Electronic Supplementary Information for:

Observation of the Room Temperature Phosphorescence of Bodipy in Visible Light-harvesting Ru(II) Polyimine Complex and Application as Triplet Photosensitizers for Triplet-triplet-Annihilation Upconversion and Photocatalytic Oxidation

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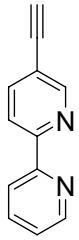
1.0 General.

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before used for synthesis. All samples in flash photolysis and upconversion experiments were deaerated with argon for ca. 15 min before measurement and the gas flow is kept during the measurement.

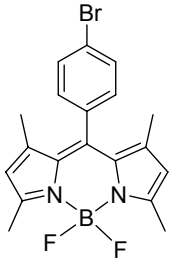
Diode pumped solid state (DPSS) laser 532 nm were used for the upconversions and the diameter of the 532 nm laser spot is ca. 3 mm. In order to repress the scattered laser, a black box was put behind the fluorescent cuvette to trap the laser beam after it passing through the cuvette. The luminescence photographs were obtained using Samsung NV 5 digital camera. The exposure time is the default value of the camera.

2.0 Synthesis and molecular structure characterization data

Synthesis of compound 2: Under argon atmosphere, compound **1** (300.0 mg, 1.283 mmol), $Pd(PPh_3)_2Cl_2$ (9.1 mg, 0.013 mmol), PPh_3 (6.8 mg, 0.026 mmol) were dissolved in triethylamine (15 mL). The flask was vacuumed and back-filled with Ar for three times, CuI (5.2 mg, 0.026 mmol) were added. After stirring, trimethylsilylacetylene (125.5 mg, 1.280 mmol) was added via syringe. The mixture was then heated to 88 °C for 8 h. The solvent was removed under reduced pressure, water was added and the mixture was extracted with dichloromethane (CH_2Cl_2, 4×20 mL). The combined organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified with column chromatography (silica gel, CH_2Cl_2: hexane = 5:1, v/v), colorless liquid was abstained. Tetrabutylammonium fluoride (3.2 mmol, 3.2 ml, 1 mol/L) was added to a solution of the above trimethylsilane protected intermediate (200 mg, 0.800 mmol) in THF (25 mL), and the solution was stirred at room temperature under argon for 3 h. CH_2Cl_2 (100 mL) and water (50 mL) were added. The organic layer was separated, and the aqueous layer was extracted with CH_2Cl_2 (3×15 mL). The combined organic layers were washed with brine (200 mL), dried over anhydrous $MgSO_4$. After filtration, the solvent was removed under reduced pressure. The residue was purified by passing through a silica plug using CH_2Cl_2/hexane (5:1, v/v) as eluent to give a white solid. 180.0 mg, yield: 78.3 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.77 (s, 1H), 8.69 (d, 1H, *J* = 3.5 Hz), 8.42–8.39 (m, 2H), 7.91 (d, 1H, *J* = 7.9 Hz), 7.83 (t, 1H, *J* = 8.0 Hz) 7.39 (m, 1H), 3.31 (s, 1H). EI-HRMS: calcd ($[C_{12}H_8N_2]^+$), *m/z* = 180.0687, found, *m/z* = 180.0689.



Synthesis of compound 3: Under argon atmosphere, 4-bromobenzaldehyde (2.2 g, 12 mmol) and 2,4-dimethylpyrrole (2.38 g, 25 mmol) were dissolved in dry CH_2Cl_2 (350 mL) under argon atmosphere. A few drops of trifluoroacetic acid (TFA) was added to the solution and reaction mixture was stirred at RT overnight. After disappearance of the benzaldehyde (monitored via TLC), a solution of DDQ (2.9 g, 12 mmol) in dry THF was added and the stirring was continued for 4 h. Absolute triethylamine (12 mL) was then added to the mixture. After stirring for 15 min, $BF_3{\cdot}OEt_2$



(12 mL) was added dropwise with ice bath cooling. After stirring for another 2 h, the reaction mixture was washed with water several times and extracted with dichloromethane. The organic phase was dried over Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel column chromatography (DCM as the elute) to obtain red solid in 22.7 % yield, (1.1 g, 2.7 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.66 (d, 2H, *J* = 8.2 Hz), 7.19 (d, 2H, *J* = 8.2 Hz), 5.99 (s, 2H), 2.55 (s, 6H), 1.42 (s, 6H); MALDI–HRMS: ($[C_{19}H_{18}BF_2N_2Br]^+$) calcd, *m/z* = 402.0714, found, *m/z* = 402.0737.

3.0 NMR and HRMS spectra

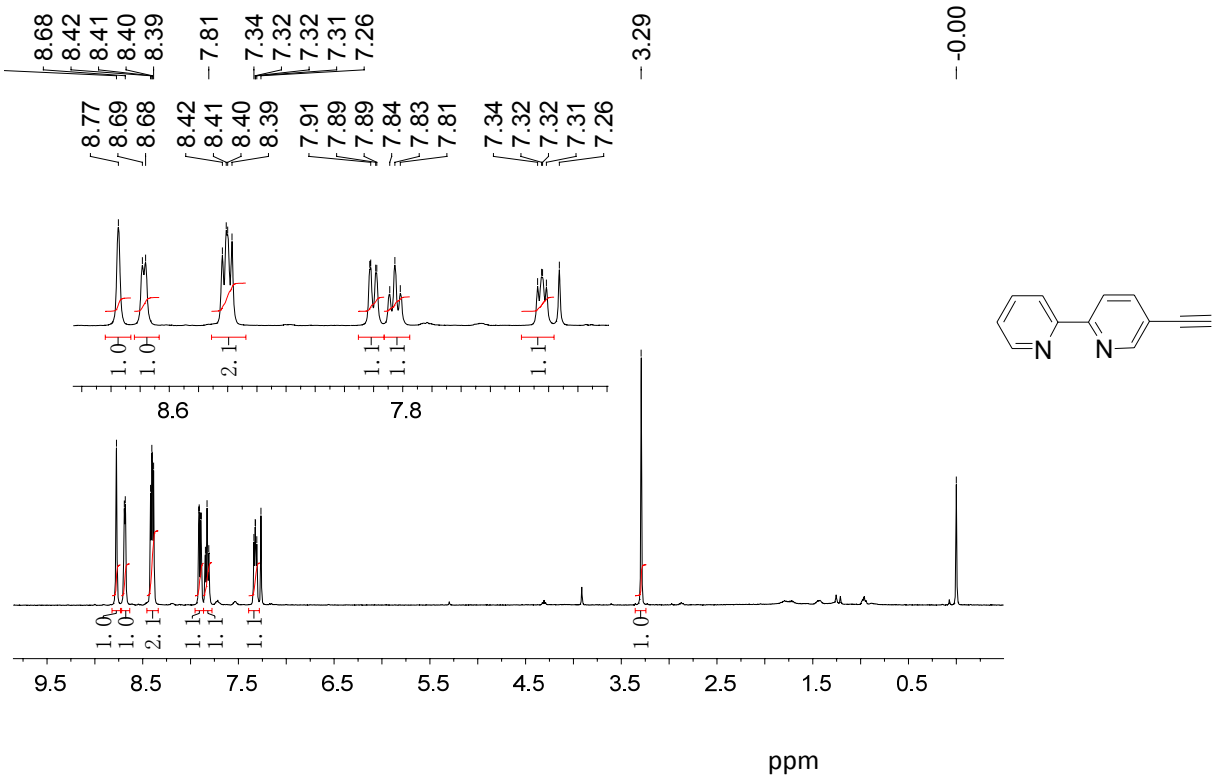


Figure S1. ^{1}H NMR of **2** (400 MHz, $CDCl_3$).

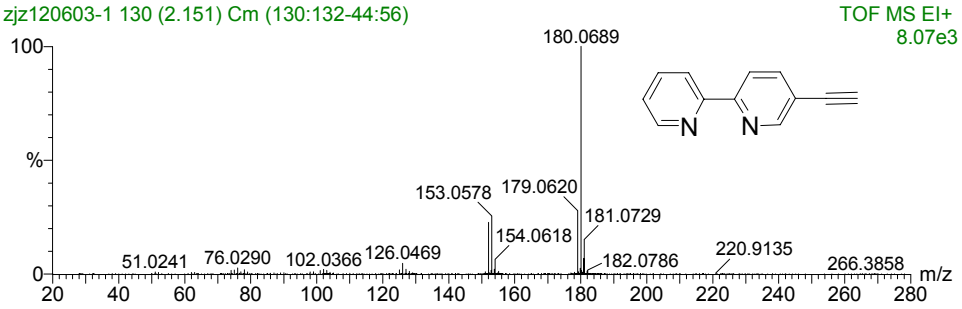


Figure S2. EI-HRMS of **2.**

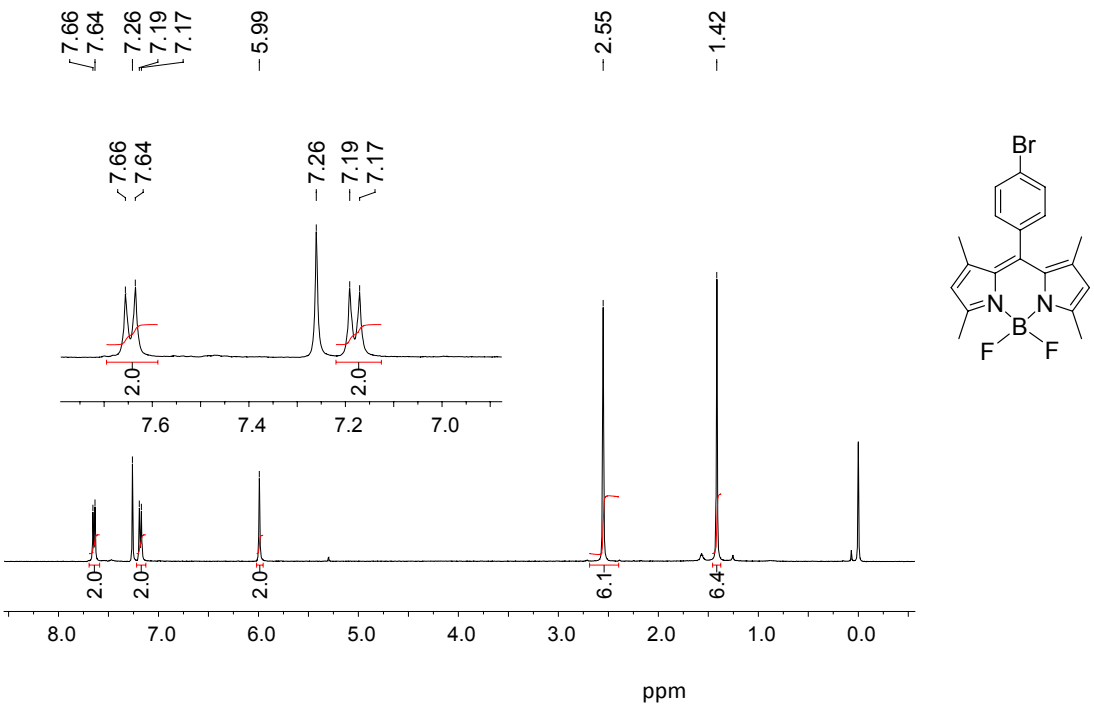


Figure S3. ^{1}H NMR of **3** (400 MHz, $CDCl_3$).

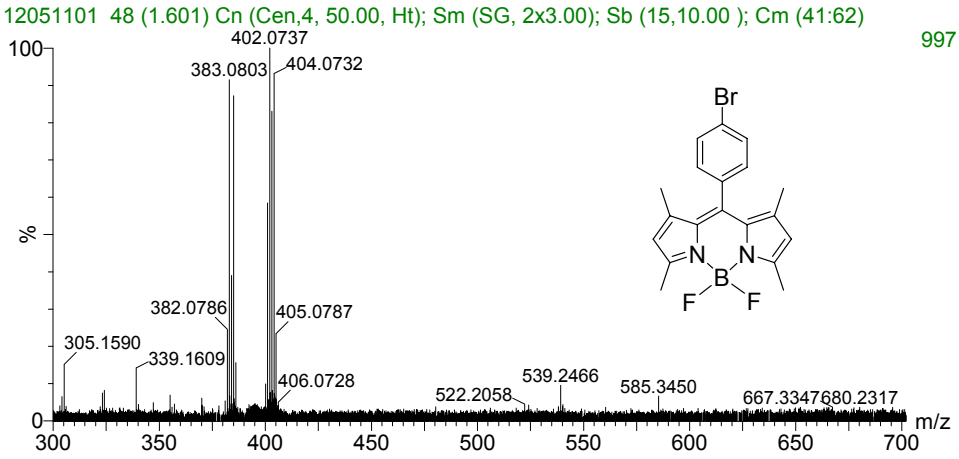


Figure S4. MALDI-HRMS of **3.**

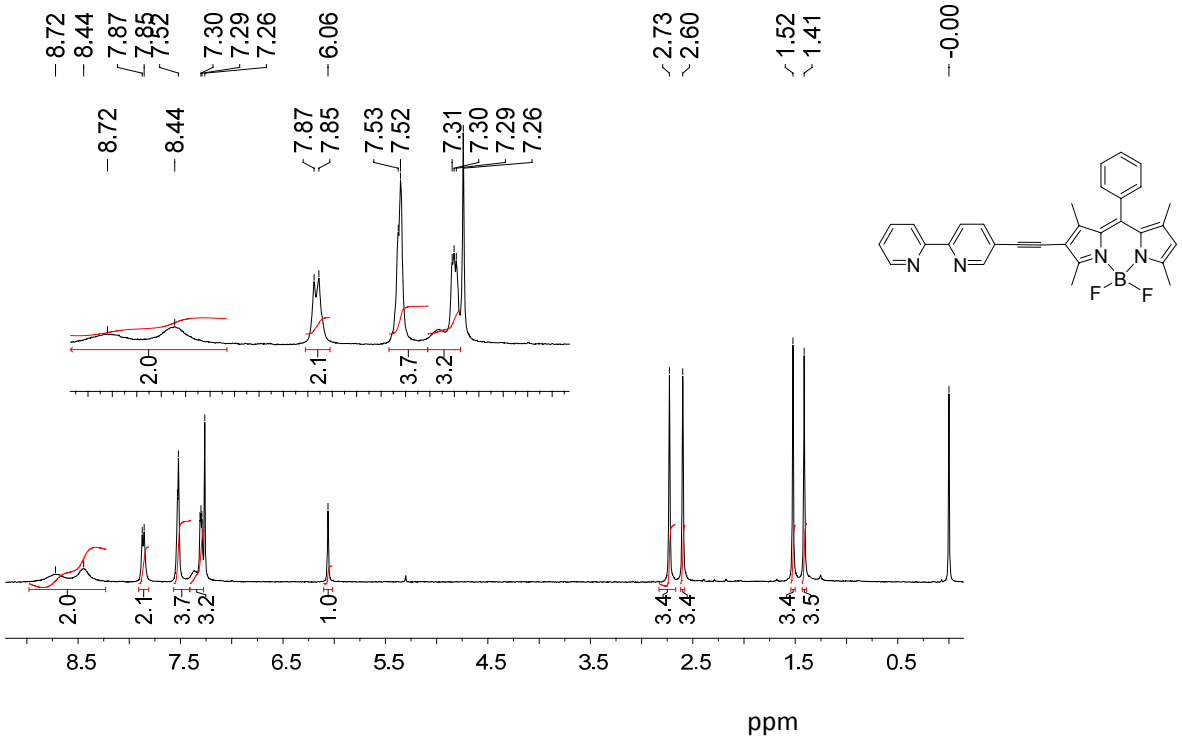


Figure S5. ^{1}H NMR of **L1** (400 MHz, $CDCl_3$).

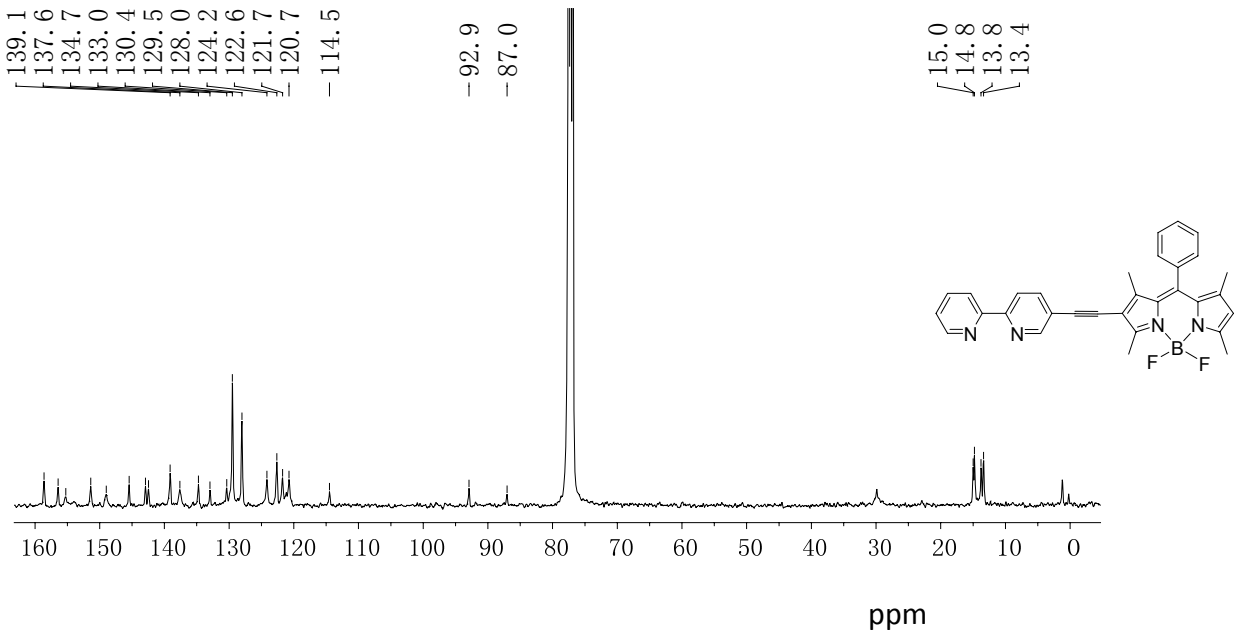


Figure S6. ^{13}C NMR of **L1** (100 MHz, $CDCl_3$).

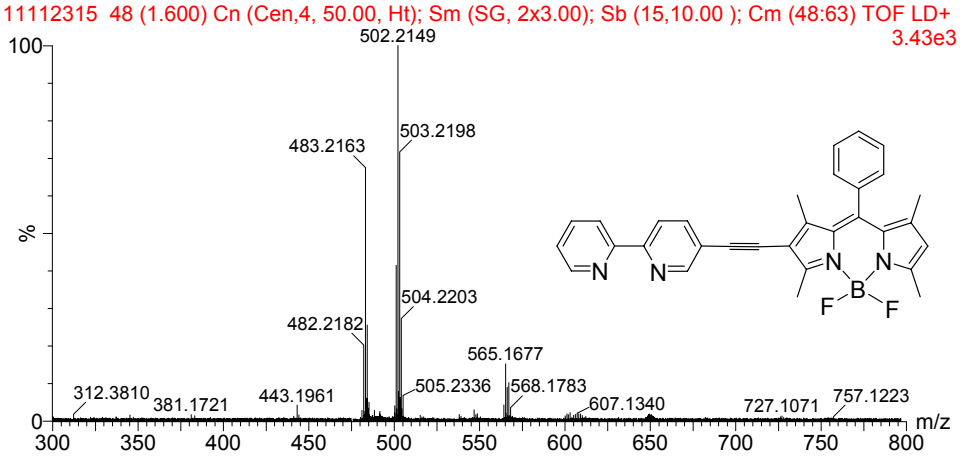


Figure S7. MALDI-HRMS of **L1.**

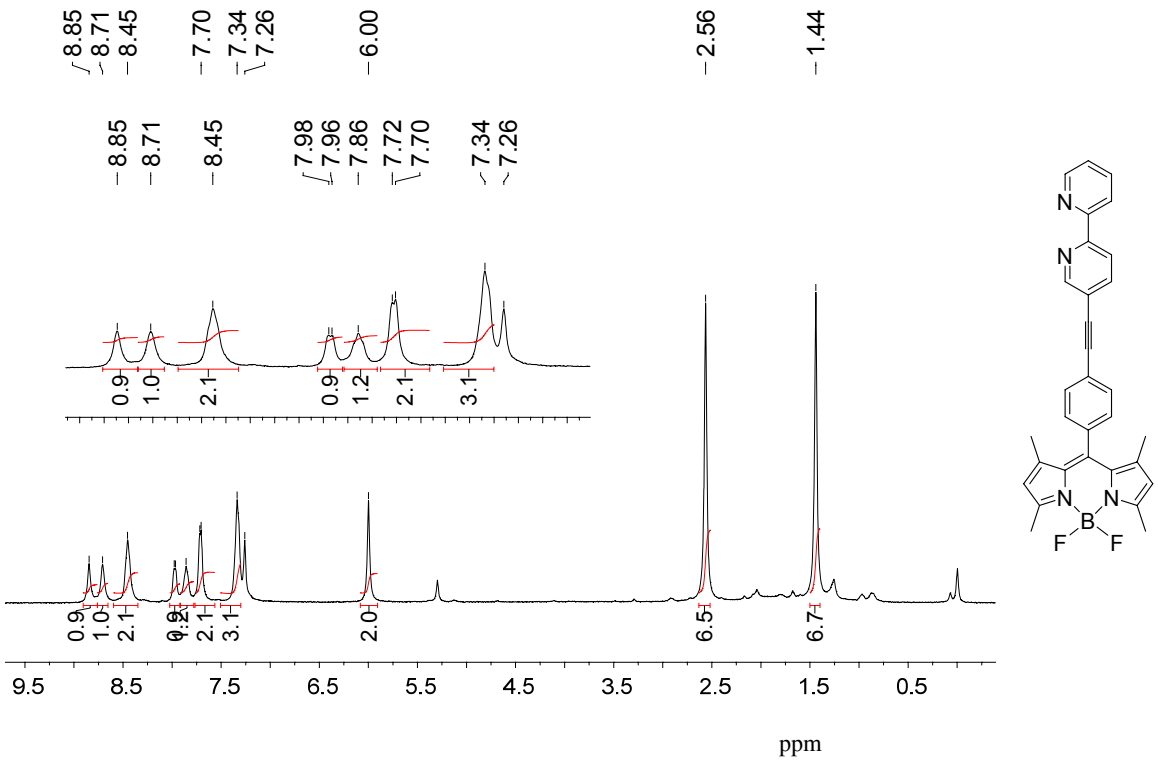


Figure S8. ^{1}H NMR of **L2** (400 MHz, $CDCl_3$).

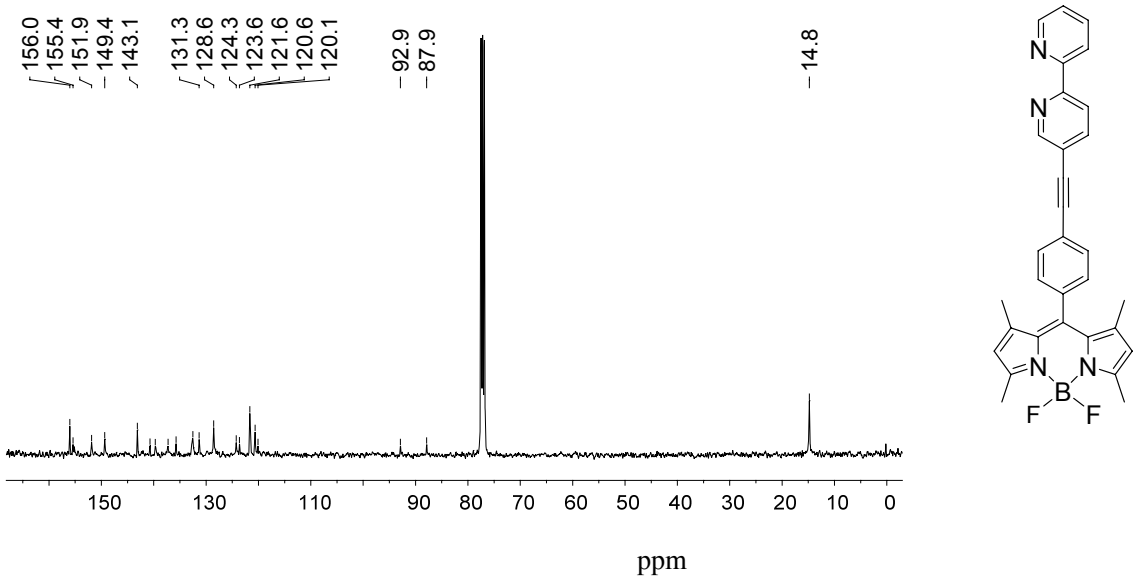


Figure S9. ^{13}C NMR of **L2** (100 MHz, $CDCl_3$).

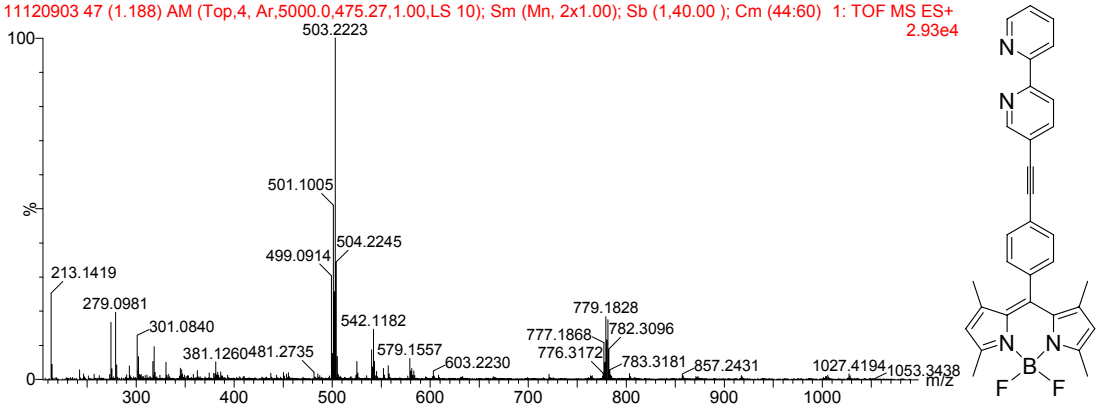


Figure S10. ESI-HRMS of **L2.**

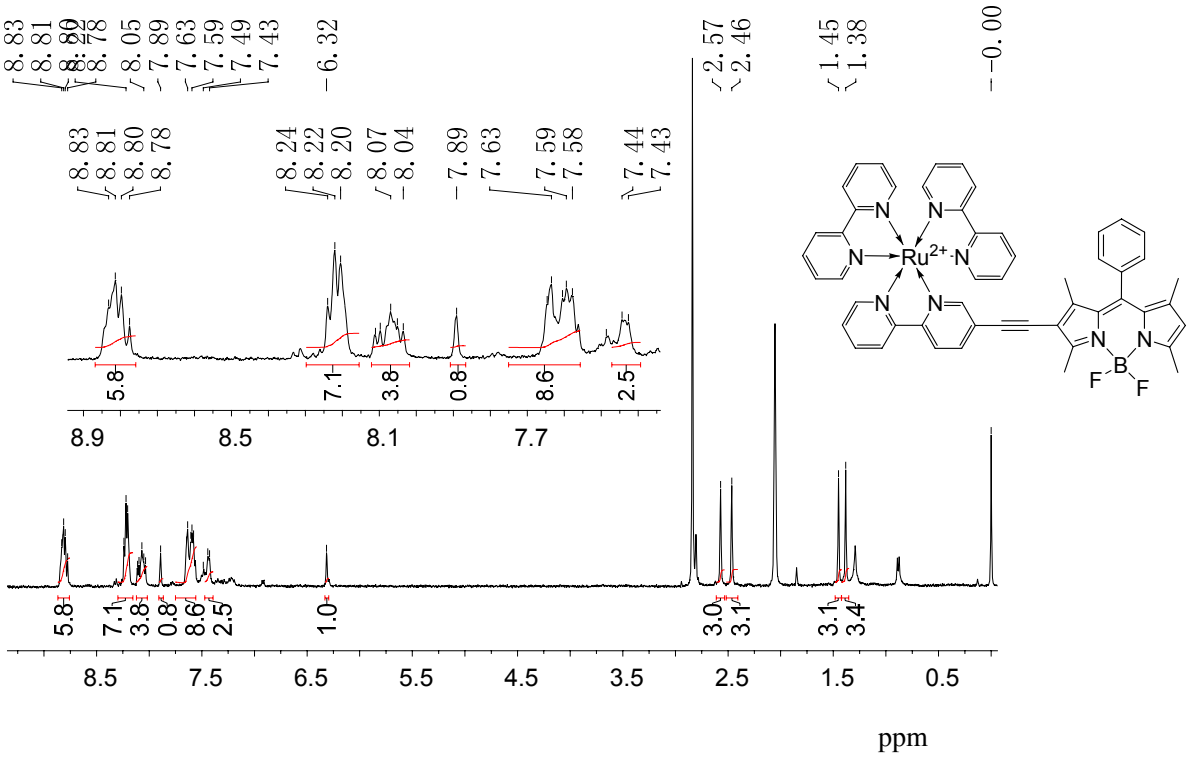


Figure S11. ^{1}HNMR of **Ru-1** (400 MHz, acetone-d_6).

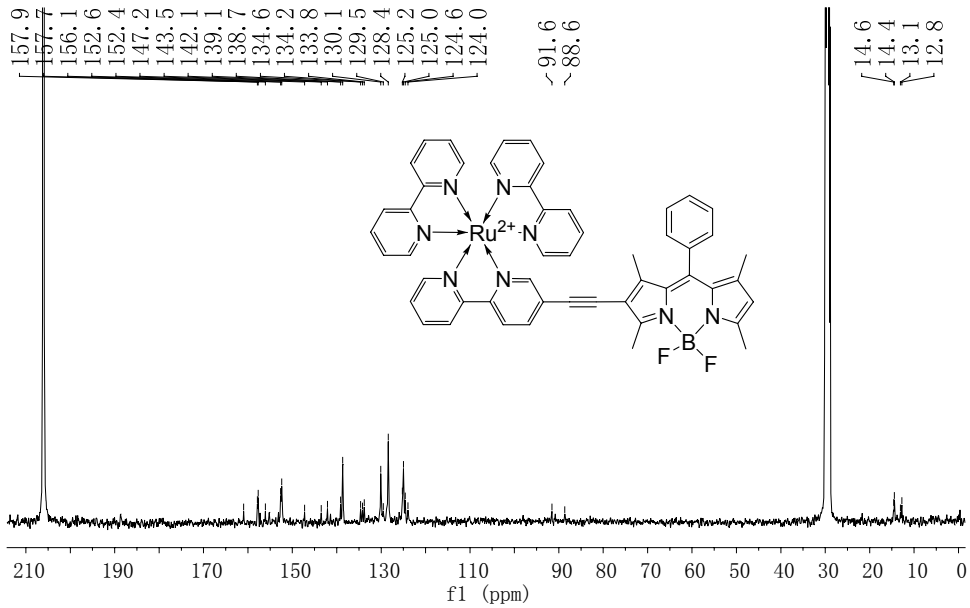


Figure S12. ^{13}CNMR of **Ru-1** (100 MHz, acetone-d_6)

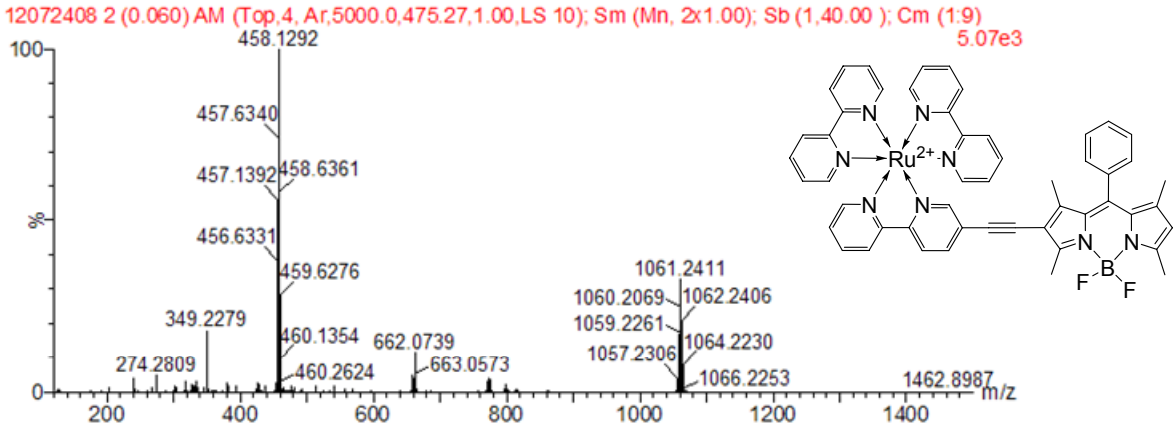


Figure S13. ESI-HRMS of **Ru-1.**

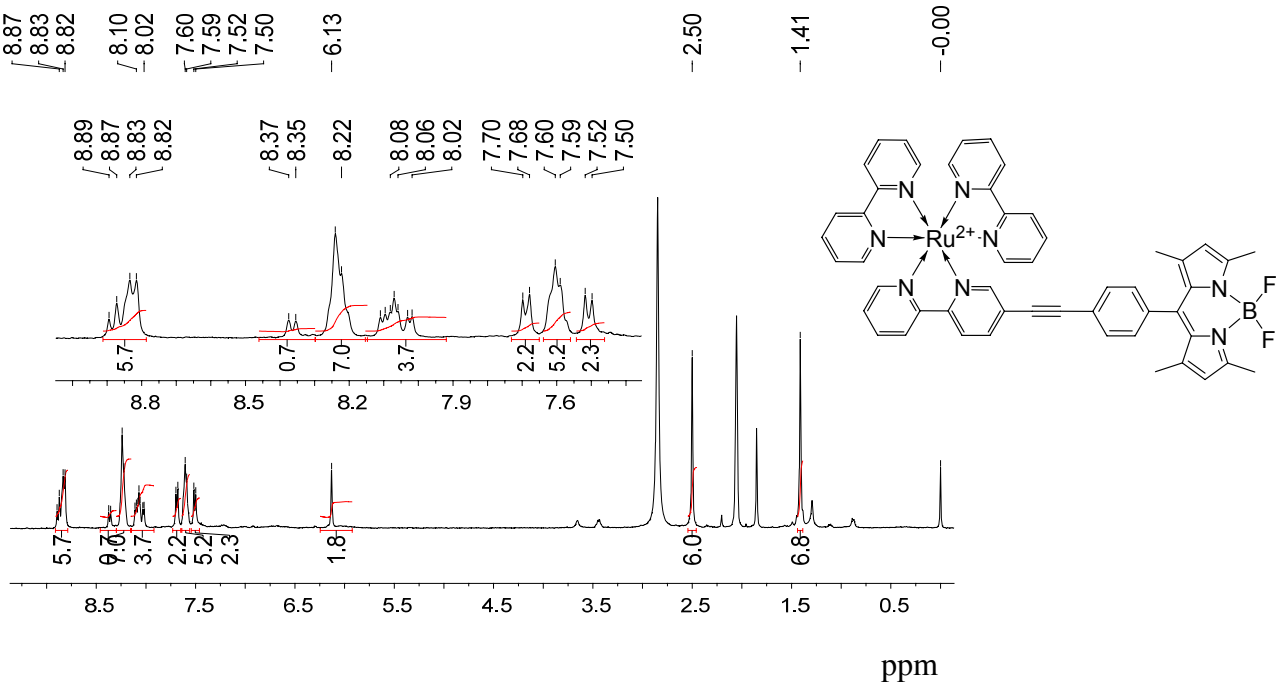


Figure S14. ^{1}HNMR of **Ru-2** (400 MHz, acetone-d_6)

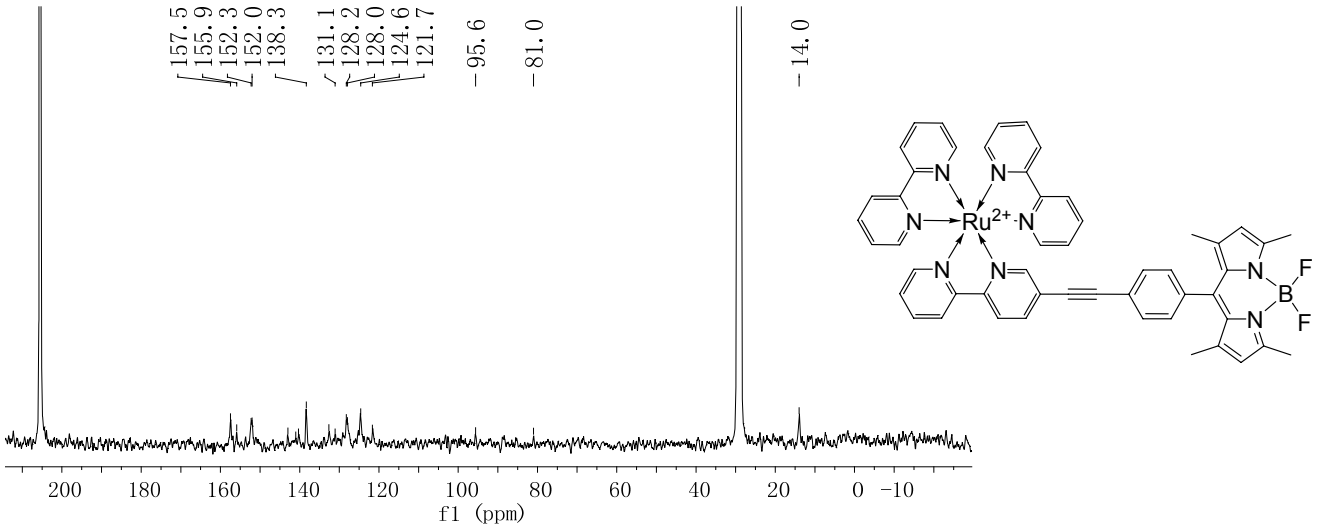


Figure S15. ^{13}CNMR of **Ru-2** (100 MHz, acetone-d_6)

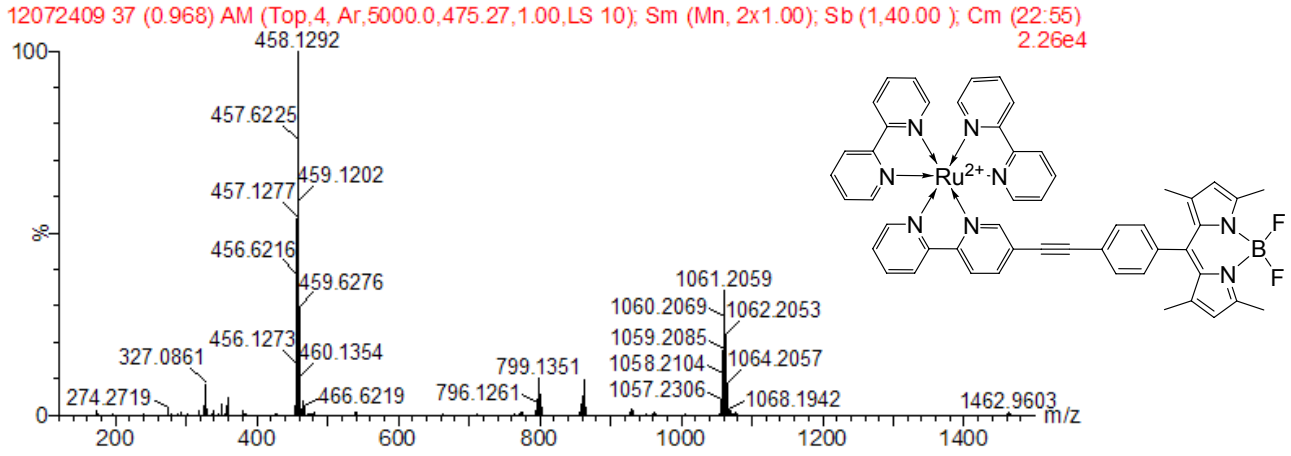


Figure S16. ESI-HRMS of **Ru-2.**

4.0 Emission spectra of Ru-3

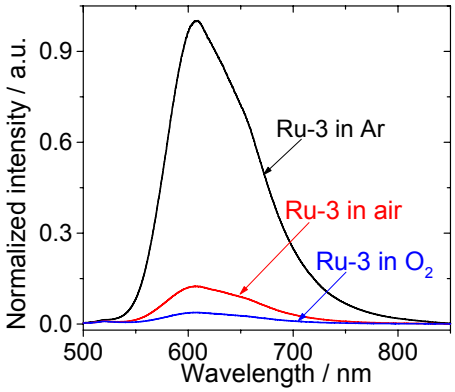


Figure S17. Emission spectra of the complexes **Ru-3** (λex = 450 nm) at different atmosphere of N_2, air and O_2. In MeCN (1.0×10^{-5} M; 20 °C).

5.0 Transient difference absorption details.

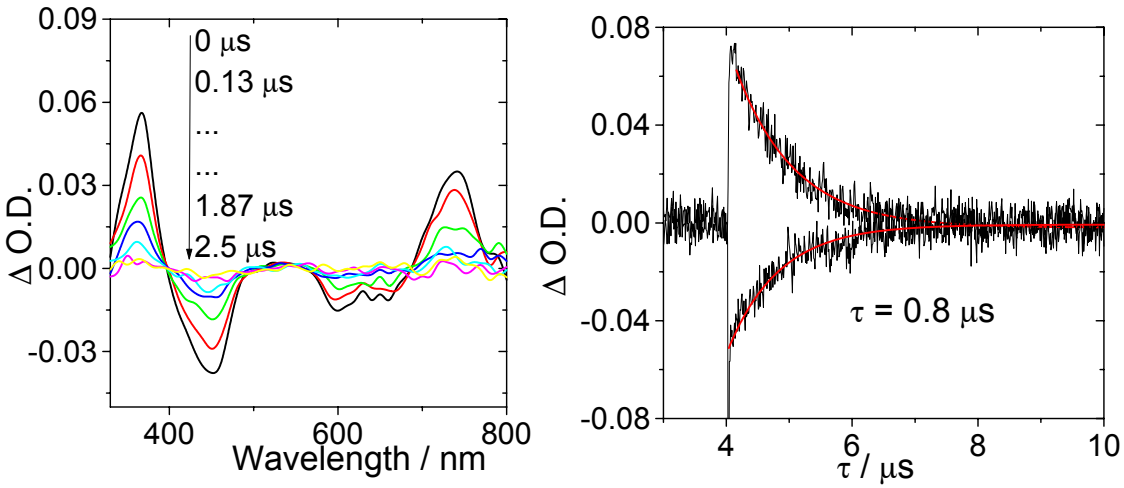


Figure S18. Nanosecond time-resolved transient difference absorption spectra of **Ru-3** after pulsed excitation (λ_{ex} = 532 nm); Decay traces of **Ru-3** at 450 nm and 370 nm. c = 1.0 × 10^{-5} M in deaerated MeCN. 20 °C.

6.0 Time-resolved emission spectra of the upconversion with Ru-2.

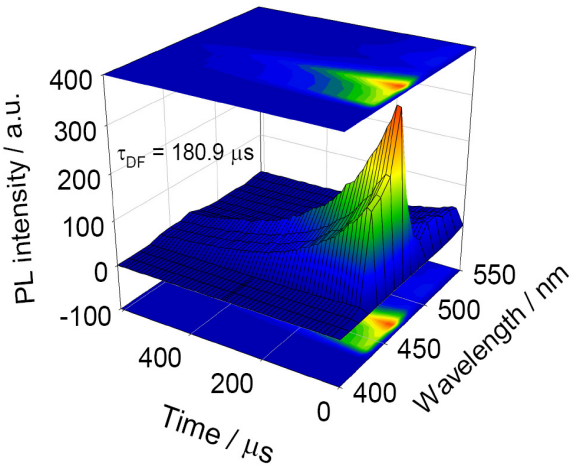


Figure S19. Time-resolved emission spectra (TRES) of the upconverted fluorescence of perylene using **Ru-2** as the triplet photosensitizer. Excited with the nanosecond pulsed OPO laser. **Ru-2**: $c = 1.0 \times 10^{-5}$ M. Py: $c = 4.1 \times 10^{-5}$ M. In deaerated MeCN. 20 °C.

7.0 Calculation details.

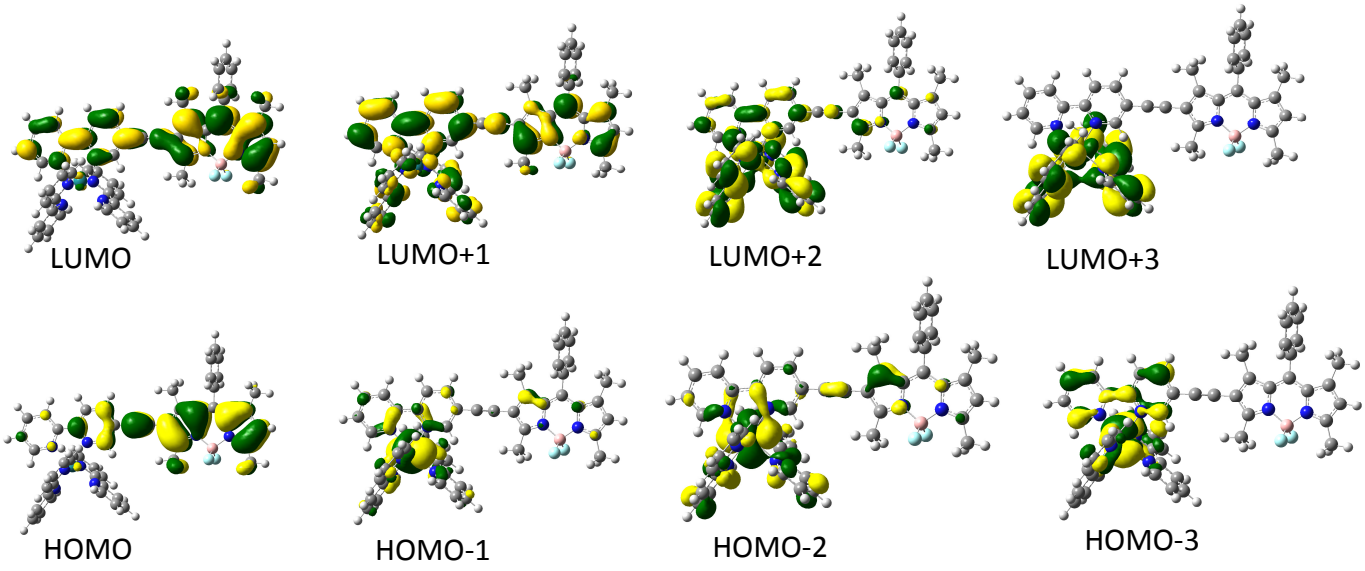


Figure S20. Frontier molecular orbitals for **Ru-1** Calculated by DFT at the B3LYP/6-31G(d) / LanL2DZ level using Gaussian 09W, MeCN as the solvent (PCM mode). Based on the optimized ground state (S_0) geometry.

Table S1. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **Ru-1**, Calculated at TDDFT//B3LYP/6-31G(d)/LanL2DZ level, MeCN as the solvent (PCM mode).

	Electronic transition	**TDDFT//B3LYP/6-31G(d)**				
		Energy (eV) [a]	***f*** [b]	**Composition**	**CI** [c]	**Character** [d]
Singlet	$S_0 \rightarrow S_1$	2.48 eV	1.1875	HOMO-1 → LUMO	0.1305	MLCT
		499 nm		HOMO → LUMO	0.6632	ILCT
	$S_0 \rightarrow S_{12}$	3.04 eV	0.1436	HOMO-3→LUMO+3	0.4392	ML'CT
		408 nm		HOMO-2→LUMO+2	0.4533	ML'CT
				HOMO-2→LUMO+1	0.2066	MLCT
Triplet	$S_0 \rightarrow T_1$	1.57 eV	0.0000[e]	HOMO→LUMO	0.5936	ILCT
		792 nm		HOMO→LUMO+1	0.2744	ILCT, LLCT
	$S_0 \rightarrow T_2$	2.14 eV	0.0000[e]	HOMO→LUMO	0.3074	ILCT
		579 nm		HOMO-4→LUMO	0.3075	ILCT, MLCT
				HOMO→LUMO+1	0.3507	ILCT, LLCT

[a] Only the selected low-lying excited states are presented. [b] oscillator strength. [c] The CI coefficients are in absolute values. [d] L stands for Bodipy localized ligand and L' stands for bpy localized ligand, [e] No spin-orbit coupling was considered, thus the *f* value is zero.

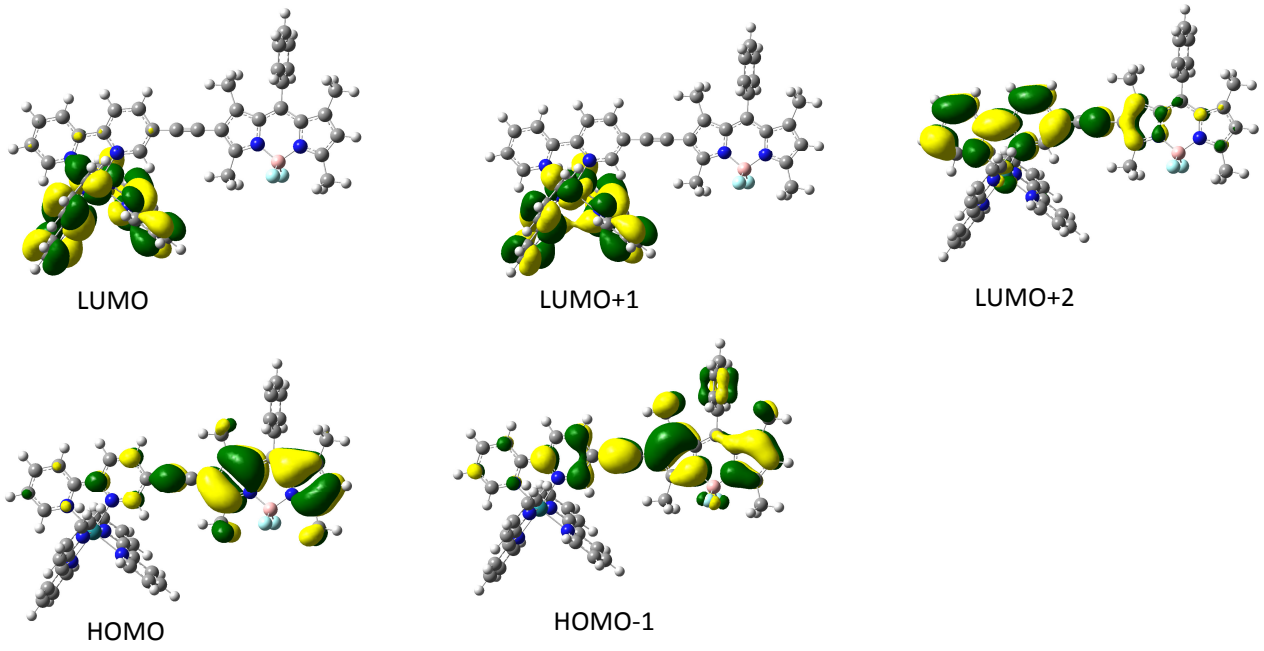


Figure S21. Frontier molecular orbitals for **Ru-1** Calculated by DFT at the B3LYP/6-31G(d) / LanL2DZ level using Gaussian 09W, Based on the optimized ground state (S_0) geometry.

Table S2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **Ru-1**, Calculated at TDDFT//B3LYP/6-31G(d)/LanL2DZ level.

	Electronic transition	**TDDFT//B3LYP/6-31G(d)**				
		Energy (eV) [a]	***f*** [b]	**Composition**	**CI** [c]	**Character** [d]
Singlet	$S_0 \rightarrow S_1$	1.45 eV	0.0068	HOMO → LUMO	0.6446	LL'CT
		854 nm		HOMO → LUMO+1	0.2823	LL'CT
	$S_0 \rightarrow S_3$	1.78 eV	0.3893	HOMO → LUMO+2	0.6993	ILCT
		697 nm				
	$S_0 \rightarrow S_7$	2.50 eV	0.6475	HOMO-1→LUMO+2	0.6555	ML'CT
		495 nm				

[a] Only the selected low-lying excited states are presented. [b] oscillator strength. [c] The CI coefficients are in absolute values. [d] L stands for Bodipy localized ligand and L' stands for bpy localized ligand, [e] No spin-orbit coupling was considered, thus the *f* value is zero.

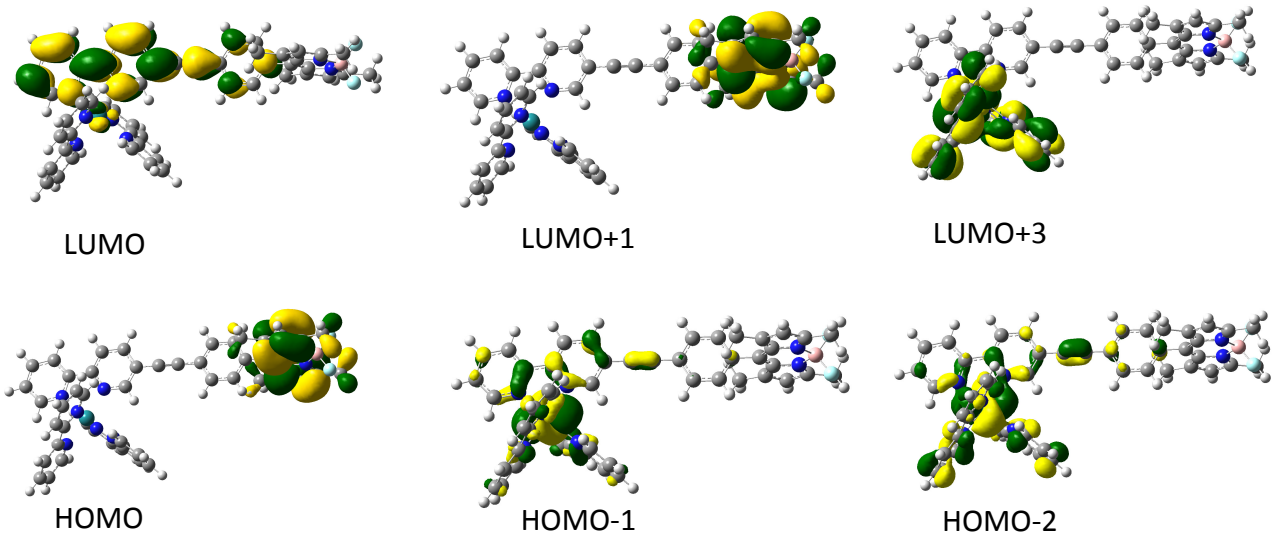


Figure S22. Frontier molecular orbitals for **Ru-2** Calculated by DFT at the B3LYP/6-31G(d) / LanL2DZ level using Gaussian 09W, MeCN as the solvent (PCM mode). Based on the optimized ground state (S_0) geometry.

Table S3. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of **Ru-2**, Calculated at TDDFT//B3LYP/6-31G(d)/LanL2DZ level, MeCN as the solvent (PCM mode).

	Electronic transition	**TDDFT//B3LYP/6-31G(d)**				
		Energy (eV) [a]	***f*** [b]	**Composition**	**CI** [c]	**Character** [d]
Singlet	$S_0 \rightarrow S_1$	2.54 eV	0.0000	HOMO → LUMO	0.7030	ILCT
		489 nm				
	$S_0 \rightarrow S_8$	2.90 eV	0.5644	HOMO-1→LUMO	0.6988	MLCT
		427 nm				
	$S_0 \rightarrow S_{15}$	3.26 eV	0.9823	HOMO-4→LUMO	0.5995	ILCT
		380 nm		HOMO-2→LUMO+3	0.2683	ML'CT
Triplet	$S_0 \rightarrow T_1$	1.52 eV	0.0000[e]	HOMO→LUMO+1	0.7106	ILCT
		816 nm		HOMO←LUMO+1	0.1188	ILCT
	$S_0 \rightarrow T_2$	2.25 eV	0.0000[e]	HOMO-4→LUMO	0.3795	ILCT
		552 nm		HOMO-2→LUMO	0.2327	MLCT
				HOMO-1→LUMO	0.4605	MLCT

[a] Only the selected low-lying excited states are presented. [b] oscillator strength. [c] The CI coefficients are in absolute values. [d] L stands for Bodipy localized ligand and L' stands for bpy localized ligand, [e] No spin-orbit coupling was considered, thus the *f* value is zero.

8.0 The *x-y-z* coordinates of the triplet optimized geometries of complexes

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

Charge = 2 Multiplicity = 1

C	-4.00425682	-0.97233612	-0.07526734
C	-4.83173204	1.16536197	0.00913356
C	-5.89552986	0.22857481	-0.06040407
C	-7.29909055	0.40386888	-0.08652687
C	-8.15760168	-0.69537870	-0.16402584
C	-9.59507575	-0.78754486	-0.20638142
C	-9.88919013	-2.14109794	-0.28293251
C	-8.67740609	-2.86656854	-0.28781461
H	-10.87636563	-2.58194331	-0.33119349
N	-5.34317523	-1.06232241	-0.11028042
N	-7.64547796	-2.00292778	-0.21673336
B	-6.14574476	-2.39262026	-0.19610047
F	-5.80653860	-3.07912489	-1.36669460
F	-5.86632261	-3.19045790	0.91862657
C	-4.86701627	2.66135694	0.07998988
H	-5.36360708	3.09889550	-0.79211945
H	-5.40825620	3.01500233	0.96353286
H	-3.84676491	3.05235390	0.12466432
C	-8.49711138	-4.34730655	-0.36095532
H	-9.46699607	-4.84886060	-0.38314875
H	-7.93241517	-4.62406834	-1.25805860
H	-7.92563249	-4.70995996	0.50003343
C	-10.62077006	0.30563925	-0.17679728
H	-10.50563765	0.99791991	-1.01738478
H	-11.62343638	-0.12884849	-0.22705869
H	-10.55342469	0.90492645	0.73726864
C	-3.09772502	-2.15719608	-0.11165553
H	-3.26629605	-2.74252889	-1.02154493
H	-2.05424505	-1.83720916	-0.07911352
H	-3.29673745	-2.81994973	0.73706166
C	-7.86530719	1.78642015	-0.03357784
C	-8.16307369	2.38265400	1.19983043
C	-8.09998121	2.49856204	-1.21825618
C	-8.68873911	3.67576025	1.24612457
C	-8.62581131	3.79133515	-1.16819198
H	-7.87048069	2.04006347	-2.17603080
H	-8.91677249	4.12914913	2.20657576
H	-8.80467137	4.33504443	-2.09145898
C	-8.92068178	4.38214717	0.06318761
H	-9.32922249	5.38795093	0.10069751
H	-7.98328805	1.83397896	2.12008281
C	6.94129238	3.50289634	0.02474866
C	6.06163553	4.58492926	0.03529706
C	4.22290416	3.02188348	0.07187660
C	6.41505249	2.21593122	0.03679455
C	2.79485537	2.66668534	0.09593483
C	0.43710587	3.18812496	0.13195879
H	-0.36948325	3.91230276	0.15672874

C	0.14714336	1.80930885	0.09539670
C	1.24045264	0.92229384	0.07215642
H	8.01604740	3.64317362	0.00692473
H	6.43304139	5.60419763	0.02507399
H	7.05958006	1.34594738	0.03172055
H	1.07450160	-0.14718869	0.04597049
N	5.09173763	1.97085445	0.06064120
N	2.51529716	1.33117981	0.07216904
C	6.39666395	-1.29046321	-1.41313301
C	6.70376556	-1.56530157	0.88519811
C	7.54727161	-2.04139924	-1.67264911
C	5.55673445	-0.69321244	-2.47014581
C	7.85695947	-2.31758003	0.69068157
H	6.33616761	-1.35065153	1.88080037
C	8.28527680	-2.56100136	-0.61323181
H	7.86651604	-2.22178307	-2.69135279
C	5.84159151	-0.79770068	-3.83501874
H	8.39882914	-2.69996767	1.54823964
H	9.17892621	-3.14512718	-0.80592642
C	3.64577310	0.56403906	-2.93865469
C	4.99553467	-0.19939477	-4.76416162
H	6.71637866	-1.33864432	-4.17286846
C	3.87649800	0.49542454	-4.30821619
H	2.78724483	1.09056402	-2.54114859
H	5.21000269	-0.27539857	-5.82489079
H	3.18887743	0.97878332	-4.99286780
N	4.45824527	-0.01447237	-2.03446635
N	5.98456595	-1.06002375	-0.13454495
H	1.78599676	-4.34164037	-1.43708289
C	2.08460037	-3.75137987	-0.57821682
C	2.75592409	-2.54873605	-0.76956524
C	1.81403686	-4.16625810	0.72468107
H	2.98435941	-2.18635109	-1.76399490
C	2.22178418	-3.36321180	1.78584474
H	1.29412220	-5.09911837	0.91543042
C	2.89092306	-2.16260076	1.52942302
H	2.02005080	-3.67297516	2.80332592
C	3.35217232	-1.24332217	2.58876265
C	3.14620535	-1.47114446	3.95285154
C	4.45877182	0.75755609	3.06348797
C	3.61618285	-0.55033698	4.88473686
H	2.62268662	-2.35724168	4.28883548
C	4.28540593	0.58573037	4.43251659
H	4.97499193	1.62366540	2.66843008
H	3.46032277	-0.71987099	5.94487617
H	4.66962250	1.33105718	5.11959854
N	4.00831300	-0.12972417	2.15665443
N	3.15289424	-1.76695859	0.25192133
Ru	4.20300414	0.05634563	0.06089332
C	-3.64143544	0.40073808	-0.00115210
C	-2.32073982	0.88886500	0.04307736
C	-1.17836706	1.31409377	0.07512187
C	1.75782044	3.60664205	0.13180115
H	1.97825138	4.66634604	0.15836027
C	4.69229424	4.34016099	0.05873168
H	3.99676696	5.16983767	0.06481064

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

Charge = 2 Multiplicity = 3

C	-3.99294875	-0.95437893	-0.06612726
C	-4.81950361	1.18326413	0.01389651
C	-5.90595354	0.22895602	-0.05781819
C	-7.30602303	0.42240878	-0.08515311
C	-8.14741724	-0.72854542	-0.16442177
C	-9.61145548	-0.83780608	-0.20869647
C	-9.88978604	-2.19377330	-0.28319099
C	-8.68004150	-2.90805426	-0.28615149
H	-10.87316586	-2.64312978	-0.33150101
N	-5.35161355	-1.04822826	-0.10403079
N	-7.63105788	-1.99797507	-0.21326055
B	-6.13706874	-2.38099286	-0.19161433
F	-5.78925239	-3.07097202	-1.36147617
F	-5.85168234	-3.18511791	0.92088085
C	-4.88080040	2.67535322	0.08113398
H	-5.38370344	3.10433774	-0.79291000
H	-5.43193323	3.02365270	0.96192372
H	-3.86752156	3.08467581	0.12787549
C	-8.45655545	-4.37624777	-0.35312719
H	-9.41045379	-4.90615321	-0.39933510
H	-7.85681463	-4.63859946	-1.23325205
H	-7.89369495	-4.72387221	0.52171582
C	-10.62876540	0.25841529	-0.17994376
H	-10.51181283	0.95084751	-1.02143844
H	-11.63394113	-0.17099265	-0.22794347
H	-10.55753153	0.86168958	0.73238604
C	-3.09434788	-2.13834627	-0.10059443
H	-3.26303751	-2.72111913	-1.01339402
H	-2.04911629	-1.82581147	-0.05929562
H	-3.30720223	-2.80595410	0.74213014
C	-7.89258866	1.79698697	-0.03819674
C	-8.20442482	2.40240085	1.18953845
C	-8.14078406	2.50944398	-1.22230008
C	-8.74998058	3.68774996	1.23303315
C	-8.68655996	3.79466310	-1.18070175
H	-7.90283993	2.05152592	-2.17875623
H	-8.98531941	4.14181368	2.19175130
H	-8.87214078	4.33237402	-2.10651595
C	-8.99220797	4.38666843	0.04758498
H	-9.41610768	5.38651257	0.08075539
H	-8.01706152	1.86076553	2.11293861
C	6.95157821	3.49974372	0.04274632
C	6.07386366	4.58316912	0.06198391
C	4.23275979	3.02284072	0.09042087
C	6.42330643	2.21342220	0.04678129
C	2.80424432	2.66997295	0.11379784
C	0.44771858	3.19590446	0.15493091
H	-0.35787684	3.92093997	0.18475669
C	0.15634027	1.81757989	0.11004080
C	1.24729945	0.92814676	0.08048710
H	8.02653892	3.63832547	0.02427737

H	6.44695515	5.60184506	0.05824217
H	7.06655048	1.34256822	0.03480234
H	1.07910547	-0.14079752	0.04770094
N	5.09976318	1.97027668	0.07091468
N	2.52272476	1.33471905	0.08194455
C	6.39639512	-1.28609587	-1.42490037
C	6.70663915	-1.57401205	0.87146029
C	7.54475648	-2.03839433	-1.69032254
C	5.55647552	-0.68064470	-2.47722087
C	7.85769841	-2.32800939	0.67099356
H	6.34117707	-1.36390290	1.86881004
C	8.28323487	-2.56545835	-0.63492428
H	7.86196908	-2.21403206	-2.71049012
C	5.83888038	-0.77828373	-3.84310469
H	8.40006874	-2.71627632	1.52558376
H	9.17515640	-3.15067495	-0.83225648
C	3.64931976	0.58602389	-2.93560638
C	4.99355216	-0.17168795	-4.76752832
H	6.71126580	-1.32029832	-4.18539008
C	3.87782817	0.52466700	-4.30588173
H	2.79343157	1.11370224	-2.53395474
H	5.20614168	-0.24240475	-5.82899752
H	3.19103248	1.01464468	-4.98663433
N	4.46078956	-0.00091213	-2.03599479
N	5.98704223	-1.06151732	-0.14437180
H	1.78353279	-4.32829598	-1.46197000
C	2.08347079	-3.74351697	-0.59982986
C	2.75653372	-2.54080042	-0.78457186
C	1.81290778	-4.16549788	0.70077270
H	2.98486728	-2.17308042	-1.77705649
C	2.22263623	-3.36933599	1.76636571
H	1.29151659	-5.09856348	0.88640617
C	2.89374526	-2.16845169	1.51655730
H	2.02084736	-3.68459629	2.78214203
C	3.35785561	-1.25661813	2.58103907
C	3.15302655	-1.49259488	3.94389753
C	4.46913354	0.73897831	3.06702698
C	3.62593797	-0.57859401	4.88097502
H	2.62823850	-2.37979992	4.27493371
C	4.29699492	0.55891761	4.43514841
H	4.98678350	1.60641087	2.67680698
H	3.47097572	-0.75449440	5.94020941
H	4.68359202	1.29908504	5.12645496
N	4.01574938	-0.14166370	2.15518780
N	3.15530875	-1.76560285	0.24120582
Ru	4.20815838	0.05728640	0.06027564
C	-3.63587169	0.42281519	0.00702778
C	-2.31396009	0.90409283	0.05344709
C	-1.17006168	1.32524164	0.08728035
C	1.76906486	3.61195291	0.15640505
H	1.99159016	4.67099160	0.18937043
C	4.70413544	4.34044319	0.08567710
H	4.01000770	5.17118990	0.09843946

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

Charge = 2 Multiplicity = 1

C	9.76947944	-2.50337482	-0.79129624
C	7.55923403	-2.67634535	-0.28597400
C	7.97940034	-1.30778434	-0.18580997
C	7.28371033	-0.13510000	0.15245859
C	7.93074969	1.11168888	0.17396119
C	7.45611956	2.43281070	0.47275288
C	8.55323221	3.27623774	0.32581429
C	9.66808670	2.50158665	-0.04993127
H	8.56148658	4.34860409	0.47300659
N	9.34377688	-1.25354939	-0.50580295
N	9.29396881	1.20682964	-0.14094066
B	10.22298705	0.02363506	-0.51680460
F	11.25855136	-0.09403524	0.42101506
F	10.76931715	0.22349379	-1.79156876
C	6.20597688	-3.28055844	-0.05000773
H	5.85322172	-3.11334556	0.97324827
H	5.44602067	-2.86336567	-0.71936906
H	6.25063013	-4.36040794	-0.22009963
C	11.06287347	2.96591767	-0.31810120
H	11.14004704	4.04527942	-0.16845453
H	11.77338023	2.46218145	0.34618892
H	11.36227910	2.72646283	-1.34431214
C	6.08191318	2.88861250	0.86718223
H	5.74011352	2.41283093	1.79250377
H	6.08450250	3.97136537	1.02413902
H	5.33605695	2.65939909	0.09859451
C	11.17961997	-2.81461718	-1.17554964
H	11.87505101	-2.48986577	-0.39412809
H	11.30206116	-3.88805039	-1.33711201
H	11.45939191	-2.28293526	-2.09163128
C	5.83090563	-0.21453180	0.49620017
C	4.85595505	-0.07982247	-0.50319475
C	5.42688340	-0.42252822	1.82341071
C	3.50289677	-0.14943753	-0.18624737
C	4.07610580	-0.49603238	2.14919788
H	6.17490486	-0.52719826	2.60354436
H	2.75471331	-0.04368584	-0.96511261
H	3.77170718	-0.65801670	3.17810751
C	3.09430507	-0.35984352	1.14664587
H	5.15966360	0.08154891	-1.53315877
C	-7.79729077	-0.89841525	2.86101520
C	-7.05922699	-1.25596851	3.98850563
C	-5.04127972	-0.82679060	2.73704450
C	-7.11571645	-0.51780626	1.70999190
C	-3.57906393	-0.75691095	2.57532061
C	-1.30387791	-0.97550077	3.35315876
H	-0.59155799	-1.20633888	4.13723685
C	-0.84964242	-0.59509068	2.07598910
C	-1.82268220	-0.30395531	1.10363465
H	-8.88126300	-0.91097838	2.86304166

H	-7.55425712	-1.55917648	4.90495393
H	-7.64818264	-0.22897263	0.81245514
H	-1.52698373	-0.00509644	0.10621478
N	-5.77229332	-0.47849830	1.63980072
N	-3.13850344	-0.38052036	1.34010658
C	-6.67047121	-0.81892296	-2.04566589
C	-6.92192052	1.46519951	-1.62939258
C	-7.71669728	-0.78101540	-2.97233654
C	-5.92112775	-2.04612792	-1.71045483
C	-7.97159434	1.56491790	-2.53596444
H	-6.57628258	2.32790909	-1.07376212
C	-8.37454731	0.42002347	-3.22142592
H	-8.01621647	-1.67852531	-3.49852289
C	-6.20611357	-3.29966257	-2.26028208
H	-8.45398507	2.52266554	-2.69477455
H	-9.18734325	0.45781749	-3.93896886
C	-4.17855018	-2.96320838	-0.45575157
C	-5.44568433	-4.40468176	-1.88900609
H	-7.01523220	-3.41655046	-2.97006473
C	-4.41147182	-4.23398230	-0.97016850
H	-3.38513818	-2.78551083	0.25943216
H	-5.66019082	-5.38081916	-2.31096836
H	-3.79173884	-5.06394489	-0.65030925
N	-4.90896473	-1.88983827	-0.81135765
N	-6.28107523	0.30706303	-1.38412996
H	-1.71730243	-0.11212115	-4.39633099
C	-2.08262831	0.53704554	-3.60872860
C	-2.89522803	0.01504728	-2.60833245
C	-1.76048381	1.89256699	-3.56957439
H	-3.16908137	-1.03241844	-2.59802499
C	-2.25843137	2.67389367	-2.53091057
H	-1.13163564	2.33757394	-4.33338816
C	-3.06873514	2.09045270	-1.55203269
H	-2.01745630	3.72845566	-2.48733729
C	-3.63528811	2.83610369	-0.41056153
C	-3.39509313	4.19386652	-0.17840864
C	-4.98392962	2.72288819	1.49253905
C	-3.97380290	4.81845163	0.92267663
H	-2.76117730	4.76160002	-0.84765451
C	-4.78453422	4.06993896	1.77427416
H	-5.60695871	2.10394667	2.12591384
H	-3.79244417	5.87157025	1.10963862
H	-5.25753915	4.51182176	2.64390296
N	-4.42832062	2.11259304	0.42904415
N	-3.38142924	0.76484914	-1.60150060
Ru	-4.65240812	0.07054716	-0.06363051
C	-2.66679514	-1.05471654	3.59423407
H	-3.01633726	-1.34938933	4.57563758
C	-5.66969739	-1.21903236	3.92371789
H	-5.08240332	-1.49506966	4.79037598
C	8.68826624	-3.39710163	-0.66325578
H	8.73973767	-4.46492789	-0.83303135
C	1.71102078	-0.43652565	1.47494066
C	0.52917618	-0.50589138	1.75546382

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

Charge = 2 Multiplicity = 3

C	-9.64692538	2.75745973	-0.29358999
C	-7.43346019	2.69230702	0.21486997
C	-7.94917903	1.32860410	0.06148913
C	-7.30096167	0.07090587	0.19091908
C	-8.07583162	-1.10585908	0.00703334
C	-7.69277365	-2.52022719	0.05038475
C	-8.85161325	-3.23747213	-0.20737965
C	-9.91026509	-2.33529816	-0.40902221
H	-8.93950917	-4.31537983	-0.25390337
N	-9.28860354	1.41919871	-0.24175540
N	-9.42117265	-1.04480170	-0.27723477
B	-10.25885240	0.23861214	-0.45668323
F	-11.29992852	0.28109895	0.48547480
F	-10.81261316	0.28723302	-1.74700423
C	-6.04451935	3.13117906	0.55906467
H	-5.68823029	2.67905291	1.49153595
H	-5.31992541	2.85930157	-0.21783885
H	-6.02072939	4.21884540	0.67647999
C	-11.33798637	-2.61940032	-0.71702703
H	-11.50781554	-3.69640823	-0.78336260
H	-11.99379870	-2.20003687	0.05569667
H	-11.63208922	-2.14997158	-1.66335816
C	-6.34172805	-3.11292273	0.30243634
H	-5.97471060	-2.89333596	1.31201823
H	-6.38981078	-4.20023948	0.18959961
H	-5.58765078	-2.73047372	-0.39492057
C	-11.03524131	3.19953707	-0.59428610
H	-11.73857540	2.79859121	0.14548504
H	-11.09803364	4.29008986	-0.59319068
H	-11.36174574	2.82182081	-1.57071767
C	-5.84704278	-0.01192786	0.52223953
C	-4.87017055	0.10502186	-0.48133977
C	-5.42243900	-0.20679987	1.84788976
C	-3.51423150	0.03184558	-0.17720315
C	-4.07008070	-0.28197254	2.16634431
H	-6.16418516	-0.29569247	2.63638384
H	-2.77172664	0.12167922	-0.96381590
H	-3.75770337	-0.42936926	3.19532611
C	-3.09468487	-0.16306104	1.15485930
H	-5.18088234	0.25277818	-1.51161821
C	7.78954530	-0.61108503	2.96140963
C	7.04065816	-0.77718007	4.12561891
C	5.03499168	-0.54110469	2.80479184
C	7.11922828	-0.41359150	1.75906610
C	3.57464857	-0.49667453	2.62119406
C	1.29354554	-0.60952487	3.40373017
H	0.57495216	-0.74164593	4.20476400
C	0.84907747	-0.37625737	2.08808758
C	1.83023853	-0.21430191	1.09352250
H	8.87330867	-0.63254676	2.97397350
H	7.52673228	-0.93242620	5.08296981
H	7.66033636	-0.28475203	0.83004592

H	1.54090288	-0.02899540	0.06693193
N	5.77663601	-0.37691264	1.67245376
N	3.14437548	-0.27004838	1.34623459
C	6.76280359	1.60763074	-1.39438362
C	6.95464791	-0.60689900	-2.11000971
C	7.84374374	1.97797792	-2.20030910
C	6.02018063	2.55446965	-0.53910567
C	8.03481891	-0.29994911	-2.93010809
H	6.57284737	-1.61767641	-2.04062160
C	8.48700632	1.01775250	-2.97572759
H	8.18252233	3.00587621	-2.22611914
C	6.33694180	3.91212762	-0.43223994
H	8.50344690	-1.08305202	-3.51521664
H	9.32636425	1.29705097	-3.60371585
C	4.24314587	2.82509561	0.95107282
C	5.57561740	4.73540119	0.39226506
H	7.17009534	4.32676115	-0.98543505
C	4.50684224	4.18273919	1.09590828
H	3.42178487	2.35499616	1.47712874
H	5.81499380	5.78981083	0.48067051
H	3.88340561	4.78341520	1.74837410
N	4.97602069	2.02262618	0.15669754
N	6.32819868	0.31637201	-1.35670595
H	1.81971336	2.18324258	-3.87676714
C	2.15528847	1.23468956	-3.47315102
C	2.96588659	1.21559152	-2.34340845
C	1.79599379	0.02201538	-4.05920454
H	3.26847898	2.13298893	-1.85418003
C	2.25807031	-1.16275906	-3.49347109
H	1.16684787	-0.00477547	-4.94258892
C	3.06844180	-1.11726046	-2.35497641
H	1.98992865	-2.11260366	-3.93839048
C	3.60094644	-2.31982270	-1.68365234
C	3.32297858	-3.62510830	-2.10077525
C	4.93275164	-3.13127523	0.05469494
C	3.87347394	-4.70160562	-1.41140375
H	2.68152373	-3.80384273	-2.95447433
C	4.69506718	-4.45098647	-0.31355559
H	5.56693286	-2.89018912	0.89876949
H	3.66251809	-5.71740526	-1.72858780
H	5.14755190	-5.25605104	0.25418290
N	4.40314475	-2.08536610	-0.60715899
N	3.41591415	0.07360715	-1.79088124
Ru	4.67417590	-0.05247431	-0.09859411
C	2.65409127	-0.66869807	3.66151909
H	2.99576431	-0.84920908	4.67284993
C	5.65202567	-0.74223015	4.04415845
H	5.05639943	-0.87067002	4.93904317
C	-8.51028228	3.53572534	-0.01538932
H	-8.49367919	4.61759299	0.01634522
C	-1.70999152	-0.23801145	1.47578670
C	-0.52741393	-0.30198512	1.75603367

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

Charge = 2 Multiplicity = 3

C	2.32693906	2.53754117	2.68519417
C	1.99647020	3.84079049	2.21547499
C	0.53926803	2.84120133	0.54986672
C	1.74754257	1.45243971	2.06877776
C	-0.34841965	2.87023968	-0.55360296
C	-1.73847578	3.96182844	-2.21943199
H	-2.12358229	4.86398118	-2.68409703
C	-1.64499921	1.56250595	-2.07118058
H	3.01148897	2.38842617	3.51172673
H	2.43888503	4.71657467	2.67952622
H	1.96032227	0.44100192	2.39537996
H	-1.92141331	0.56628852	-2.39740715
N	0.86220461	1.57123785	1.04706054
N	-0.75475631	1.62348819	-1.04906070
C	2.21809576	-1.91761708	0.54240600
C	0.45355997	-2.29768458	2.03279484
C	2.94843585	-2.96295377	1.11246395
C	2.70145364	-1.09490825	-0.58346131
C	1.13444274	-3.34541219	2.64342849
H	-0.53375705	-2.00008089	2.36291458
C	2.40272026	-3.68172404	2.17277139
H	3.93107280	-3.21841881	0.73742628
C	3.95196897	-1.25684890	-1.18422854
H	0.67223676	-3.87893999	3.46573650
H	2.96404935	-4.49333679	2.62308629
C	2.20223133	0.67349357	-2.04056109
C	4.31986984	-0.42679195	-2.24030425
H	4.63473470	-2.02066646	-0.83522506
C	3.43215693	0.55544995	-2.67675242
H	1.47636650	1.41850270	-2.34002743
H	5.28865007	-0.54758835	-2.71304091
H	3.67840799	1.22263068	-3.49444335
N	1.84292919	-0.13270957	-1.02477072
N	0.98133894	-1.59871998	1.01334042
H	-0.94647056	-3.83539801	-3.46277692
C	-1.36732863	-3.27046855	-2.63924013
C	-0.61610461	-2.26733015	-2.03680315
C	-2.65234220	-3.52046826	-2.16114257
H	0.38628102	-2.03433839	-2.37507259
C	-3.14390581	-2.76281204	-1.10128896
H	-3.26816660	-4.29515169	-2.60522001
C	-2.34271330	-1.76675360	-0.53814237
H	-4.13951086	-2.95106929	-0.72072918
C	-2.76574969	-0.91048563	0.58605154
C	-4.02344654	-0.98362872	1.18915321
C	-2.14253714	0.82057636	2.03881317
C	-4.33171481	-0.12772948	2.24375402
H	-4.75756551	-1.69927539	0.84225558
C	-3.37658496	0.79036708	2.67726284
H	-1.36530214	1.51239537	2.33714238

H	-5.30556221	-0.18022041	2.71852186
H	-3.57387034	1.47558755	3.49333063
N	-1.84147327	-0.01010563	1.02378771
N	-1.08921252	-1.53245054	-1.01503628
Ru	0.00103879	0.00824776	-0.00252372
C	-0.85821936	4.04882970	-1.17042299
H	-0.54948361	5.01910750	-0.79860791
C	1.12257161	3.98440412	1.16788673
H	0.87588631	4.97212627	0.79603393
C	-2.15223854	2.68257051	-2.68893702
H	-2.84429789	2.57805322	-3.51623366