Synthesis and Photophysical Properties of Orthogonal Rhodium(III)-Carbon Bonded Porphyrin-Aza-BODIPY Conjugates

Table of contents

I. Experimental details

I.1 Materials and methods

Unless otherwise noted, all reagents were purchased from commercial suppliers and directly used without further purification. Hexane for chromatography was distilled from anhydrous calcium chloride. Benzene and benzene-d_6 were distilled from sodium and were stored in a Teflon-capped tube under nitrogen gas prior to use. All reactions carried out in Telfon screw-capped tube under N_2 with the mixture degassed for three freeze-thaw-pump cycles were wrapped with aluminum foil to prevent undesired photochemical reactions. The reaction mixtures in Teflon-screw-capped tubes were heated in heat blocks on heaters. The crude mixture was dried under high vacuum.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 400 MHz and 700 MHz spectrometer, respectively. Chemical Shifts were referenced with the residual solvent protons $CDCl_3$ (δ = 7.26 ppm) in ^{1}H NMR spectra, δ = 77.16 ppm in ^{13}C NMR spectra as the internal standards. Chemical shifts (δ) were reported as part per million (ppm) in (δ) scale downfield from tetramethylsilane (TMS). Coupling constants (J) were reported in Hertz (Hz). MALDI-TOF MS data were measured on Bruker Daltonics autoflex^{II}. High resolution mass spectra (HRMS) were recorded on a ThermoFinnigan MAT 95 XL mass spectrometer. Fast atom bombardment spectra were measured with 3-nitrobenzyl alcohol (NBA) as the matrix.

II. Supplementary data

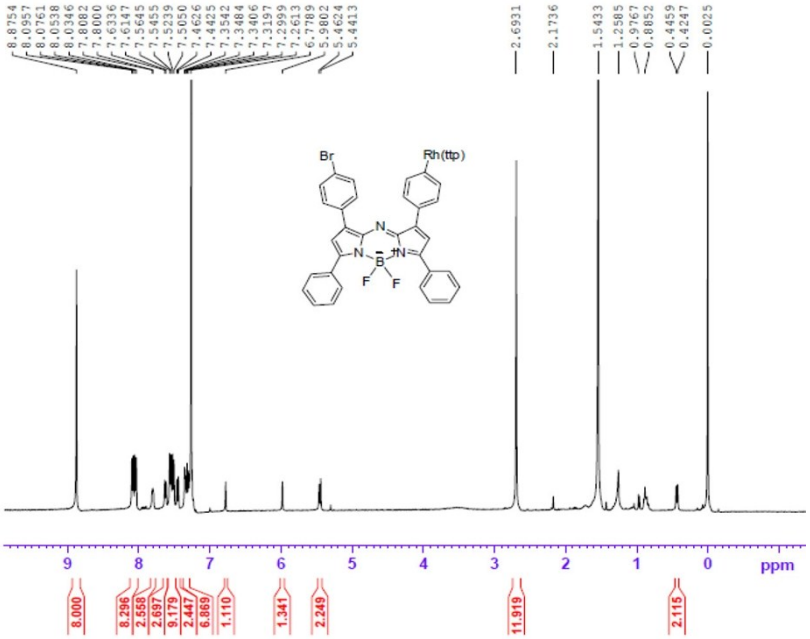

Fig. S1 ^{1}H NMR spectrum (400 MHz) of **1a** in $CDCl_3$.

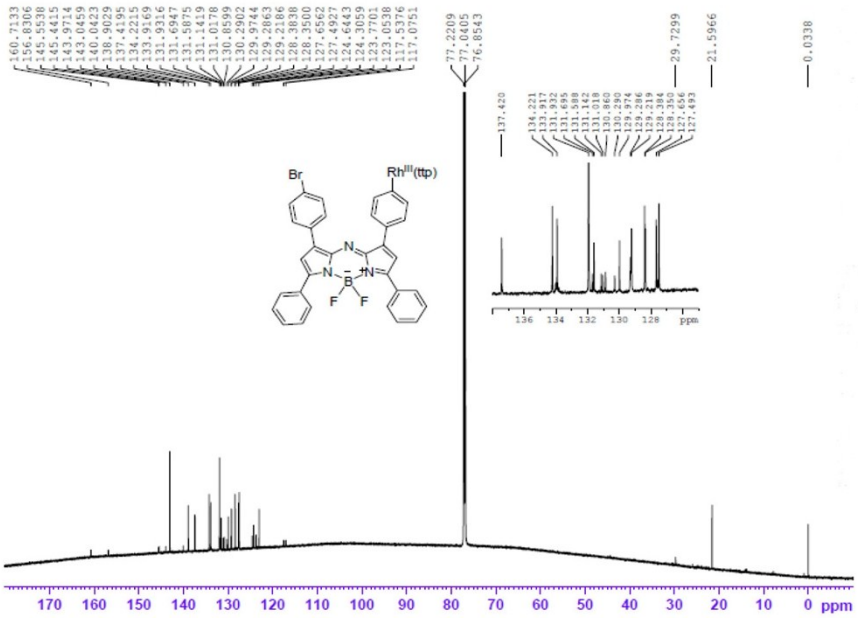

Fig. S2 ^{13}C NMR spectrum (175 MHz) of **1a** in $CDCl_3$.

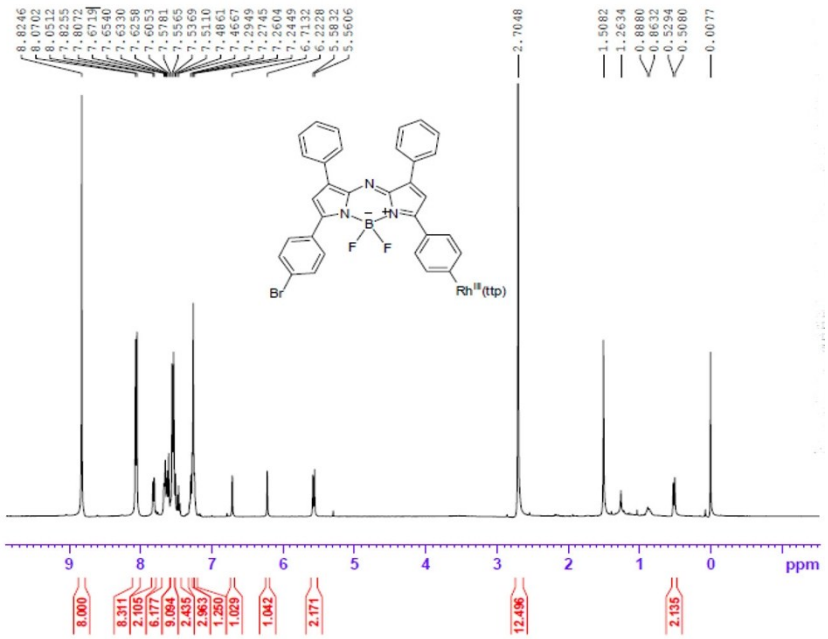

Fig. S3 ^{1}H NMR spectrum (400 MHz) of **1b** in $CDCl_3$.

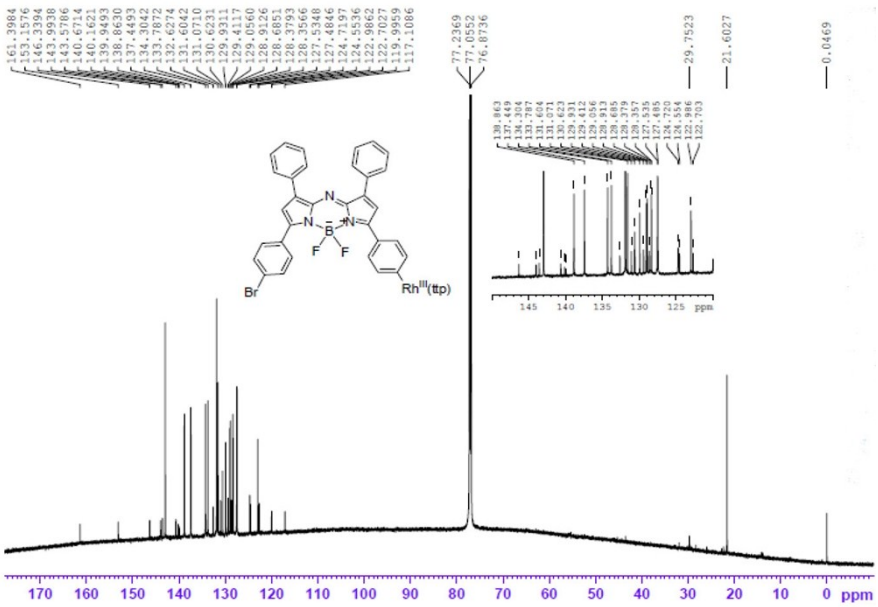

Fig. S4 ^{13}C NMR spectrum (175 MHz) of **1b** in $CDCl_3$.

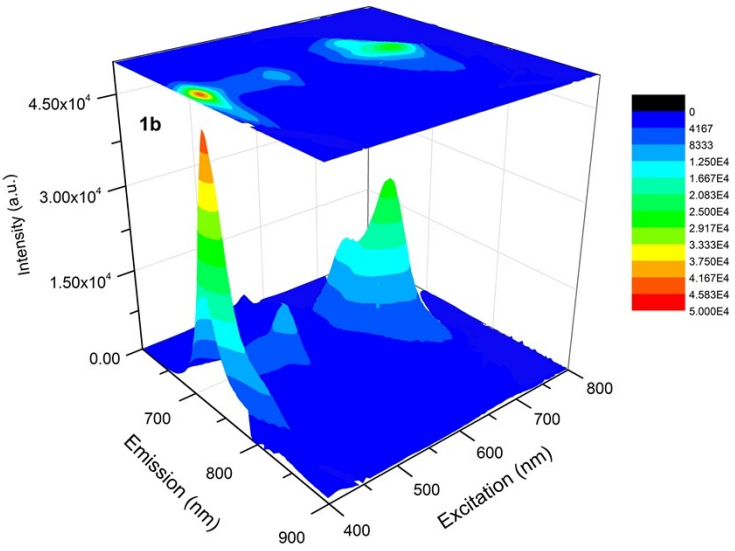

Fig. S5 3D-EEM spectra of **1b** in degassed toluene.

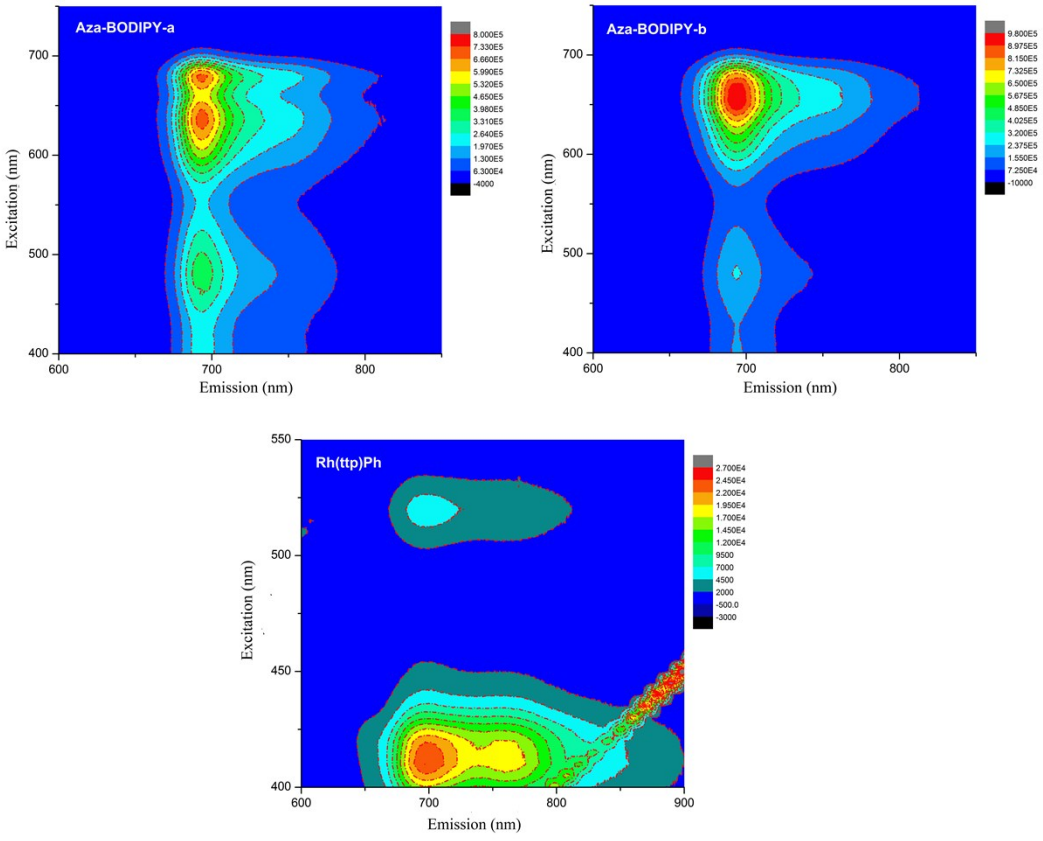

Fig. S6 3D-EEM spectra of **aza-BODIPYs** in air-saturated and **Rh^{III}(ttp)Ph** in degassed toluene.

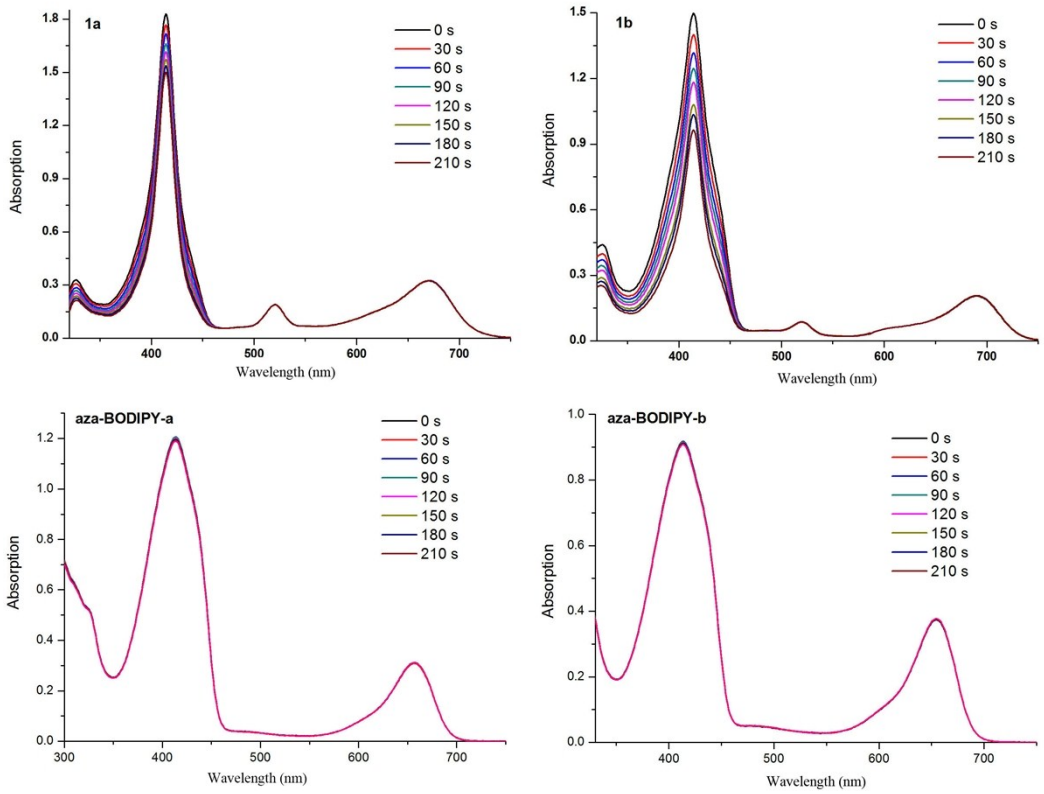

Fig. S7 Changes in the absorption spectra of DPBF upon irradiation (λ_{irr}=690 nm) in the presence of **1a** and **1b** and upon irradiation (λ_{irr}=671 nm) in the presence of **aza-BODIPYs** with 30 s interval in dichloromethane. The absorbance at the irradiation wavelength was adjusted to 0.1 – 0.3.

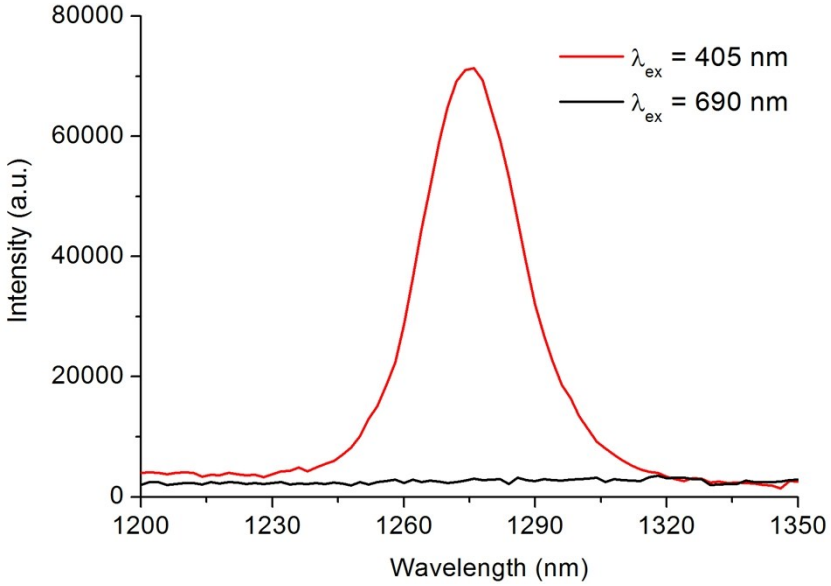

Fig. S8 The $^1O_2$ phosphorescence spectra of **Rh^{III}(ttp)Ph** in air-saturated dichloromethane upon irradiation with 405 nm (red) and 690 nm (black).

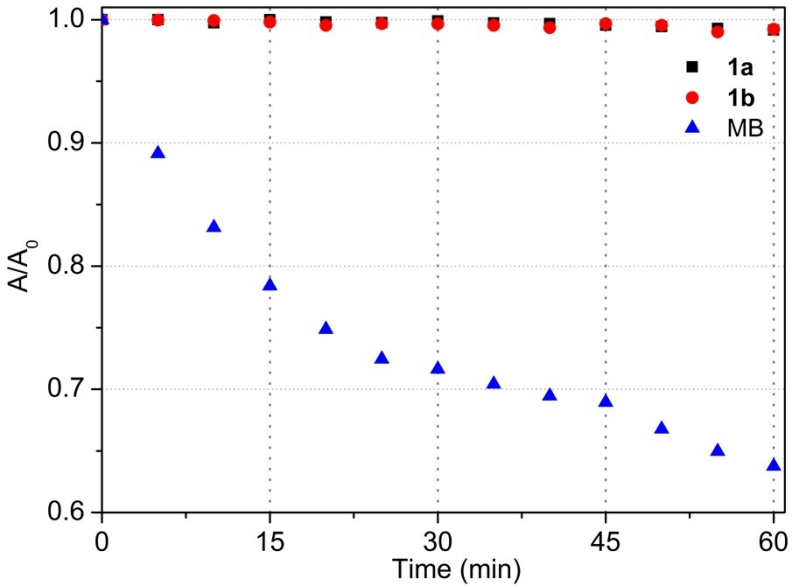

Fig. S9 Photostability of **1a**, **1b** and MB in dichloromethane at 5 min intervals determined using a laser beam (671 nm, 100 mW cm^{-2}) over an irradiation period of 60 min.

Table S1 Absorbance data in different solvents.

Compound	Solvent	Absorption/λ_{max} [nm](logε[$M^{-1}cm^{-1}$])
aza-BODIPY-a	Toluene	484 (3.87) , 662 (4.79)
	DCM	480 (4.06), 655 (4.93)
	Chloroform	484 (4.15), 658 (5.03)
aza-BODIPY-b	Toluene	483 (4.00), 663 (4.93)
	DCM	481 (4.00), 658 (4.89)
	Chloroform	497 (4.09), 658 (4.92)
Rh^{III}(ttp)Ph	Toluene	416 (5.01),521 (4.06)
	DCM	414 (5.01), 520 (4.03)
	Chloroform	414 (5.22), 521 (4.24)
1a	Toluene	415 (5.25), 521 (4.41), 674 (4.67)
	DCM	414 (5.02), 520 (4.16), 671 (4.40)
	THF	415 (5.21), 526 (4.30), 681 (4.48)
	Chloroform	415 (5.14), 521 (4.25), 674 (4.49)
	CH_3CN	417 (5. 31), 531 (4.39), 666 (4.62)
1b	Toluene	417 (5.28), 520 (4.47), 696 (4.87)
	DCM	414 (5.29), 520 (4.47), 690 (4.82)
	THF	415 (5.01), 525 (4.15), 703 (4.53)
	Chloroform	416 (5.35), 521 (4.50), 699 (4.89)
	CH_3CN	417 (5.14), 529 (4.21), 685 (4.62)

Table S2 TD-DFT spectra of the B3LYP optimized geometries of **Rh^{III}(ttp)Ph**, **1a** and **1b** calculated with the CAM-B3LYP functional and 6-31G(d) basis sets.

				Rh^{III}(ttp)Ph			
Band[a]	**#[b]**		**Calc[c]**			**Exp[d]**	**Wavefunction=[e]**
--	1	---	---	---	---	---	Ground state
Q	2	19.8	504.0	(0.01)	18.0	555	**54% $1a_{2u} \rightarrow 1e_{gx}$; 45% $1a_{1u} \rightarrow$ 1egy;** …
Q	3	19.9	502.3	(0.00)	18.0	555	**52% $1a_{2u} \rightarrow$ 1egy; 45% $1a_{1u} \rightarrow 1e_{gx}$;** …
B	10	28.0	356.6	(1.13)	24.2	413	**48% $1a_{1u} \rightarrow$ 1egy; 41% $1a_{2u} \rightarrow 1e_{gx}$;** …
B	11	28.1	355.9	(1.18)	24.2	413	**47% $1a_{1u} \rightarrow 1e_{gx}$; 43% $1a_{2u} \rightarrow$ 1egy;** …
				1a			
Band	**#**		**Calc**			**Exp**	**Wavefunction=**
--	1	---	---	---	---	---	Ground state
BDY	2	17.2	580.4	(0.76)	671	14.9	97% H–2 → L; …
Q	3	19.7	508.2	(0.01)	554	18.1	**55% $1a_{2u} \rightarrow 1e_{gx}$; 42% $1a_{1u} \rightarrow 1e_{gy}$;** …
Q	4	19.7	506.5	(0.01)	554	18.1	**52% $1a_{2u} \rightarrow 1e_{gy}$; 42% $1a_{1u} \rightarrow 1e_{gx}$;** …
B	14	27.8	360.0	(1.07)	416	24.0	**32% $1a_{1u} \rightarrow 1e_{gy}$; 26% $1a_{2u} \rightarrow 1e_{gx}$; 13% $1a_{1u} \rightarrow 1e_{gx}$; 11% $1a_{2u} \rightarrow 1e_{gy}$;** …
B	15	27.9	358.9	(1.22)	416	24.0	**35% $1a_{1u} \rightarrow 1e_{gx}$; 30% $1a_{2u} \rightarrow 1e_{gy}$; 15% $1a_{1u} \rightarrow 1e_{gy}$; 12% $1a_{2u} \rightarrow 1e_{gx}$;** …
				1b			
Band[a]	**#**		**Calc**			**Exp**	**Wavefunction=**
--	1	---	---	---	---	---	Ground state
BDY	2	17.0	588.6	(0.84)	690	14.5	97% H–2 → L; …
Q	3	19.8	505.6	(0.01)	554	18.1	**54% $1a_{2u} \rightarrow 1e_{gx}$; 44% $1a_{1u} \rightarrow 1e_{gy}$;** …
Q	4	19.8	503.9	(0.01)	554	18.1	**52% $1a_{2u} \rightarrow 1e_{gy}$; 46% $1a_{1u} \rightarrow 1e_{gx}$;** …
B	15	28.0	357.7	(1.18)	417	24.0	**47% $1a_{1u} \rightarrow 1e_{gy}$; 39% $1a_{2u} \rightarrow 1e_{gx}$;** …
B	16	28.0	356.9	(1.28)	417	24.0	**49% $1a_{1u} \rightarrow 1e_{gx}$; 44% $1a_{2u} \rightarrow 1e_{gy}$;** …

a − Band assignment described in the text. BDY refers to the main π → π* band of the BODIPY moiety, while Q and B refer to the main π → π* bands associated with the Rh(ttp) moiety. b − The number of the state assigned in terms of ascending energy within the TD-DFT calculation. c − Calculated band energies ($10^3.cm^{-1}$), wavelengths (nm) and oscillator strengths in parentheses (f). d − Observed energies ($10^3.cm^{-1}$) and wavelengths (nm). e − The wave functions based on the eigenvectors predicted by TD-DFT. One-electron transitions associated with the four frontier π-MOs of Gouterman's 4-orbital model[1] are highlighted in bold. H and L refer to the HOMO and LUMO, respectively.

Table S3 Cartesian coordinated of the B3LYP optimized geometries of **Rh^{III}(ttp)Ph**, **1a** and **1b**.

Rh^{III}(ttp)Ph

C	0.953168	7.121832	-1.26542
Rh	0.000178	0.003769	-0.24416
N	-1.68351	-1.15546	-0.37127
N	1.685356	1.163354	-0.35354
C	-3.00372	-0.70606	-0.44895
C	-1.73431	-2.54899	-0.31603
C	-3.89921	-1.85255	-0.45604
C	-3.12215	-2.98015	-0.37431
C	3.004827	0.714454	-0.4477
C	1.734388	2.557787	-0.33251
C	3.895913	1.862276	-0.51971
C	3.118981	2.990051	-0.43984
C	-0.9112	-4.89628	-0.15786
C	-0.67514	-5.75275	-1.25656
C	-0.9437	-7.13125	-1.16316
C	-1.44747	-7.67493	0.034838
C	-3.42604	0.63712	-0.47883
C	0.632608	3.431843	-0.28065
C	3.427155	-0.62899	-0.47784
C	0.709797	-3.00224	-0.29962
C	2.554118	-1.7334	-0.42513
C	2.983882	-3.12192	-0.36848
C	1.855425	-3.89771	-0.28409
C	-0.70968	3.01189	-0.3163
C	-1.85414	3.908798	-0.35039
C	-2.98185	3.13207	-0.43395
C	-2.55404	1.741822	-0.42546
N	-1.15963	1.690976	-0.36049
N	1.159102	-1.68252	-0.37727
C	-1.68374	-6.82887	1.136186
C	-1.4208	-5.44965	1.038335
C	5.456642	-1.47271	-1.73632
C	7.686602	-1.42308	-0.74478
C	7.143165	-0.85913	0.426086
C	5.762878	-0.59842	0.511294
C	6.837724	-1.72732	-1.82702
C	0.914156	4.907376	-0.216
C	0.68045	5.74258	-1.33146
C	1.459116	7.687656	-0.07862
C	1.693955	6.862788	1.038951
C	1.426812	5.482672	0.968476
C	-4.90254	0.907213	-0.56892
C	-5.61163	1.431182	0.535284

C	-6.99444	1.67886	0.449887
C	-7.68931	1.41142	-0.74589
C	-6.99065	0.89172	-1.8532
C	-5.60904	0.638953	-1.76301
C	-0.63234	-3.422	-0.25342
C	4.902223	-0.90326	-0.56755
C	-0.00368	-0.01519	1.771779
C	1.186141	-0.26664	2.489071
C	-1.1963	0.222638	2.489041
C	1.180249	-0.27941	3.898025
C	-0.00915	-0.04172	4.611985
C	-1.19589	0.20886	3.898006
H	-0.2925	-5.33571	-2.18515
H	-0.76232	-7.77533	-2.02044
H	-1.6529	-8.74026	0.108674
H	-2.06909	-7.23924	2.066578
H	0.297002	5.30844	-2.25183
H	0.773512	7.749256	-2.13531
H	1.667746	8.753617	-0.02597
H	2.081738	7.290265	1.960604
H	1.604926	4.848661	1.833838
H	-5.08056	1.6353	1.461992
H	-7.52504	2.076728	1.311701
H	-8.75726	1.604755	-0.81365
H	-7.51698	0.684973	-2.78208
H	-5.07254	0.241837	-2.6215
H	4.805741	-1.70403	-2.57615
H	8.753464	-1.62228	-0.8126
H	7.789029	-0.62458	1.268942
H	5.347855	-0.16728	1.419186
H	7.24765	-2.15895	-2.73708
H	-4.97563	-1.79342	-0.51021
H	-3.4481	-4.00921	-0.36379
H	4.967709	1.804449	-0.63318
H	3.440864	4.019832	-0.47663
H	4.012381	-3.44952	-0.37339
H	1.796231	-4.97292	-0.20966
H	-1.79423	4.986133	-0.32257
H	-4.00772	3.461337	-0.49855
H	-1.59922	-4.79944	1.8915
H	2.118239	-0.45532	1.967987
H	-2.12704	0.417667	1.967852
H	2.108359	-0.47719	4.431506
H	-0.01132	-0.05225	5.699608
H	-2.12657	0.393971	4.431581

1a

C	5.33653	-0.16063	-0.01147
N	6.40224	-1.09366	-0.03863
C	7.58887	-0.38637	-0.10201
C	7.2802	1.00503	-0.09998
C	5.88901	1.17055	-0.03052
B	6.15096	-2.61377	-0.1382
F	6.83481	-3.10213	-1.31541
F	6.66437	-3.31894	1.0158
C	3.9255	-4.04808	-0.24442
C	2.53307	-3.75101	-0.23156
C	2.34209	-2.36186	-0.18651
C	3.68474	-1.79593	-0.15498
N	4.62922	-2.85937	-0.22057
N	4.04175	-0.51607	-0.05833
C	5.17119	2.45147	0.0024
C	1.04737	-1.6777	-0.1775
C	8.95674	-0.92538	-0.16268
C	9.34741	-2.14741	0.44048
C	10.68355	-2.57465	0.37458
C	11.65401	-1.8049	-0.29512
C	11.27646	-0.59065	-0.90318
C	9.94541	-0.15519	-0.8338
C	4.46406	-5.41836	-0.24892
C	5.68694	-5.78475	-0.86557
C	6.11039	-7.12366	-0.85912
C	5.33716	-8.121	-0.23487
C	4.12239	-7.76825	0.38704
C	3.6893	-6.43493	0.37514
C	3.9012	2.58758	0.61358
C	3.25185	3.83218	0.66674
C	3.87516	4.95374	0.0973
C	5.13164	4.8552	-0.52104
C	5.76936	3.60617	-0.5631
C	-0.12902	-2.40614	-0.4987
C	-1.39535	-1.81526	-0.4521
C	-1.54948	-0.46128	-0.06852
C	-0.38247	0.28249	0.22939
C	0.88871	-0.31135	0.16902
BR	2.97922	6.70035	0.15584
C	-2.67883	6.72034	3.29057
RH	-3.37559	0.3486	0.05541
N	-4.19876	-1.3439	0.8704
N	-2.80659	2.1502	-0.73454
C	-4.15047	-1.72283	2.21422

C	-4.78883	-2.40098	0.17276
C	-4.72347	-3.05134	2.35589
C	-5.12521	-3.46126	1.10925
C	-2.73052	2.4718	-2.09061
C	-2.45087	3.30099	-0.02411
C	-2.32984	3.86214	-2.22976
C	-2.17664	4.37448	-0.96615
C	-5.64645	-3.70908	-1.76868
C	-7.0207	-3.93428	-1.54077
C	-7.65904	-5.08068	-2.05035
C	-6.9452	-6.04328	-2.79593
C	-3.63608	-0.95545	3.27623
C	-2.37096	3.42246	1.37804
C	-3.07157	1.63387	-3.17035
C	-4.53935	-1.50006	-2.13477
C	-3.64895	0.35875	-3.02263
C	-4.11323	-0.47091	-4.12288
C	-4.67691	-1.59753	-3.57929
C	-2.61841	2.36275	2.27489
C	-2.43606	2.44183	3.7158
C	-2.7601	1.21552	4.23944
C	-3.15633	0.36065	3.1328
N	-3.05499	1.07899	1.93999
N	-3.91521	-0.29148	-1.81533
C	-5.56758	-5.81589	-3.01977
C	-4.92971	-4.66894	-2.51866
C	-3.9238	2.51035	-5.39893
C	-2.38593	3.16653	-7.19705
C	-1.30814	2.81665	-6.3516
C	-1.53187	2.32543	-5.05438
C	-3.69604	3.01	-6.69475
C	-2.02885	4.76351	1.96106
C	-2.97944	5.46183	2.73803
C	-1.41662	7.32045	3.09407
C	-0.46658	6.61924	2.31674
C	-0.7679	5.36727	1.75626
C	-3.63071	-1.55664	4.653
C	-2.41146	-1.90531	5.27707
C	-2.39636	-2.46684	6.56484
C	-3.59617	-2.69434	7.27743
C	-4.81139	-2.33761	6.65393
C	-4.83037	-1.78124	5.36116
C	-4.96935	-2.48375	-1.22247
C	-2.84514	2.15952	-4.5593
C	-7.62637	-7.28735	-3.33754
C	-3.57252	-3.31457	8.66299

C	-1.08223	8.67411	3.69426
C	-2.1369	3.6807	-8.60365
H	1.76031	-4.50191	-0.27102
H	8.01972	1.79099	-0.0696
H	8.61842	-2.75123	0.96654
H	10.96449	-3.51208	0.84786
H	12.68567	-2.14502	-0.34549
H	12.01334	0.00756	-1.43351
H	9.66194	0.76905	-1.32983
H	6.29366	-5.03464	-1.35665
H	7.0481	-7.38527	-1.3427
H	5.67494	-9.15465	-0.22981
H	3.52162	-8.52626	0.88345
H	2.76473	-6.17267	0.88152
H	3.43011	1.71874	1.05829
H	2.28457	3.92043	1.15038
H	5.60022	5.72736	-0.96542
H	6.73118	3.526	-1.06174
H	-0.05733	-3.44648	-0.80491
H	-2.25768	-2.4168	-0.71359
H	-0.45643	1.32638	0.51533
H	1.76918	0.27905	0.39455
H	-7.59356	-3.20498	-0.97272
H	-8.72168	-5.22546	-1.86625
H	-4.99021	-6.54207	-3.58947
H	-3.96098	5.02273	2.89988
H	-3.43369	7.23843	3.87859
H	0.51684	7.05287	2.14701
H	-0.01933	4.85255	1.15907
H	-1.47644	-1.74313	4.74594
H	-1.44377	-2.73093	7.02075
H	-5.75029	-2.49236	7.18188
H	-5.77905	-1.50671	4.90572
H	-4.94224	2.40783	-5.03154
H	-0.28663	2.92928	-6.71048
H	-0.68743	2.0602	-4.42259
H	-4.54533	3.28188	-7.31846
H	-4.79658	-3.59371	3.28609
H	-5.58464	-4.39925	0.83696
H	-2.21862	4.37853	-3.1711
H	-1.91672	5.38513	-0.69132
H	-4.0261	-0.21365	-5.16728
H	-5.14376	-2.41989	-4.09941
H	-2.09852	3.319	4.24622
H	-2.75074	0.9152	5.27616
H	-3.86812	-4.51909	-2.70109

H	-7.48215	-7.38165	-4.42217
H	-8.7046	-7.27063	-3.14287
H	-7.21793	-8.1972	-2.87616
H	-3.29949	-4.37832	8.61615
H	-4.5517	-3.24515	9.15038
H	-2.83716	-2.81985	9.31072
H	-0.22922	8.60396	4.38299
H	-1.9304	9.08577	4.25282
H	-0.80974	9.399	2.91516
H	-1.35398	4.44986	-8.61605
H	-3.0443	4.11523	-9.0384
H	-1.80599	2.8701	-9.26844

1b

C	-4.03993	-3.34845	-0.38005
N	-3.22068	-2.18859	-0.32357
C	-1.89997	-2.60233	-0.32949
C	-1.88075	-4.03661	-0.41939
C	-3.18746	-4.52075	-0.46724
B	-3.83464	-0.77885	-0.14952
F	-3.29632	-0.19254	1.06036
F	-3.51108	0.08926	-1.2596
C	-6.35088	0.07356	-0.05047
C	-7.62505	-0.5597	-0.07309
C	-7.44984	-1.95477	-0.1106
C	-6.02474	-2.16044	-0.13484
N	-5.37323	-0.90697	-0.07352
N	-5.36477	-3.32076	-0.2828
C	-3.61197	-5.92323	-0.58259
C	-8.5045	-2.97846	-0.12452
C	-0.69681	-1.77829	-0.25316
C	-0.63335	-0.41765	-0.65201
C	0.56037	0.30741	-0.55215
C	1.7405	-0.28403	-0.04342
C	1.68952	-1.64459	0.34673
C	0.50041	-2.37246	0.23865
C	-6.15169	1.53173	-0.01774
C	-5.05305	2.16186	0.61742
C	-4.94037	3.56164	0.63812
C	-5.92507	4.34319	0.01536
C	-7.02648	3.75245	-0.62468
C	-7.13262	2.35365	-0.63318
C	-4.89255	-6.27849	-1.07893
C	-5.25977	-7.62823	-1.20708
C	-4.36267	-8.65115	-0.84184

C	-3.08871	-8.31101	-0.34263
C	-2.71916	-6.96366	-0.21465
C	-9.81994	-2.634281	-0.531954
C	-10.8505	-3.58672	-0.527951
C	-10.5906	-4.9097	-0.11638
C	-9.28864	-5.26576	0.28766
C	-8.25553	-4.31429	0.28406
BR	-5.75859	6.3001	0.03302
C	1.46112	7.22429	-2.51312
RH	3.42244	0.77865	0.13761
N	4.60203	-0.66977	-0.70762
N	2.45261	2.35905	1.00621
C	4.84861	-0.84836	-2.07098
C	5.26515	-1.70213	-0.03815
C	5.69249	-2.01758	-2.25418
C	5.96012	-2.53084	-1.01011
C	2.16718	2.51269	2.36391
C	1.92394	3.47575	0.35348
C	1.46892	3.77181	2.56606
C	1.32726	4.36502	1.33719
C	6.04725	-3.10128	1.87611
C	7.21356	-2.90879	2.64725
C	7.9452	-4.00669	3.13711
C	7.53354	-5.33207	2.87958
C	4.3822	-0.03062	-3.11695
C	1.95692	3.72643	-1.03216
C	2.5284	1.63013	3.39949
C	4.58775	-1.12026	2.28533
C	3.32053	0.48206	3.2129
C	3.73496	-0.4162	4.27774
C	4.5167	-1.39187	3.71196
C	2.5568	2.86817	-1.97427
C	2.56365	3.09649	-3.41016
C	3.22557	2.04412	-3.99049
C	3.63608	1.14641	-2.92313
N	3.21881	1.66905	-1.69738
N	3.84448	0.02822	1.99983
C	6.36116	-5.52153	2.11236
C	5.63342	-4.42728	1.61545
C	2.95269	2.37484	5.79027
C	1.13118	2.55896	7.42619
C	0.23479	2.13065	6.41983
C	0.68568	1.83466	5.12273
C	2.49598	2.67905	7.08666
C	1.30349	4.98187	-1.53669
C	2.07561	6.0465	-2.04889

C	0.05716	7.37297	-2.491
C	-0.7127	6.3039	-1.97849
C	-0.1016	5.12957	-1.50734
C	4.72784	-0.41763	-4.52782
C	3.74131	-0.93733	-5.3945
C	4.06099	-1.29675	-6.71572
C	5.37362	-1.14621	-7.21703
C	6.35496	-0.61756	-6.34964
C	6.03964	-0.26284	-5.02521
C	5.26979	-1.92685	1.35265
C	2.05443	1.94954	4.78884
C	0.63535	2.87134	8.82678
C	8.32552	-6.51935	3.39741
C	5.72106	-1.55954	-8.63603
C	-0.61012	8.63058	-3.01794
H	-8.56511	-0.03501	0.00938
H	-0.97904	-4.6214	-0.51498
H	-1.50742	0.07163	-1.0623
H	0.55807	1.34132	-0.87622
H	2.5678	-2.13813	0.74669
H	0.49295	-3.40386	0.58079
H	-4.29069	1.56763	1.10584
H	-4.095	4.02758	1.13375
H	-7.77877	4.36327	-1.1129
H	-7.9703	1.8981	-1.15294
H	-5.5868	-5.49633	-1.3631
H	-6.2429	-7.88084	-1.59687
H	-4.65002	-9.695	-0.94296
H	-2.39196	-9.09273	-0.04983
H	-1.74233	-6.715223	0.192482
H	-10.0303	-1.62363	-0.872572
H	-11.8499	-3.30276	-0.8488
H	-11.3886	-5.6483	-0.11077
H	-9.07919	-6.28231	0.61215
H	-7.25698	-4.59423	0.59946
H	7.5538	-1.89724	2.85595
H	8.84376	-3.82933	3.72464
H	6.01469	-6.53241	1.90423
H	3.15946	5.95822	-2.07021
H	2.07999	8.03443	-2.89387
H	-1.79745	6.38933	-1.94772
H	-0.71683	4.3193	-1.12331
H	2.72447	-1.06362	-5.03009
H	3.28263	-1.6969	-7.36289
H	7.37192	-0.47916	-6.71187
H	6.81038	0.14998	-4.37832

H	4.00821	2.48181	5.551
H	-0.82359	2.02744	6.65265
H	-0.0216	1.50287	4.36628
H	3.20792	3.0141	7.83838
H	6.03688	-2.38361	-3.20935
H	6.57237	-3.38517	-0.76506
H	1.15566	4.15274	3.52619
H	0.87728	5.31928	1.10975
H	3.45251	-0.31256	5.31423
H	4.98819	-2.22933	4.20327
H	2.11615	3.94861	-3.8985
H	3.42933	1.88644	-5.03874
H	4.73231	-4.59919	1.03139
H	1.43383	3.28784	9.45127
H	0.25891	1.9673	9.32543
H	-0.18896	3.59657	8.80623
H	9.10249	-6.20539	4.10357
H	8.82052	-7.0553	2.57529
H	7.67595	-7.24103	3.90988
H	6.61103	-1.03313	-9.00044
H	4.89626	-1.35093	-9.32846
H	5.93007	-2.63768	-8.69316
H	0.10256	9.4595	-3.09905
H	-1.43154	8.95179	-2.36507
H	-1.03688	8.46198	-4.01709

References

1 M. Gouterman, In *The Porphyrins*, vol. III, Dolphin D. (Ed.) Academic Press: New York, **1978**, 1-165.