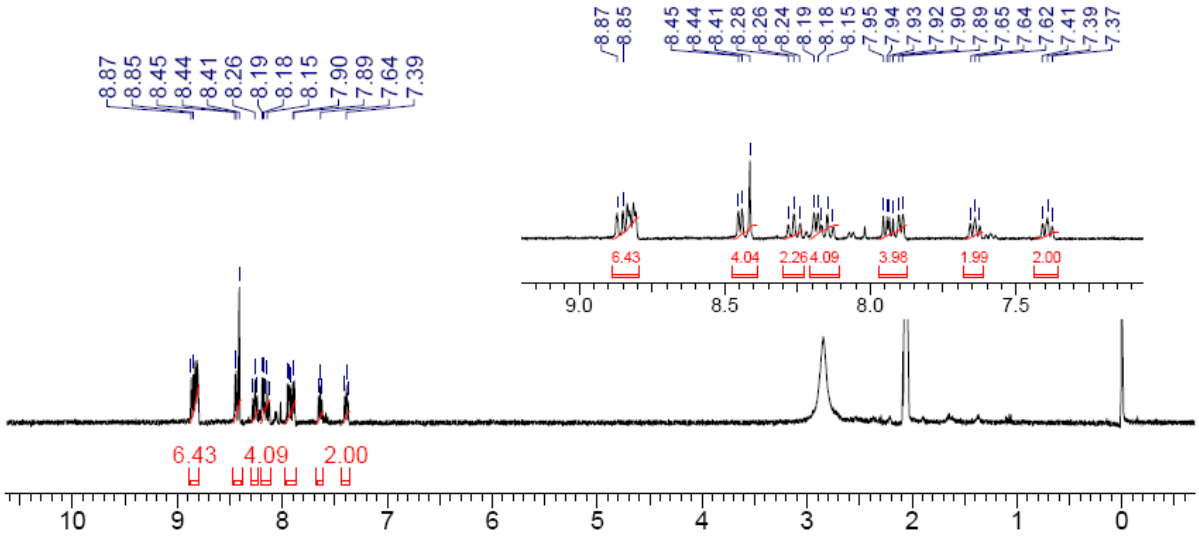


Figure S7. ^{1}H NMR of **1** (acetone-d_6, 400 MHz).

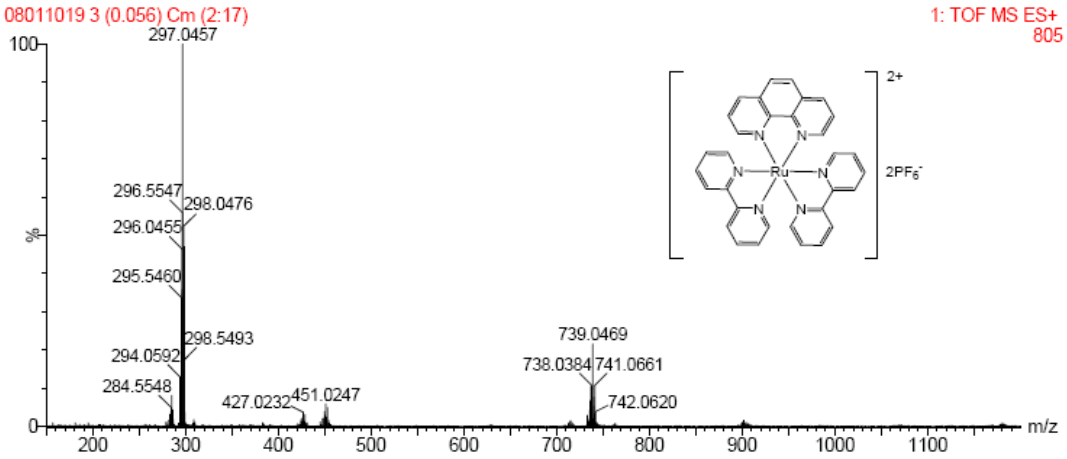


Figure S8. TOF ESI MS of **1.**

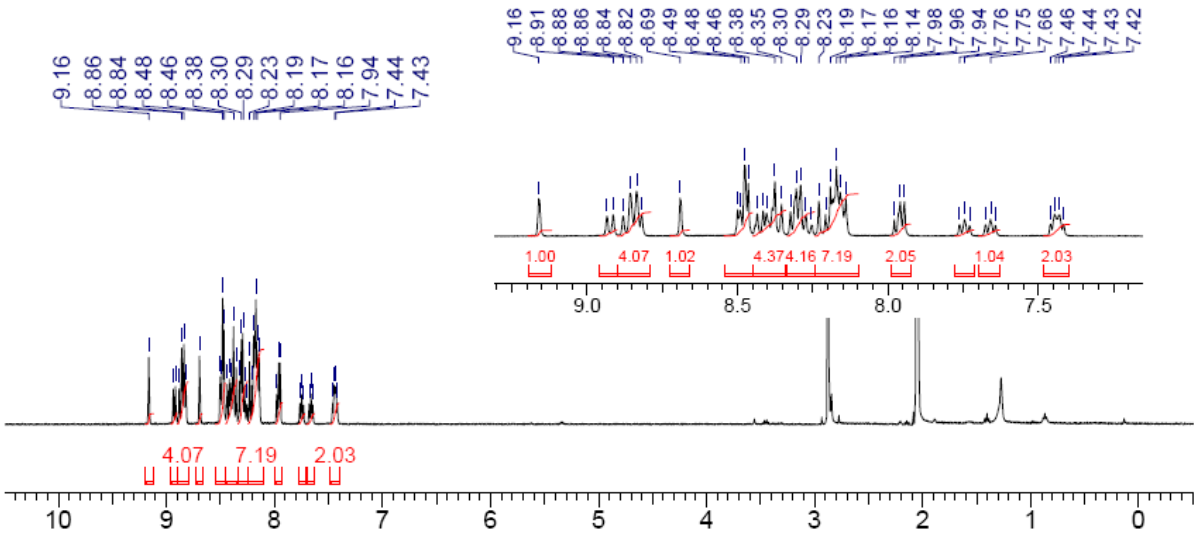


Figure S9. ^{1}H NMR of **3** (acetone-d_6, 400 MHz).

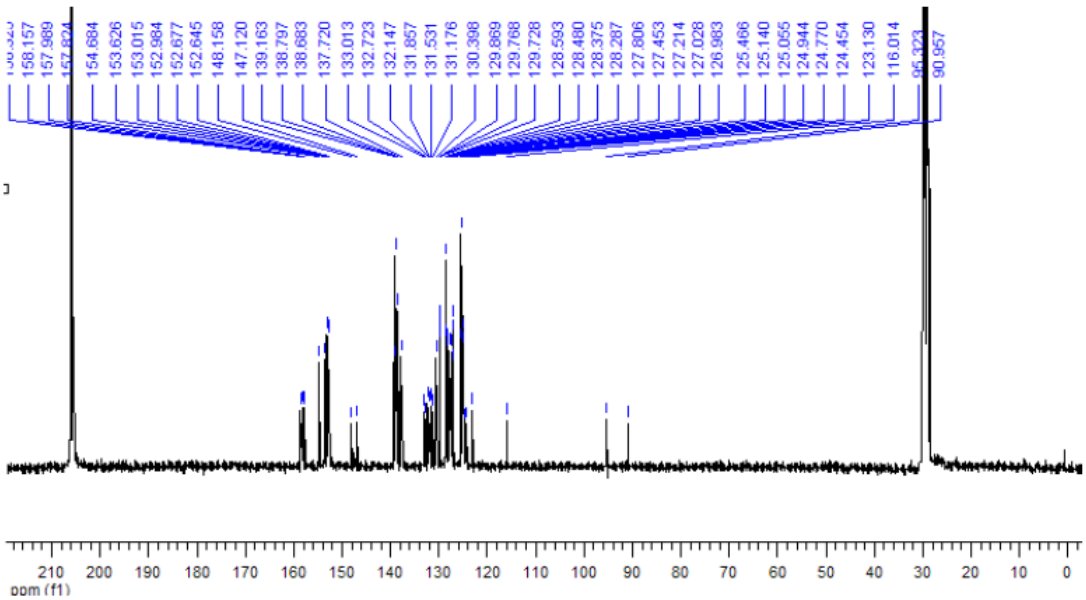


Figure S10. ^{13}C NMR of **3** (acetone-d_6, 100 MHz).

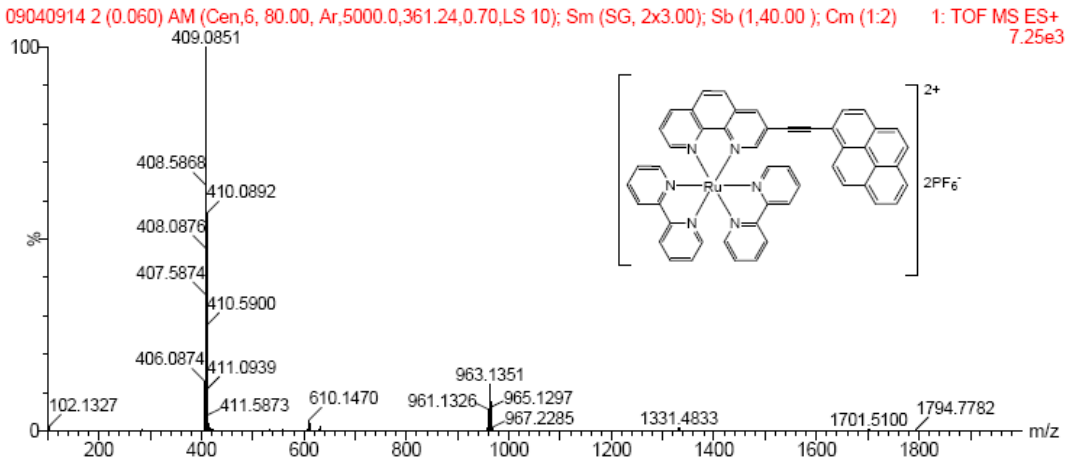


Figure S11. TOF ESI MS of **3.**

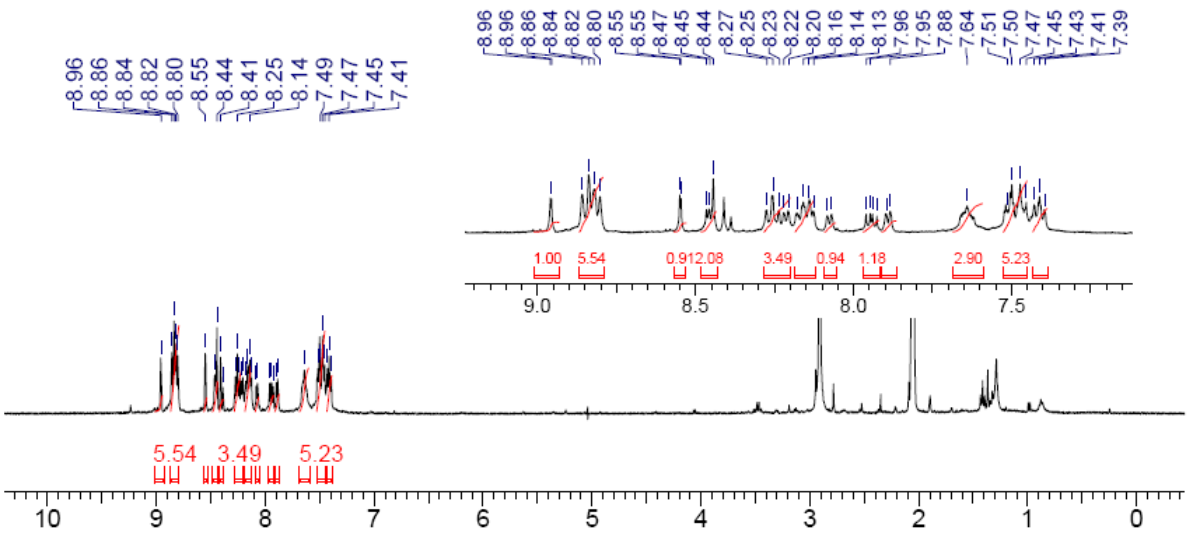


Figure S12. ^{1}H NMR of **2** (acetone-d_6, 400 MHz).

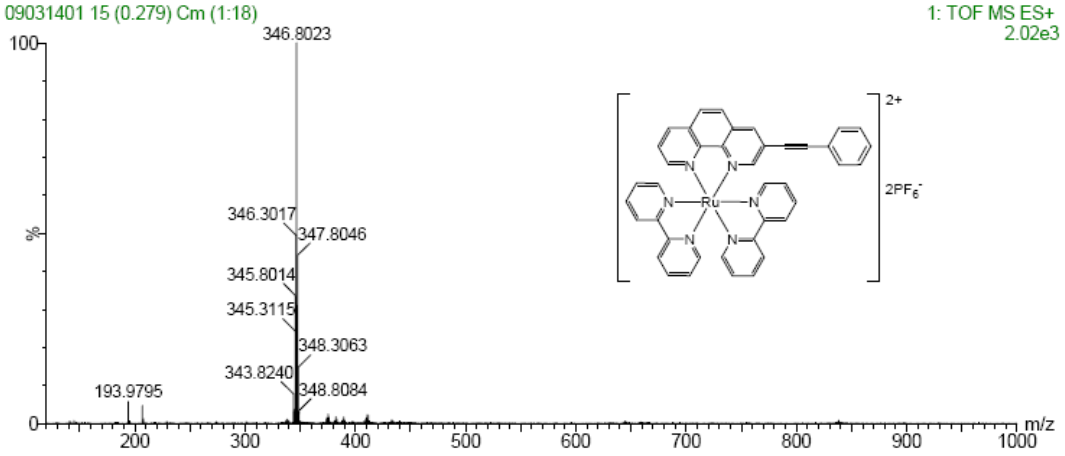


Figure S13. TOF ESI MS of **2.**

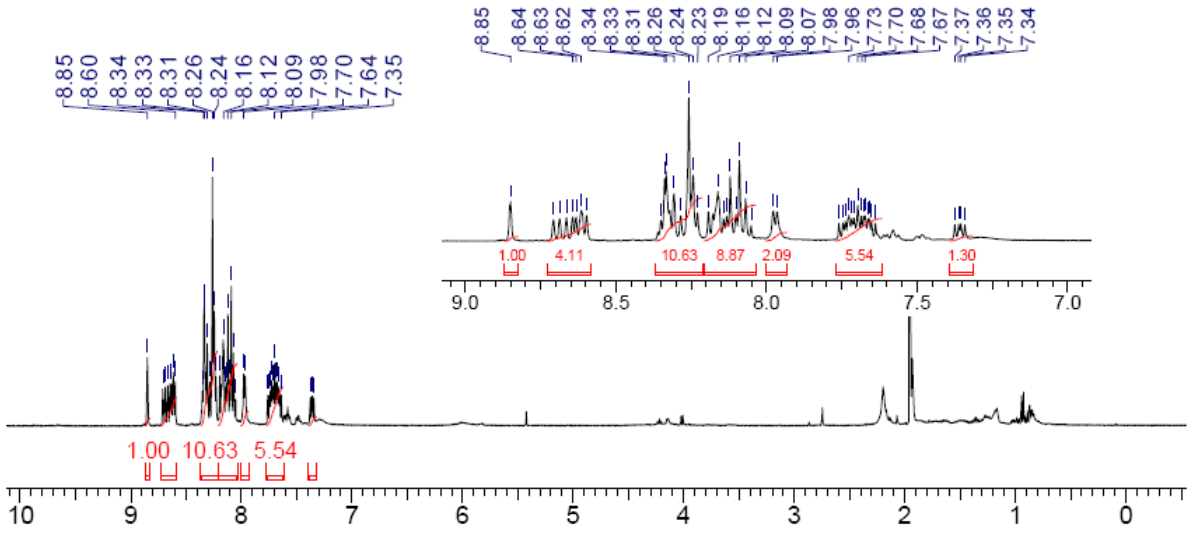


Figure S14. ^{1}H NMR of **4** (acetone-d_6, 400 MHz).

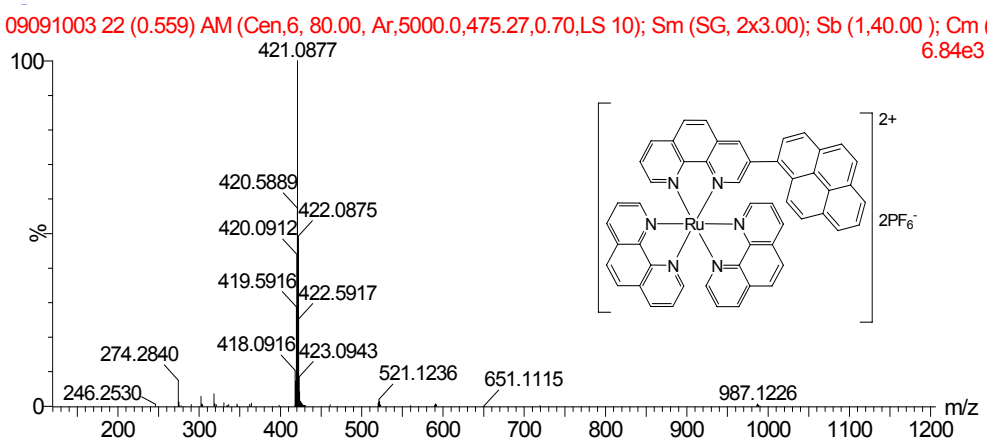


Figure S15. TOF ESI MS of **4.**

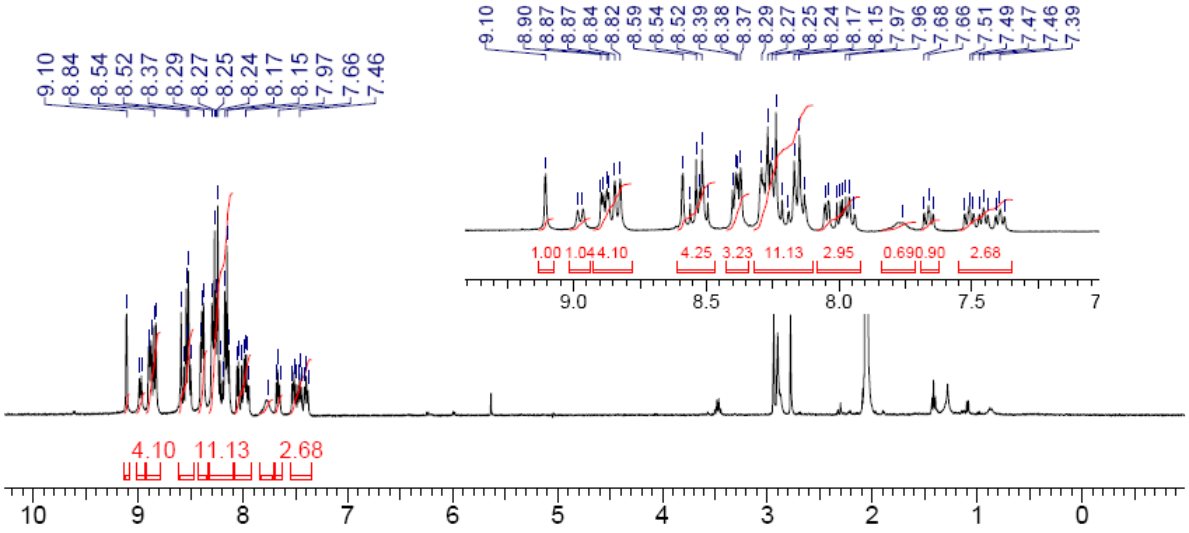


Figure S16. ^{1}H NMR of **5** (acetone-d_6, 400 MHz).

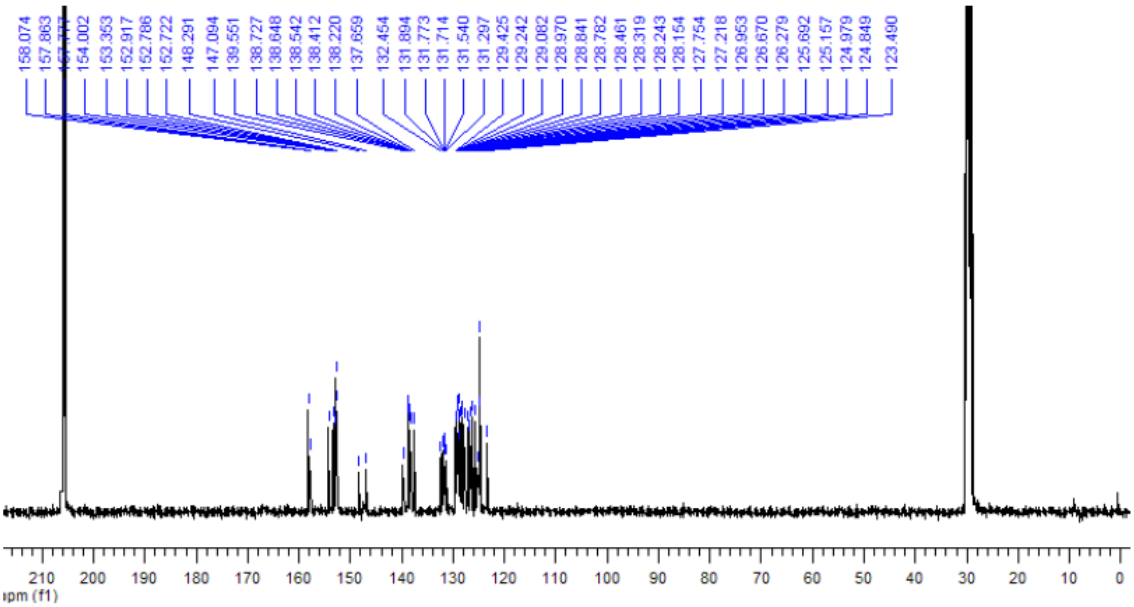


Figure S17. ^{13}C NMR of **5** (acetone-d_6, 100 MHz).

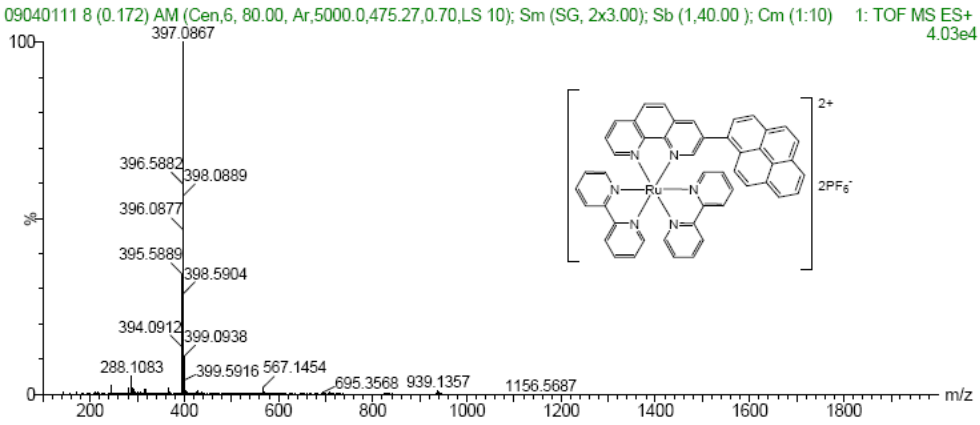
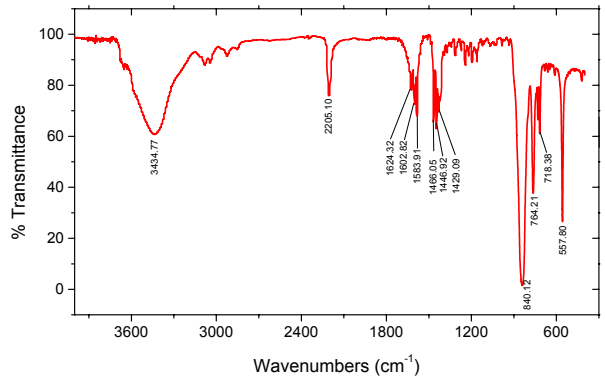
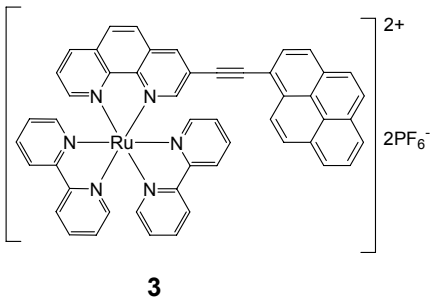


Figure S18. TOF ESI MS of **5.**





3

Figure S19-1. FT-IR of **3** (KBr disk).

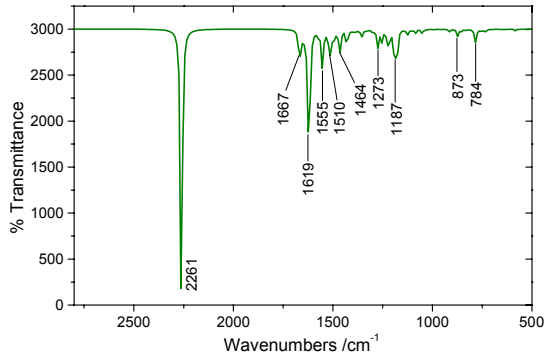
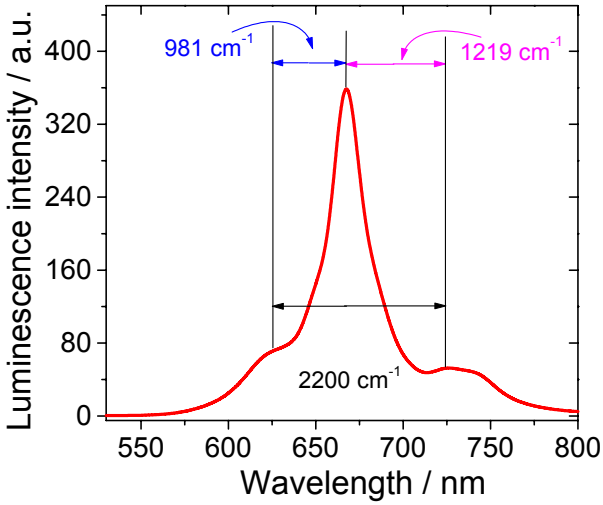
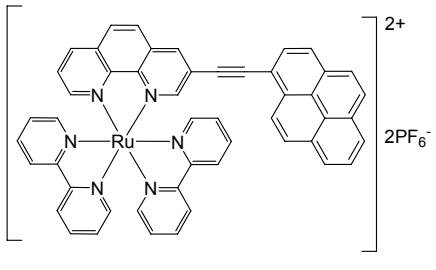


Figure S19-2. FT-IR of **3** (calculated by DFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.)





3

Figure S19-3. Room-temperature Fluorescence spectra of **3**. λex = 418 nm 1.0×10^{-5} mol/L solution in deoxygenated acetonitrile. 25°C.

The emission of complex **3** is centered at 626 nm, 667 nm and 726 nm. The vibration progression of 2200 cm^{-1} of the emission spectrum (energy difference between 726 nm and 626 nm) is due to the C≡C triple bond stretching vibration. The vibration progression of 981 cm^{-1} of the emission spectrum (energy difference between 667 nm and 626 nm) is due to the pyrene C–H wagging vibration. The vibration progression of 1219 cm^{-1} of the emission spectrum (energy difference between 667 nm and 726 nm) is due to the phenanthroline C–H rocking vibration.

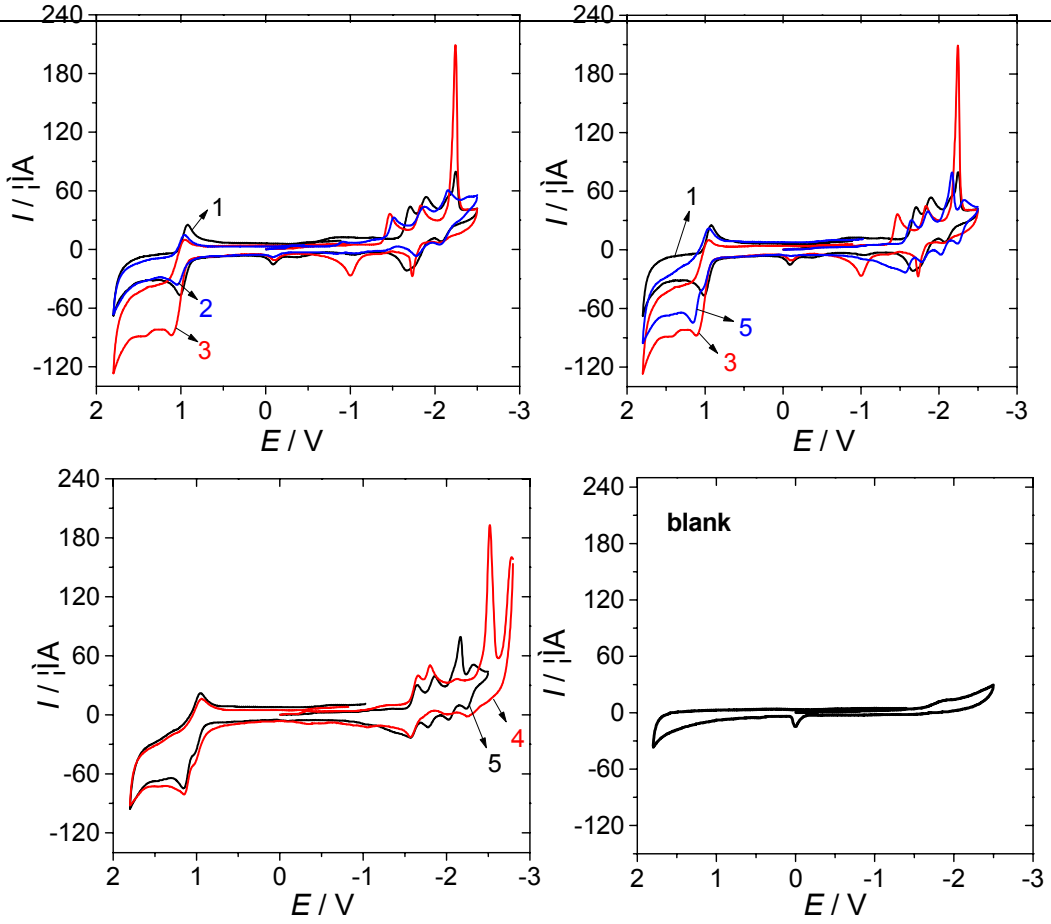
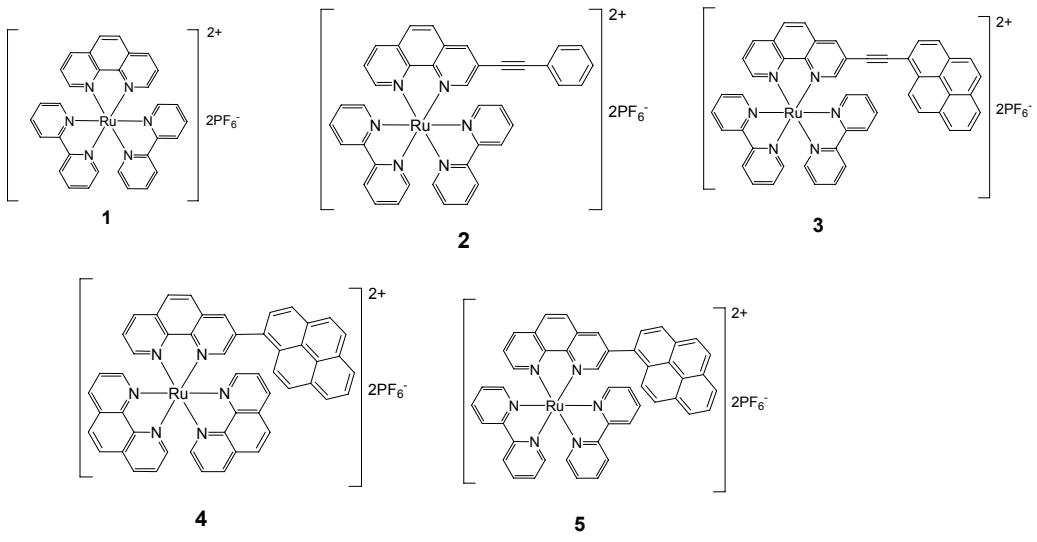


Figure S20. Cyclic voltammogram of $[(bpy)_2Ru(1,10\text{-phenanthroline})]^{2+}(PF_6)_2$ **1** and its derivatives **2**, **3**, **4**, **5** in argon-purged acetonitrile. 1.0 mM complex in 0.05 M n-Bu_4NPF_6 / CH_3CN at a scan rate of 200 mV/s.

Table S1. Electro potential of the complexes **1-5.**

complex	E_{ap} or $E_{1/2}$ (V)	E_{cp} or $E_{1/2}$ (V)
1	0.97	-1.68, -1.90, -2.25
2	1.01	-1.52(irr), -1.83, -2.10
3	1.45(irr), 1.04	-1.00(irr), -1.47(irr), -1.78, -2.24
4	1.15(irr), 0.97	-1.61, -1.80(irr), -2.06, -2.52(irr)
5	1.16(irr), 0.99	-1.61, -1.82, -2.10, -2.29



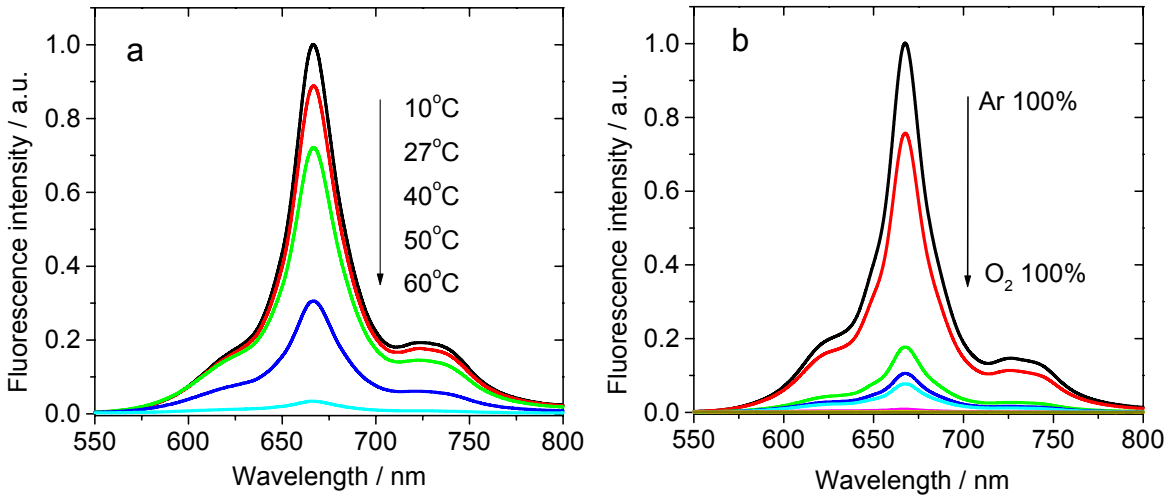
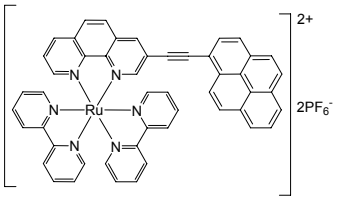


Figure S21. (a) Effect of elevated temperature (10–60°C) on the luminescence spectrum of complex **3** in deoxygenated acetonitrile solution (3.0×10^{-6} mol dm^{-3}, λ_{ex} = 421 nm). (b) The quenching of complex **3** with increasing the O_2 partial pressure at room temperature (1.0×10^{-5} mol dm^{-3} acetonitrile solution, λ_{ex} = 418 nm). Both of the spectrums are normalized.



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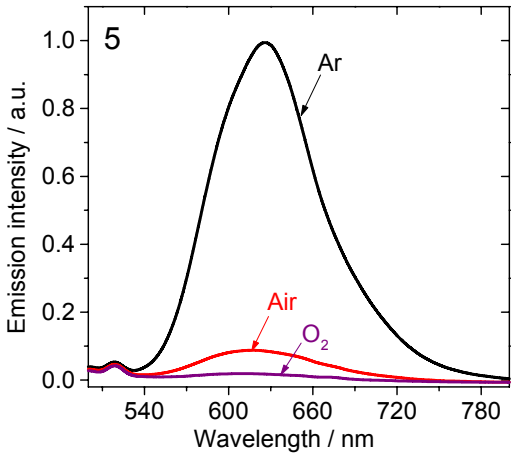
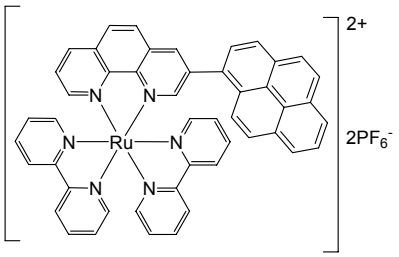




5

Figure S22. Room-temperature emission spectra of complex **5** under Ar, air and O_2 atmosphere. λ_{ex} = 450 nm, 1.0×10^{-5} mol/L complexes solution in acetonitrile. The spectra were normalized.

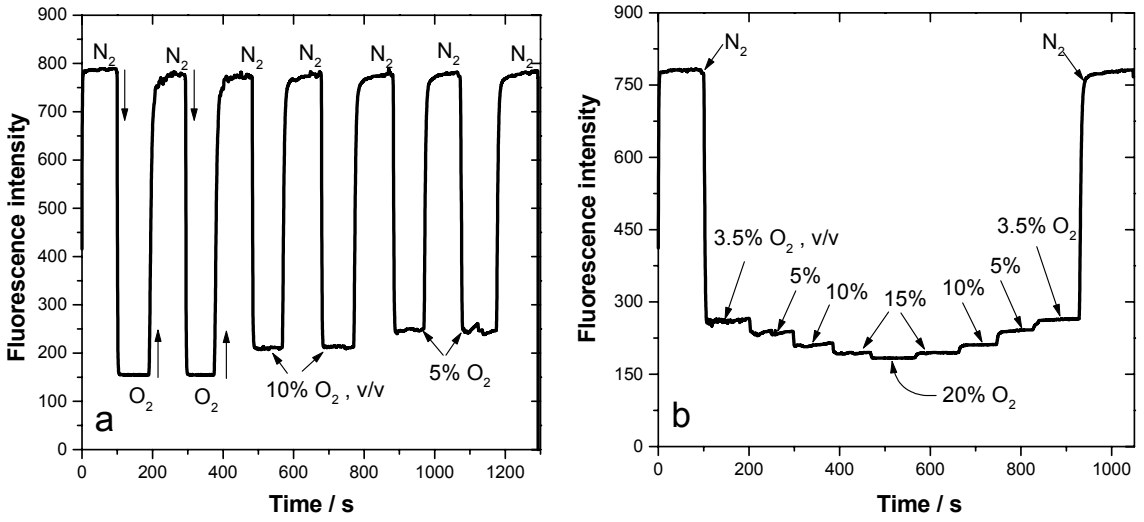
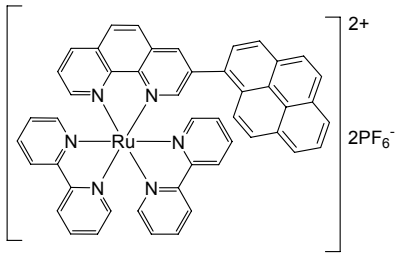


Figure S23. Phosphorescent intensity response of sensing films of the complex **5** in IMPES-C. a) Emission intensity response to O_2/N_2 saturation cycles; b) Emission intensity response to step variations of O_2 concentrations. λ_{ex}= 475 nm, λ_{em} = 641 nm. Measured with home assembled optical fiber/flow cell system.

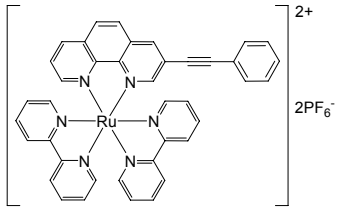


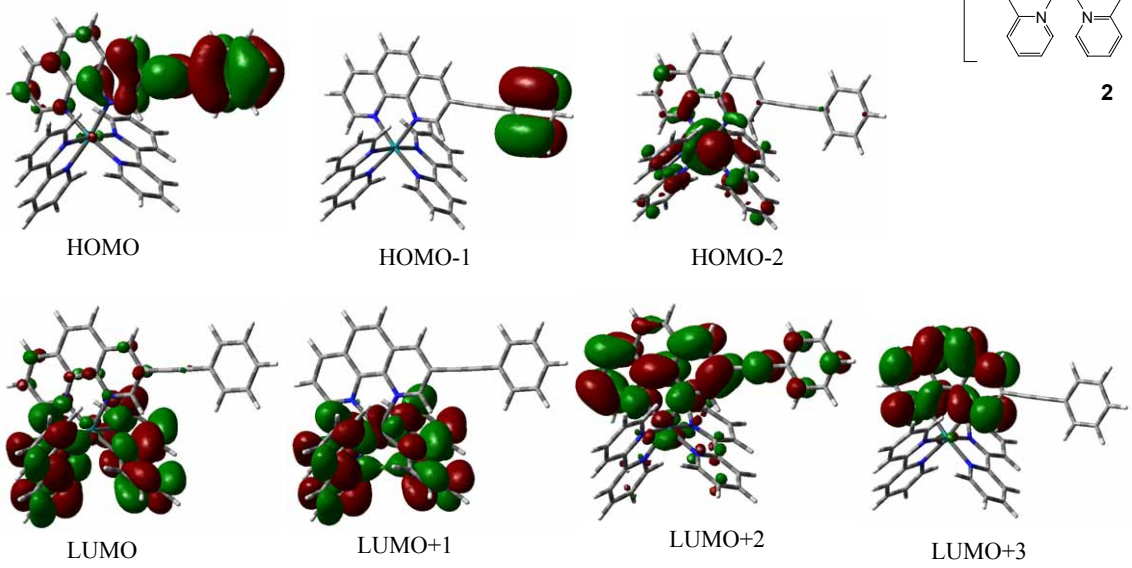
5

Table S2. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **2,** Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ , based on the Optimized Ground State Geometries.

2	**Electronic transition**	**TDDFT//B3LYP/6-31G(d)**				
		Energy (eV) [a]	***f*** [b]	**Composition** [c]	**CI** [d]	**character**
Singlet						
	$S_0 \rightarrow S_1$	2.40 eV (516 nm)	0.01	HOMO→LUMO	0.63	LL′CT [e]
				HOMO→LUMO+1	0.30	LL′CT/LMCT
	$S_0 \rightarrow S_3$	2.68 eV (462 nm)	0.44	HOMO−2→LUMO+2	0.13	MLCT
				HOMO→LUMO+2	0.63	ILCT/LMCT
				HOMO→LUMO+3	0.11	ILCT
Triplet						
	$S_0 \rightarrow T_1$ [f]	1.98 eV (627 nm)	0.00	HOMO−7→LUMO+2	0.13	ILCT
				HOMO−5→LUMO+3	0.11	ILCT/MLCT
				HOMO→LUMO	0.22	LL′CT
				HOMO→LUMO+2	0.65	ILCT/LMCT
				HOMO→LUMO+3	0.17	ILCT
				HOMO→LUMO+8	0.13	ILCT/LMCT
				HOMO→LUMO+9	0. 14	ILCT

[a] only the selected low-lying excited states are presented. [b] oscillator strength. [c] only the main configurations are presented. [d] the CI coefficients are in absolute values. [e] L: phenanthroline, L′: bispyridine. [f] no spin-orbital coupling effect was considered, thus the *f* values are zero.



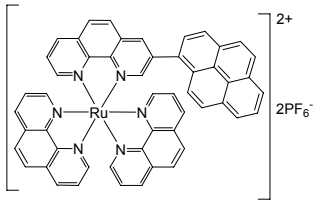


Scheme S4. Qualitative scheme of frontier molecular orbitals of complex **2** calculated by DFT/TDDFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.

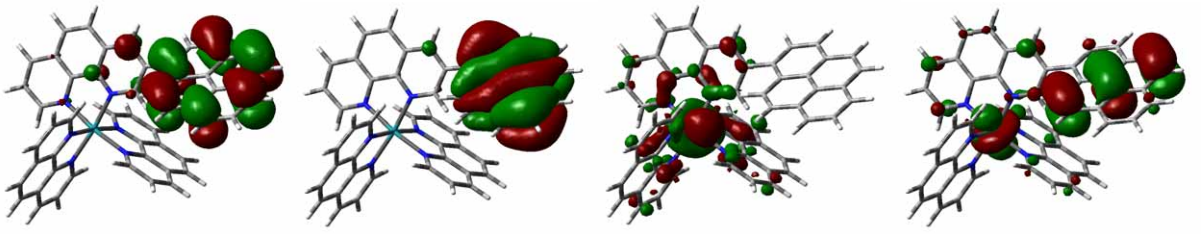
Table S3. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **4,** Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ , based on the Optimized Ground State Geometries.

4	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy (eV) [a]	*f* [b]	Composition [c]	CI [d]	character
Singlet	$S_0 \rightarrow S_1$	1.65 eV (752 nm)	0.01	HOMO→LUMO	0.65	LL′CT/LMCT
				HOMO→LUMO+1	0.27	LL′CT/LMCT
	$S_0 \rightarrow S_4$	1.87 eV (663 nm)	0.15	HOMO→LUMO+2	0.39	LL′CT
				HOMO→LUMO+3	0.51	ILCT/LL′CT
				HOMO→LUMO+4	0.15	LL′CT
				HOMO→LUMO+5	0.18	ILCT
Triplet	$S_0 \rightarrow T_1$ [f]	1.57 eV (788 nm)	0.00	HOMO→LUMO	0.42	LL′CT/LMCT
				HOMO→LUMO+1	0.12	LL′CT/LMCT
				HOMO→LUMO+2	0.15	LL′CT
				HOMO→LUMO+3	0.47	ILCT/LL′CT
				HOMO→LUMO+4	0.12	LL′CT
				HOMO→LUMO+5	0.19	ILCT
				HOMO→LUMO+8	0.13	ILCT/LL′CT
				HOMO→LUMO+9	0.16	ILCT

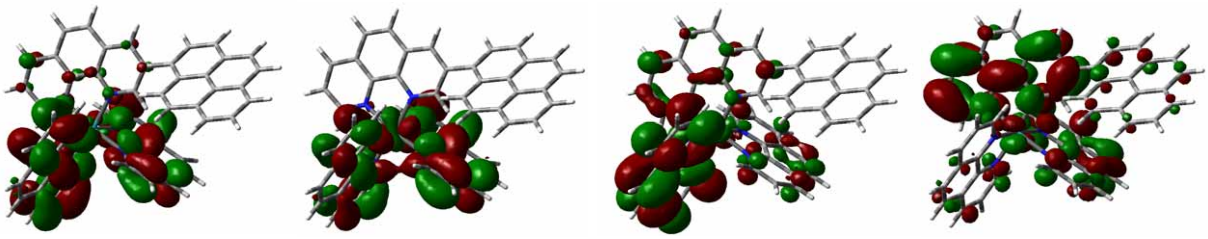
[a] only the selected low-lying excited states are presented. [b] oscillator strength. [c] only the main configurations are presented. [d] the CI coefficients are in absolute values. [e] L: phenanthroline, L′: bispyridine. [f] no spin-orbital coupling effect was considered, thus the *f* values are zero.



4



HOMO-200 199 198 197



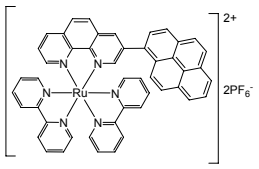
LUMO-201 202 203 204

Scheme S5. Qualitative scheme of frontier molecular orbitals of complex **4** calculated by DFT/TDDFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.

Table S4. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **5,** Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ , based on the Optimized Ground State Geometries.

5	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy (eV) [a]	*f* [b]	Composition [c]	CI [d]	character
Singlet	$S_0 \rightarrow S_1$	1.44 eV (862 nm)	0.00	HOMO→LUMO	0.62	LL′CT [e]
				HOMO→LUMO+1	0.34	LL′CT/LMCT
	$S_0 \rightarrow S_3$	1.72 eV (723 nm)	0.14	HOMO→LUMO+2	0.63	ILCT/LMCT
				HOMO→LUMO+3	0.26	ILCT
	$S_0 \rightarrow S_{19}$	3.01 eV (412 nm)	0.12	HOMO-5→LUMO	0.14	LL′CT/MLCT
				HOMO-4→LUMO+1	0.11	LL′CT/MLCT
				HOMO→LUMO+8	0.62	ILCT
				HOMO→LUMO+9	0.13	ILCT
	$S_0 \rightarrow S_{20}$	3.02 eV (411 nm)	0.16	HOMO-6→LUMO	0.26	ML′CT/LL′CT
				HOMO-5→LUMO	0.47	ML′CT/LL′CT
				HOMO-4→LUMO+1	0.28	ML′CT/LL′CT
				HOMO-3→LUMO+2	0.23	MLCT
				HOMO→LUMO+8	0.19	ILCT
Triplet	$S_0 \rightarrow T_1$ [f]	1.42 eV (872 nm)	0.00	HOMO→LUMO	0.60	LL′CT
				HOMO→LUMO+1	0.25	LL′CT/LMCT
				HOMO→LUMO+2	0.28	ILCT/LMCT

[a] only the selected low-lying excited states are presented. [b] oscillator strength. [c] only the main configurations are presented. [d] the CI coefficients are in absolute values. [e] L: phenanthroline, L′: bispyridine. [f] no spin-orbital coupling effect was considered, thus the *f* values are zero.



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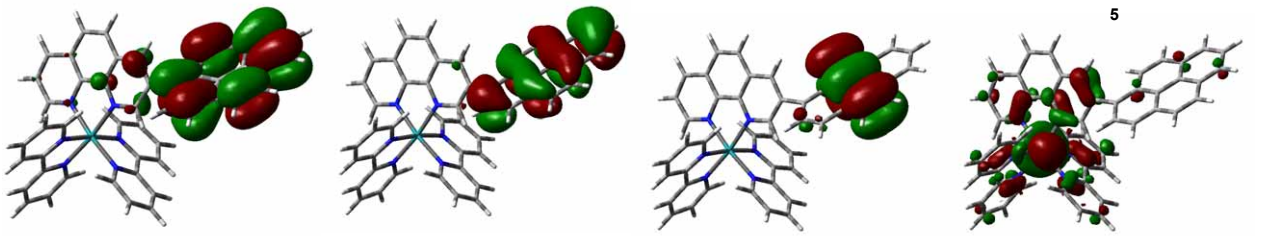
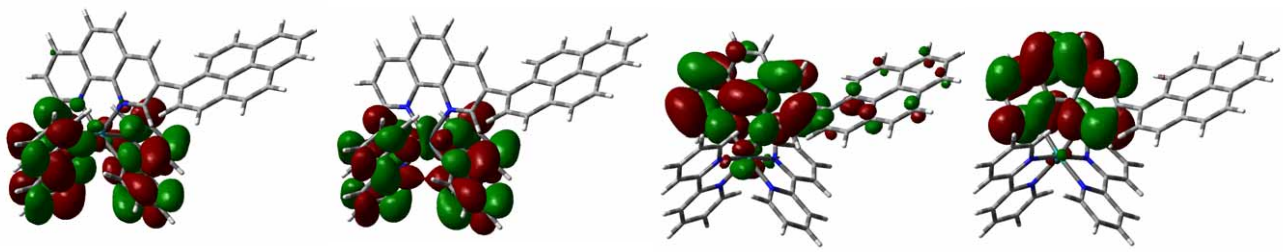


HOMO-188 187 186 185



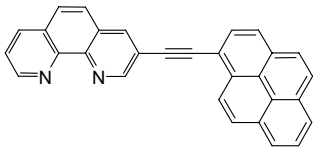
LUMO-189 190 191 192

Scheme S6. Qualitative scheme of frontier molecular orbitals of complex **5** calculated by DFT/TDDFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.

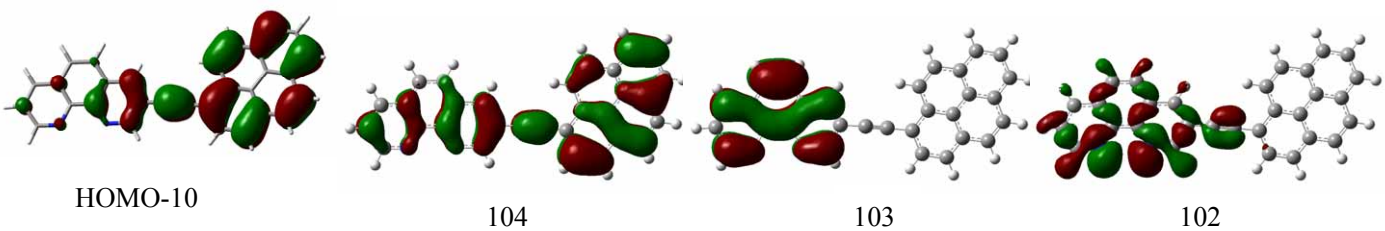
Table S5. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of ligand of **3**, Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ , based on the Optimized Ground State Geometries.

Ligand of **3**	**Electronic transition**	**TDDFT//B3LYP/6-31G(d)**			
		Energy (eV) [a]	***f*** [b]	**Composition** [c]	**CI** [d]
Singlet					
	$S_0 \rightarrow S_1$	2.96 eV (419 nm)	1.18	HOMO→LUMO	0.64
	$S_0 \rightarrow S_2$	3.41 eV (364 nm)	0.01	HOMO−2→LUMO	0.20
				HOMO→LUMO+1	0.65
	$S_0 \rightarrow S_7$	3.94 eV (315 nm)	0.25	HOMO−4→LUMO	0.41
				HOMO−1→LUMO	0.39
Triplet					
	$S_0 \rightarrow T_1$ [e]	1.82 eV (682 nm)	0.00	HOMO−6→LUMO+5	0.11
				HOMO−4→LUMO+3	0.10
				HOMO−1→LUMO+2	0.15
				HOMO−1→LUMO+3	0.11
				HOMO→LUMO	0.75
				HOMO→LUMO+2	0.24

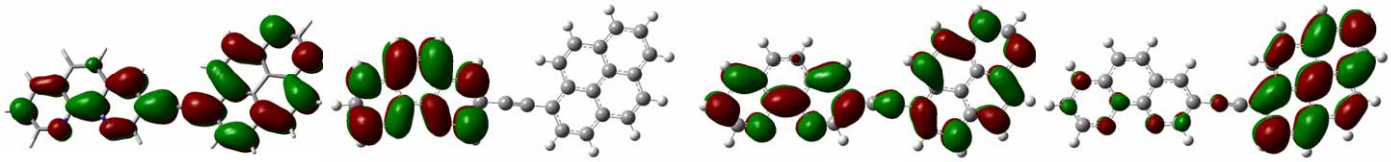
[a] only the selected low-lying excited states are presented. [b] oscillator strength. [c] only the main configurations are presented. [d] the CI coefficients are in absolute values. [e] no spin-orbital coupling effect was considered, thus the *f* values are zero.



Ligand of complex **3**



HOMO-10 104 103 102



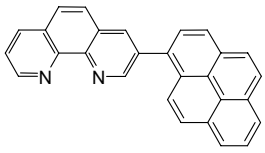
LUMO-106 108 109

Scheme S7. Qualitative scheme of frontier molecular orbitals of the ligand of **3** calculated by DFT/TDDFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.

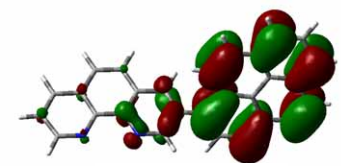
Table S6. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of the ligand of **4**, Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ , based on the Optimized Ground State Geometries.

Ligand of **4**	**Electronic transition**	**TDDFT//B3LYP/6-31G(d)**			
		Energy (eV) [a]	***f*** [b]	**Composition** [c]	**CI** [d]
Singlet					
	$S_0 \rightarrow S_1$	3.31eV (374 nm)	0.46	HOMO→LUMO	0.60
				HOMO→LUMO+1	0.18
				HOMO→LUMO+2	0.22
				HOMO−1→LUMO	0.39
Triplet					
	$S_0 \rightarrow T_1$	2.04eV (606 nm)	0.00	HOMO−7→LUMO+6	0.11
				HOMO−6→LUMO+5	0.12
				HOMO−2→LUMO+3	0.14
				HOMO→LUMO	0.74
				HOMO→LUMO+2	0.29

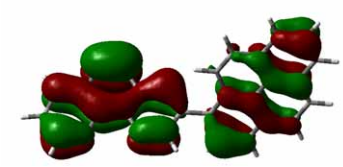
[a] only the selected low-lying excited states are presented. [b] oscillator strength. [c] only the main configurations are presented. [d] the CI coefficients are in absolute values.



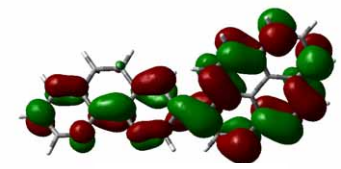
Ligand of complex **4**



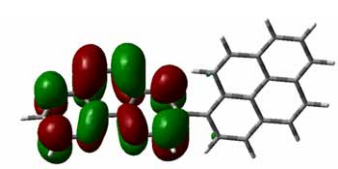
HOMO-99



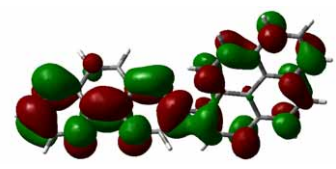
98



LUMO-100



101



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Scheme S8. Qualitative scheme of frontier molecular orbitals of the ligand of **4** calculated by DFT/TDDFT at the B3LYP/6-31G((d)/ LanL2DZ level using Gaussian 03.

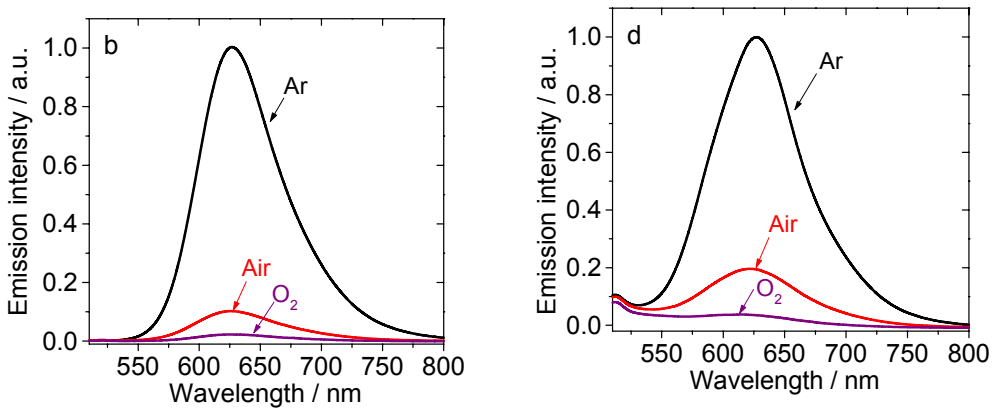


Figure S24. Room-temperature emission spectra of complexes **2** and **4** under Ar, air and O_2 atmosphere. (a) complex **2**, λ_{ex} = 450 nm, (b) complex **4**, λ_{ex} = 445 nm. 1.0× 10^{-5} mol/L complexes solution in acetonitrile. The spectra were normalized.

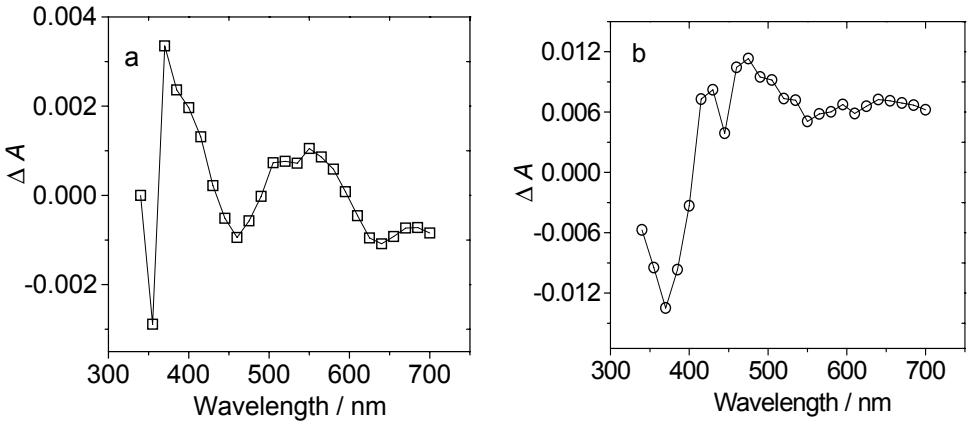


Figure S25. Time-resolved transient absorption spectra measured in deoxygenated acetonitrile at room temperature after pulsed excitation (λex = 532 nm). (a) complex **2**, (b) complex **4**.

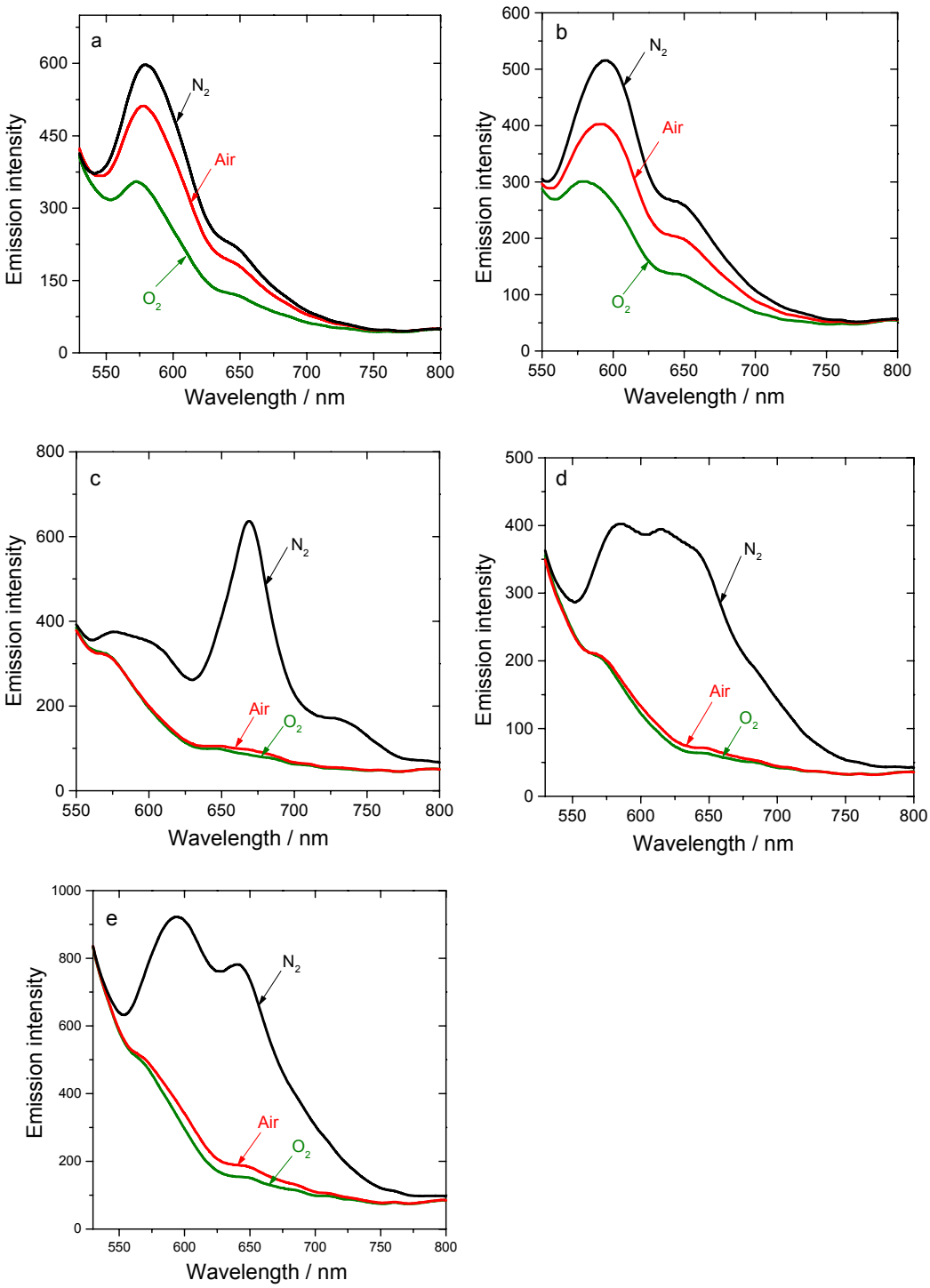


Figure S26. Emission spectra of the oxygen sensing films used in the study. (a), complex **1**, λex = 475 nm, λem = 578 nm; (b) complex **2**, λex = 477 nm, λem = 596 nm; (c) complex **3**, λex = 476 nm, λem = 669 nm; (d) complex **4**, λex = 475 nm, λem = 615 nm; (e) complex **5**, λex = 475 nm, λem = 641 nm

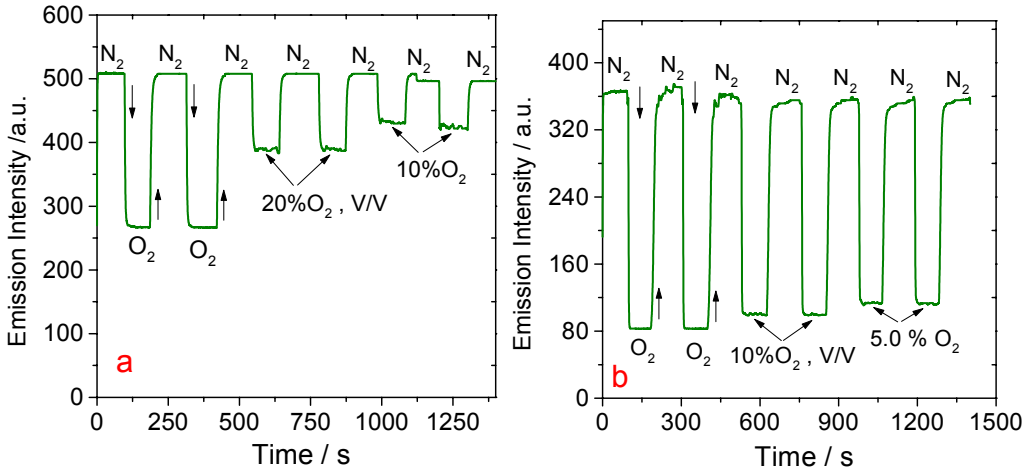


Figure S27. Phosphorescent intensity response of sensing films of the complexes in IMPES-C to O_2/N_2 saturation cycles. (a) complex **2**, λ_{ex}= 477 nm, λ_{em}= 596 nm; (b) complex **4**, λ_{ex}= 475 nm, λ_{em} = 615 nm. In order to compare the quenching properties of the films, the y axel are set from 0. Measured with optical fiber/flow cell system.

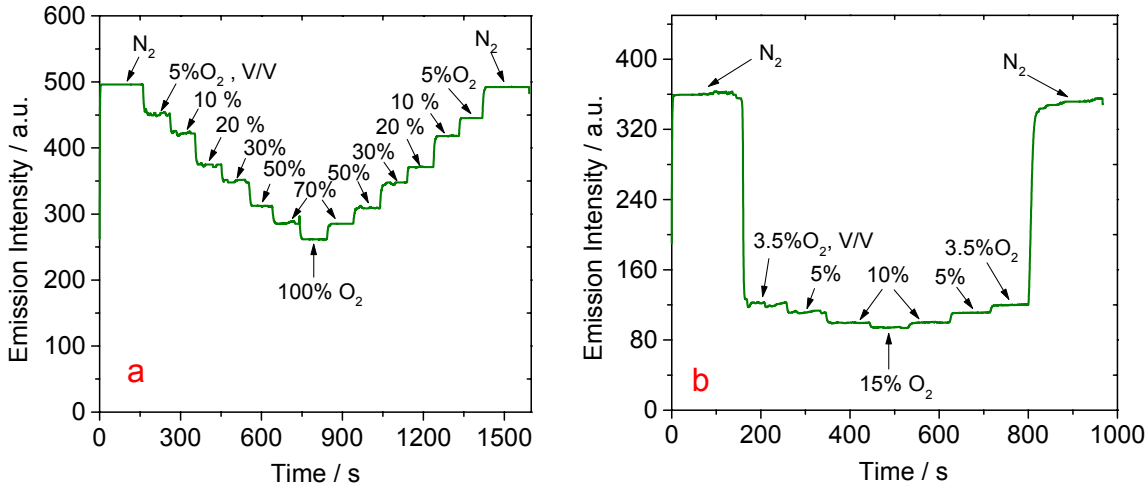
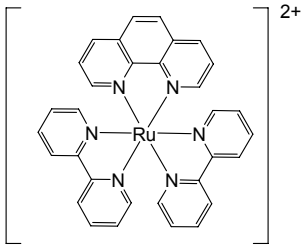


Figure S28. Phosphorescent intensity response of sensing films of the complexes in IMPES-C to step variations of O_2 concentrations. (a) complex **2**, λ_{ex}= 477 nm, λ_{em}= 596 nm; (b) complex **4**, λ_{ex}= 475 nm, λ_{em}=615 nm. In order to

compare the quenching efficiencies of the films, the y axels are set from 0 for all the figures. Measured with home assembled optical fiber/flow cell system. The numbers indicate the O_2 concentration in mixed O_2/N_2 gas (V/V).

Z-matrix, number of imaginary frequencies and total energy of $[(bpy)_2Ru(1,10\text{-phenanthroline})]^{2+}$ and its derivatives (there are no imaginary frequencies for all the structures).

complex 1 （DFT//B3LYP/6-31G(d)/ LanL2DZ）



Symbolic Z-matrix:

Charge = 2 Multiplicity = 1

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C	3	B3	2	A2	1	D1	0
C	1	B4	2	A3	3	D2	0
C	3	B5	2	A4	1	D3	0
C	4	B6	3	A5	2	D4	0
C	7	B7	4	A6	3	D5	0
C	6	B8	3	A7	2	D6	0
C	8	B9	7	A8	4	D7	0
H	10	B10	8	A9	7	D8	0
C	10	B11	8	A10	7	D9	0
C	12	B12	10	A11	8	D10	0
H	6	B13	3	A12	2	D11	0
H	1	B14	2	A13	3	D12	0
H	2	B15	1	A14	5	D13	0
H	5	B16	1	A15	2	D14	0
H	9	B17	6	A16	3	D15	0
H	12	B18	10	A17	8	D16	0
H	13	B19	12	A18	10	D17	0
N	13	B20	12	A19	10	D18	0
N	5	B21	1	A20	2	D19	0
H	22	B22	5	A21	1	D20	0
C	5	B23	1	A22	2	D21	0
C	24	B24	5	A23	1	D22	0
C	24	B25	5	A24	1	D23	0
C	25	B26	24	A25	5	D24	0
H	25	B27	24	A26	5	D25	0
C	27	B28	25	A27	24	D26	0

C	26	B29	24	A28	5	D27	0
H	27	B30	25	A29	24	D28	0
H	29	B31	27	A30	25	D29	0
C	30	B32	26	A31	24	D30	0
C	30	B33	26	A32	24	D31	0
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H	33	B35	30	A34	26	D33	0
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H	34	B37	30	A36	26	D35	0
H	35	B38	33	A37	30	D36	0
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H	53	B55	52	A54	50	D53	0
C	54	B56	52	A55	50	D54	0
H	54	B57	52	A56	50	D55	0
H	55	B58	53	A57	52	D56	0
H	57	B59	54	A58	52	D57	0
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Variables:

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B9	1.41325

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B26	1.39452
B27	1.08461
B28	1.39233
B29	1.47753
B30	1.08526
B31	1.08318
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B33	2.3345
B34	1.39231
B35	1.08323
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B37	1.08353
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B47	1.39231
B48	1.08527
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A34	120.49786
A35	92.12448

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A38	119.82092
A39	30.75638
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D39	-152.10199
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D41	-105.21028
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D43	-132.71062
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D45	3.85292
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D49	179.86371
D50	-1.51724
D51	178.37318
D52	179.87962
D53	-0.27747
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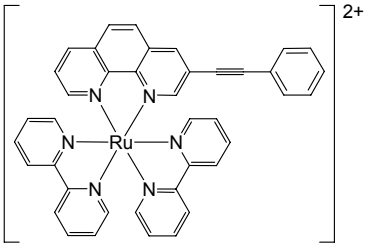
.....

SCF Done: E(RB+HF-LYP) = -1655.96186472 Hartree
Number of Imaginary frequencies: 0

complex 2 （DFT//B3LYP/6-31G(d)/ LanL2DZ）



Symbolic Z-matrix:
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C	3	B5	2	A4	1	D3	0
C	4	B6	3	A5	2	D4	0
C	7	B7	4	A6	3	D5	0
C	6	B8	3	A7	2	D6	0
C	8	B9	7	A8	4	D7	0
H	10	B10	8	A9	7	D8	0
C	10	B11	8	A10	7	D9	0
C	12	B12	10	A11	8	D10	0
H	6	B13	3	A12	2	D11	0
H	1	B14	2	A13	3	D12	0
H	2	B15	1	A14	5	D13	0
H	5	B16	1	A15	2	D14	0
H	9	B17	6	A16	3	D15	0
H	13	B18	12	A17	10	D16	0
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H	26	B29	24	A28	23	D27	0
H	28	B30	26	A29	24	D28	0
C	29	B31	25	A30	23	D29	0

C	29	B32	25	A31	23	D30	0
C	32	B33	29	A32	25	D31	0
H	32	B34	29	A33	25	D32	0
C	33	B35	29	A34	25	D33	0
H	33	B36	29	A35	25	D34	0
H	34	B37	32	A36	29	D35	0
H	36	B38	33	A37	29	D36	0
N	33	B39	29	A38	25	D37	0
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H	21	B41	5	A40	1	D39	0
C	21	B42	5	A41	1	D40	0
C	43	B43	21	A42	5	D41	0
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C	45	B46	43	A45	21	D44	0
H	45	B47	43	A46	21	D45	0
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H	67	B70	65	A69	64	D68	0
C	68	B71	66	A70	65	D69	0
H	68	B72	66	A71	65	D70	0
H	70	B73	67	A72	65	D71	0
H	72	B74	68	A73	66	D72	0

Variables:

B1	1.3839
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B9	1.40563
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B11	1.40006
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B13	1.08591
B14	1.08456
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B16	1.08431
B17	1.08581
B18	1.08389
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B27	1.39222
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B29	1.08527
B30	1.08324
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B35	1.39097
B36	1.08346
B37	1.08527
B38	1.08461
B39	1.34684
B40	1.34695
B41	5.12658
B42	4.66761
B43	1.3909
B44	1.3944

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B46	1.39232
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B48	1.39894
B49	1.08319
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B51	1.39907
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B65	1.41178
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B67	1.39076
B68	1.08531
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B71	1.39847
B72	1.08564
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B74	1.08591
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A7	121.14731
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A9	120.16033
A10	120.09461
A11	117.50182
A12	118.45191
A13	121.2521
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D16	-179.81396
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D18	0.01209
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D20	-150.77139
D21	-43.57454
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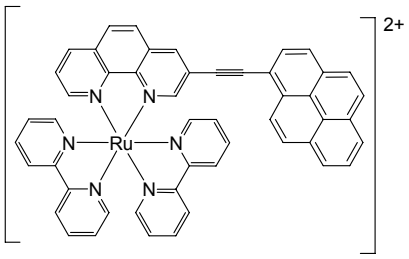
D69	-0.05945
D70	179.96515
D71	179.93371
D72	-179.95982

.....

SCF Done: E(RB+HF-LYP) = -1963.17416954 Hartree
Number of Imaginary frequencies: 0

Complex 3 （DFT//B3LYP/6-31G(d)/ LanL2DZ）



Symbolic Z-matrix:
Charge = 2 Multiplicity = 1

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	1	B5	2	A4	3	D3	0
C	5	B6	4	A5	3	D4	0
C	7	B7	5	A6	4	D5	0
C	8	B8	7	A7	5	D6	0
C	9	B9	8	A8	7	D7	0
N	7	B10	5	A9	4	D8	0
C	11	B11	7	A10	5	D9	0
C	12	B12	11	A11	7	D10	0
C	13	B13	12	A12	11	D11	0
Ru	11	B14	7	A13	5	D12	0
C	15	B15	11	A14	7	D13	0
C	16	B16	15	A15	11	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
C	19	B19	18	A18	17	D17	0
N	16	B20	15	A19	11	D18	0
C	20	B21	19	A20	18	D19	0
C	22	B22	20	A21	19	D20	0
C	23	B23	22	A22	20	D21	0
C	24	B24	23	A23	22	D22	0
C	25	B25	24	A24	23	D23	0
N	26	B26	25	A25	24	D24	0
C	15	B27	11	A26	7	D25	0
C	28	B28	15	A27	11	D26	0
C	29	B29	28	A28	15	D27	0
N	30	B30	29	A29	28	D28	0
C	31	B31	30	A30	29	D29	0
C	28	B32	15	A31	11	D30	0

C	32	B33	31	A32	30	D31	0
N	34	B34	32	A33	31	D32	0
C	35	B35	34	A34	32	D33	0
C	36	B36	35	A35	34	D34	0
C	37	B37	36	A36	35	D35	0
C	38	B38	37	A37	36	D36	0
H	1	B39	6	A38	5	D37	0
H	3	B40	2	A39	1	D38	0
H	9	B41	8	A40	7	D39	0
H	10	B42	9	A41	8	D40	0
H	12	B43	11	A42	7	D41	0
H	13	B44	12	A43	11	D42	0
H	14	B45	13	A44	12	D43	0
H	16	B46	15	A45	11	D44	0
H	17	B47	16	A46	15	D45	0
H	18	B48	17	A47	16	D46	0
H	19	B49	18	A48	17	D47	0
H	23	B50	22	A49	20	D48	0
H	24	B51	23	A50	22	D49	0
H	25	B52	24	A51	23	D50	0
H	26	B53	25	A52	24	D51	0
H	28	B54	15	A53	11	D52	0
H	29	B55	28	A54	15	D53	0
H	30	B56	29	A55	28	D54	0
H	33	B57	28	A56	15	D55	0
H	36	B58	35	A57	34	D56	0
H	37	B59	36	A58	35	D57	0
H	38	B60	37	A59	36	D58	0
H	39	B61	38	A60	37	D59	0
C	2	B62	1	A61	6	D60	0
C	63	B63	2	A62	1	D61	0
C	64	B64	63	A63	2	D62	0
C	65	B65	64	A64	63	D63	0
C	65	B66	64	A65	63	D64	0
C	66	B67	65	A66	64	D65	0
C	66	B68	65	A67	64	D66	0
C	67	B69	65	A68	64	D67	0
H	67	B70	65	A69	64	D68	0
C	68	B71	66	A70	65	D69	0
C	70	B72	67	A71	65	D70	0
C	69	B73	66	A72	65	D71	0
H	69	B74	66	A73	65	D72	0
H	70	B75	67	A74	65	D73	0
C	72	B76	68	A75	66	D74	0

C	72	B77	68	A76	66	D75	0
C	73	B78	70	A77	67	D76	0
H	74	B79	69	A78	66	D77	0
C	77	B80	72	A79	68	D78	0
C	78	B81	72	A80	68	D79	0
C	79	B82	73	A81	70	D80	0
H	79	B83	73	A82	70	D81	0
C	81	B84	77	A83	72	D82	0
H	81	B85	77	A84	72	D83	0
H	82	B86	78	A85	72	D84	0
H	83	B87	79	A86	73	D85	0
H	85	B88	81	A87	77	D86	0

Variables:

B1	1.40444
B2	1.42756
B3	1.32774
B4	1.3719
B5	1.40296
B6	1.42715
B7	1.41915
B8	1.43752
B9	1.36287
B10	1.36984
B11	1.33756
B12	1.40264
B13	1.38523
B14	2.12637
B15	3.09638
B16	1.39077
B17	1.39455
B18	1.39213
B19	1.39908
B20	1.34699
B21	1.47751
B22	1.39903
B23	1.3923
B24	1.39449
B25	1.39091
B26	1.34693
B27	4.90328
B28	1.39448
B29	1.39062
B30	1.3469
B31	1.36356

B32	1.39202
B33	1.47735
B34	1.36336
B35	1.3468
B36	1.39086
B37	1.39435
B38	1.39223
B39	1.08521
B40	1.08395
B41	1.08596
B42	1.08588
B43	1.08433
B44	1.0845
B45	1.08624
B46	1.08361
B47	1.08461
B48	1.08527
B49	1.08325
B50	1.08322
B51	1.08527
B52	1.0846
B53	1.08357
B54	1.08527
B55	1.08462
B56	1.08351
B57	1.08318
B58	1.08332
B59	1.08459
B60	1.08525
B61	1.0832
B62	1.4053
B63	1.22374
B64	1.40851
B65	1.42985
B66	1.41625
B67	1.42787
B68	1.43068
B69	1.38008
B70	1.08567
B71	1.42655
B72	1.41204
B73	1.36577
B74	1.08523
B75	1.08636

B76	1.42612
B77	1.42765
B78	1.43075
B79	1.08703
B80	1.40639
B81	1.40563
B82	1.36574
B83	1.08647
B84	1.39343
B85	1.08682
B86	1.08669
B87	1.08677
B88	1.08567
A1	117.1692
A2	123.6392
A3	118.86487
A4	120.18461
A5	117.69742
A6	119.98433
A7	118.71421
A8	121.19757
A9	117.61923
A10	118.35613
A11	122.83714
A12	119.34539
A13	113.07092
A14	97.02531
A15	156.6391
A16	118.63202
A17	118.85403
A18	119.86424
A19	33.77534
A20	123.60696
A21	123.62261
A22	119.81676
A23	118.85926
A24	118.67732
A25	122.79671
A26	170.76277
A27	61.3989
A28	118.64641
A29	122.88523
A30	118.90235
A31	57.4435

A32	115.55368
A33	115.50921
A34	118.9286
A35	122.8546
A36	118.6553
A37	118.83977
A38	120.10275
A39	119.45934
A40	118.41248
A41	120.37628
A42	116.34566
A43	119.38967
A44	120.76685
A45	82.13043
A46	119.83188
A47	120.87834
A48	119.67049
A49	120.47959
A50	120.26376
A51	121.53261
A52	121.2679
A53	177.68006
A54	121.54367
A55	121.14898
A56	119.7022
A57	115.88536
A58	119.80376
A59	120.88987
A60	119.67473
A61	122.98177
A62	179.50192
A63	179.17337
A64	121.21761
A65	118.98159
A66	118.57928
A67	122.72235
A68	121.15807
A69	118.68526
A70	119.91136
A71	120.87448
A72	121.23214
A73	118.59352
A74	120.05729
A75	120.21601

A76	120.12401
A77	121.78771
A78	120.06673
A79	119.24813
A80	119.12148
A81	121.10383
A82	118.5228
A83	120.75088
A84	119.19775
A85	119.14213
A86	120.20023
A87	119.84302
D1	-0.09936
D2	0.11456
D3	0.08218
D4	-179.67488
D5	179.51503
D6	0.20993
D7	-0.13409
D8	-0.66123
D9	179.59949
D10	0.41028
D11	-0.02627
D12	-0.09922
D13	-163.85814
D14	-90.26657
D15	1.01319
D16	0.08887
D17	0.0227
D18	-88.53994
D19	179.84003
D20	-1.60163
D21	179.82918
D22	-0.01858
D23	0.1343
D24	-0.16406
D25	-58.99658
D26	152.6088
D27	-0.31256
D28	-0.12201
D29	0.13944
D30	-27.02733
D31	179.72199
D32	-1.95525

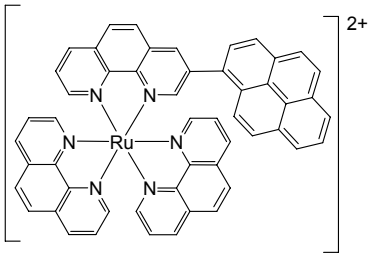
D33	-179.69301
D34	0.11012
D35	-0.21562
D36	0.14307
D37	180.
D38	-179.94213
D39	179.90218
D40	-179.98716
D41	-179.84856
D42	179.90247
D43	179.86588
D44	90.50062
D45	-178.93883
D46	-179.88232
D47	-179.86287
D48	-0.3219
D49	179.9373
D50	-180.
D51	179.9605
D52	-37.73838
D53	179.58334
D54	-179.98006
D55	-179.40403
D56	179.99592
D57	179.94295
D58	-179.79261
D59	-179.81152
D60	-179.86142
D61	6.4694
D62	175.28328
D63	177.67322
D64	-2.33062
D65	-179.948
D66	0.02746
D67	179.96289
D68	-0.07994
D69	179.97937
D70	0.
D71	-180.
D72	0.01145
D73	179.97012
D74	0.00796
D75	-179.98956
D76	-179.98327

D77	-179.97683
D78	179.99606
D79	-180.
D80	-179.9875
D81	-0.00605
D82	0.0132
D83	-179.98994
D84	179.97883
D85	179.97863
D86	179.99456

.....

SCF Done: E(RB+HF-LYP) = -2346.69665205 Hartree
Number of Imaginary frequencies: 0

complex 4 （DFT//B3LYP/6-31G(d)/ LanL2DZ）



Symbolic Z-matrix:
Charge = 2 Multiplicity = 1

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	1	B4	2	A3	3	D2	0
C	3	B5	2	A4	1	D3	0
C	4	B6	3	A5	2	D4	0
C	7	B7	4	A6	3	D5	0
C	6	B8	3	A7	2	D6	0
C	8	B9	7	A8	4	D7	0
H	10	B10	8	A9	7	D8	0
C	10	B11	8	A10	7	D9	0
C	12	B12	10	A11	8	D10	0
H	1	B13	2	A12	3	D11	0
H	2	B14	1	A13	5	D12	0
H	5	B15	1	A14	2	D13	0
H	13	B16	12	A15	10	D14	0

N	5	B17	1	A16	2	D15	0
N	13	B18	12	A17	10	D16	0
Ru	18	B19	5	A18	1	D17	0
H	20	B20	18	A19	5	D18	0
C	20	B21	18	A20	5	D19	0
C	22	B22	20	A21	18	D20	0
C	23	B23	22	A22	20	D21	0
H	23	B24	22	A23	20	D22	0
C	22	B25	20	A24	18	D23	0
C	24	B26	23	A25	22	D24	0
H	24	B27	23	A26	22	D25	0
C	26	B28	22	A27	20	D26	0
C	27	B29	24	A28	23	D27	0
C	29	B30	26	A29	22	D28	0
C	30	B31	27	A30	24	D29	0
H	30	B32	27	A31	24	D30	0
C	31	B33	29	A32	26	D31	0
C	29	B34	26	A33	22	D32	0
H	32	B35	30	A34	27	D33	0
C	34	B36	31	A35	29	D34	0
H	34	B37	31	A36	29	D35	0
H	35	B38	29	A37	26	D36	0
H	37	B39	34	A38	31	D37	0
N	22	B40	20	A39	18	D38	0
N	35	B41	29	A40	26	D39	0
H	20	B42	18	A41	5	D40	0
C	20	B43	18	A42	5	D41	0
C	44	B44	20	A43	18	D42	0
C	44	B45	20	A44	18	D43	0
C	45	B46	44	A45	20	D44	0
H	45	B47	44	A46	20	D45	0
C	46	B48	44	A47	20	D46	0
C	46	B49	44	A48	20	D47	0
C	47	B50	45	A49	44	D48	0
C	47	B51	45	A50	44	D49	0
H	50	B52	46	A51	44	D50	0
C	50	B53	46	A52	44	D51	0
C	51	B54	47	A53	45	D52	0
H	51	B55	47	A54	45	D53	0
C	54	B56	50	A55	46	D54	0
H	54	B57	50	A56	46	D55	0
C	55	B58	51	A57	47	D56	0
H	55	B59	51	A58	47	D57	0
H	57	B60	54	A59	50	D58	0

H	59	B61	55	A60	51	D59	0
N	57	B62	54	A61	50	D60	0
N	59	B63	55	A62	51	D61	0
H	12	B64	10	A63	8	D62	0
C	12	B65	10	A64	8	D63	0
C	66	B66	12	A65	10	D64	0
C	66	B67	12	A66	10	D65	0
C	67	B68	66	A67	12	D66	0
H	67	B69	66	A68	12	D67	0
C	68	B70	66	A69	12	D68	0
C	69	B71	67	A70	66	D69	0
C	69	B72	67	A71	66	D70	0
C	71	B73	68	A72	66	D71	0
C	72	B74	69	A73	67	D72	0
C	73	B75	69	A74	67	D73	0
H	73	B76	69	A75	67	D74	0
C	74	B77	71	A76	68	D75	0
H	74	B78	71	A77	68	D76	0
C	75	B79	72	A78	69	D77	0
C	75	B80	72	A79	69	D78	0
H	76	B81	73	A80	69	D79	0
H	78	B82	74	A81	71	D80	0
C	80	B83	75	A82	72	D81	0
C	81	B84	75	A83	72	D82	0
C	85	B85	81	A84	75	D83	0
H	84	B86	80	A85	75	D84	0
H	85	B87	81	A86	75	D85	0
H	86	B88	85	A87	81	D86	0
H	9	B89	6	A88	3	D87	0
H	6	B90	3	A89	2	D88	0

Variables:

B1	1.38859
B2	1.41511
B3	1.41945
B4	1.40658
B5	1.4396
B6	1.4258
B7	1.4166
B8	1.36818
B9	1.41228
B10	1.08456
B11	1.39917
B12	1.42175
B13	1.083

B14	1.08454
B15	1.08173
B16	1.08107
B17	1.34692
B18	1.34252
B19	2.11841
B20	3.21678
B21	3.13369
B22	1.40739
B23	1.38721
B24	1.08295
B25	2.34076
B26	1.41627
B27	1.08441
B28	1.42823
B29	1.43906
B30	1.41812
B31	1.36837
B32	1.08445
B33	1.41639
B34	2.34114
B35	1.08446
B36	1.38743
B37	1.08445
B38	1.08147
B39	1.08305
B40	1.34608
B41	1.34643
B42	6.37272
B43	5.36058
B44	1.36836
B45	1.43914
B46	1.43912
B47	1.08448
B48	1.41829
B49	1.41629
B50	1.4164
B51	1.4183
B52	1.08444
B53	1.38737
B54	1.38738
B55	1.08447
B56	1.4075
B57	1.08306

B58	1.40752
B59	1.08307
B60	1.08155
B61	1.0816
B62	1.34654
B63	1.34644
B64	2.65107
B65	2.47455
B66	1.38899
B67	1.41009
B68	1.40784
B69	1.08501
B70	1.42533
B71	1.43336
B72	1.43728
B73	1.44173
B74	1.43114
B75	1.36551
B76	1.08515
B77	1.36738
B78	1.0845
B79	1.43204
B80	1.43013
B81	1.08534
B82	1.08649
B83	1.40775
B84	1.40833
B85	1.39607
B86	1.08537
B87	1.08584
B88	1.08435
B89	1.08452
B90	1.08454
A1	119.46407
A2	117.54383
A3	119.80445
A4	123.92413
A5	120.1804
A6	120.53689
A7	121.15652
A8	117.8433
A9	119.64037
A10	120.67833
A11	117.42556

A12	120.93729
A13	120.7064
A14	121.18668
A15	120.03859
A16	122.17347
A17	123.27341
A18	128.36785
A19	145.56824
A20	164.72161
A21	154.22543
A22	119.85438
A23	119.22541
A24	63.19391
A25	119.3795
A26	120.7755
A27	147.59976
A28	123.78834
A29	120.22597
A30	121.12069
A31	118.48872
A32	117.54664
A33	147.58483
A34	120.39716
A35	119.37349
A36	119.85436
A37	147.77886
A38	120.93787
A39	32.03873
A40	31.14942
A41	94.6686
A42	94.25129
A43	82.64935
A44	38.46739
A45	121.11301
A46	120.38849
A47	118.67248
A48	123.77309
A49	123.79246
A50	118.66546
A51	119.85005
A52	119.37447
A53	119.38164
A54	119.84103
A55	119.86272

A56	120.92335
A57	119.87128
A58	120.92428
A59	121.13618
A60	121.21979
A61	122.2003
A62	122.16728
A63	80.63985
A64	99.39991
A65	153.58845
A66	32.00387
A67	120.73086
A68	119.94054
A69	119.449
A70	118.91425
A71	121.78809
A72	123.43747
A73	119.3128
A74	121.1507
A75	118.33045
A76	121.76385
A77	119.05652
A78	120.19656
A79	120.36904
A80	120.40932
A81	120.17013
A82	119.14373
A83	119.47469
A84	120.64766
A85	119.11105
A86	119.30669
A87	119.8778
A88	120.36423
A89	118.46168
D1	-0.16293
D2	-0.20812
D3	179.65752
D4	-179.70702
D5	-0.97182
D6	-179.62824
D7	-179.77746
D8	-179.13852
D9	-0.07764
D10	0.09768

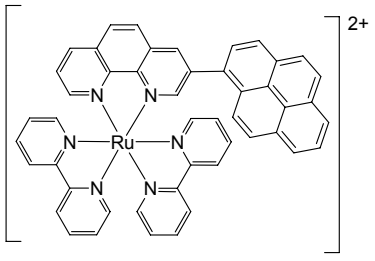
D11	179.91995
D12	179.78213
D13	-179.6502
D14	178.5328
D15	0.13612
D16	-0.17371
D17	179.41598
D18	-93.4216
D19	-103.5273
D20	-163.3497
D21	0.98851
D22	-179.18962
D23	-162.49706
D24	-0.18052
D25	179.77618
D26	0.04104
D27	179.83463
D28	179.63053
D29	-179.86623
D30	0.01409
D31	-179.87194
D32	-0.4517
D33	179.84148
D34	-0.10441
D35	179.89192
D36	-0.12354
D37	179.93613
D38	-161.97351
D39	-0.35026
D40	-32.12284
D41	-35.92989
D42	-83.69604
D43	95.98372
D44	-0.05789
D45	179.97752
D46	-0.21283
D47	179.94491
D48	179.96371
D49	-0.06554
D50	-0.24626
D51	179.74858
D52	179.91508
D53	-0.21674
D54	-0.15949

D55	179.91818
D56	-0.2719
D57	179.72569
D58	-179.83563
D59	-179.9003
D60	0.0544
D61	0.08741
D62	138.8122
D63	154.07185
D64	145.61777
D65	140.30874
D66	-3.66817
D67	175.56742
D68	179.39857
D69	-1.11401
D70	179.16675
D71	174.69749
D72	-178.58339
D73	179.35331
D74	-0.3859
D75	-179.91367
D76	-2.74085
D77	-1.19693
D78	178.26677
D79	-179.8613
D80	178.83411
D81	-179.86543
D82	-179.90544
D83	-0.04787
D84	179.93141
D85	179.44067
D86	179.85456
D87	179.80038
D88	0.22044

……

SCF Done: E(RB+HF-LYP) = -2422.47930765 Hartree
Number of Imaginary frequencies: 0

complex 5 （DFT//B3LYP/6-31G(d)/ LanL2DZ）



Symbolic Z-matrix:

Charge = 2 Multiplicity = 1

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	1	B5	2	A4	3	D3	0
C	5	B6	4	A5	3	D4	0
C	7	B7	5	A6	4	D5	0
C	8	B8	7	A7	5	D6	0
C	9	B9	8	A8	7	D7	0
N	7	B10	5	A9	4	D8	0
C	11	B11	7	A10	5	D9	0
C	12	B12	11	A11	7	D10	0
C	13	B13	12	A12	11	D11	0
Ru	11	B14	7	A13	5	D12	0
C	15	B15	11	A14	7	D13	0
C	16	B16	15	A15	11	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
C	19	B19	18	A18	17	D17	0
N	16	B20	15	A19	11	D18	0
C	20	B21	19	A20	18	D19	0
C	22	B22	20	A21	19	D20	0
C	23	B23	22	A22	20	D21	0
C	24	B24	23	A23	22	D22	0
C	25	B25	24	A24	23	D23	0
N	26	B26	25	A25	24	D24	0
C	15	B27	11	A26	7	D25	0
C	28	B28	15	A27	11	D26	0
C	29	B29	28	A28	15	D27	0
N	30	B30	29	A29	28	D28	0
C	31	B31	30	A30	29	D29	0
C	28	B32	15	A31	11	D30	0
C	32	B33	31	A32	30	D31	0
N	34	B34	32	A33	31	D32	0
C	35	B35	34	A34	32	D33	0
C	36	B36	35	A35	34	D34	0
C	37	B37	36	A36	35	D35	0
C	38	B38	37	A37	36	D36	0
H	1	B39	2	A38	3	D37	0
H	3	B40	2	A39	1	D38	0
H	9	B41	8	A40	7	D39	0
H	10	B42	9	A41	8	D40	0

H	12	B43	11	A42	7	D41	0
H	13	B44	12	A43	11	D42	0
H	14	B45	13	A44	12	D43	0
H	16	B46	15	A45	11	D44	0
H	17	B47	16	A46	15	D45	0
H	18	B48	17	A47	16	D46	0
H	19	B49	18	A48	17	D47	0
H	23	B50	22	A49	20	D48	0
H	24	B51	23	A50	22	D49	0
H	25	B52	24	A51	23	D50	0
H	26	B53	25	A52	24	D51	0
H	28	B54	15	A53	11	D52	0
H	29	B55	28	A54	15	D53	0
H	30	B56	29	A55	28	D54	0
H	33	B57	28	A56	15	D55	0
H	36	B58	35	A57	34	D56	0
H	37	B59	36	A58	35	D57	0
H	38	B60	37	A59	36	D58	0
H	39	B61	38	A60	37	D59	0
C	2	B62	1	A61	6	D60	0
C	63	B63	2	A62	1	D61	0
C	63	B64	2	A63	1	D62	0
C	64	B65	63	A64	2	D63	0
C	64	B66	63	A65	2	D64	0
C	65	B67	63	A66	2	D65	0
H	65	B68	63	A67	2	D66	0
C	66	B69	64	A68	63	D67	0
C	68	B70	65	A69	63	D68	0
C	67	B71	64	A70	63	D69	0
H	67	B72	64	A71	63	D70	0
H	68	B73	65	A72	63	D71	0
C	70	B74	66	A73	64	D72	0
C	70	B75	66	A74	64	D73	0
C	71	B76	68	A75	65	D74	0
H	72	B77	67	A76	64	D75	0
C	75	B78	70	A77	66	D76	0
C	76	B79	70	A78	66	D77	0
C	77	B80	71	A79	68	D78	0
H	77	B81	71	A80	68	D79	0
C	79	B82	75	A81	70	D80	0
H	79	B83	75	A82	70	D81	0
H	80	B84	76	A83	70	D82	0
H	81	B85	77	A84	71	D83	0
H	83	B86	79	A85	75	D84	0

Variables:

B1	1.39553
B2	1.41994
B3	1.3328
B4	1.36834
B5	1.40863
B6	1.42991
B7	1.41748
B8	1.43712
B9	1.36369
B10	1.36897
B11	1.3368
B12	1.40384
B13	1.38398
B14	2.12812
B15	3.09748
B16	1.39078
B17	1.39456
B18	1.39222
B19	1.39907
B20	1.34696
B21	1.4775
B22	1.39897
B23	1.39225
B24	1.39449
B25	1.39094
B26	1.34698
B27	4.9018
B28	1.39445
B29	1.39071
B30	1.34687
B31	1.36346
B32	1.39205
B33	1.4772
B34	1.36339
B35	1.3469
B36	1.39081
B37	1.39451
B38	1.39223
B39	1.08556
B40	1.08414
B41	1.08592
B42	1.08593
B43	1.08439

B44	1.08457
B45	1.08622
B46	1.08357
B47	1.08461
B48	1.08527
B49	1.08322
B50	1.08324
B51	1.08528
B52	1.08462
B53	1.08352
B54	1.08523
B55	1.08461
B56	1.08354
B57	1.08318
B58	1.08348
B59	1.08461
B60	1.08525
B61	1.08319
B62	1.47786
B63	1.42408
B64	1.40754
B65	1.43383
B66	1.43821
B67	1.38566
B68	1.0876
B69	1.42836
B70	1.40575
B71	1.36408
B72	1.08471
B73	1.08644
B74	1.42644
B75	1.42873
B76	1.43412
B77	1.08714
B78	1.40528
B79	1.4048
B80	1.36271
B81	1.08655
B82	1.39314
B83	1.08679
B84	1.08664
B85	1.0867
B86	1.08569
A1	116.79271

A2	124.15518
A3	118.51641
A4	120.63384
A5	117.72287
A6	119.93671
A7	118.79876
A8	121.13457
A9	117.48298
A10	118.32755
A11	122.75756
A12	119.41931
A13	113.11058
A14	97.26515
A15	156.66646
A16	118.63425
A17	118.84443
A18	119.85868
A19	33.78849
A20	123.59255
A21	123.63825
A22	119.83725
A23	118.86518
A24	118.64771
A25	122.82373
A26	171.06793
A27	61.39124
A28	118.64752
A29	122.88334
A30	118.8998
A31	57.44336
A32	115.53789
A33	115.51004
A34	118.93812
A35	122.84761
A36	118.65454
A37	118.84546
A38	119.93137
A39	119.50096
A40	118.45153
A41	120.37934
A42	116.34104
A43	119.35121
A44	120.78075
A45	82.12144

A46	119.83198
A47	120.88324
A48	119.67701
A49	120.49147
A50	120.2575
A51	121.53074
A52	121.29744
A53	177.66721
A54	121.53088
A55	121.19326
A56	119.68699
A57	115.89913
A58	119.81036
A59	120.88497
A60	119.68801
A61	123.79726
A62	122.73967
A63	117.81133
A64	118.66795
A65	123.54368
A66	121.78304
A67	119.11873
A68	120.23841
A69	120.63129
A70	121.72277
A71	119.3639
A72	120.06027
A73	120.36315
A74	120.22283
A75	121.72379
A76	119.93455
A77	119.49152
A78	119.16698
A79	121.10583
A80	118.42743
A81	120.6629
A82	119.23541
A83	119.09459
A84	120.3366
A85	119.87028
D1	0.26851
D2	0.28111
D3	-0.53023
D4	179.61959

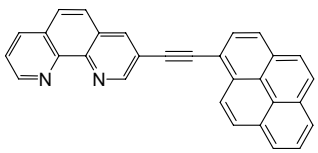
D5	179.09314
D6	0.10847
D7	0.31908
D8	-1.18594
D9	179.92762
D10	0.23032
D11	-0.03774
D12	0.72397
D13	-164.45857
D14	-90.1024
D15	1.18455
D16	0.03631
D17	0.0537
D18	-88.10699
D19	-179.97009
D20	-1.80076
D21	179.74196
D22	-0.01489
D23	0.13861
D24	-0.16677
D25	-60.03045
D26	152.21564
D27	-0.43185
D28	-0.09142
D29	0.02385
D30	-27.25386
D31	-179.8606
D32	-1.82534
D33	179.8699
D34	0.27555
D35	-0.19894
D36	0.0134
D37	178.10376
D38	179.47304
D39	-179.82356
D40	179.85224
D41	179.99065
D42	179.92951
D43	179.93234
D44	90.90302
D45	-178.74784
D46	-179.88965
D47	-179.80354
D48	-0.41987

D49	179.93455
D50	179.97676
D51	179.92901
D52	-39.46885
D53	179.49549
D54	-179.90469
D55	-179.35698
D56	-179.78941
D57	179.90152
D58	-179.87555
D59	-179.70521
D60	-178.16189
D61	-48.8829
D62	130.00619
D63	176.60615
D64	-5.91401
D65	-176.68014
D66	-0.18751
D67	-179.3927
D68	-0.54568
D69	179.82985
D70	-1.65803
D71	178.07417
D72	-1.10649
D73	179.03478
D74	179.01462
D75	179.7874
D76	179.75282
D77	-179.6039
D78	179.63193
D79	-0.52723
D80	0.
D81	179.9829
D82	179.6792
D83	179.80398
D84	-179.83877

.....

SCF Done: E(RB+HF-LYP) = -2270.53597843 Hartree
Number of Imaginary frequencies: 0

Ligand of Complex **3** （**DFT//B3LYP/6-31G(d)/ LanL2DZ**）



Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C
C 1 B1
C 2 B2 1 A1
N 3 B3 2 A2 1 D1
C 4 B4 3 A3 2 D2
C 1 B5 2 A4 3 D3
C 5 B6 4 A5 3 D4
C 7 B7 5 A6 4 D5
C 8 B8 7 A7 5 D6
C 9 B9 8 A8 7 D7
N 7 B10 5 A9 4 D8
C 11 B11 7 A10 5 D9
C 12 B12 11 A11 7 D10
C 13 B13 12 A12 11 D11
H 1 B14 2 A13 3 D12
H 3 B15 2 A14 1 D13
H 9 B16 8 A15 7 D14
H 10 B17 9 A16 8 D15
H 12 B18 11 A17 7 D16
H 13 B19 12 A18 11 D17
H 14 B20 13 A19 12 D18
C 2 B21 1 A20 6 D19
C 22 B22 2 A21 1 D20
C 23 B23 22 A22 2 D21
C 24 B24 23 A23 22 D22
C 24 B25 23 A24 22 D23
C 25 B26 24 A25 23 D24
C 25 B27 24 A26 23 D25
C 26 B28 24 A27 23 D26
H 26 B29 24 A28 23 D27
C 27 B30 25 A29 24 D28
C 29 B31 26 A30 24 D29
C 28 B32 25 A31 24 D30
H 28 B33 25 A32 24 D31
H 29 B34 26 A33 24 D32
C 31 B35 27 A34 25 D33
C 31 B36 27 A35 25 D34
C 32 B37 29 A36 26 D35
H 33 B38 28 A37 25 D36
C 36 B39 31 A38 27 D37

C	37	B40	31	A39	27	D38
C	38	B41	32	A40	29	D39
H	38	B42	32	A41	29	D40
C	40	B43	36	A42	31	D41
H	40	B44	36	A43	31	D42
H	41	B45	37	A44	31	D43
H	42	B46	38	A45	32	D44
H	44	B47	40	A46	36	D45

B1	1.39191707
B2	1.42762925
B3	1.31542172
B4	1.35520030
B5	1.40771328
B6	1.45534350
B7	1.42604016
B8	1.43457146
B9	1.36058157
B10	1.35359131
B11	1.32246328
B12	1.41063895
B13	1.37892016
B14	1.08663311
B15	1.08901662
B16	1.08741589
B17	1.08726480
B18	1.08973629
B19	1.08592622
B20	1.08764880
B21	1.41918138
B22	1.21836099
B23	1.42045919
B24	1.42332132
B25	1.41000633
B26	1.42761354
B27	1.43426102
B28	1.38543410
B29	1.08540559
B30	1.42811516
B31	1.40601763
B32	1.36255701
B33	1.08530375
B34	1.08704998
B35	1.42749382

B36	1.42889450
B37	1.43459645
B38	1.08743011
B39	1.40476173
B40	1.40438775
B41	1.36240650
B42	1.08728564
B43	1.39340886
B44	1.08726497
B45	1.08725863
B46	1.08731412
B47	1.08655761
A1	116.91831616
A2	124.45244858
A3	118.64416627
A4	119.95665959
A5	118.92789919
A6	118.78931524
A7	120.21767553
A8	120.96280130
A9	118.82368526
A10	118.10675602
A11	124.17056437
A12	118.23836788
A13	120.21214464
A14	118.73678258
A15	118.46691647
A16	120.69232999
A17	116.06795434
A18	120.27847389
A19	121.14223005
A20	122.79605947
A21	178.27425412
A22	178.55102766
A23	121.44379990
A24	119.09141635
A25	119.05642774
A26	122.34578853
A27	121.24724538
A28	118.60036307
A29	119.97476541
A30	120.99239786
A31	121.35953838
A32	118.14022077

A33	119.81456927
A34	120.16343501
A35	120.15004820
A36	122.17411406
A37	120.14736389
A38	119.17132694
A39	119.09383458
A40	121.31721296
A41	118.28370304
A42	120.75853263
A43	119.10580488
A44	119.08921672
A45	120.37771534
A46	119.76979972
D1	0.00000000
D2	0.00000000
D3	0.00000000
D4	-180.00000000
D5	-180.00000000
D6	0.00000000
D7	0.00000000
D8	0.00000000
D9	-180.00000000
D10	0.00000000
D11	0.00000000
D12	180.00000000
D13	180.00000000
D14	180.00000000
D15	-180.00000000
D16	180.00000000
D17	180.00000000
D18	180.00000000
D19	-180.00000000
D20	179.36408107
D21	1.25037553
D22	179.38718338
D23	-0.61280680
D24	-180.00000000
D25	0.00000000
D26	180.00000000
D27	0.00000000
D28	-180.00000000
D29	0.00000000
D30	180.00000000

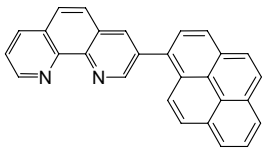
D31	0.00000000
D32	180.00000000
D33	0.00000000
D34	180.00000000
D35	-180.00000000
D36	180.00000000
D37	-180.00000000
D38	-180.00000000
D39	-180.00000000
D40	0.00000000
D41	0.00000000
D42	-180.00000000
D43	-180.00000000
D44	-180.00000000
D45	-180.00000000

1 2 1.5 6 1.5 15 1.0
2 3 1.5 22 1.0
3 4 1.5 16 1.0
4 5 1.5
5 6 1.5 7 1.5
6 10 1.5
7 8 1.5 11 1.5
8 9 1.5 14 1.5
9 10 1.5 17 1.0
10 18 1.0
11 12 1.5
12 13 1.5 19 1.0
13 14 1.5 20 1.0
14 21 1.0
15
16
17
18
19
20
21
22 23 3.0
23 24 1.0
24 25 1.5 26 1.5
25 27 1.5 28 1.5
26 29 1.5 30 1.0
27 31 1.5 32 1.5
28 33 2.0 34 1.0

29 32 1.5 35 1.0
30
31 36 1.5 37 1.5
32 38 1.5
33 36 1.5 39 1.0
34
35
36 40 1.5
37 41 1.5 42 1.5
38 42 2.0 43 1.0
39
40 44 1.5 45 1.0
41 44 1.5 46 1.0
42 47 1.0
43
44 48 1.0
45
46
47
48

SCF Done: E(RB+HF-LYP) = -1262.34930599 Hartree
Number of Imaginary frequencies: 0

Ligand of Complex **5** （**DFT//B3LYP/6-31G(d)/ LanL2DZ**）



Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

0 1

C								
C		1	B1					
C		2	B2	1	A1			
N		3	B3	2	A2	1	D1	
C		4	B4	3	A3	2	D2	
C		1	B5	2	A4	3	D3	
C		5	B6	4	A5	3	D4	
C		7	B7	5	A6	4	D5	

C	8	B8	7	A7	5	D6
C	9	B9	8	A8	7	D7
N	7	B10	5	A9	4	D8
C	11	B11	7	A10	5	D9
C	12	B12	11	A11	7	D10
C	13	B13	12	A12	11	D11
H	1	B14	2	A13	3	D12
H	3	B15	2	A14	1	D13
H	9	B16	8	A15	7	D14
H	10	B17	9	A16	8	D15
H	12	B18	11	A17	7	D16
H	13	B19	12	A18	11	D17
H	14	B20	13	A19	12	D18
C	2	B21	1	A20	6	D19
C	22	B22	2	A21	1	D20
C	22	B23	2	A22	1	D21
C	23	B24	22	A23	2	D22
C	23	B25	22	A24	2	D23
C	24	B26	22	A25	2	D24
H	24	B27	22	A26	2	D25
C	25	B28	23	A27	22	D26
C	27	B29	24	A28	22	D27
C	26	B30	23	A29	22	D28
H	26	B31	23	A30	22	D29
H	27	B32	24	A31	22	D30
C	29	B33	25	A32	23	D31
C	29	B34	25	A33	23	D32
C	30	B35	27	A34	24	D33
H	31	B36	26	A35	23	D34
C	34	B37	29	A36	25	D35
C	35	B38	29	A37	25	D36
C	36	B39	30	A38	27	D37
H	36	B40	30	A39	27	D38
C	38	B41	34	A40	29	D39
H	38	B42	34	A41	29	D40
H	39	B43	35	A42	29	D41
H	40	B44	36	A43	30	D42
H	42	B45	38	A44	34	D43

B1	1.38709041
B2	1.42166294
B3	1.31961967
B4	1.35290254
B5	1.41070649

B6	1.45706214
B7	1.42560775
B8	1.43471570
B9	1.36084770
B10	1.35316524
B11	1.32279690
B12	1.41035572
B13	1.37894866
B14	1.08735913
B15	1.08987533
B16	1.08748450
B17	1.08738140
B18	1.08975652
B19	1.08596281
B20	1.08769155
B21	1.48548461
B22	1.42001613
B23	1.40363597
B24	1.43264832
B25	1.43953832
B26	1.38882145
B27	1.08645103
B28	1.42922178
B29	1.40229422
B30	1.36184000
B31	1.08408930
B32	1.08718408
B33	1.42739851
B34	1.42966217
B35	1.43629599
B36	1.08748392
B37	1.40440681
B38	1.40409333
B39	1.36082631
B40	1.08732163
B41	1.39314115
B42	1.08730350
B43	1.08729803
B44	1.08732598
B45	1.08662204
A1	116.38973410
A2	125.03338192
A3	118.39009691
A4	120.39841568

A5	119.05051137
A6	118.76220896
A7	120.23053371
A8	120.94583548
A9	118.83925077
A10	118.11256992
A11	124.16264879
A12	118.22901344
A13	120.37311370
A14	118.80185886
A15	118.46577593
A16	120.67458512
A17	116.06509552
A18	120.28680113
A19	121.14199137
A20	123.34362458
A21	122.90306747
A22	118.00000734
A23	119.15482912
A24	123.01087250
A25	121.83803672
A26	118.71279500
A27	120.28598474
A28	120.73763810
A29	121.73903103
A30	118.69587640
A31	119.92695112
A32	120.24474113
A33	120.24864110
A34	122.04886850
A35	120.03520652
A36	119.33197203
A37	119.14756059
A38	121.31685567
A39	118.20071678
A40	120.72190314
A41	119.09739261
A42	119.04788230
A43	120.48331328
A44	119.79795650
D1	-0.11466506
D2	0.05914482
D3	0.18956557
D4	179.75850341

D5	-179.66156882
D6	-0.01019160
D7	-0.06813523
D8	0.29354113
D9	-179.95550348
D10	0.02212986
D11	-0.01668849
D12	-178.49444101
D13	-179.34337129
D14	179.90297502
D15	179.95059491
D16	-179.98603251
D17	179.97568785
D18	179.98408305
D19	177.42918593
D20	54.82949190
D21	-124.97730542
D22	-177.62429028
D23	4.22950592
D24	177.99113555
D25	-0.09303342
D26	179.25953585
D27	0.13519303
D28	-179.62914130
D29	1.56875770
D30	-179.00945355
D31	0.94923230
D32	-179.26518188
D33	-178.99393726
D34	-179.57450910
D35	-179.83845784
D36	179.71570334
D37	-179.71846389
D38	0.30198560
D39	-0.02680814
D40	-179.90503300
D41	-179.85341293
D42	-179.90315927
D43	179.96734734

SCF Done: E(RB+HF-LYP) = -1186.11355554 Hartree
Number of Imaginary frequencies: 0.