Electronic Supplementary Information for:

Switching of the Photophysical Properties of Bodipy-derived Trans Bis(tributylphosphine) Pt(II) bisacetylide Complexes with Rhodamine as the Acid-Activatable Unit

*Poulomi Majumdar, Xiaoneng Cui, Kejing Xu and Jianzhang Zhao**

State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, E-208 West Campus, 2 Ling-Gong Road, Dalian 116024, P. R. China.

E-mail: zhaojzh@dlut.edu.cn Web: http://finechem2.dlut.edu.cn/photochem

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1.0 General

Singlet oxygen ($^1O_2$) quantum yields (Φ_Δ)

Φ_Δ value of the triplet photosensitizers were measured with methylene blue (Φ_Δ = 0.57 in dichloromethane) as standard.[39] Quantum yields for singlet oxygen ($^1O_2$) generation in CH_2Cl_2 were determined by monitoring the photooxidation of 1,3-diphenylisobenzofuran (DPBF) sensitized by the Pt(II) complexes. 1,3-Diphenylisobenzofuran (DPBF) was used as the $^1O_2$ scavenger, due to its fast reaction with $^1O_2$. The absorbance of DPBF was adjusted to around 1.0 at 414 nm in air saturated CH_2Cl_2. Then, the photosensitizer was added to cuvette and photosensitizer's absorbance was adjusted to around 0.2–0.3. Then, the cuvette was exposed to monochromatic light at the specific wavelength for 10 seconds depending on the efficiency of the triplet photosensitizers. The photosensitizer and MB were irradiated at the same wavelength. Absorbance was measured six times after each irradiation. Then, the slope of the curves of absorbance maxima of DPBF at 414 nm versus irradiation time for each photosensitizer were calculated. Singlet oxygen quantum yield (Φ_Δ) were calculated according to the equation (eqn (1)):

$$\Phi_{\Delta sam} = \Phi_{\Delta \mathrm{std}} \left(\frac{m_{\mathrm{sam}}}{m_{\mathrm{std}}} \right) \left(\frac{F_{\mathrm{std}}}{F_{\mathrm{sam}}} \right) \qquad \text{(eqn } \mathbf{1}\text{)}$$

where "sam" and "std" designate the "Pt(II) photosensitizers" and "MB", respectively. "m" is the slope of difference in change in absorbance of DPBF (at 414 nm) with the irradiation time, "F" is the absorption correction factor, which is given by $F = 1 - 10^{-\mathrm{OD}}$ (OD is the optical density, i.e. absorbance at the irradiation wavelength).

2.0 NMR and HR MS spectra

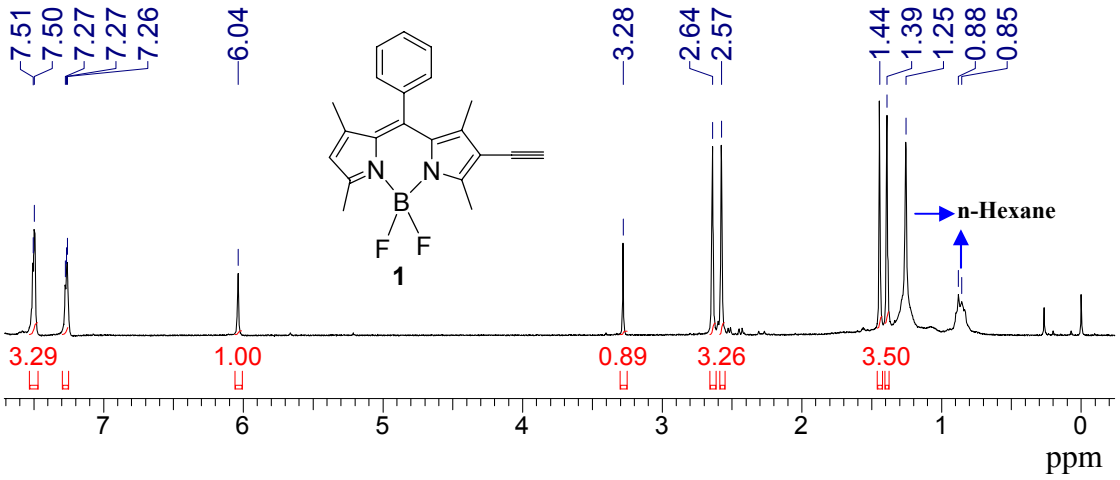

Fig. S1 ^{1}H NMR of compound **1** (400 MHz, $CDCl_3$).

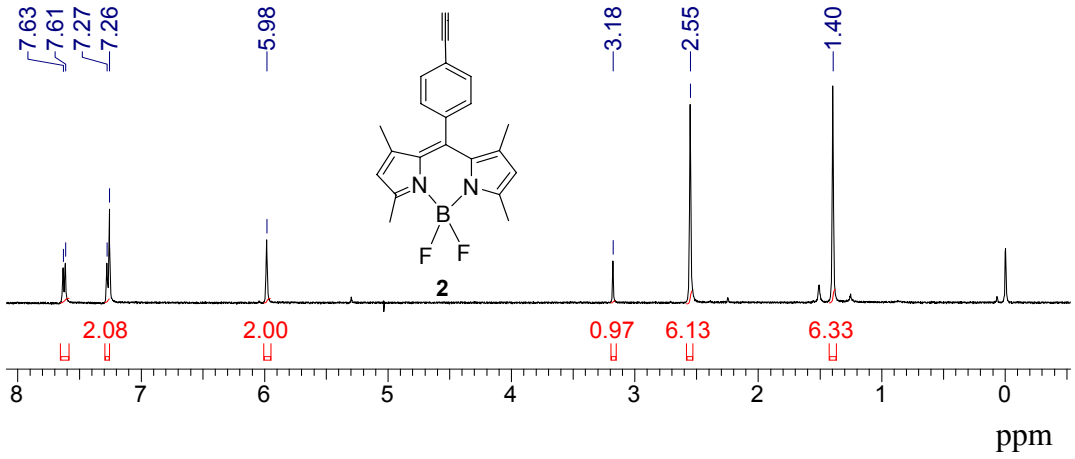

Fig. S2 ^{1}H NMR of compound **2** (400 MHz, $CDCl_3$).

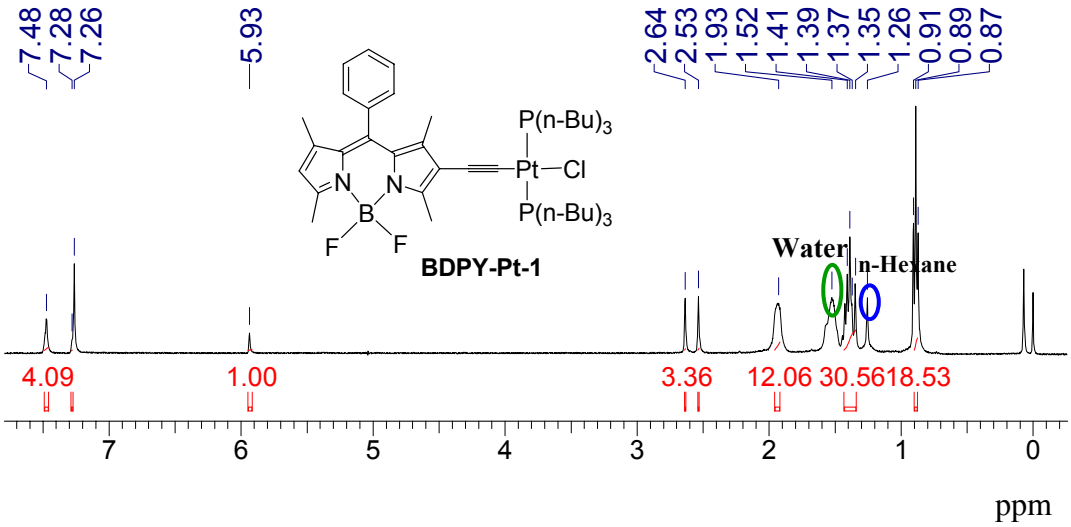

Fig. S3 ^{1}H NMR (400 MHz, $CDCl_3$) of complex **BDPY-Pt-1**.

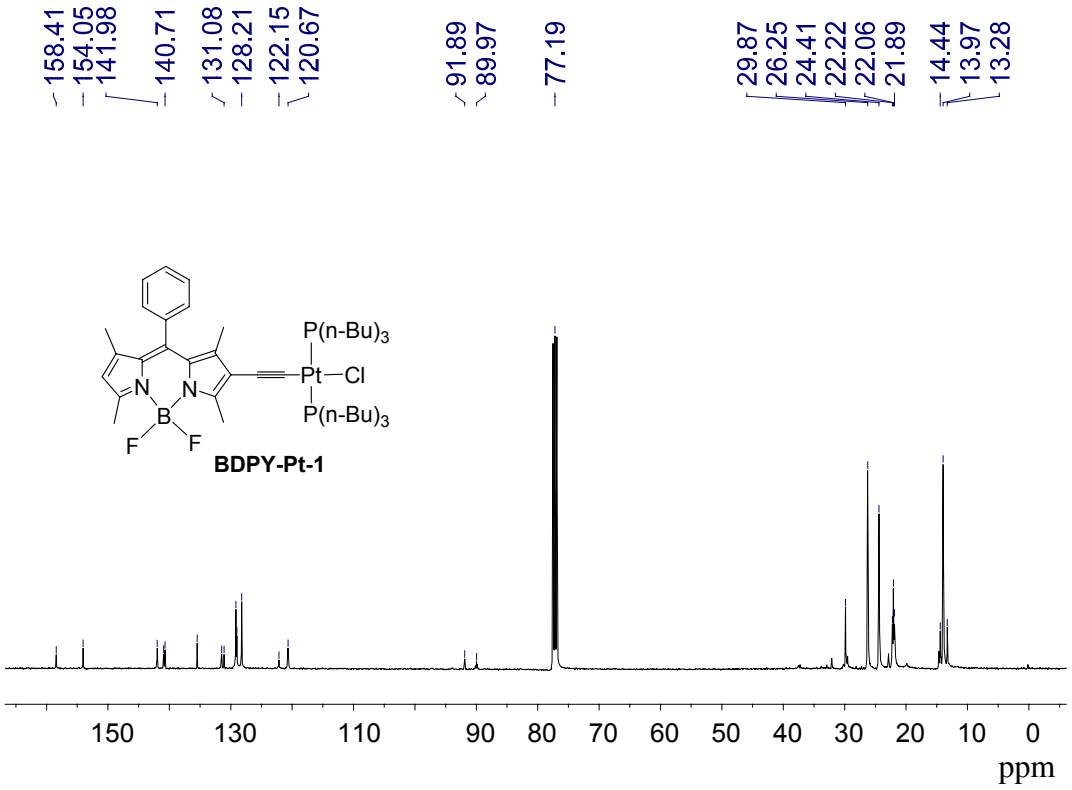

Fig. S4 ^{13}C NMR (100 MHz, $CDCl_3$) of **BDPY-Pt-1.**

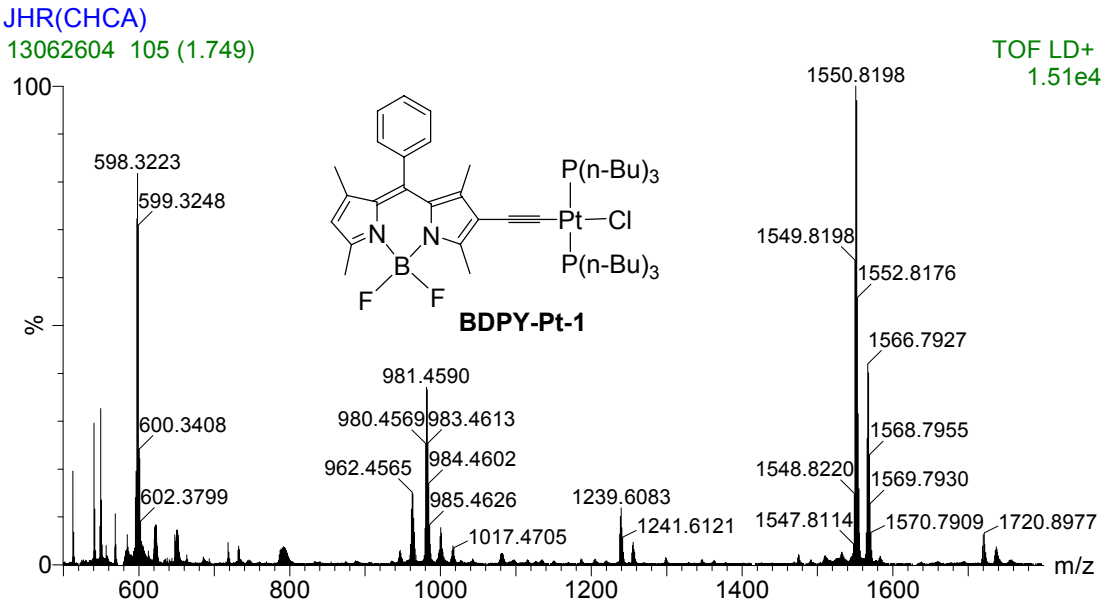

Fig. S5 MALDI-HRMS of **BDPY-Pt-1.**

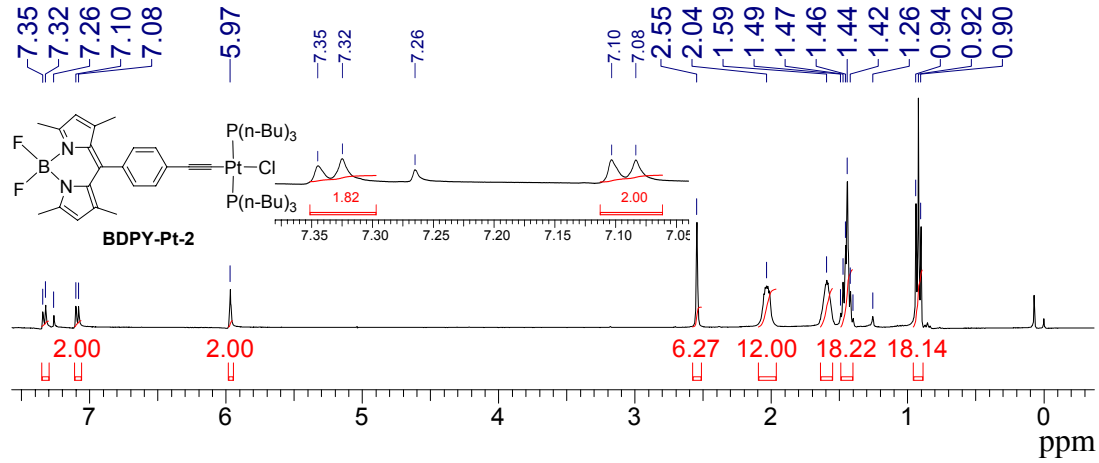

Fig. S6 ^{1}H NMR (400 MHz, $CDCl_3$) of complex **BDPY-Pt-2**.

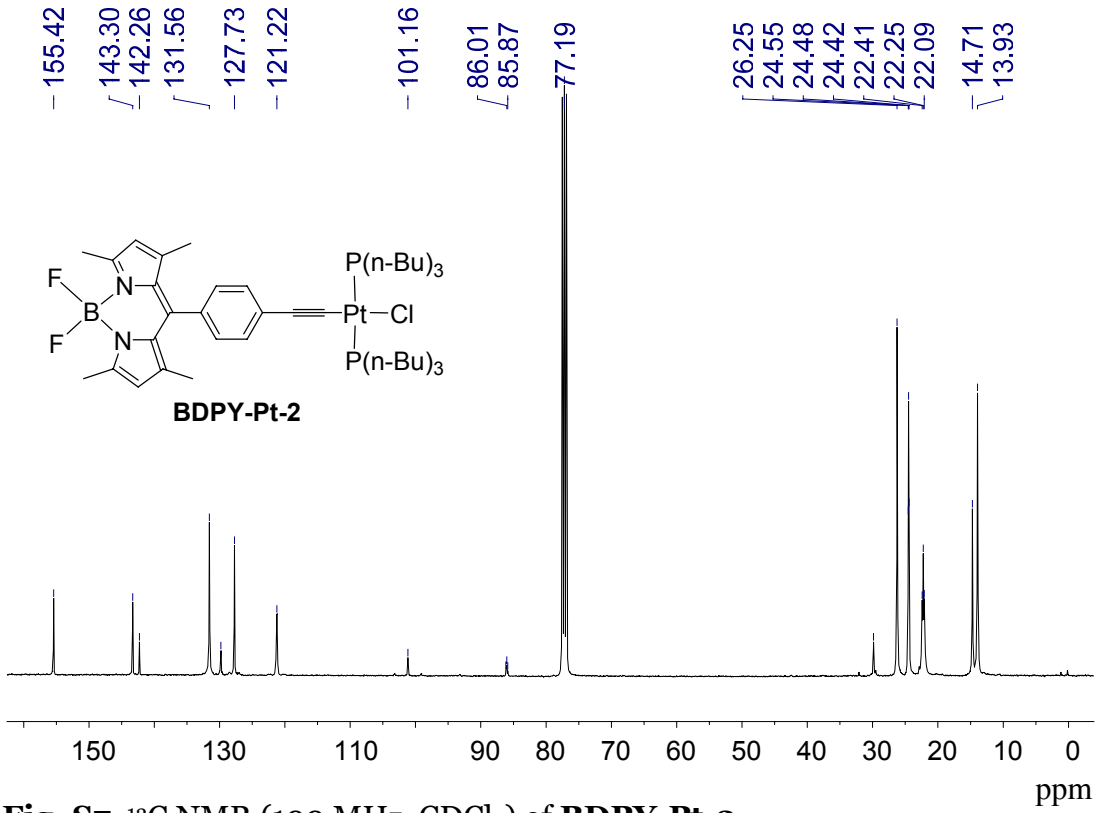

Fig. S7 ^{13}C NMR (100 MHz, $CDCl_3$) of **BDPY-Pt-2**.

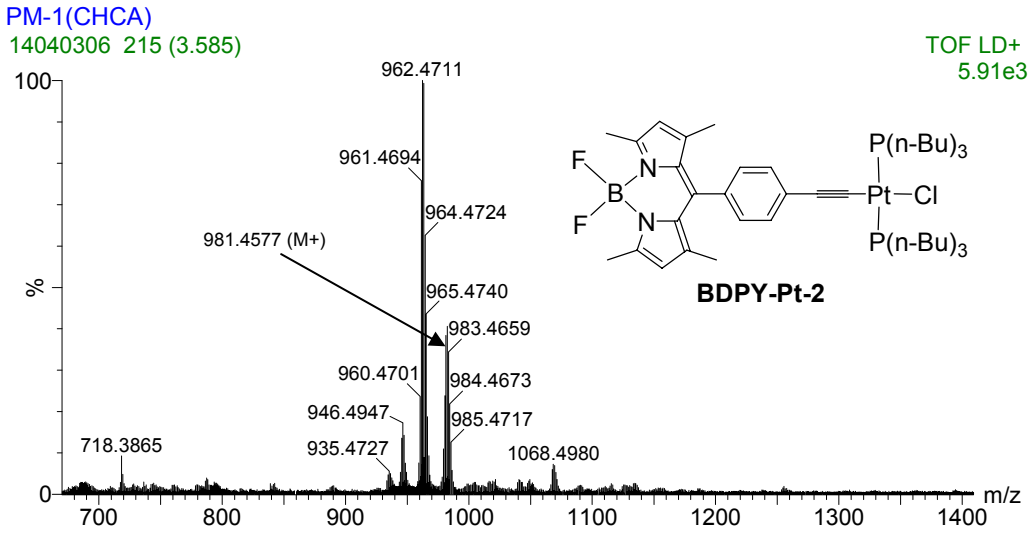

Fig. S8 MALDI-HRMS of **BDPY-Pt-2**.

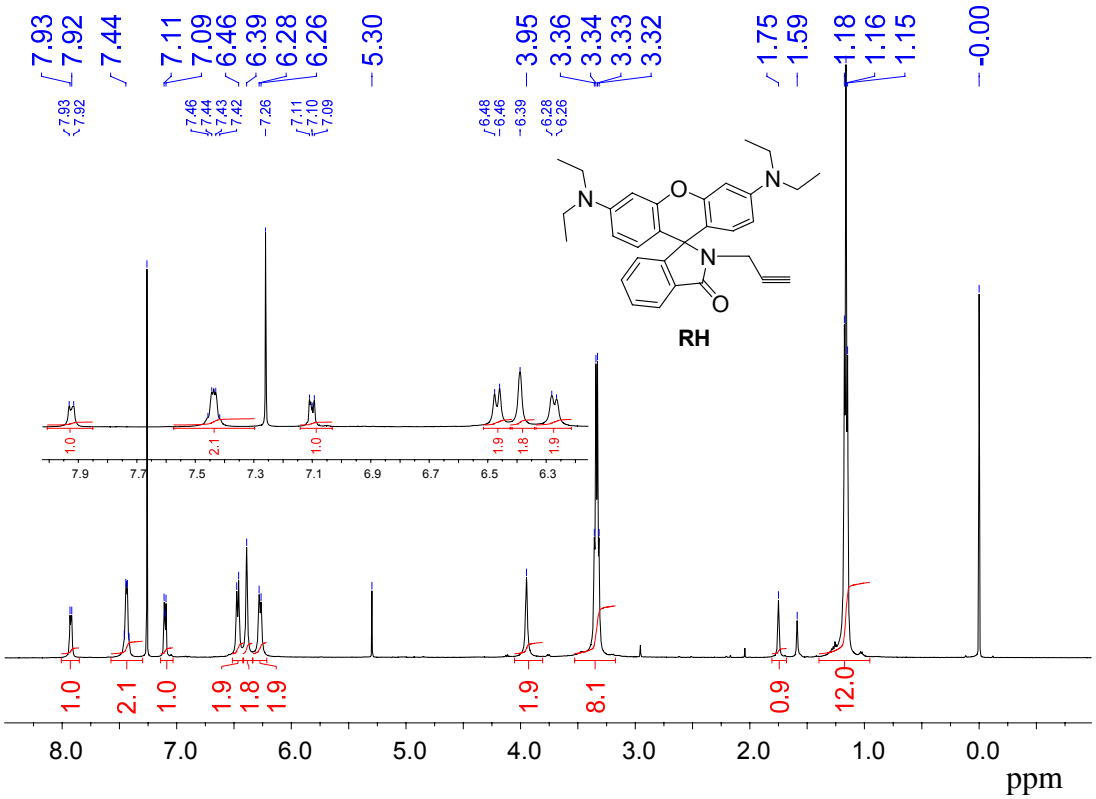

Fig. S9 ^{1}H NMR (500 MHz, $CDCl_3$) of **RH**.

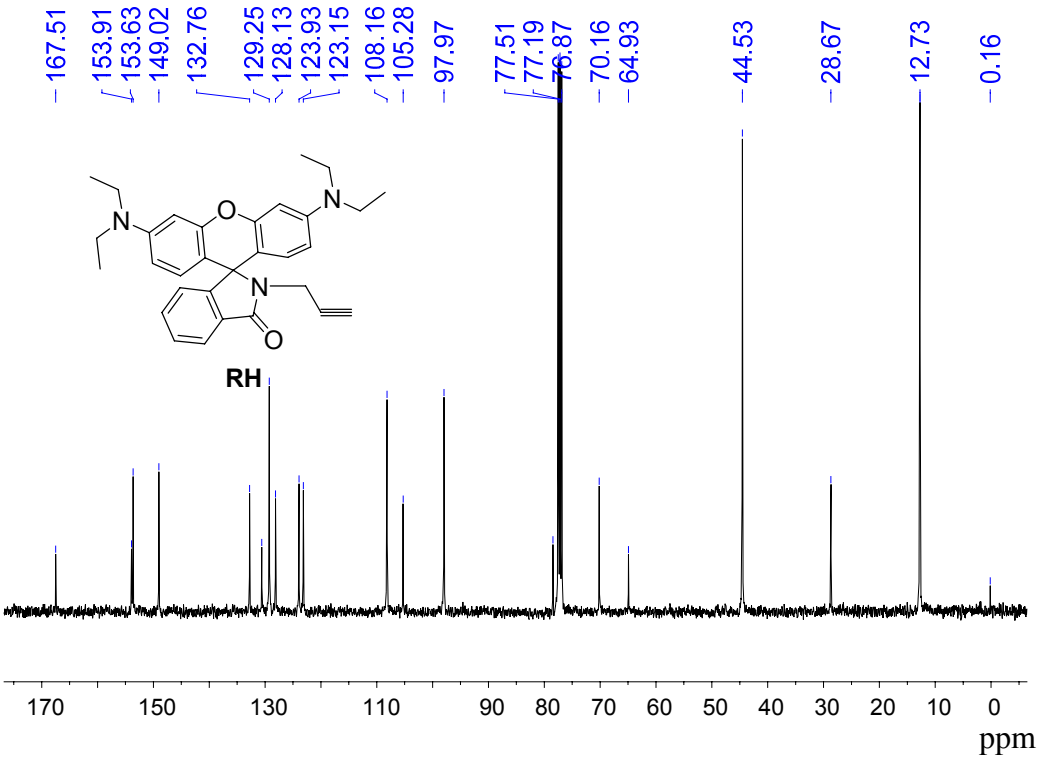

Fig. S10 ^{13}C NMR (125 MHz, $CDCl_3$) of **RH**.

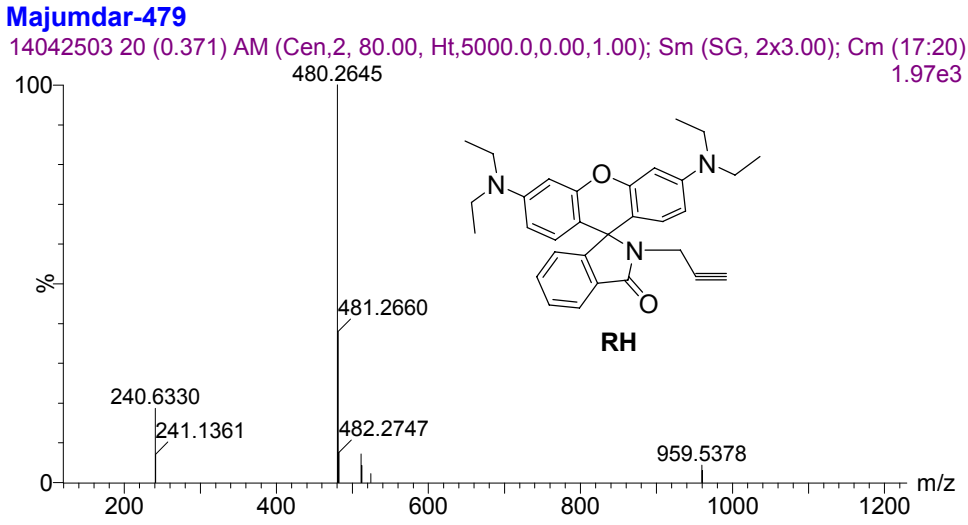

Fig. S11 TOF ES+ HRMS of **RH**.

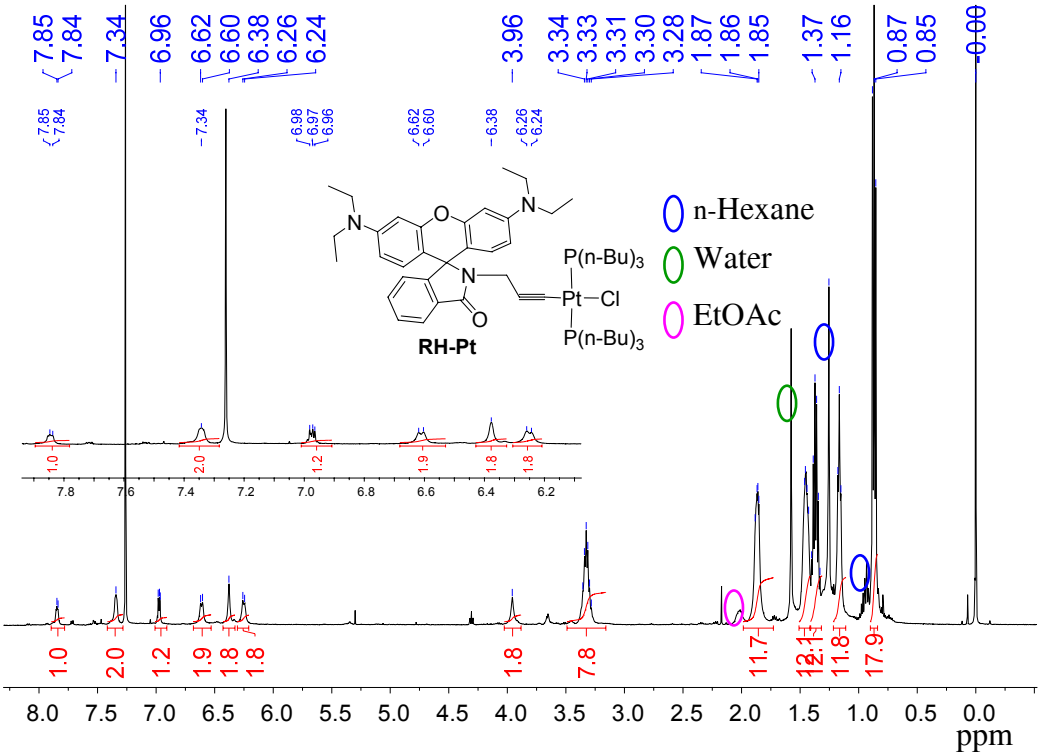

Fig. S12 ^{1}H NMR (500 MHz, $CDCl_3$) of **RH-Pt**.

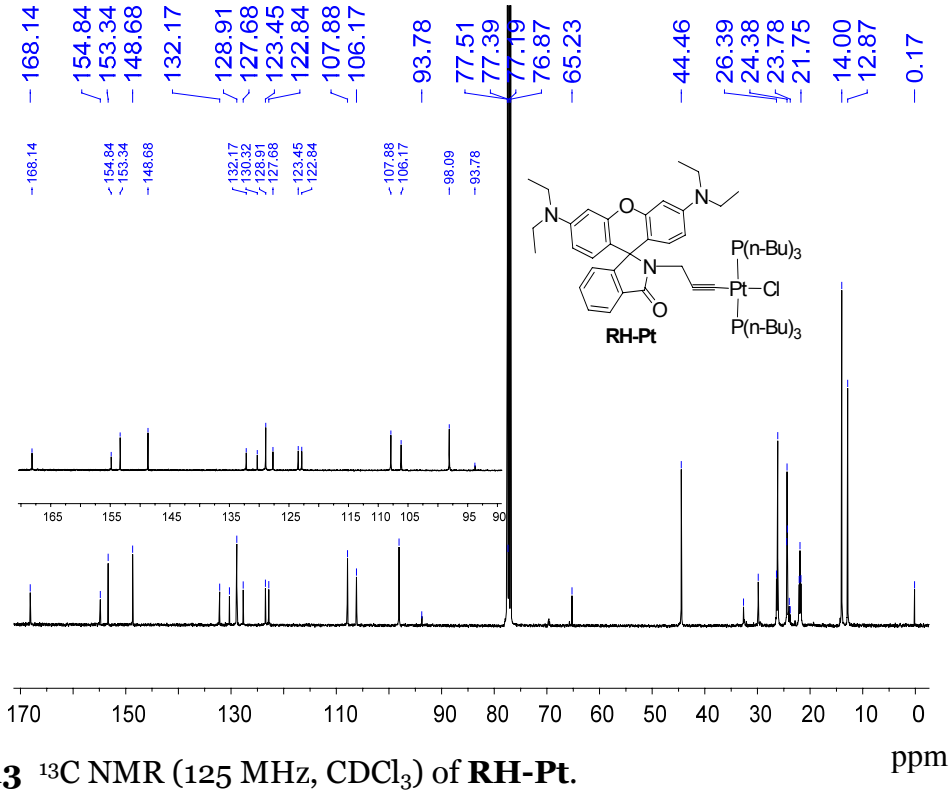

Fig. S13 ^{13}C NMR (125 MHz, $CDCl_3$) of **RH-Pt**.

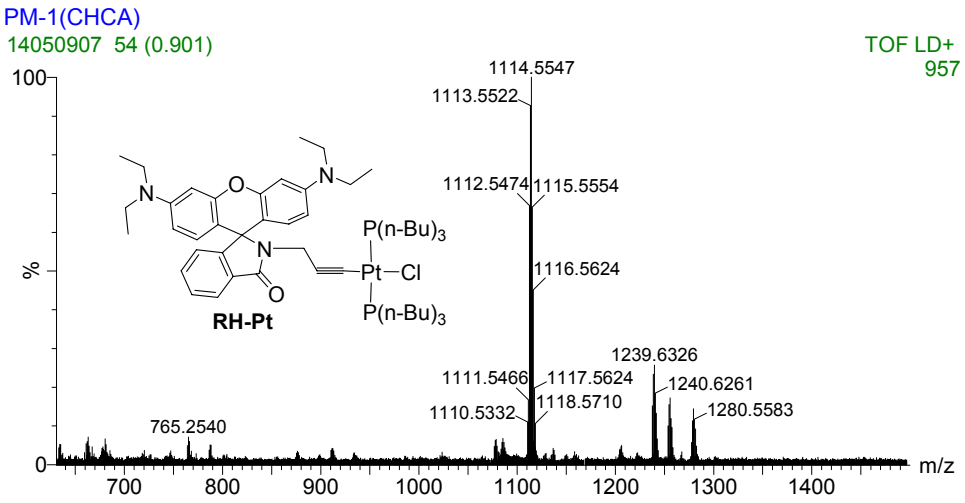

Fig. S14 MALDI-HRMS of **RH-Pt**.

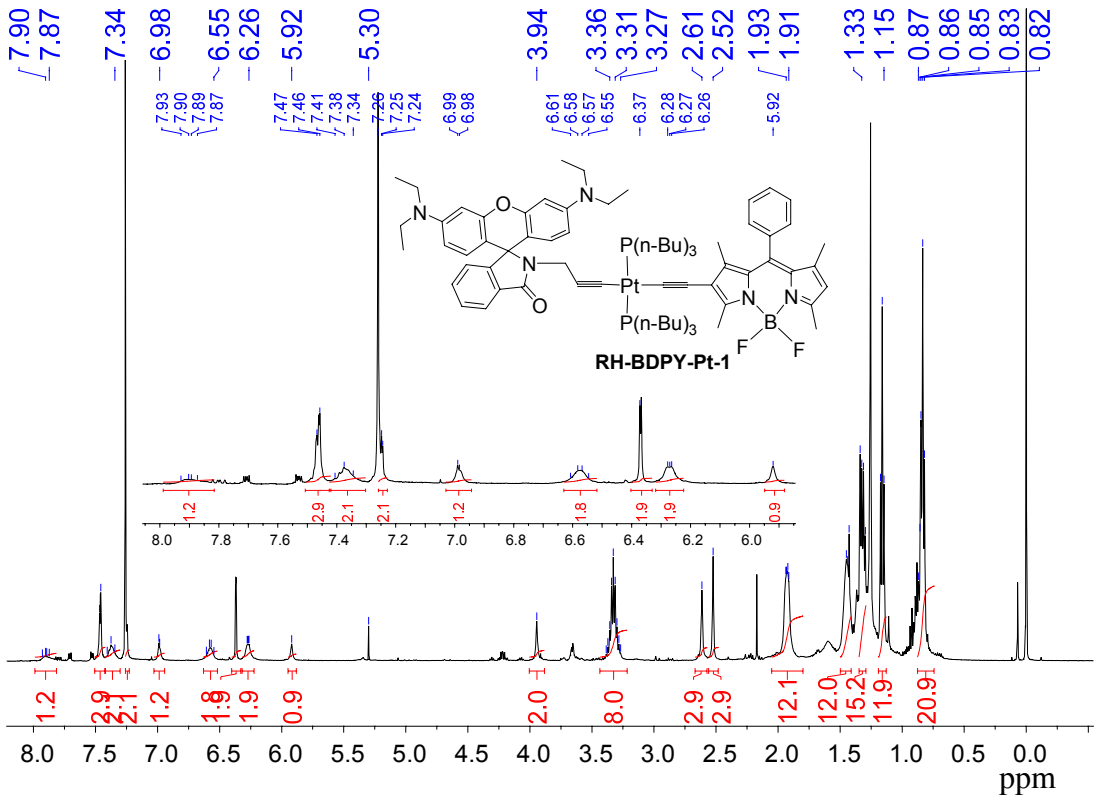

Fig. S15 ^{1}H NMR (500 MHz, $CDCl_3$) of **RH-BDPY-Pt-1**.

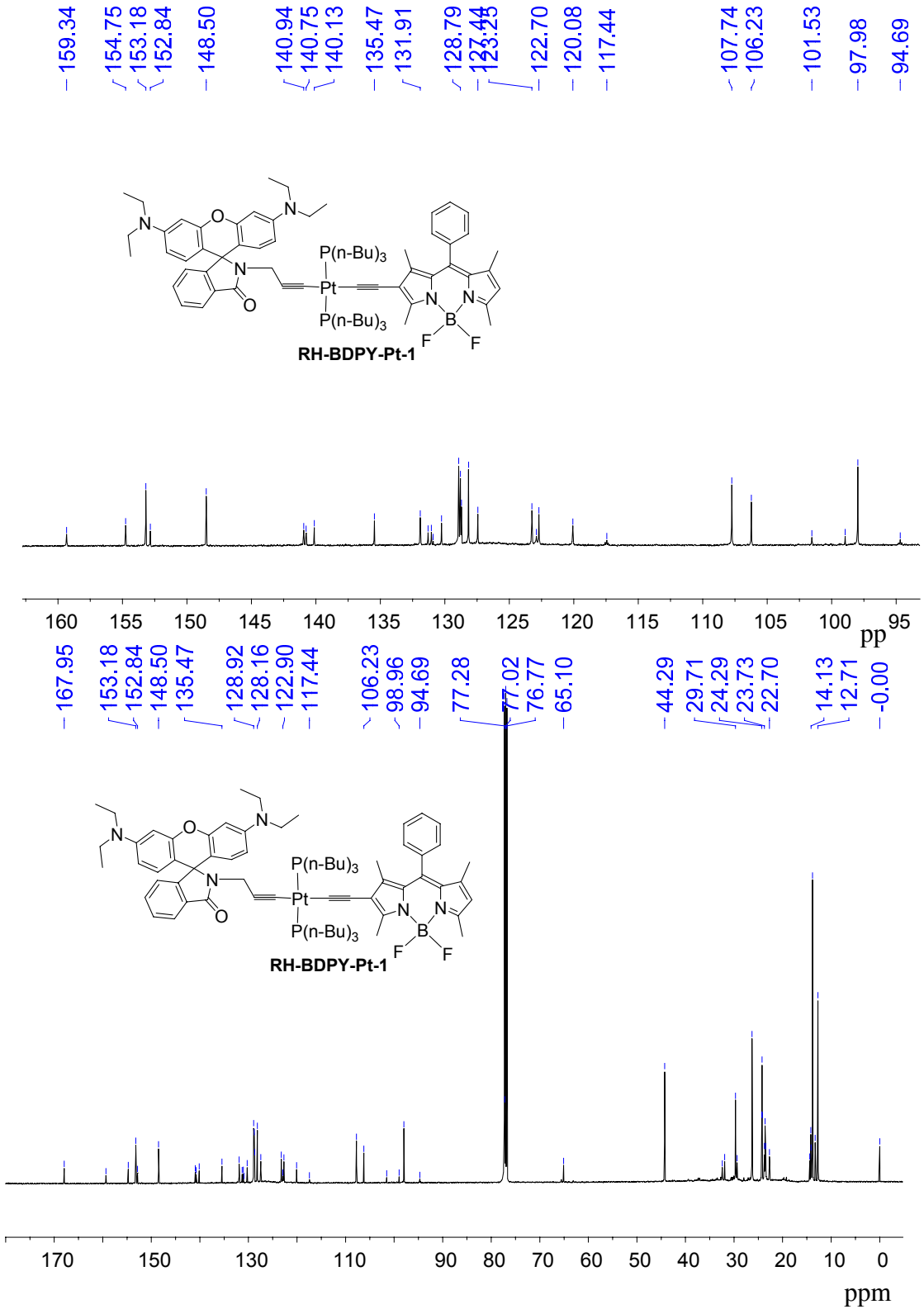

Fig. S16 ^{13}C NMR (125 MHz, $CDCl_3$) of **RH-BDPY-Pt-1**.

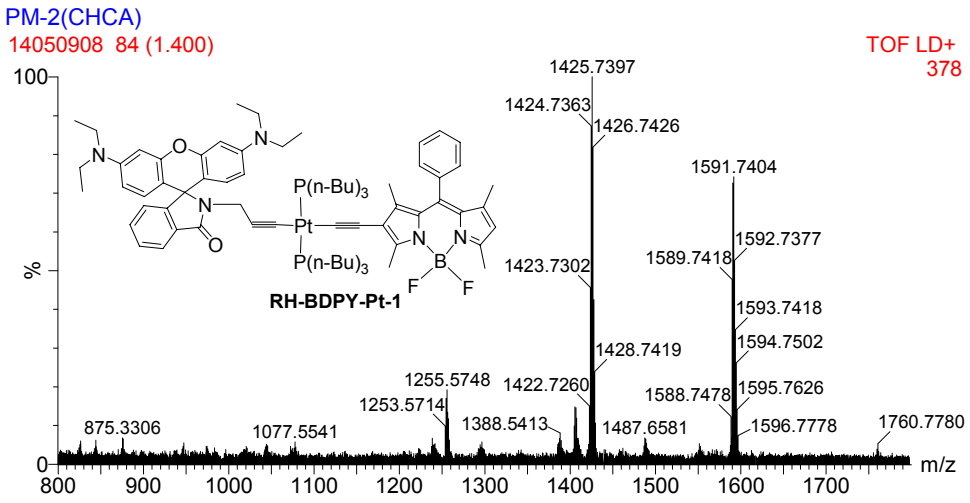

Fig. S17 MALDI-HRMS of **RH-BDPY-Pt-1**.

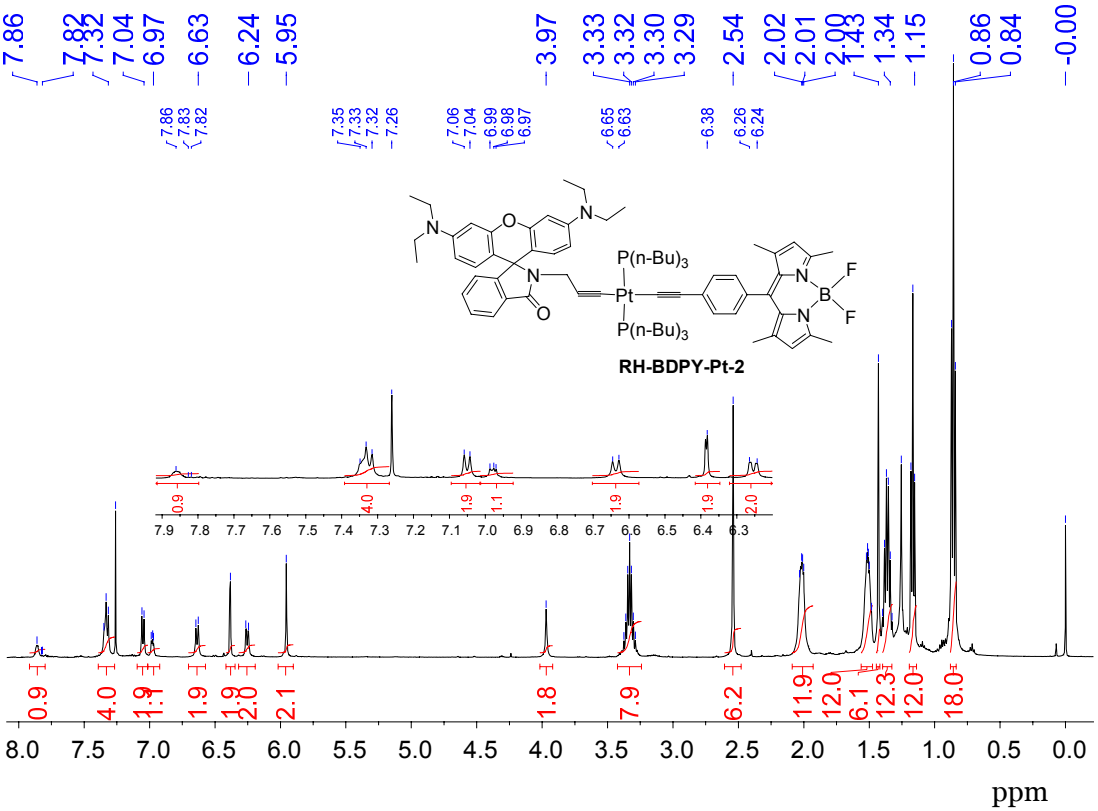

Fig. S18 ^{1}H NMR (500 MHz, $CDCl_3$) of **RH-BDPY-Pt-2**.

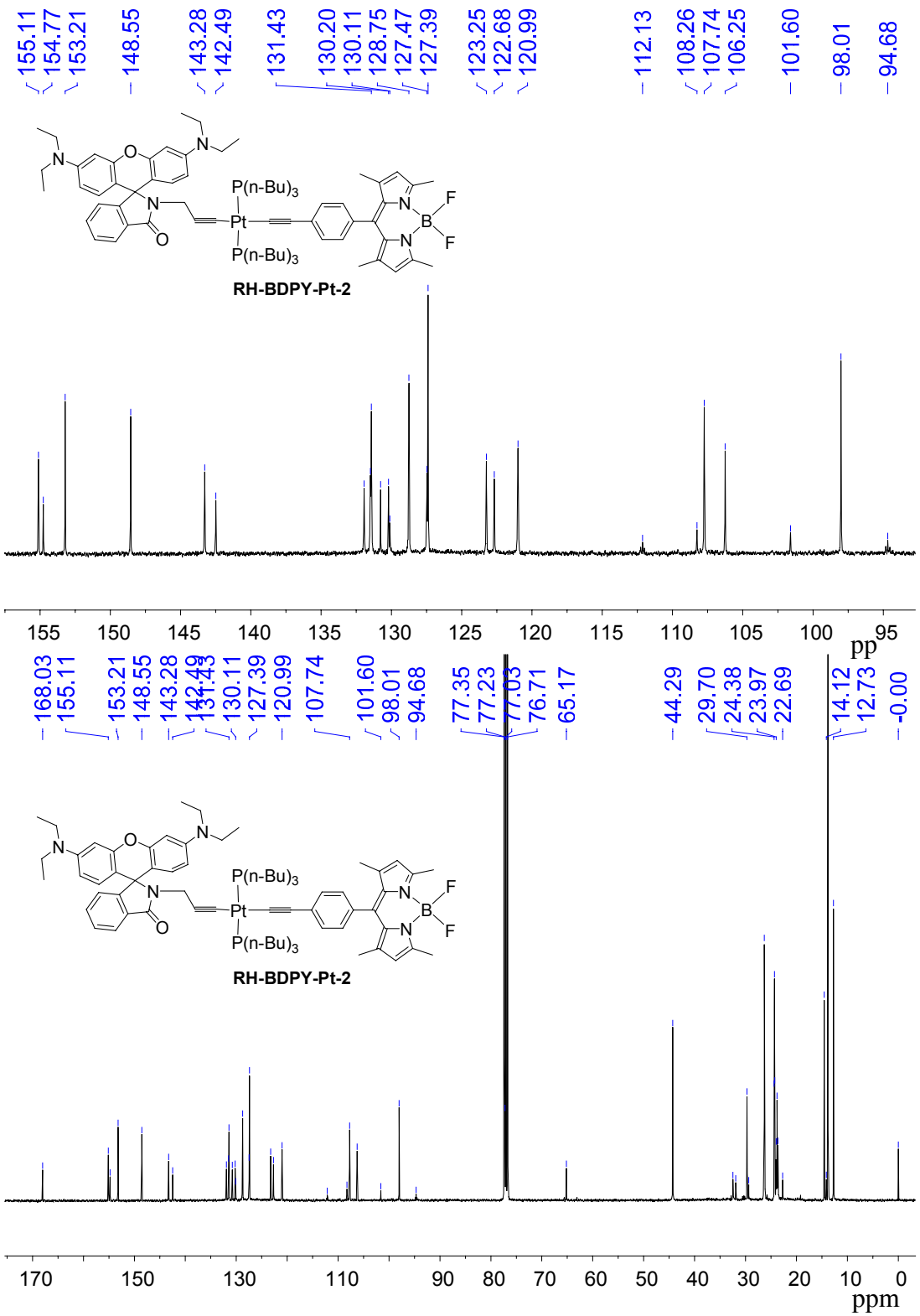

Fig. S19 ^{13}C NMR (125 MHz, $CDCl_3$) of **RH-BDPY-Pt-2**.

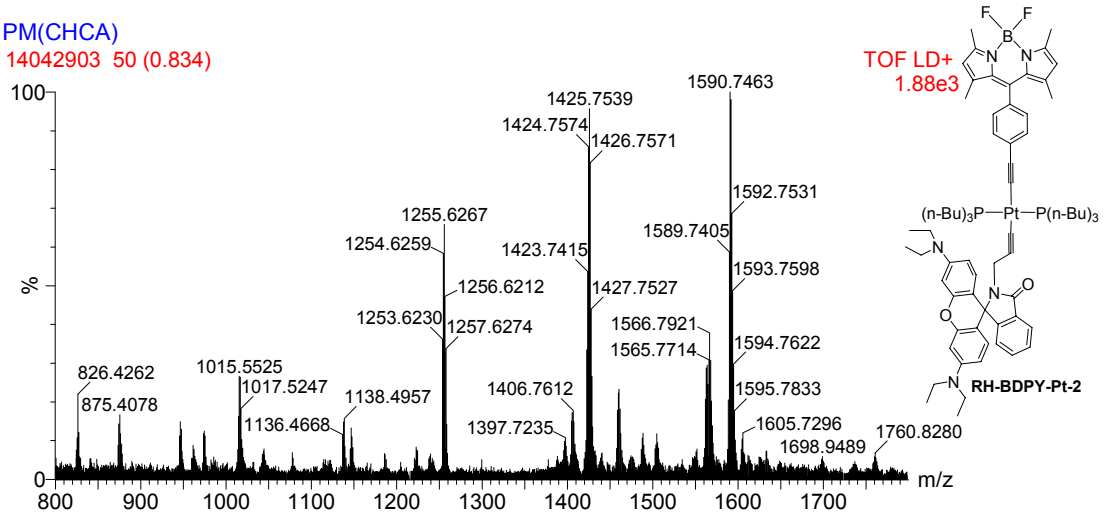

Fig. S20 MALDI-HRMS of **RH-BDPY-Pt-2**.

3.0 UV-Vis absorption spectra of the complex in different solvents

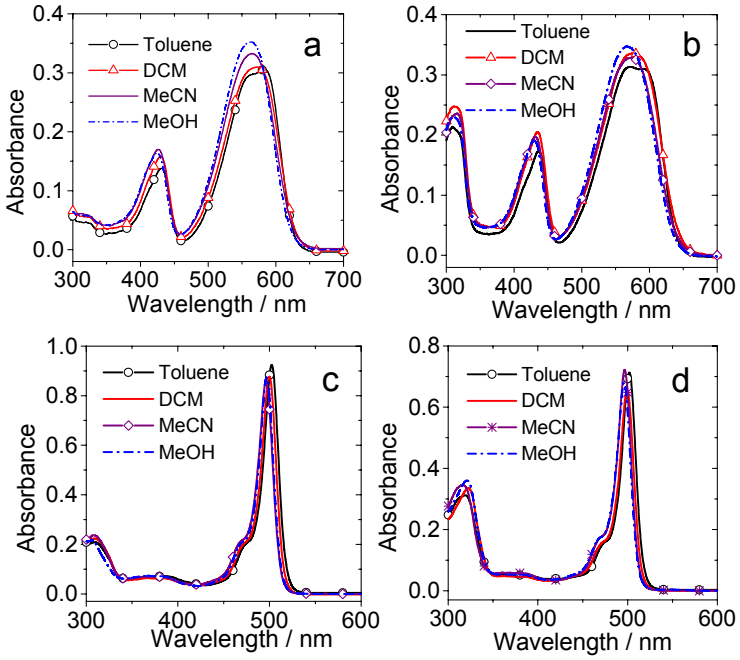

Fig. S21 Solvent-polarity-dependence of the absorption of the complexes (a) **BDPY-Pt-1**, (b) **RH-BDPY-Pt-1**, (c) **BDPY-Pt-2**, (d) **RH-BDPY-Pt-2**. c = 1.0 ×10^{-5} M. 20 °C.

4.0 Emission Spectra, decay curve and Cyclic voltammogram of the complexes

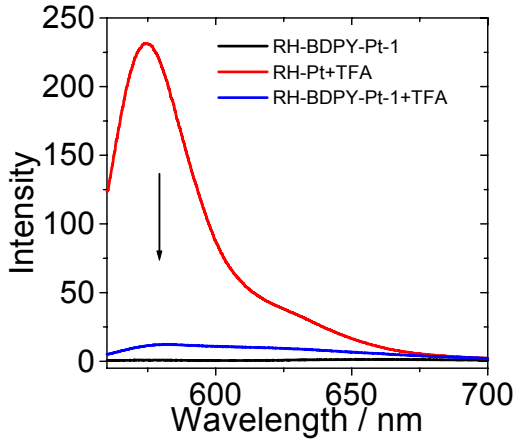

Fig. S22 Emission of complexes. (a) **RH-BDPY-Pt-1 (***c* = 1.8×10⁻⁵ M), **RH-Pt** (*c* = 1.0×10⁻⁵ M) + **TFA** (333 eqv.) and **RH-BDPY-Pt-1**(*c* = 1×10⁻⁵ M) +**TFA**(333 eqv.) (λ_{ex} = 550 nm). in deaerated dichloromethane. 20 °C.

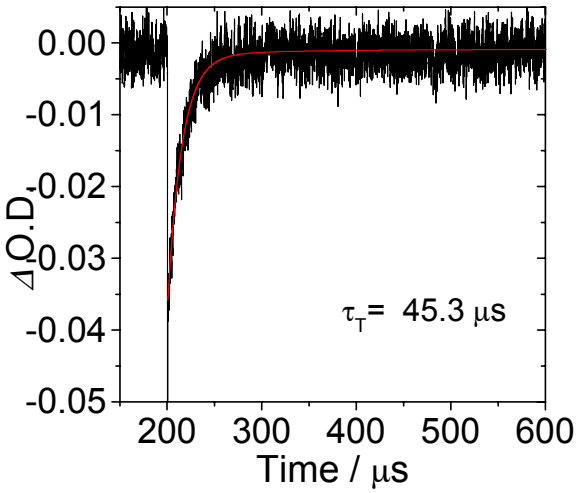

Fig. S23 The decay curve of complexes **BDPY-Pt-1+TFA** (333 eqv.) at 580 nm (upon λ_{ex} = 532 nm pulsed laser excitation). *c* = 1.0 ×10⁻⁵ M in deaerated dichloromethane at 20 °C.

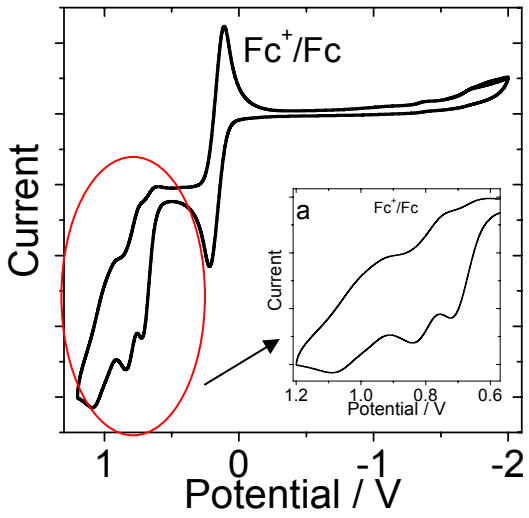

Fig. S24 Cyclic voltammogram of (a) **RH-Pt** in deaerated CH_2Cl_2 solutions containing 1.0 mM photosensitizers with the ferrocene(Fc) as internal reference, 0.10 M Bu_4NPF_6 as supporting electrode, $Ag/AgNO_3$ as reference electrode. Scan rates: 0.1 mV/s.

5.0 DFT Calculations

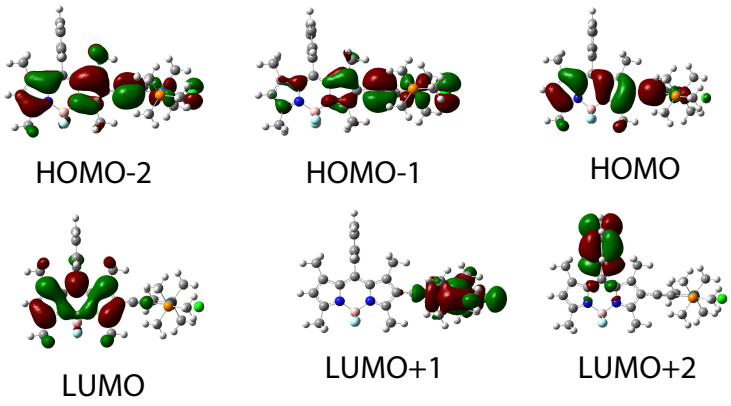

Fig. S25 Electron density maps of the frontier molecular orbitals of complex **BDPY-Pt-1** based on the optimized ground state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/GENCP/LANL2DZ level with Gaussian 09W.

Table S1: Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **BDPY-Pt-1**, Calculated by TDDFT//B3LYP/LANL2DZ, based on the DFT//B3LYP/LANL2DZ Optimized Ground State Geometries

	TDDFT//B3LYP/LANL2DZ					
	Electronic transition	Energy [eV/nm][a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	2.36 / 525	0.458	H →L	0.684	MLCT
	$S_0 \rightarrow S_3$	3.06 / 405	0.539	H−2 →L	0.627	MLCT
Triplet	$S_0 \rightarrow T_1$	1.42 / 867	0.668	H →L	0.000	MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [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.

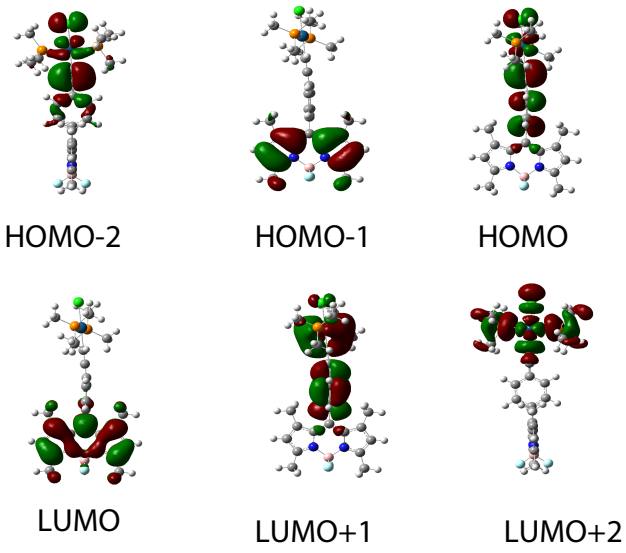

Fig. S26 Electron density maps of the frontier molecular orbitals of complex **BDPY-Pt-2** based on the optimized ground state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/GENCP/LANL2DZ level with Gaussian 09W.

Table S2. Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **BDPY-Pt-2**, Calculated by TDDFT//B3LYP/LANL2DZ, based on the DFT//B3LYP/LANL2DZ Optimized Ground State Geometries

	TDDFT//B3LYP/ LANL2DZ					
	Electronic transition	Energy [eV/nm] [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	2.26 / 548	0.001	H →L	0.703	MLCT
	$S_0 \rightarrow S_2$	2.80 / 442	0.566	H–1 →L	0.696	ILCT
	$S_0 \rightarrow S_6$	3.61 / 342	1.013	H →L+1	0.681	ILCT
Triplet	$S_0 \rightarrow T_1$	1.53 / 809	0.000	H →L	0.710	MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [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.

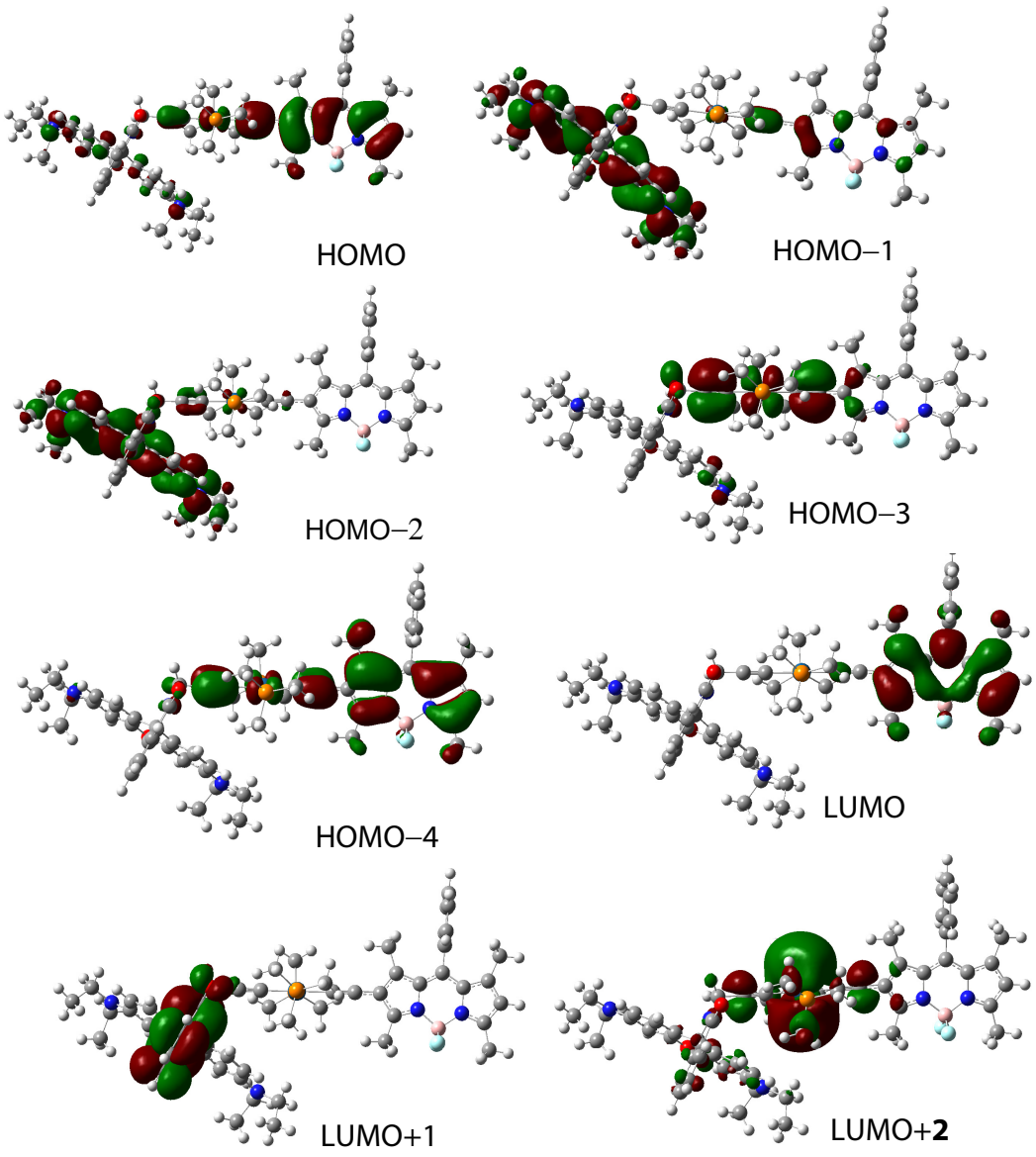

Fig. S27 Electron density maps of the frontier molecular orbital of the complex **RH-BDPY-Pt-1** in dichloromethane. Based on ground state optimized geometry by the DFT calculations at the B3LYP/GENECP level with Gaussian 09W.

Table S3. Electronic excitation energies (eV) and corresponding oscillator strengths (*f*), main configurations and CI coefficients of the low-lying electronic excited states of the complex **RH-BDPY-Pt-1** in dichloromethane calculated by TDDFT//B3LYP/GENECP based on the DFT//B3LYP/ GENECP optimized ground state geometries

TDDFT//B3LYP/ GENECP						
	Electronic transition	Energy [eV/nm][a]	f [b]	Composition [c]	CI[d]	Character
Singlet	$S_0 \rightarrow S_1$	2.28/543	0.417	H→L	0.667	MLCT/ILCT
	$S_0 \rightarrow S_5$	3.04/408	0.585	H−4→L	0.682	MLCT/ILCT
				H→L	0.149	MLCT/ILCT
	$S_0 \rightarrow S_{10}$	3.63/341	0.004	H−1→L+1	0.633	ILCT
				H→L+1	0.306	LLCT
	$S_0 \rightarrow S_{18}$	4.06/305	0.104	H−1→L+2	0.538	MLCT
				H−2→L+2	0.281	MLCT
				H−3→L+1	0.249	MLCT
Triplet	$S_0 \rightarrow T_1$	1.40/883	0.000	H→L	0.619	MLCT/ILCT
	$S_0 \rightarrow T_2$	2.05/606	0.000	H−4→L	0.582	MLCT/ILCT
	$S_0 \rightarrow T_3$	2.44/509	0.000	H−1→L	0.640	LLCT
	$S_0 \rightarrow T_4$	2.56/484	0.000	H−2→L	0.577	LLCT
	$S_0 \rightarrow T_5$	2.64/470	0.000	H−3→L	0.597	MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [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.

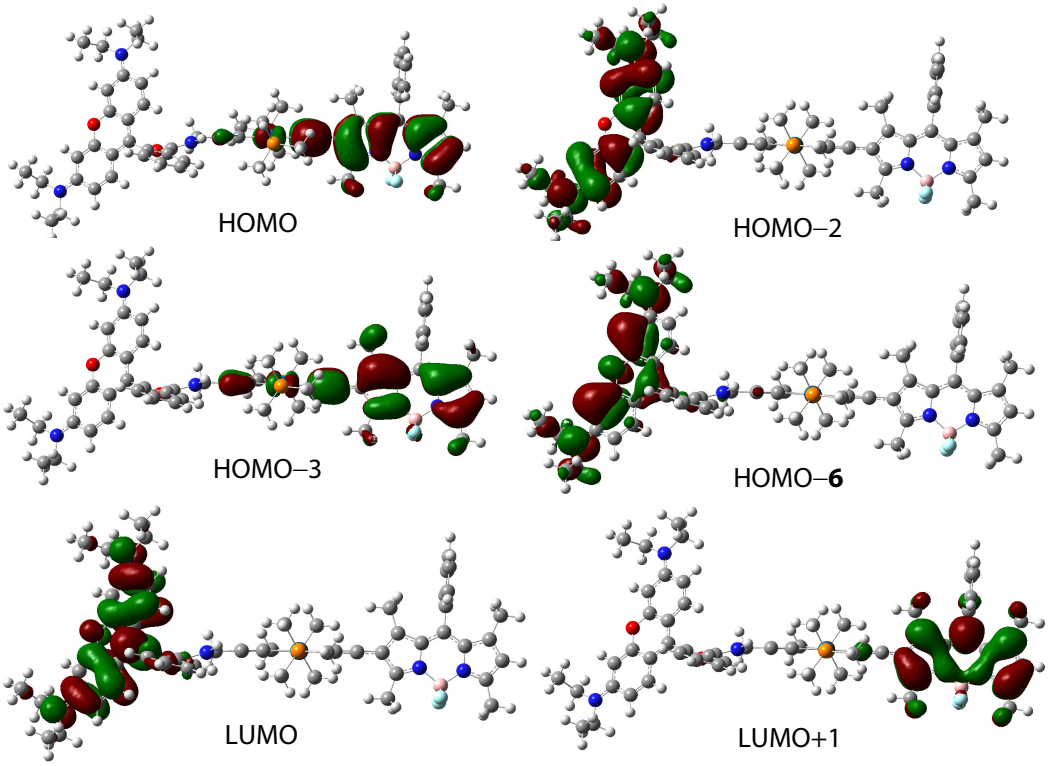

Fig. S28 Electron density maps of the frontier molecular orbital of the complex **RH(o)-BDPY-Pt-1** in dichloromethane. Based on ground state optimized geometry by the DFT calculations at the B3LYP/GENECP level with Gaussian 09W.

Table S4. Electronic excitation energies (eV) and corresponding oscillator strengths (*f*), main configurations and CI coefficients of the low-lying electronic excited states of the complex **RH(o)-BDPY-Pt-1** in dichloromethane calculated by TDDFT//B3LYP/GENECP based on the DFT//B3LYP/ GENECP optimized ground state geometries.

TDDFT//B3LYP/ GENECP						
	Electronic transition	Energy [eV/nm][a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.98/626	0.001	H→L	0.7061	LLCT
	$S_0 \rightarrow S_2$	2.30/530	0.453	H→L+1	0.6837	ILCT
				H–3→L+1	0.1731	MLCT/ILCT
	$S_0 \rightarrow S_4$	2.60/476	0.994	H–2→L	0.7043	ILCT
	$S_0 \rightarrow S_8$	3.06/404	0.601	H–3→L+1	0.6758	MLCT/ILCT
				H→L+1	0.1803	ILCT
	$S_0 \rightarrow S_{18}$	3.63/342	0.169	H–6→L	0.1321	ILCT
Triplet	$S_0 \rightarrow T_1$	1.43/870	0.000	H→L+1	0.6631	ILCT
				H–3→L+1	0.2563	MLCT/ILCT
	$S_0 \rightarrow T_2$	1.74/714	0.000	H–2→L	0.7033	ILCT
	$S_0 \rightarrow T_3$	1.98/626	0.000	H→L	0.7060	LLCT
	$S_0 \rightarrow T_4$	2.09/594	0.000	H–3→L+1	0.6321	MLCT/ILCT
	$S_0 \rightarrow T_5$	2.39/518	0.000	H–2→L	0.7037	ILCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [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.

Table S5. Electronic excitation energies (eV) and corresponding oscillator strengths (*f*), main configurations and CI coefficients of the low-lying electronic excited states of the complex **RHO-Pt** in dichloromethane calculated by TDDFT//B3LYP/GENECP based on the DFT//B3LYP/ GENECP optimized ground state geometries.

TDDFT//B3LYP/ GENECP						
	Electronic transition	Energy [eV/nm][a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	2.60/476	0.9513	H→L	0.6972	ILCT
	$S_0 \rightarrow S_4$	3.10/399	0.0231	H–3→L	0.6733	ILCT
	$S_0 \rightarrow S_8$	3.62/342	0.1707	H–7→L	0.4561	MLCT
	$S_0 \rightarrow S_{11}$	3.90/318	0.0366	H→L+1	0.6339	LLCT
Triplet	$S_0 \rightarrow T_1$	1.74/714	0.0000	H→L	0.7045	ILCT
	$S_0 \rightarrow T_2$	2.47/503	0.0000	H–3→L	0.6824	ILCT
	$S_0 \rightarrow T_3$	2.66/467	0.0000	H–1→L	0.6914	MLCT
	$S_0 \rightarrow T_4$	2.76/449	0.0000	H–1→L	0.1182	MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [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.

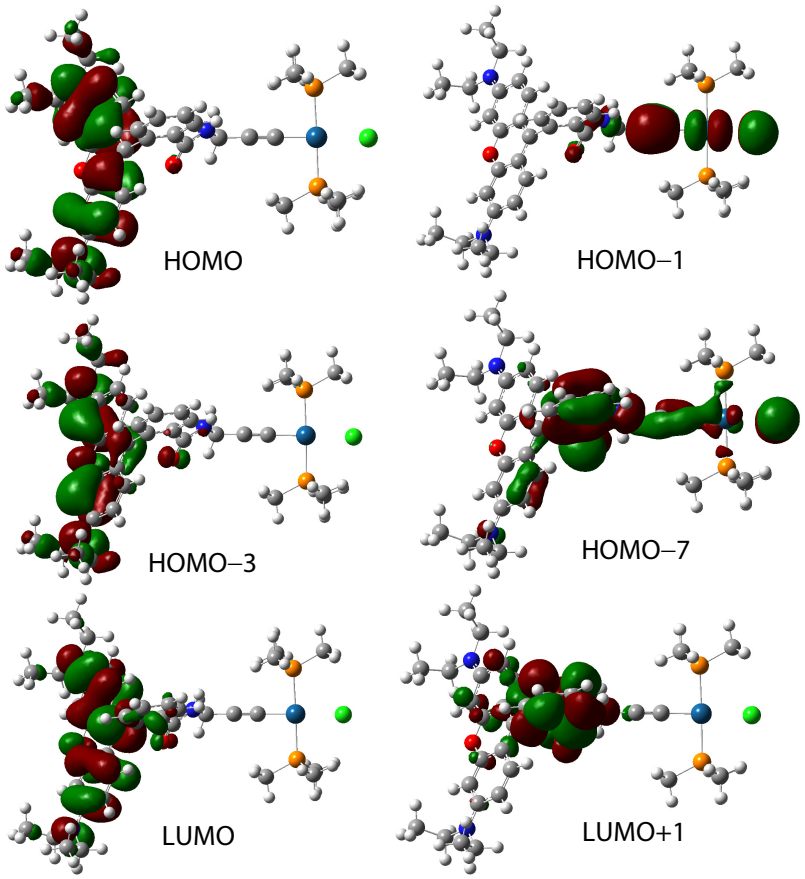

Fig. S29 Electron density maps of the frontier molecular orbital of the complex **RH(o)-Pt** in dichloromethane Based on ground state optimized geometry by the DFT calculations at the B3LYP/GENECP level with Gaussian 09W.

6.0 The x -y- z coordinates of the optimized geometries of complexes

BDPY-Pt-1 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	2.75414	9.89495	-11.42985
P	0.6833	10.54654	-9.07646
C	-0.0519	12.19226	-8.75219
H	-0.12324	12.3637	-7.66857
H	-1.04555	12.22832	-9.19294
H	0.56765	12.96851	-9.1959
C	-0.33914	9.36561	-8.11622
H	0.09851	8.37027	-8.16805
H	-1.33985	9.34057	-8.5394
H	-0.38963	9.68161	-7.06425
C	2.30514	10.57203	-8.21397
H	2.7684	9.5913	-8.2715
H	2.96267	11.29724	-8.68593
H	2.1551	10.84456	-7.15856
P	0.77976	9.50729	-13.70209
C	1.49523	7.84956	-14.02661
H	1.56289	7.67708	-15.11024
H	0.86678	7.08143	-13.58163
H	2.48979	7.79964	-13.58807
C	-0.83586	9.50656	-14.56902
H	-1.28546	10.49304	-14.50722
H	-1.50434	8.78746	-14.10366
H	-0.68475	9.23816	-15.62551
C	1.82681	10.67343	-14.65332
H	1.40391	11.67467	-14.60119
H	2.82641	10.68305	-14.2252
H	1.87864	10.35888	-15.70551
C	3.97783	9.81435	-11.44898
C	6.47534	8.62071	-11.32437
C	6.36076	10.85273	-11.74196
C	5.57575	9.70911	-11.47396
C	7.72118	10.42777	-11.75581
C	8.92189	11.12188	-11.98693
C	10.16072	10.45817	-11.95783
C	11.51057	10.93135	-12.14378
C	11.50974	8.66708	-11.78139
N	7.73264	9.05479	-11.42622
N	10.22369	9.07113	-11.71195
B	9.00314	8.15373	-11.43693
F	9.09003	7.6044	-10.14856

F	8.96414	7.11441	-12.38901
C	5.77922	12.23493	-11.96737
H	6.12727	12.93793	-11.21099
H	6.0611	12.63398	-12.94014
H	4.69432	12.16509	-11.91331
C	11.92321	7.24347	-11.6109
H	13.00051	7.17069	-11.72566
H	11.6235	6.87576	-10.63008
H	11.42765	6.61771	-12.35683
C	12.00375	12.3204	-12.43055
H	11.71912	13.01613	-11.64288
H	13.08887	12.28581	-12.49968
H	11.60043	12.70309	-13.36762
C	6.1238	7.16668	-11.17973
H	6.55825	6.76893	-10.26287
H	5.04058	7.06117	-11.15245
H	6.53004	6.59247	-12.01206
C	8.88124	12.59161	-12.26447
C	8.7973	13.05195	-13.58363
C	8.92682	13.51227	-11.21093
C	8.75369	14.42488	-13.84782
C	8.89466	14.88556	-11.47652
H	9.00171	13.15848	-10.18952
H	8.68297	14.77324	-14.87151
H	8.93634	15.59247	-10.6563
C	8.80519	15.34421	-12.79488
H	8.77592	16.40823	-12.99969
H	8.75186	12.3405	-14.39972
Cl	-1.53797	10.17764	-11.36275
Pt	0.73682	10.02781	-11.39831
C	12.30916	9.8027	-12.00112
H	13.37791	9.80736	-12.05265

BDPY-Pt-2 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-10.13944	2.2579	-2.16761
Pt	-8.1705	2.20045	-1.72852
P	-7.85734	1.17746	-3.82795
C	-8.43274	2.23467	-5.21897
H	-8.33461	1.71101	-6.17597
H	-7.83944	3.15349	-5.24769
H	-9.47907	2.49952	-5.0468
C	-6.13793	0.71952	-4.28869
H	-5.73877	0.01402	-3.5555
H	-5.50766	1.6124	-4.27614

H	-6.11377	0.26632	-5.28534
C	-8.81069	-0.38412	-4.01829
H	-8.45545	-1.11958	-3.29031
H	-9.86525	-0.17641	-3.81983
H	-8.69658	-0.79212	-5.02837
P	-8.50386	3.22556	0.36718
C	-10.22965	3.66808	0.81746
H	-10.26093	4.13495	1.80758
H	-10.84808	2.76697	0.81628
H	-10.63653	4.35645	0.07252
C	-7.92536	2.17969	1.76589
H	-6.87324	1.92966	1.60663
H	-8.50469	1.25189	1.79043
H	-8.04087	2.70336	2.72095
C	-7.56762	4.79779	0.55902
H	-6.50909	4.6035	0.36778
H	-7.92666	5.52799	-0.17239
H	-7.69191	5.20683	1.5675
C	-11.33569	2.27842	-2.44748
C	-19.4603	0.68528	-4.45634
C	-17.30848	0.3463	-3.72964
C	-17.48214	1.70445	-4.12917
C	-16.57626	2.80179	-4.14053
C	-17.02243	4.07318	-4.59789
C	-16.34047	5.31997	-4.72264
C	-18.52017	5.54122	-5.41047
N	-18.8091	1.86774	-4.56561
N	-18.34872	4.2528	-5.02943
B	-19.45136	3.17392	-5.07945
F	-19.91138	3.00747	-6.39608
F	-20.53282	3.54065	-4.26205
C	-16.08976	-0.34026	-3.18753
H	-15.25672	-0.34269	-3.90049
H	-15.7155	0.13046	-2.27142
H	-16.33826	-1.38094	-2.95456
C	-19.81042	6.08054	-5.9192
H	-19.70593	7.14276	-6.15304
H	-20.13077	5.53887	-6.81714
H	-20.60575	5.94729	-5.17624
C	-14.91571	5.66497	-4.40362
H	-14.20034	5.07223	-4.98543
H	-14.74312	6.72191	-4.63187
H	-14.67036	5.50267	-3.34772
C	-20.88915	0.49949	-4.82831
H	-21.05726	0.78306	-5.87374
H	-21.18171	-0.543	-4.68168
H	-21.53497	1.14741	-4.22327

C	-15.17005	2.62307	-3.66582
C	-14.83236	2.85234	-2.32255
C	-14.15483	2.22299	-4.54898
C	-13.51984	2.68729	-1.8737
C	-12.84102	2.05688	-4.10396
H	-14.40184	2.0425	-5.59195
H	-13.27901	2.8695	-0.82949
H	-12.06893	1.74699	-4.80359
C	-12.51996	2.28873	-2.76429
H	-15.60882	3.16206	-1.6279
Cl	-5.94515	2.13276	-1.23695
C	-18.54917	-0.29282	-3.93665
H	-18.7591	-1.32294	-3.73749
C	-17.28045	6.23986	-5.23265
H	-17.08946	7.27117	-5.44433

RH-BDPY-Pt-1 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-4.59129877	-1.09896594	0.08096644
P	-3.75887040	1.29653031	-1.74198957
C	-2.87485012	2.82592595	-1.22966388
H	-3.25958754	3.69718511	-1.77081164
H	-1.80922466	2.70077985	-1.43787873
H	-3.00691840	2.98089909	-0.15463638
C	-3.63276026	1.28290779	-3.57711639
H	-4.23439230	0.46071638	-3.97602736
H	-2.58867786	1.12023765	-3.85594529
H	-3.98803034	2.22926757	-3.99918141
C	-5.53007748	1.66491315	-1.41601627
H	-6.14709357	0.83901767	-1.77897417
H	-5.69265483	1.75910689	-0.33937193
H	-5.82693514	2.59270133	-1.91641147
P	-2.00636424	-2.60407771	0.25368426
C	-2.86979804	-4.13419839	-0.29111426
H	-2.49485024	-5.00911041	0.25068111
H	-2.71237347	-4.27948998	-1.36403343
H	-3.94085843	-4.01751403	-0.10731597
C	-0.22441811	-2.96603718	-0.01512323
H	0.37834095	-2.13633462	0.36225880
H	-0.02775698	-3.06487141	-1.08527378
H	0.05650742	-3.89089406	0.50013852
C	-2.19773638	-2.60307157	2.08348496
H	-1.61661598	-1.77920299	2.50867130

H	-3.25226265	-2.44711084	2.32504644
H	-1.85359665	-3.54891280	2.51535649
C	-5.66692907	-1.37810155	0.60094671
C	-7.90008059	-2.55504738	0.58892497
C	-7.43984518	-1.26390956	2.41169529
C	-6.92150606	-1.70293978	1.18149040
C	-8.73115649	-1.86426683	2.54464399
C	-9.70131718	-1.78856141	3.55707566
C	-10.91830480	-2.48672303	3.45186534
C	-12.04797360	-2.57766734	4.33077458
C	-12.40765893	-3.83625165	2.47153324
N	-8.96499869	-2.64439994	1.40158151
N	-11.18773212	-3.27602961	2.32625916
B	-10.24604052	-3.47794842	1.11014426
F	-10.86045291	-3.01696812	-0.05826445
F	-9.91532102	-4.82920225	0.97300287
C	-6.71243106	-0.34284393	3.34326885
H	-7.27814654	0.57332629	3.54400046
H	-6.51475227	-0.80909086	4.31497685
H	-5.75345501	-0.06445650	2.89605368
C	-13.00958782	-4.74328366	1.44752949
H	-13.99970940	-5.07687604	1.76798662
H	-13.09906021	-4.23285085	0.48244603
H	-12.37276745	-5.61936484	1.28386727
C	-12.27744580	-1.93107560	5.66573025
H	-12.26113336	-0.83771185	5.60300598
H	-13.25367588	-2.23284822	6.05787149
H	-11.51520754	-2.21466089	6.39932100
C	-7.81021811	-3.25995581	-0.72286832
H	-8.64747885	-2.97756663	-1.36983918
H	-6.86819155	-3.00934082	-1.21582745
H	-7.87054430	-4.34507310	-0.58371820
C	-9.43755137	-0.95314786	4.76903931
C	-8.79696025	-1.50751254	5.88575613
C	-9.83056186	0.39205878	4.80257760
C	-8.55336026	-0.72783312	7.01838581
C	-9.58554969	1.17042542	5.93588801
H	-10.32742047	0.82637511	3.93939884
H	-8.05646824	-1.16834839	7.87839184
H	-9.89406251	2.21214350	5.95026782
C	-8.94687308	0.61230251	7.04585408
H	-8.75677828	1.21828762	7.92732336
H	-8.49139364	-2.54997285	5.86470946
C	-12.95827971	-3.42102574	3.69901634
H	-13.92864127	-3.71530363	4.07824311
C	2.32886003	-2.06493749	4.12440450
C	2.56411939	-2.44810557	2.79536194

C	2.43082616	-3.81019992	2.51678481
C	2.08371269	-4.74532625	3.49261173
C	1.83253416	-4.35018990	4.82034045
C	1.98117848	-2.96748734	5.11453342
H	2.42566074	-1.01530586	4.38928644
H	2.01577773	-5.77675612	3.17405410
H	1.82595074	-2.59472749	6.11865036
C	2.92150413	-1.42907714	1.72258871
C	3.58527035	-1.42719502	-0.74401708
C	3.79451793	-2.03747604	-1.96895401
C	3.59553461	-3.43607985	-2.12927251
C	3.21395666	-4.15595170	-0.98112695
C	3.00870621	-3.51062350	0.23879763
C	3.17934816	-2.13365856	0.39838259
H	3.74349874	-0.35469665	-0.66448245
H	4.11380562	-1.42366106	-2.80119384
H	3.06075066	-5.22659683	-0.99512066
O	2.63717682	-4.34127983	1.26731590
C	3.68347079	0.79642034	2.23023179
C	4.09120145	-0.53287773	2.14168962
C	4.56136114	1.81376010	2.59587754
C	5.40841367	-0.88456922	2.41935599
C	6.29888724	0.12834161	2.78790233
C	5.88291170	1.46519795	2.87646090
H	4.21242751	2.84052709	2.65606917
H	5.73804131	-1.91766506	2.35264334
H	7.33233907	-0.12457986	3.00993997
H	6.59728799	2.23124233	3.16525591
N	1.84385975	-0.39880042	1.58634193
C	0.46510581	-0.70113919	1.26135416
H	0.30015176	-1.77565765	1.37424316
H	-0.18628398	-0.17846520	1.97089965
C	0.10421754	-0.25577160	-0.16957253
C	3.53598304	-5.49355470	-3.50667442
H	2.64208513	-5.77644923	-2.93873398
C	4.21798402	-3.30788879	-4.52467535
H	3.67528957	-2.35659489	-4.58108126
C	1.32793366	-6.68496552	5.47315132
H	0.81701701	-6.79583436	4.50909972
C	1.21612559	-4.84452430	7.17031889
H	0.64834714	-3.90656151	7.17236923
C	2.24134694	0.88580824	1.88154852
O	1.51911319	1.87739712	1.84897683
N	1.44128284	-5.26289382	5.78856832
N	3.75354935	-4.05662269	-3.35876044
H	3.29309324	-5.67906918	-4.55839765
H	3.91794828	-3.87425500	-5.41228496

C	4.72258621	-6.37730807	-3.09437562
H	5.59785645	-6.18049377	-3.72238392
H	5.00889487	-6.19960935	-2.05301661
H	4.46031280	-7.43680503	-3.20056432
C	5.73152606	-3.05144370	-4.57175146
H	6.06998144	-2.50747190	-3.68443124
H	6.29003329	-3.99189471	-4.62283083
H	5.98718951	-2.45556593	-5.45617482
C	2.48595788	-4.68943214	8.02008323
H	3.01542935	-5.64298259	8.11743385
H	3.17597896	-3.96560590	7.57511859
H	2.22740646	-4.34059719	9.02717435
H	0.66061654	-7.13037166	6.21849253
H	0.56006502	-5.59059544	7.63110439
C	2.65635946	-7.45558517	5.45388223
H	3.35930803	-7.01924002	4.73753531
H	3.13189270	-7.44681194	6.44016310
H	2.48351012	-8.50048965	5.16945239
C	-1.39435679	-0.45551541	-0.46279151
Pt	-2.86943842	-0.65212790	-0.75141379

RH-BDPY-Pt-2 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.43658174	7.29920261	-7.23112397
C	-0.82922322	5.92253038	-5.93762948
C	0.44873226	5.32056200	-6.18850409
C	1.00424946	4.09632930	-5.77833553
C	2.30877152	3.73409109	-6.15514953
C	3.09079877	2.56179476	-5.88621240
C	4.28374937	4.01362466	-7.16673546
N	1.18938035	6.20497120	-6.98619151
N	3.08449357	4.59427985	-6.94599717
B	2.63839428	5.97656040	-7.48880196
F	2.67018086	5.97845592	-8.88997615
F	3.48287247	6.98293618	-7.00140350
C	-1.99087163	5.40388388	-5.14170477
H	-2.39685782	4.47754957	-5.56234768
H	-1.71475051	5.18365424	-4.10518279
H	-2.79137262	6.14993610	-5.12996341
C	5.36326259	4.65823741	-7.97489746
H	6.23755392	4.00550699	-8.03175892
H	5.01225000	4.87403924	-8.98971665
H	5.66183692	5.61470055	-7.53190049
C	2.73536556	1.33611181	-5.09663622

H	1.83858335	0.84188596	-5.48483189
H	3.56230144	0.62043112	-5.13553625
H	2.53647057	1.56722829	-4.04450075
C	0.91907509	8.45098518	-8.05248678
H	1.18884980	8.12251560	-9.06200191
H	0.14502654	9.21878423	-8.12309503
H	1.81933869	8.89205944	-7.61095368
C	0.19903269	3.17182069	-4.92465133
C	0.29369427	3.23003743	-3.52659888
C	-0.66746206	2.23319129	-5.50321212
C	-0.46058709	2.37589517	-2.72698078
C	-1.42165295	1.37587585	-4.70622231
H	-0.75148886	2.17523927	-6.58507341
H	-0.37725865	2.43582601	-1.64609775
H	-2.08769651	0.65483706	-5.17041119
H	0.96119095	3.95148845	-3.06319329
C	4.31194629	2.76069707	-6.52411518
H	5.14931419	2.07472251	-6.53381067
C	-2.11588727	0.55708231	-2.47607779
C	-1.33849529	1.42771855	-3.29728296
C	-0.81158221	7.14871319	-6.59644759
H	-1.61474062	7.87403126	-6.62273809
P	-2.30349875	-1.27918621	1.17648970
C	-3.04415219	-0.96716015	2.83072613
H	-2.25919177	-0.92586394	3.59338392
H	-3.75082043	-1.76446651	3.07473308
H	-3.57788667	-0.01200010	2.81426114
C	-1.38535819	-2.86091818	1.38032391
H	-0.80435783	-3.06439962	0.47589166
H	-2.10417139	-3.67176484	1.52444398
H	-0.70959743	-2.81214588	2.24069834
C	-0.98458517	-0.00591777	1.03912014
H	-0.42847810	-0.14896934	0.11012592
H	-1.43773678	0.98886264	1.01756266
H	-0.30407002	-0.07715802	1.89436998
P	-5.52396216	-1.75395326	-2.25469817
C	-5.33475867	-0.86403968	-3.85172922
H	-6.16750520	-1.11109396	-4.51874160
H	-4.39090778	-1.14924907	-4.32262075
H	-5.31605055	0.21371242	-3.67235304
C	-5.65840100	-3.52394459	-2.73792901
H	-5.81794704	-4.12473997	-1.83906478
H	-4.72440653	-3.84348569	-3.20957481
H	-6.48679060	-3.67531795	-3.43811883
C	-7.21599332	-1.30461265	-1.69029325
H	-7.43677594	-1.84963701	-0.76918451
H	-7.25799686	-0.23123922	-1.48236516

H	-7.95834499	-1.55314256	-2.45587152
C	-7.89106348	-7.20109008	3.64668461
C	-7.08599184	-7.21844696	2.49604473
C	-7.67588799	-7.74535832	1.34396872
C	-8.98470526	-8.23061636	1.32332219
C	-9.79281919	-8.19446907	2.47881658
C	-9.19368982	-7.67048068	3.65927687
H	-7.47514555	-6.80442395	4.56916798
H	-9.34311429	-8.62898704	0.38351372
H	-9.74449388	-7.63290943	4.59006615
C	-5.66545922	-6.67276208	2.50723580
C	-3.66662793	-6.55833147	0.91808747
C	-3.05151656	-6.72623306	-0.31143424
C	-3.77124895	-7.25217008	-1.42170576
C	-5.11457751	-7.61386590	-1.18844645
C	-5.70303695	-7.43079013	0.06472191
C	-5.00956945	-6.89368627	1.15151774
H	-3.08060251	-6.15234525	1.73837489
H	-2.00886398	-6.45263720	-0.40651310
H	-5.73430524	-8.05072471	-1.96011346
O	-7.01529495	-7.83503193	0.14161519
C	-4.42253969	-6.23807461	4.51811194
C	-4.82791960	-7.25106539	3.65098089
C	-3.64448564	-6.50011301	5.64414324
C	-4.45914578	-8.57207372	3.88895994
C	-3.67788966	-8.84719589	5.01667774
C	-3.27283534	-7.82371040	5.88769962
H	-3.34230748	-5.69322317	6.30545680
H	-4.76811936	-9.37099270	3.22069320
H	-3.37973109	-9.87160287	5.22220447
H	-2.66675821	-8.06653790	6.75579255
N	-5.65806010	-5.22378870	2.88745662
C	-6.39787998	-4.19622949	2.15743997
H	-7.19695083	-4.70523510	1.60652724
H	-6.88577117	-3.55826315	2.90520118
C	-5.58310092	-3.36585859	1.25989556
C	-3.92942680	-7.97835572	-3.78373933
H	-4.94130192	-7.55658523	-3.80065595
C	-1.77849257	-7.05260760	-2.88348338
H	-1.55669149	-6.10425561	-2.38095137
C	-11.68831828	-9.21303228	1.25205878
H	-11.40558271	-8.60154780	0.38688234
C	-11.92653341	-8.60167374	3.67337699
H	-11.76225562	-7.65225971	4.19562430
C	-4.96052490	-4.94058413	4.03044377
O	-4.82950176	-3.82553727	4.53987474
N	-11.10650755	-8.62759952	2.46086290

N	-3.18733510	-7.38868050	-2.66862398
H	-3.44740376	-7.64141533	-4.70650546
H	-1.65311499	-6.86169367	-3.95370973
C	-4.00151052	-9.51255271	-3.77901404
H	-3.00294996	-9.95390147	-3.86142720
H	-4.46423450	-9.88959655	-2.86126230
H	-4.59916647	-9.86138501	-4.62937755
C	-0.77878982	-8.12946208	-2.43740317
H	-0.89300330	-8.36400529	-1.37405603
H	-0.91649266	-9.05529357	-3.00557400
H	0.24737339	-7.77949514	-2.60056406
C	-11.70026476	-9.77611223	4.63630698
H	-11.95631287	-10.72959150	4.16276825
H	-10.65653187	-9.82938590	4.96267916
H	-12.32989525	-9.65799060	5.52606103
H	-12.77520421	-9.12351423	1.34128199
H	-12.97312435	-8.59095120	3.35378811
C	-11.31838222	-10.68185551	0.99882519
H	-10.23453958	-10.81460319	0.92017238
H	-11.68106302	-11.32411976	1.80796975
H	-11.77184733	-11.02569885	0.06171029
C	-4.92221534	-2.62720563	0.54423685
Pt	-3.87385435	-1.41344664	-0.59282312
C	-2.78593080	-0.18494852	-1.76180253

RHO-BDPY-Pt-1(open amide form) ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 1 Multiplicity = 1

C	-4.91909087	-0.36277610	-0.75472885
P	-2.79819185	-2.60746034	-1.42191144
C	-1.53920664	-2.99025265	-2.70676998
H	-1.56208483	-4.05840761	-2.94801139
H	-0.54673042	-2.71513952	-2.34160284
H	-1.75618804	-2.41454993	-3.61177983
C	-2.36043455	-3.72068921	-0.02240452
H	-3.11757861	-3.63682608	0.76258459
H	-1.39387232	-3.41710909	0.38850256
H	-2.30191182	-4.76145151	-0.35845255
C	-4.34293441	-3.33716234	-2.10253392
H	-5.15452127	-3.21485780	-1.38209910
H	-4.61907475	-2.81209197	-3.02144180
H	-4.19564166	-4.39955310	-2.32317818
P	-2.90841179	1.90032297	-0.01868361
C	-4.36464980	2.43808807	0.96765769

H	-4.30623257	3.51057832	1.18057819
H	-4.38762424	1.88473303	1.91126843
H	-5.27957050	2.21498460	0.41495891
C	-1.48106291	2.42219357	1.01674082
H	-0.55153292	2.19077115	0.49247146
H	-1.49172189	1.86508811	1.95823874
H	-1.53654898	3.49477140	1.22974610
C	-2.87880648	3.06914250	-1.44216611
H	-1.98004471	2.89281464	-2.04011878
H	-3.75648178	2.89962296	-2.07248003
H	-2.88158212	4.10661369	-1.09071448
C	-6.14859611	-0.36747354	-0.75766439
C	-8.37775771	-0.75896318	0.36277932
C	-8.43891102	-0.03643196	-1.79836906
C	-7.56858112	-0.37967899	-0.74889283
C	-9.76774457	-0.21526777	-1.30107920
C	-11.02479788	-0.03073922	-1.89794351
C	-12.21178258	-0.28413940	-1.18482074
C	-13.59164016	-0.17766829	-1.55749128
C	-13.42421783	-0.89004360	0.59514890
N	-9.67569252	-0.65883847	0.02833968
N	-12.16022116	-0.72518877	0.14437377
B	-10.87218877	-0.97969743	0.96549945
F	-10.81486583	-2.31814005	1.37590198
F	-10.84022883	-0.14409632	2.08981374
C	-7.97788665	0.42025467	-3.14880062
H	-8.32347190	-0.24249652	-3.94955141
H	-8.34219087	1.42438047	-3.39193213
H	-6.88410756	0.43822039	-3.16657855
C	-13.73747633	-1.35146016	1.98178574
H	-14.81852131	-1.41330570	2.12755632
H	-13.29521263	-2.33499238	2.17361855
H	-13.31674427	-0.66416010	2.72376368
C	-14.20141743	0.24727355	-2.86132697
H	-13.88592812	-0.39291583	-3.69183141
H	-15.29235934	0.19891524	-2.79052250
H	-13.92403165	1.27187448	-3.13093712
C	-7.90876196	-1.20391164	1.70727535
H	-8.28725484	-2.20528336	1.93887990
H	-6.81689104	-1.21518531	1.73278081
H	-8.28149640	-0.53395695	2.48983922
C	-11.10647464	0.44402098	-3.31353981
C	-11.15876107	1.81570549	-3.59762905
C	-11.13265633	-0.47674713	-4.37032884
C	-11.23607170	2.25927738	-4.91964809
C	-11.21007026	-0.03102637	-5.69165924
H	-11.09215355	-1.54103547	-4.15586893

H	-11.27552471	3.32473525	-5.12810415
H	-11.22942649	-0.75354499	-6.50271922
C	-11.26212334	1.33728220	-5.96898272
H	-11.32237255	1.68305841	-6.99703722
H	-11.13780268	2.53363149	-2.78249647
C	-14.32351703	-0.55963532	-0.43478891
H	-15.40253934	-0.59909120	-0.35674020
C	0.35061066	-0.35676302	-0.73706310
C	-0.87366168	-0.33977232	-0.72458057
Pt	-2.89640887	-0.35209875	-0.73187545
C	6.91919096	0.56636704	-0.97307292
C	6.93272455	0.50467936	0.44910005
C	7.29034453	1.71014900	1.11663489
C	7.59181731	2.88175915	0.45137390
C	7.54342039	2.93601199	-0.96458959
C	7.21126782	1.71695183	-1.65413355
H	6.67772285	-0.33227216	-1.53028089
H	7.86188765	3.73883067	1.05162813
H	7.19871583	1.69243301	-2.73507651
C	6.45735123	-1.65560870	3.50085931
C	6.55641027	-1.52235766	4.85873848
C	6.92980096	-0.27253179	5.46758875
C	7.20942391	0.81089228	4.59646179
C	7.09771231	0.65390578	3.22960972
C	6.73012542	-0.57588944	2.61380085
H	6.16212486	-2.61073027	3.08133362
H	6.34669904	-2.38475172	5.47644711
H	7.50879438	1.78229101	4.96344630
O	7.36557440	1.75499541	2.47474836
C	7.42998835	1.12932973	7.43521923
H	6.92562600	1.95730387	6.92599011
C	6.69860922	-1.26076611	7.72590693
H	5.82213101	-1.79563489	7.34859068
C	8.18582318	5.31780697	-0.93513811
H	7.53907629	5.43864851	-0.05982445
C	7.73778764	4.14573902	-3.11612507
H	6.87431192	3.56806169	-3.45905880
N	7.79442440	4.08749310	-1.64463491
N	6.99697376	-0.13726362	6.81975202
C	6.62965644	-0.64536650	1.20924022
C	5.88639698	-4.42386986	-0.71332206
C	4.85128043	-3.49604893	-0.60975714
C	5.05288999	-2.24951127	-0.00131285
C	6.32299280	-1.94517326	0.53530952
C	7.14540227	-4.11353285	-0.20185389
H	5.70540151	-5.38668695	-1.18126546
H	3.86372320	-3.76627830	-0.97255753

H	7.96034310	-4.82706155	-0.27796673
C	3.93835480	-1.24942735	0.15323906
O	3.93476251	-0.43237261	1.07426775
N	2.94381914	-1.29226862	-0.77730293
H	3.03664502	-1.89865376	-1.57859872
C	7.35743056	-2.88347246	0.42201043
H	8.33766578	-2.64367201	0.82412539
H	7.05069299	1.12997336	8.45997731
H	6.39329028	-0.82298317	8.67986097
C	8.94819338	1.34399641	7.44447967
H	9.45438805	0.57322343	8.03327025
H	9.36614357	1.32618397	6.43321559
H	9.17945855	2.31681013	7.89167638
C	7.86911852	-2.22518912	7.94830616
H	8.21117204	-2.66895221	7.00785805
H	8.72033155	-1.71708200	8.41131844
H	7.55736756	-3.03648507	8.61495794
C	9.66347320	5.37349953	-0.52913196
H	9.93675718	4.53910510	0.12415626
H	10.31663492	5.34372646	-1.40628557
H	9.86235122	6.30664453	0.00889998
C	9.01640857	3.67976789	-3.82185299
H	9.86993369	4.31122123	-3.55744932
H	9.26790862	2.64618839	-3.56315787
H	8.87960018	3.73594306	-4.90721571
H	7.52649619	5.18480057	-3.38191647
H	7.95383610	6.15427366	-1.59894965
C	1.83017903	-0.35199269	-0.74143880
H	1.87602810	0.26391941	0.13231754
H	2.23024416	0.18371216	-1.57682387

RHO-BDPY-Pt-2(open amide form) ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 1 Multiplicity = 1

C	6.06861835	-17.40365658	-9.20399709
C	4.36480873	-15.88937059	-9.18599317
C	5.29000237	-15.57734477	-10.23085427
C	5.31430115	-14.54802026	-11.18499336
C	6.35846940	-14.45272142	-12.12431185
C	6.61218446	-13.51631710	-13.17930095
C	8.26235505	-15.07919695	-13.11837369
N	6.31620110	-16.53575241	-10.19996634
N	7.39848434	-15.39203264	-12.12644419

B	7.53770225	-16.59224830	-11.15786263
F	8.72743914	-16.48897923	-10.42505540
F	7.53247115	-17.79680439	-11.87364929
C	3.10156815	-15.18885825	-8.78815246
H	3.28099797	-14.14996702	-8.49086458
H	2.37018417	-15.16127418	-9.60326946
H	2.65181288	-15.71520278	-7.94099654
C	9.49146664	-15.87931211	-13.40629429
H	10.03937508	-15.44672816	-14.24677012
H	10.14889469	-15.91093639	-12.53078249
H	9.23213131	-16.91623654	-13.64600457
C	5.81582301	-12.31905543	-13.60914315
H	5.70429109	-11.58706736	-12.80237945
H	6.31618194	-11.82616302	-14.44831182
H	4.80438742	-12.59081158	-13.92943399
C	6.95712430	-18.55785468	-8.88152287
H	7.96987645	-18.21421243	-8.64512079
H	6.55358358	-19.10791685	-8.02855966
H	7.04255381	-19.23366934	-9.73951634
C	4.21341287	-13.53630807	-11.20654983
C	3.06714715	-13.75475622	-11.98328290
C	4.31643335	-12.35942722	-10.45180439
C	2.03929168	-12.80948521	-12.00433463
C	3.28741786	-11.41539704	-10.47434515
H	5.20254466	-12.18511852	-9.84784544
H	1.15523258	-12.98952331	-12.60950959
H	3.37786123	-10.50707777	-9.88527623
H	2.98171226	-14.66554429	-12.56934099
C	7.80007882	-13.92758559	-13.78077278
H	8.29324511	-13.44938794	-14.61746359
C	0.26403313	-9.77938712	-11.51967663
P	-0.08719957	-6.94992601	-10.15852342
C	0.00083837	-5.17000434	-10.61301581
H	0.49744393	-4.60381482	-9.81772454
H	-1.00819650	-4.78067260	-10.76894126
H	0.57095772	-5.05902329	-11.54048791
C	-0.97220770	-6.95512828	-8.54413094
H	-0.98903232	-7.97115281	-8.13926165
H	-2.00193066	-6.62186685	-8.69858325
H	-0.47795285	-6.28911930	-7.82881035
C	1.64800379	-7.36672584	-9.71435144
H	1.69958462	-8.40157841	-9.36927528
H	2.28344092	-7.26902382	-10.59923450
H	2.01167046	-6.69289587	-8.93156610
P	-2.29269882	-9.70290890	-13.29829496
C	-2.09522396	-11.52140398	-13.10654260
H	-2.59913129	-12.04814450	-13.92361353

H	-2.53147740	-11.83483670	-12.15335125
H	-1.03246589	-11.77201394	-13.09812330
C	-4.11679541	-9.48177020	-13.37277206
H	-4.34572203	-8.42686547	-13.53772450
H	-4.55904694	-9.78364819	-12.41873764
H	-4.54201431	-10.08998508	-14.17784144
C	-1.73194820	-9.37359718	-15.02178866
H	-1.90787884	-8.32246260	-15.26791089
H	-0.66019319	-9.57654191	-15.10241793
H	-2.27386961	-10.00702508	-15.73239594
C	1.11764920	-10.65432394	-11.38724189
C	-3.39366769	-6.02631305	-12.07263434
C	-2.56033560	-6.91523364	-11.95153494
Pt	-1.15298455	-8.35134758	-11.73096487
C	2.09757712	-11.66878489	-11.22233701
C	4.85864675	-17.03807856	-8.54311915
H	4.40282113	-17.53654799	-7.71326902
C	-8.32292772	-1.79316011	-13.26506023
C	-9.02369463	-2.92419123	-13.77128039
C	-9.33769511	-2.88629552	-15.15930757
C	-8.98141366	-1.83997014	-15.98658933
C	-8.25604725	-0.73474432	-15.47418551
C	-7.95653524	-0.74591161	-14.06632482
H	-8.08182242	-1.76109893	-12.20809273
H	-9.27752971	-1.90346346	-17.02394106
H	-7.44000344	0.09048762	-13.61596093
C	-10.61324464	-6.24678453	-12.97142828
C	-11.30655230	-7.22134393	-13.63547861
C	-11.59487001	-7.11514535	-15.04181381
C	-11.14485790	-5.94570841	-15.70571534
C	-10.44260919	-4.97817472	-15.01569061
C	-10.15084015	-5.06961221	-13.62527809
H	-10.40625489	-6.36923131	-11.91427188
H	-11.63974833	-8.08575751	-13.07777275
H	-11.32634662	-5.77467371	-16.75724983
O	-10.03330240	-3.90106378	-15.74113126
C	-12.59558900	-7.96359870	-17.13123031
H	-11.71995909	-7.57662135	-17.66297991
C	-12.71895789	-9.32100522	-15.01599970
H	-11.93554317	-9.65740204	-14.33060583
C	-8.21137086	0.32062921	-17.70368922
H	-8.04989657	-0.67638373	-18.12671342
C	-7.09562090	1.43579725	-15.74341234
H	-6.35026270	1.06607037	-15.03302642
N	-7.85525398	0.29004194	-16.27453000
N	-12.25805647	-8.10161642	-15.70379095
C	-9.41814312	-4.03937814	-13.00119119

C	-8.83304721	-4.09004098	-8.73728874
C	-7.77473270	-4.43800256	-9.57510542
C	-7.91874468	-4.42426045	-10.96930006
C	-9.16789844	-4.07414832	-11.52677896
C	-10.05940696	-3.72420890	-9.28974844
H	-8.70144293	-4.11574134	-7.65989980
H	-6.83773129	-4.76344886	-9.13235222
H	-10.89090893	-3.44929878	-8.64781868
C	-6.79935197	-4.83245895	-11.88939614
O	-7.02662843	-5.30693203	-13.00254748
N	-5.53013528	-4.64462698	-11.43042657
H	-5.38174854	-4.15166868	-10.56245881
C	-10.22367093	-3.72212404	-10.67547002
H	-11.18079445	-3.44092368	-11.10547316
H	-12.76089640	-8.97246745	-17.51704350
H	-12.80289635	-10.09966675	-15.77858899
C	-13.82684543	-7.09362361	-17.41098913
H	-14.72729009	-7.52457373	-16.96323942
H	-13.70487651	-6.08002696	-17.01678094
H	-13.98851512	-7.02165693	-18.49196957
C	-14.05517639	-9.16854725	-14.28051218
H	-14.01014015	-8.38273837	-13.51969349
H	-14.86462299	-8.92134985	-14.97391428
H	-14.31257664	-10.11020769	-13.78368717
C	-9.63646860	0.80762772	-17.99234321
H	-10.38699384	0.18186158	-17.49958332
H	-9.77951718	1.83763336	-17.65244528
H	-9.82385078	0.77856106	-19.07115435
C	-7.95763135	2.53031864	-15.10387082
H	-8.64382619	2.97313509	-15.83201778
H	-8.55306013	2.14195094	-14.27134627
H	-7.31381232	3.32873669	-14.71928000
H	-6.52937411	1.85292048	-16.58025810
H	-7.49018214	0.97737640	-18.19634555
C	-4.38308178	-4.95421052	-12.24289874
H	-4.54447831	-5.22340333	-13.26582904
H	-4.06634537	-3.93362008	-12.18837154

RHO- Pt(open amide form) ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:
Charge = 1 Multiplicity = 1

P	1.90580966	-11.05682066	-12.30149220
C	1.99384760	-9.27689899	-12.75598459
H	2.49045316	-8.71070947	-11.96069332
H	0.98481273	-8.88756725	-12.91191004
H	2.56396695	-9.16591794	-13.68345669

C	1.02080153	-11.06202293	-10.68709972
H	1.00397691	-12.07804746	-10.28223043
H	-0.00892143	-10.72876150	-10.84155203
H	1.51505638	-10.39601395	-9.97177913
C	3.64101302	-11.47362049	-11.85732022
H	3.69259385	-12.50847306	-11.51224406
H	4.27645015	-11.37591847	-12.74220328
H	4.00467969	-10.79979052	-11.07453488
P	-0.29968959	-13.80980355	-15.44126374
C	-0.10221473	-15.62829863	-15.24951138
H	-0.60612206	-16.15503915	-16.06658231
H	-0.53846817	-15.94173135	-14.29632003
H	0.96054334	-15.87890859	-15.24109208
C	-2.12378618	-13.58866485	-15.51574084
H	-2.35271280	-12.53376012	-15.68069328
H	-2.56603771	-13.89054284	-14.56170642
H	-2.54900508	-14.19687973	-16.32081022
C	0.26106103	-13.48049183	-17.16475744
H	0.08513039	-12.42935725	-17.41087967
H	1.33281604	-13.68343656	-17.24538671
H	-0.28086038	-14.11391973	-17.87536472
C	-1.40065846	-10.13320770	-14.21560312
C	-0.56732637	-11.02212829	-14.09450372
Pt	0.84002468	-12.45824223	-13.87393365
C	-6.32991849	-5.90005476	-15.40802901
C	-7.03068540	-7.03108588	-15.91424917
C	-7.34468588	-6.99319017	-17.30227635
C	-6.98840443	-5.94686479	-18.12955811
C	-6.26303802	-4.84163897	-17.61715429
C	-5.96352601	-4.85280626	-16.20929360
H	-6.08881319	-5.86799358	-14.35106151
H	-7.28452048	-6.01035811	-19.16690984
H	-5.44699421	-4.01640703	-15.75892971
C	-8.62023541	-10.35367918	-15.11439706
C	-9.31354307	-11.32823858	-15.77844739
C	-9.60186078	-11.22204000	-17.18478259
C	-9.15184867	-10.05260306	-17.84868412
C	-8.44959996	-9.08506937	-17.15865939
C	-8.15783092	-9.17650686	-15.76824687
H	-8.41324566	-10.47612596	-14.05724066
H	-9.64673910	-12.19265216	-15.22074153
H	-9.33333739	-9.88156836	-18.90021861
O	-8.04029317	-8.00795843	-17.88410004
C	-10.60257977	-12.07049335	-19.27419909
H	-9.72694986	-11.68351600	-19.80594869
C	-10.72594866	-13.42789987	-17.15896848
H	-9.94253394	-13.76429669	-16.47357461

C	-6.21836163	-3.78626544	-19.84665800
H	-6.05688734	-4.78327838	-20.26968220
C	-5.10261167	-2.67109740	-17.88638112
H	-4.35725347	-3.04082428	-17.17599520
N	-5.86224475	-3.81685271	-18.41749878
N	-10.26504724	-12.20851107	-17.84675973
C	-7.42513389	-8.14627279	-15.14415997
C	-6.84003798	-8.19693563	-10.88025752
C	-5.78172347	-8.54489721	-11.71807420
C	-5.92573545	-8.53115510	-13.11226884
C	-7.17488921	-8.18104297	-13.66974774
C	-8.06639773	-7.83110355	-11.43271722
H	-6.70843370	-8.22263599	-9.80286858
H	-4.84472206	-8.87034351	-11.27532100
H	-8.89789970	-7.55619343	-10.79078746
C	-4.80634274	-8.93935360	-14.03236492
O	-5.03361920	-9.41382668	-15.14551626
N	-3.53712605	-8.75152163	-13.57339535
H	-3.38873931	-8.25856333	-12.70542759
C	-8.23066170	-7.82901869	-12.81843880
H	-9.18778522	-7.54781833	-13.24844194
H	-10.76788717	-13.07936210	-19.66001228
H	-10.80988712	-14.20656140	-17.92155777
C	-11.83383620	-11.20051826	-19.55395791
H	-12.73428086	-11.63146838	-19.10620820
H	-11.71186728	-10.18692161	-19.15974972
H	-11.99550589	-11.12855158	-20.63493835
C	-12.06216716	-13.27544190	-16.42348096
H	-12.01713092	-12.48963302	-15.66266227
H	-12.87161376	-13.02824450	-17.11688306
H	-12.31956741	-14.21710234	-15.92665595
C	-7.64345937	-3.29926693	-20.13531199
H	-8.39398461	-3.92503307	-19.64255210
H	-7.78650795	-2.26926129	-19.79541406
H	-7.83084155	-3.32833359	-21.21412313
C	-5.96462212	-1.57657601	-17.24683960
H	-6.65081696	-1.13375956	-17.97498656
H	-6.56005090	-1.96494371	-16.41431505
H	-5.32080309	-0.77815796	-16.86224878
H	-4.53636488	-2.25397417	-18.72322688
H	-5.49717291	-3.12951825	-20.33931433
C	-2.39007255	-9.06110517	-14.38586752
H	-2.55146908	-9.33029798	-15.40879782
H	-2.07333614	-8.04051473	-14.33134032
Cl	2.43718583	-14.06782644	-13.63578463