Electronic Supplementary Information for:

Trans bis(alkylphosphine) platinum(II)-alkynyl complexes showing broadband visible light absorption and long-lived triplet excited states

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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.

Fluorescence lifetimes were measured on a OB920 luminescence lifetime spectrometer (TCSPC. Edinburgh, UK). The nanosecond time-resolved transient absorption spectra were detected by LP920 Edinburgh analytical instruments (Edinburgh Instruments, U.K.) and recorded on a Tektronix TDS 3012B oscilloscope. The lifetime values (by monitoring the decay trace of the transients) were obtained with the LP900 software. All samples in flash photolysis experiments were deaerated with argon for ca. 15 min before measurement and the gas flow is kept during the measurement.

The free energy changes of the electron transfer process (charge separation, CS), can be
calculated with the Weller equation (eq. 1 and eq. 2)

$$\Delta G^{0}{}_{\mathrm{CS}} = e[E_{OX} - E_{RED}] - E_{00} + \Delta G_{\mathrm{S}} \qquad \text{(Eq. 1)}$$

$$\Delta G_{\mathrm{S}} = -\frac{e^2}{4\pi\varepsilon_{\mathrm{S}}\varepsilon_0 R_{\mathrm{CC}}} - \frac{e^2}{8\pi\varepsilon_0}\left(\frac{1}{R_D} + \frac{1}{R_{\mathrm{A}}}\right)\left(\frac{1}{\varepsilon_{REF}} - \frac{1}{\varepsilon_S}\right) \qquad \text{(Eq. 2)}$$

Where ΔG_{S} is the static Coulombic energy, which is described by eq. 2. Where ΔG_{S} is the static Coulombic energy, which is described by eq. 2. e = electronic charge, E_{OX} = half-wave potential for one-electron oxidation of the electron-donor unit, E_{RED} = half-wave potential for one-electron reduction of the electron-acceptor unit; note herein the anodic and cathodic peak potentials were used because in some cases the oxidation is irreversible therefore the formal potential $E_{1/2}$ cannot be derived; E_{00} = energy level approximated with the fluorescence emission wavelength (for the singlet excited state), or the T_1 state energy level of Bodipy. ε_{S} = static dielectric constant of the solvent, R_{CC} center-to-center separation distance determined by DFT optimization of the geometry, R_{D} is the radius of the BODIPY-based donor, R_{A} is the radius of the electron acceptor, $\varepsilon_{\mathrm{REF}}$ is the static dielectric constant of the solvent used for the electrochemical studies, ε_0 permittivity of free space. The solvents used in the calculation of free energy of the electron transfer is CH_2Cl_2 (ε =9.1).

2.0 NMR and HRMS spectra

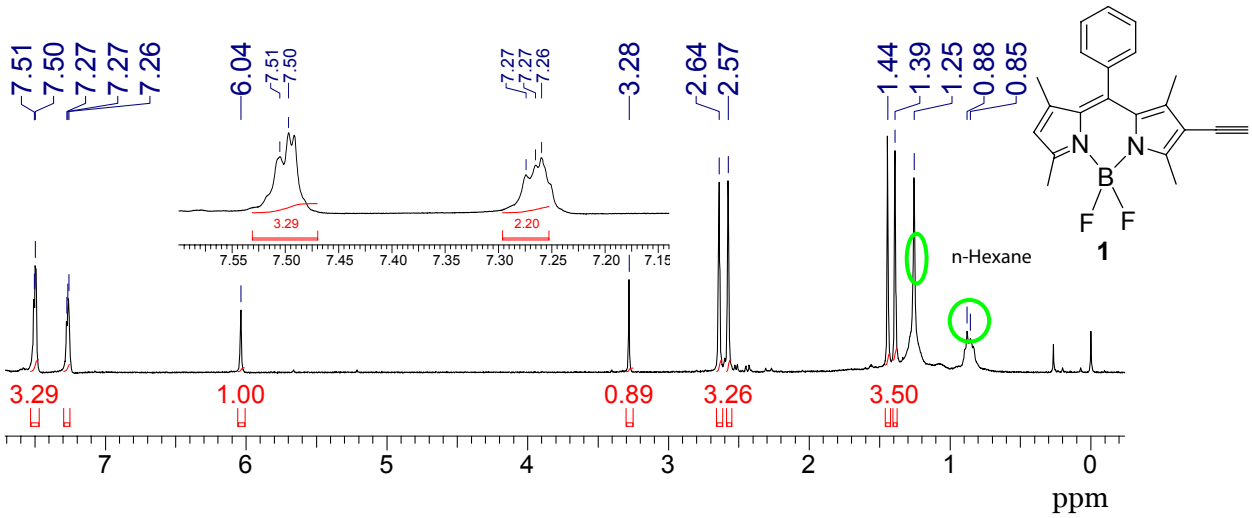


Fig. S1 ^{1}H NMR of compound **1** (400 MHz, $CDCl_3$).

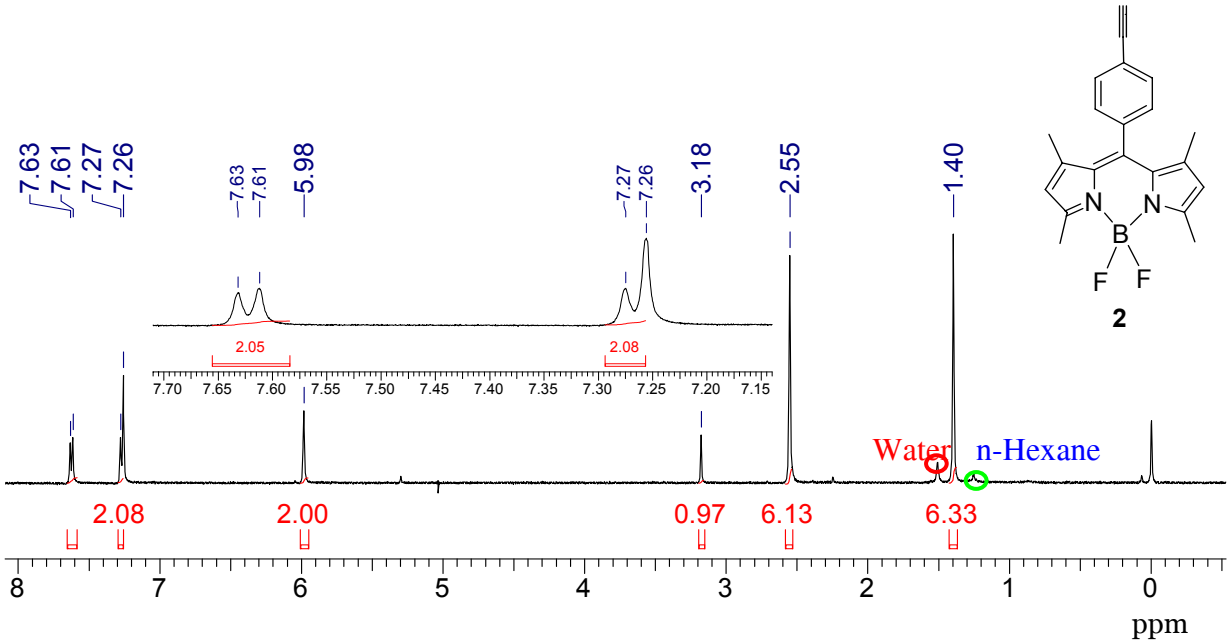


Fig. S2 ^{1}H NMR of compound **2** (400 MHz, $CDCl_3$).

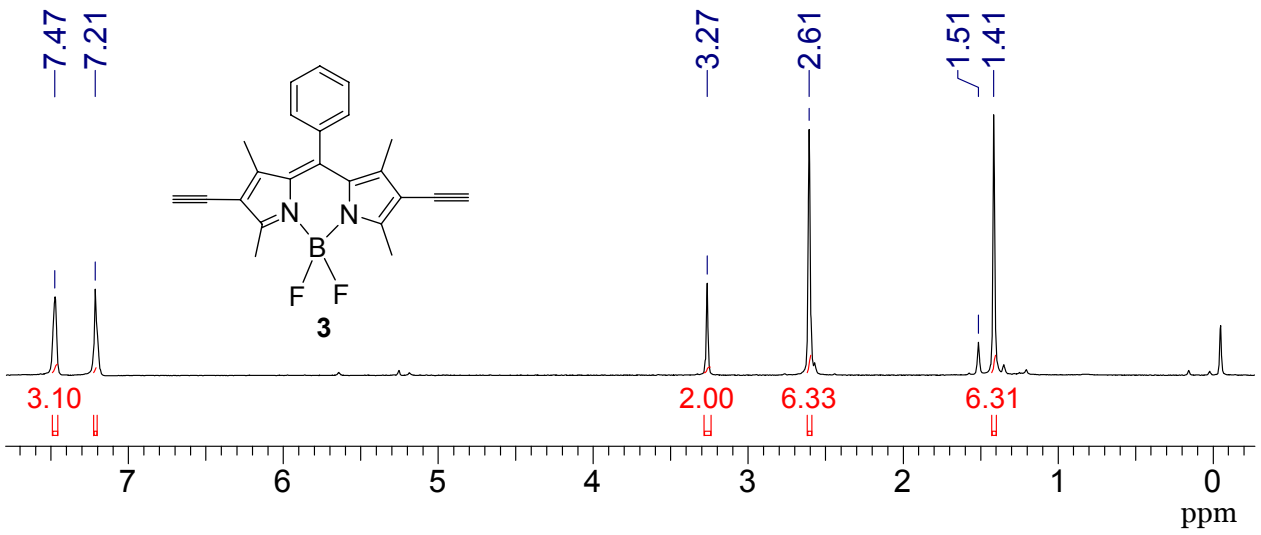


Fig. S3 ^{1}H NMR of compound **3** (400 MHz, $CDCl_3$).

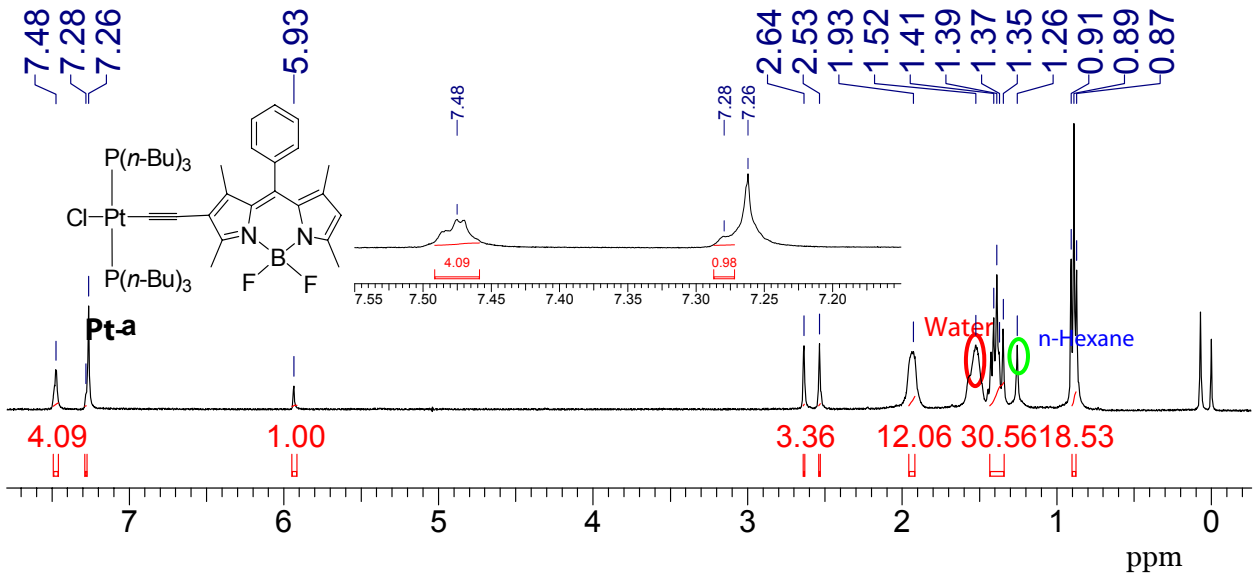


Fig. S4 ^{1}H NMR (400 MHz, $CDCl_3$) of complex **Pt-a**.

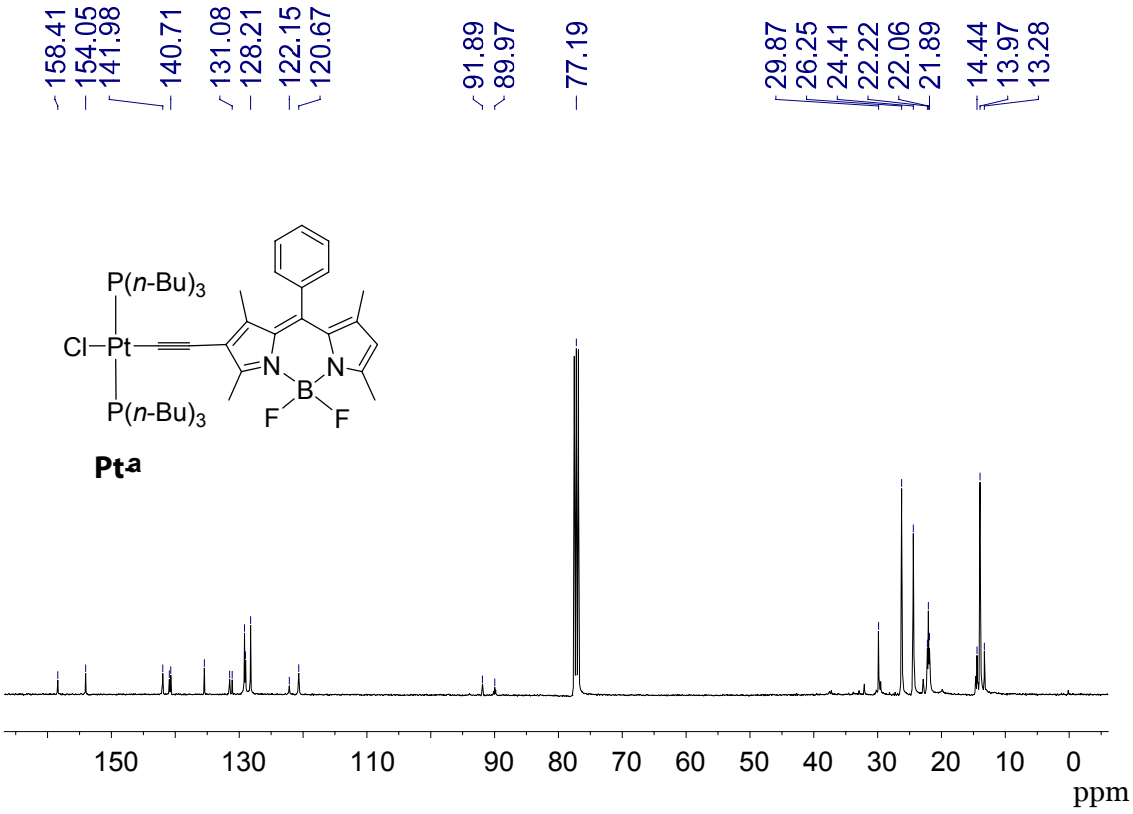


Fig. S5 ^{13}C NMR (100 MHz, $CDCl_3$) of **Pt-a.**

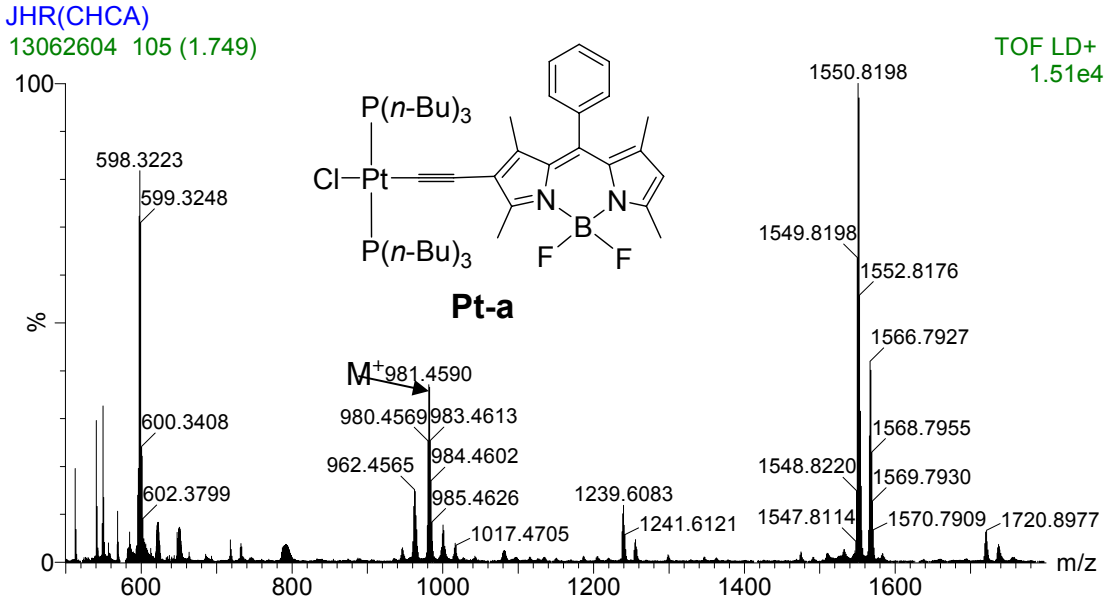


Fig. S6 MALDI-HRMS of **Pt-a.**

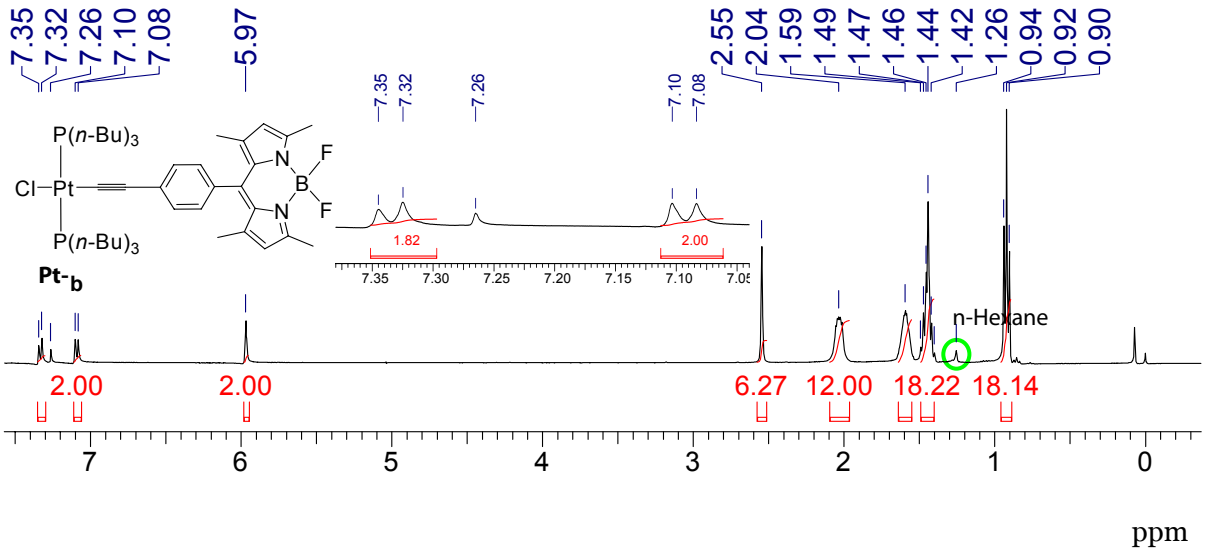


Fig. S7 ^{1}H NMR (400 MHz, $CDCl_3$) of complex **Pt-b**.

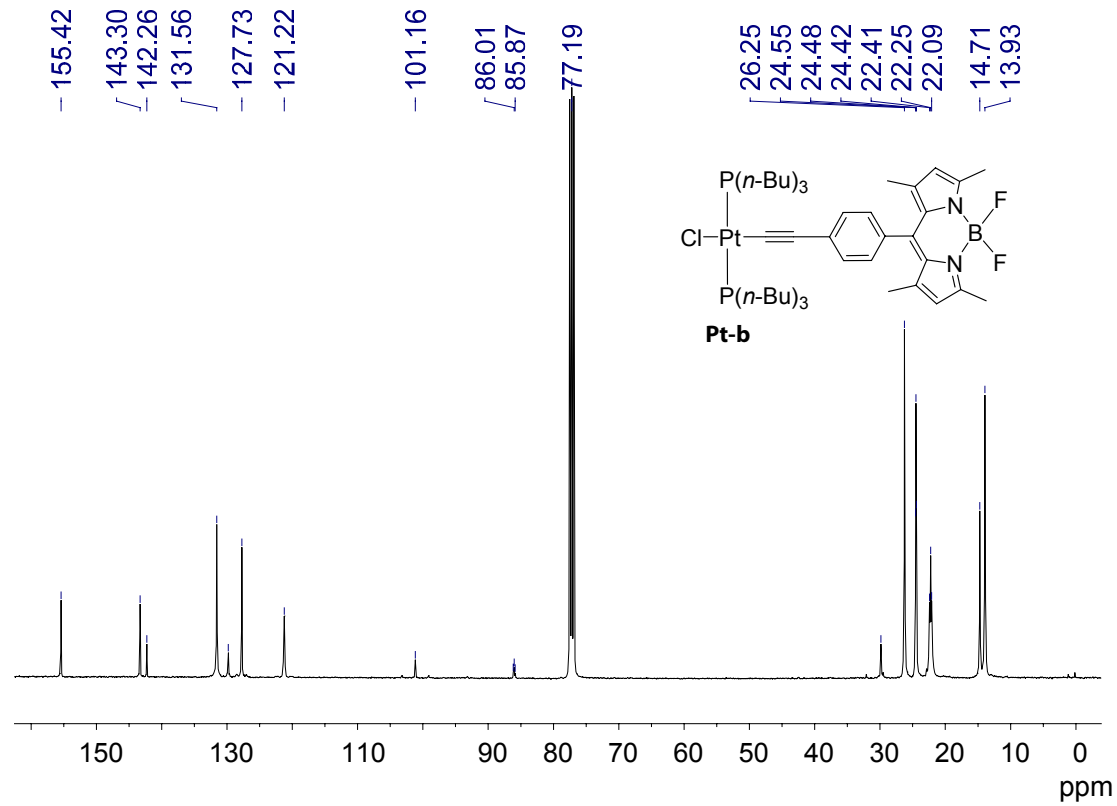


Fig. S8 ^{13}C NMR (100 MHz, $CDCl_3$) of **Pt-b**.

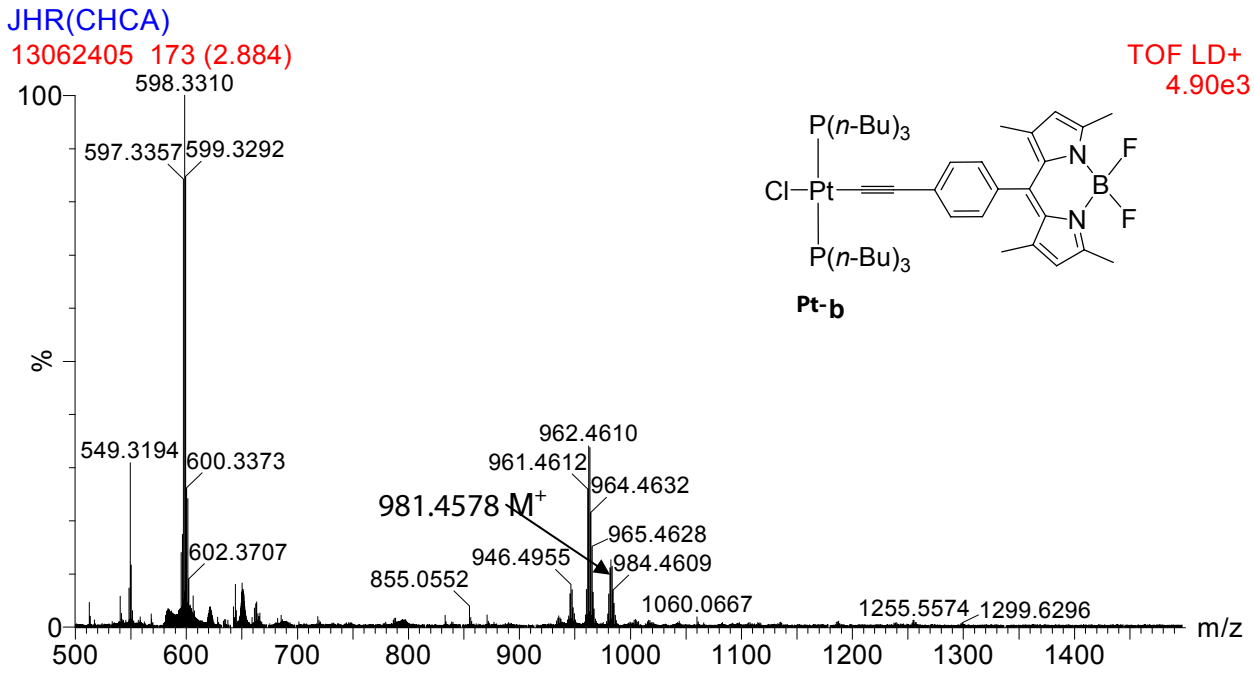


Fig. S9 MALDI-HRMS of **Pt-b**.

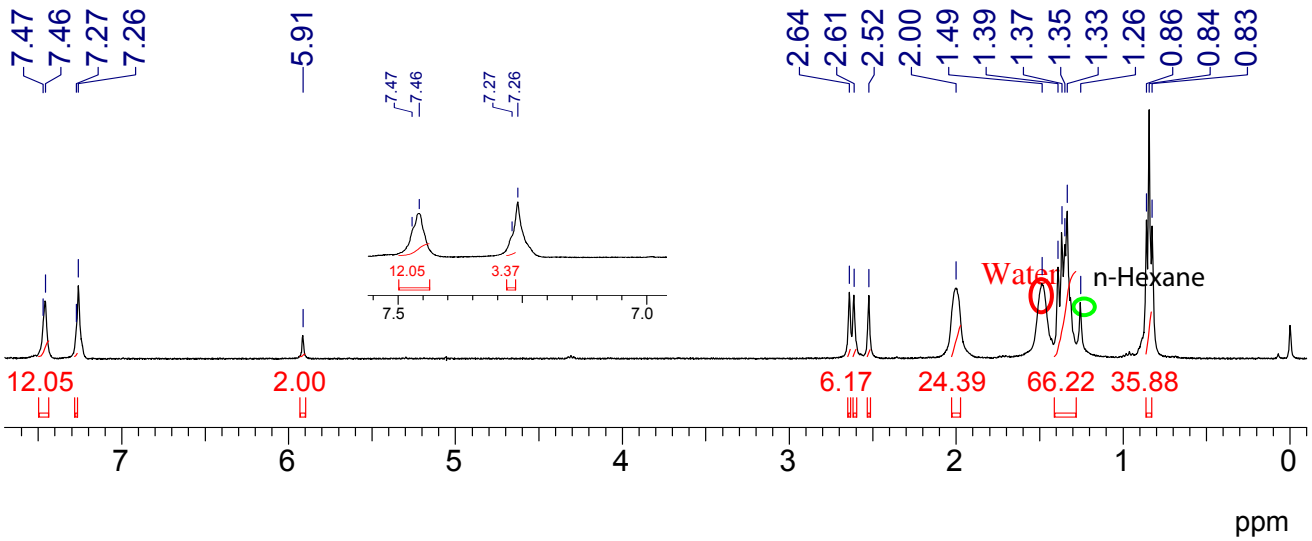
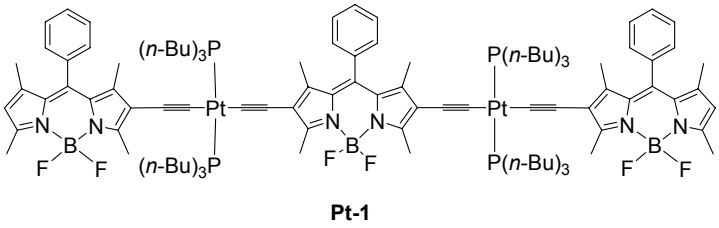


Fig. S10 ^{1}H NMR (400 MHz, $CDCl_3$) of **Pt-1**.



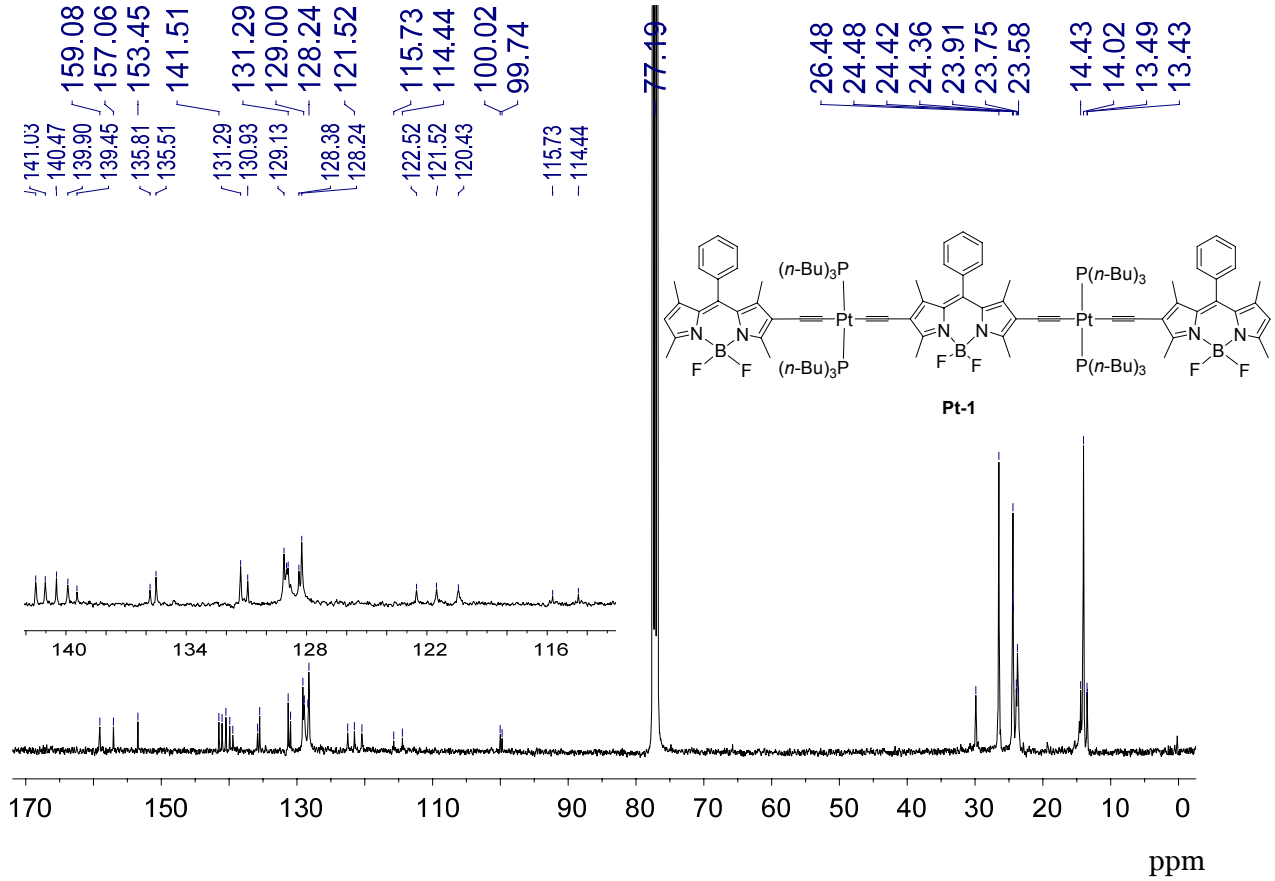


Fig. S11 ^{13}C NMR (100 MHz, $CDCl_3$) of **Pt-1**.

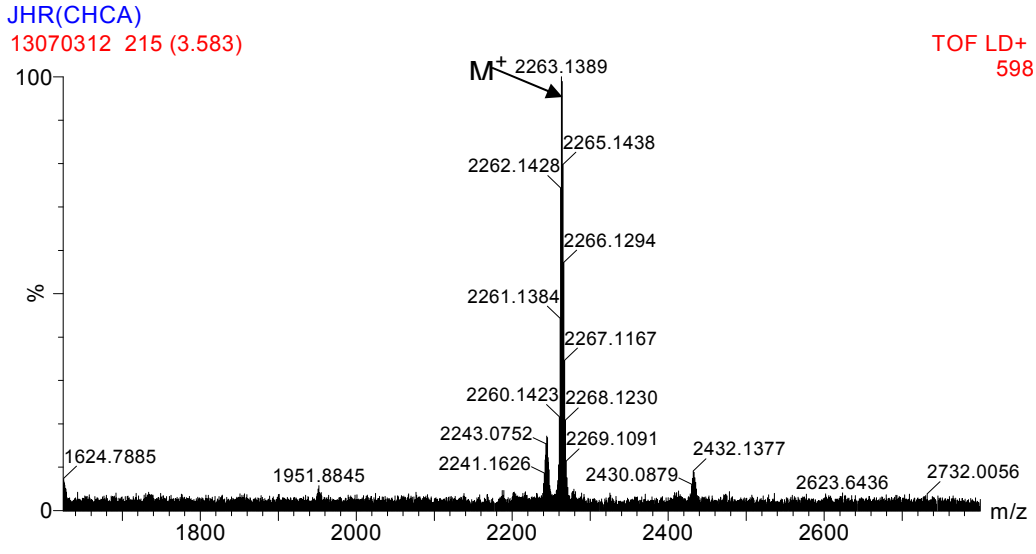


Fig. S12 MALDI-HRMS of **Pt-1**.

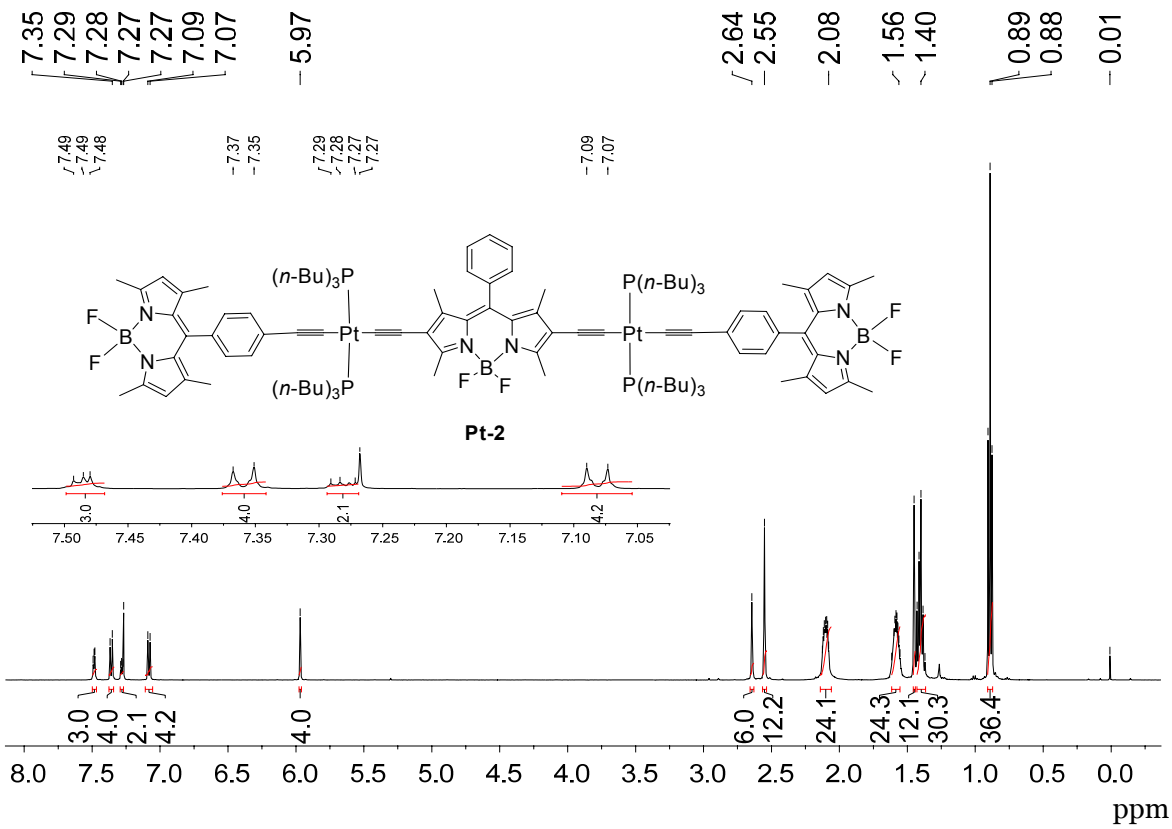


Fig. S13 ^{1}H NMR (500 MHz, $CDCl_3$) of **Pt-2**.

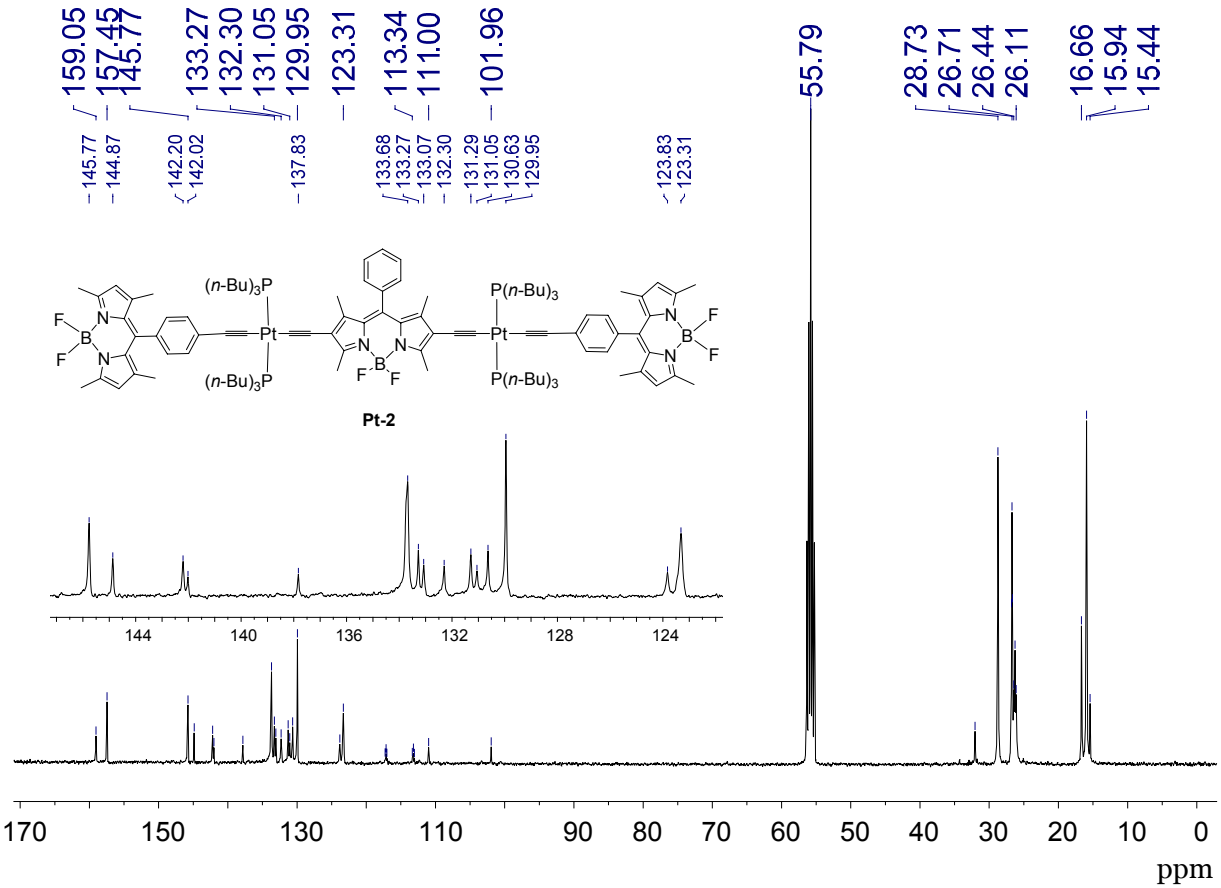


Fig. S14 ^{13}C NMR (100 MHz, $CDCl_3$) of **Pt-2**.

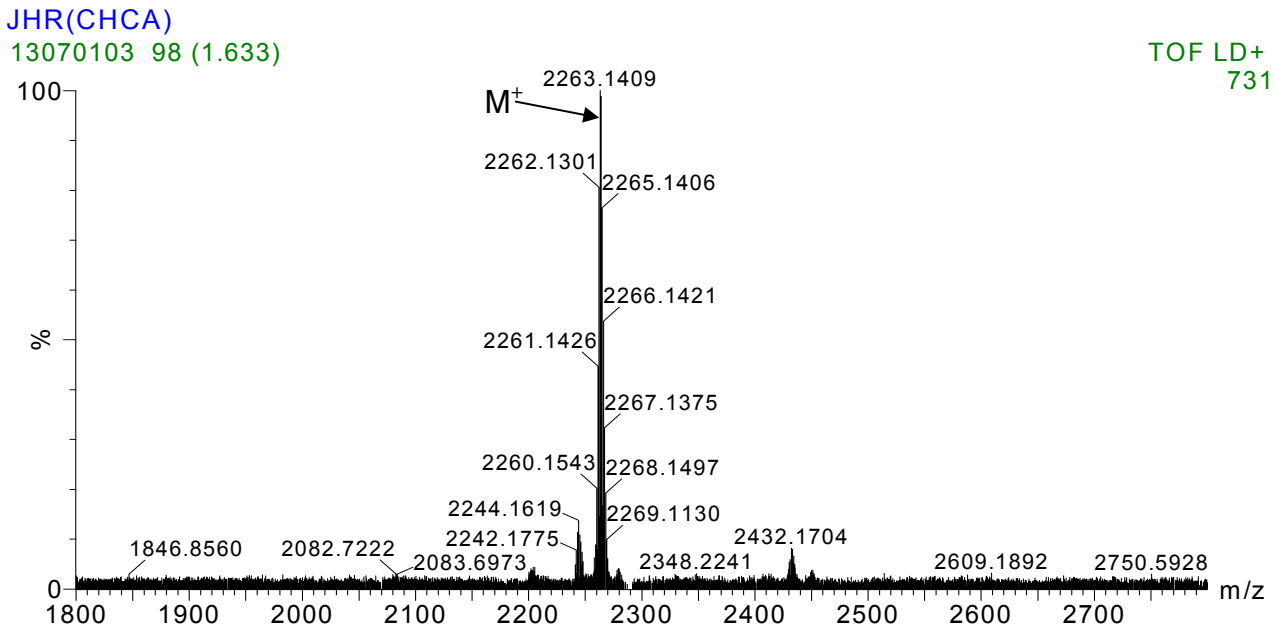
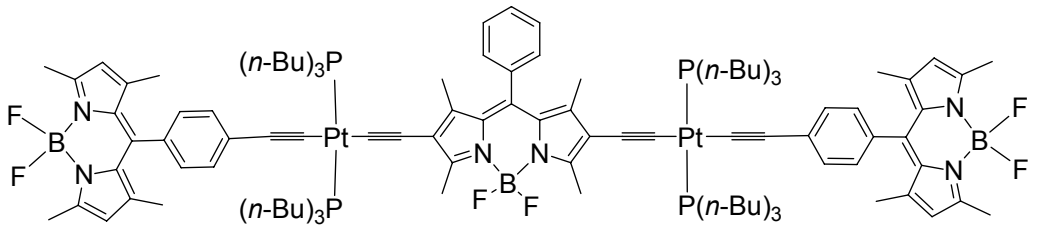


Fig. S 15 MALDI-HRMS of **Pt-2**.



Pt-2

3.0 Crystallographic data.

Table S1. Summary of unit cell, space group, data collection and structure refinement parameters for **Pt-b**.

Compound	**Pt-b**
Empirical formula	$C_{45}H_{72}BClF_2N_2P_2Pt$
Formula weight	982.33
Temperature (K)	173 K
Wavelength (Å)	0.71073
Volume	4964.0(9)
Space group	P21/c
a (Å)	10.0654(11)
b (Å)	36.749(4)
c (Å)	13.9440(15)
(°)	90
(°)	105.757(2)
(°)	90
Dx, g cm^{-3}	1.314
	4
Mu (mm^{-1})	2.982
Data completeness	0.994
Theta(max)	27.610
R(reflections)	0.0635(6050)
*w*R2(reflections)	0.1551(11457)

4.0 Nanosecond and Femtosecond Time-resolved Transient difference absorption spectra

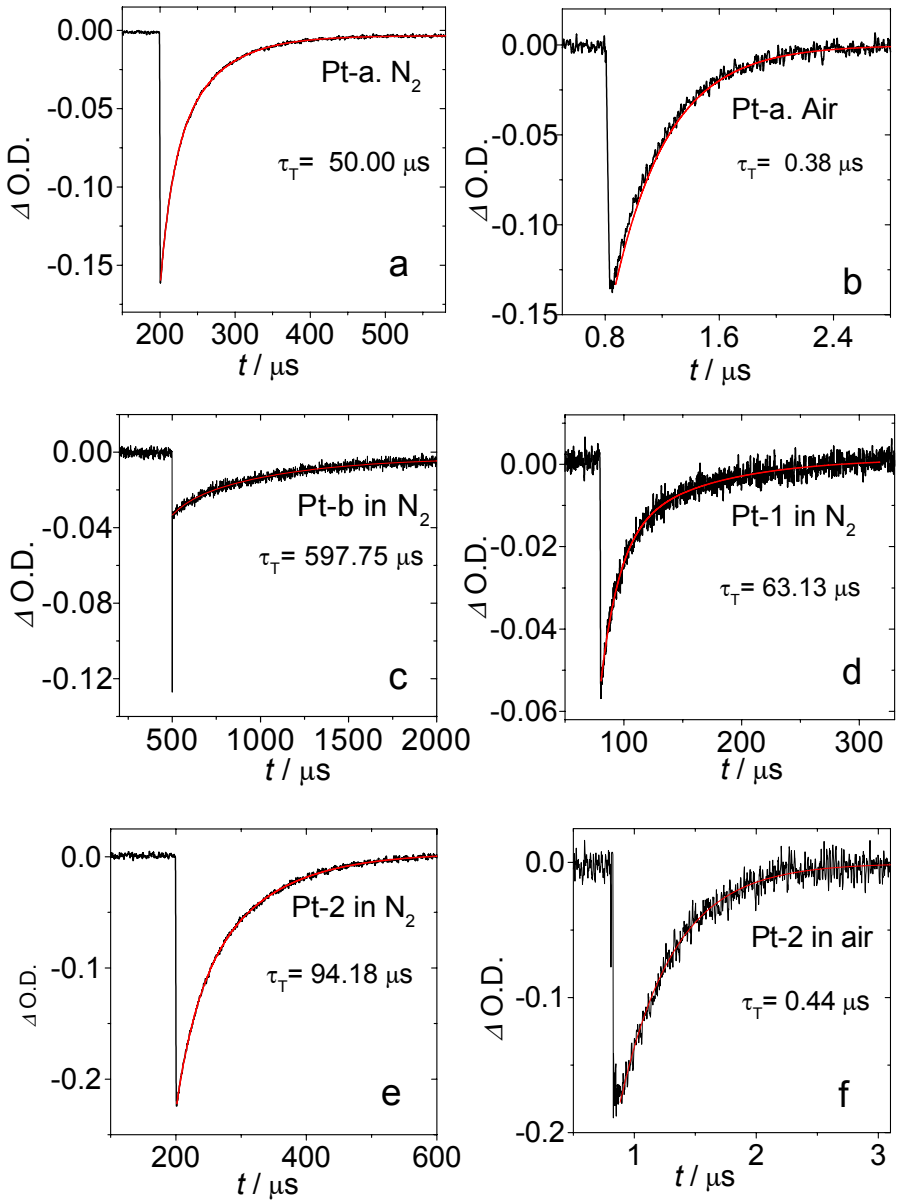


Fig. S16 Triplet excited state decay traces of (a, b) **Pt-a** (584 nm); (c) **Pt-b** (504 nm), (d) **Pt-1** (644 nm) and (e, f) **Pt-2** (640 nm) under different atmosphere (annotated in the figures). c = 1.0 ×10^{-5} M in toluene at 20 °C.

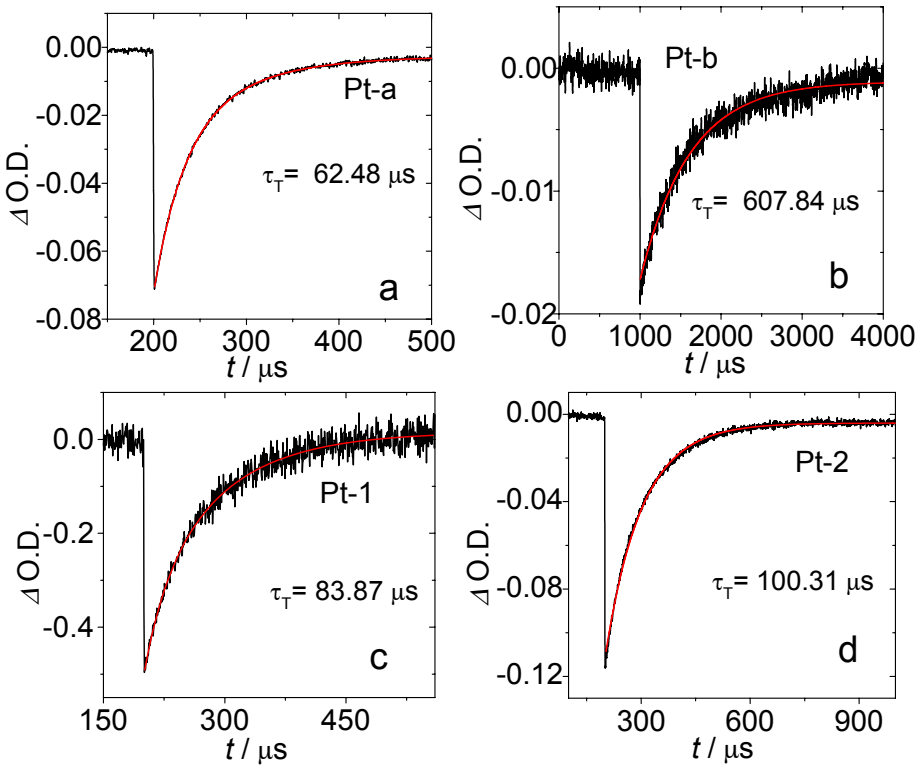


Fig. S17 Triplet excited state decay traces of (a) **Pt-a** (584 nm), (b) **Pt-b** (504 nm), (c) **Pt-1** (644 nm), (d) **Pt-2** (640 nm). c = 5.0 ×10^{-6} M in deaerated toluene at 20 °C.

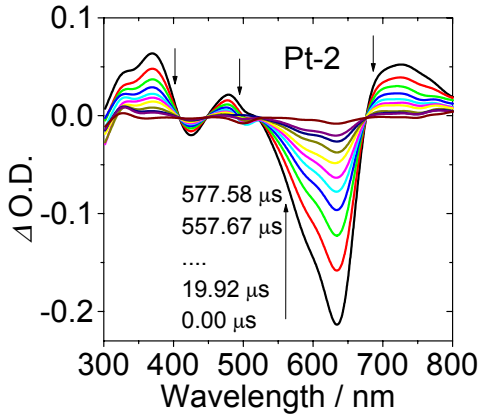


Fig. S18 Nanosecond time-resolved transient difference absorption spectra of complex **Pt-2**, after nanosecond pulsed laser excitation (λ_{ex}=503 nm). c = 1.0 ×10^{-5} M in deaerated toluene, 20 °C.

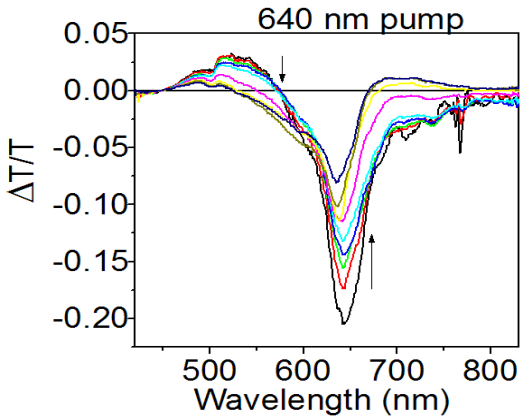


Fig. S19 Picosecond ultrafast transient difference absorption spectra of **Pt-2** upon femtosecond pulsed laser excitation at 640 nm. c = 1.0 ×10^{-5} M in toluene at 20 °C.

5.0 TTA upconversion details

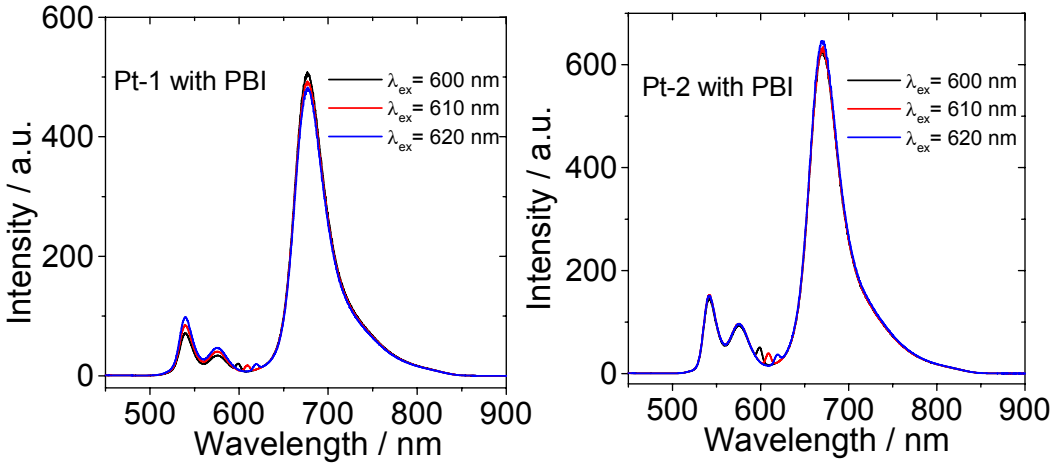


Fig. S20 Upconversions with (a) **Pt-1** and (b) **Pt-2** upon excitation with the light of a spectrofluorometer (RF5301 PC, Shimadzu, Japan). Excitation wavelength λ_{ex} = 600 nm, 610 nm, 620 nm, c [sensitizers] = 1.0×10^{-5} M , for **Pt-1**, c [PBI] = 2.6×10^{-5} M; for **Pt-2**, c [PBI] = 4.0×10^{-5} M, in deaerated toluene. 20 °C.

6.0 Time-resolved emission spectra (TRES) of Pt-a and Pt-b

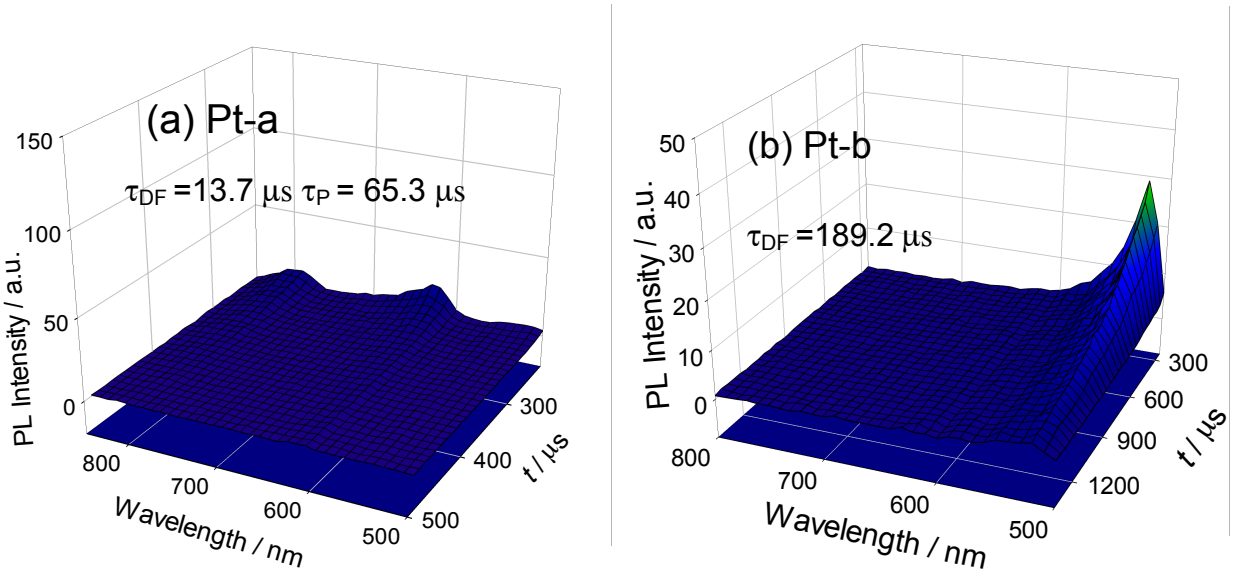


Fig. S21 TRES of **Pt-a**, **Pt-b** alone. (a) **Pt-a**, the fluorescence and phosphorescence region was measured (500 nm – 850 nm), τ_{DF} = 13.7 μs monitored at 627 nm; τ_P = 65.3 μs monitored at 805 nm. (b) **Pt-b**, the fluorescence region was measured (500 nm – 800 nm) , τ_{DF} = 189.2 μs monitored at 516 nm. c = 1.0 × 10^{-5} M. In deaerated toluene. Excited with nanosecond pulsed OPO laser synchronized with spectrofluorometer (for **Pt-a** λ_{ex} = 560 nm, for **Pt-b,** λ_{ex} = 503 nm), 25°C.

7.0 DFT calculations

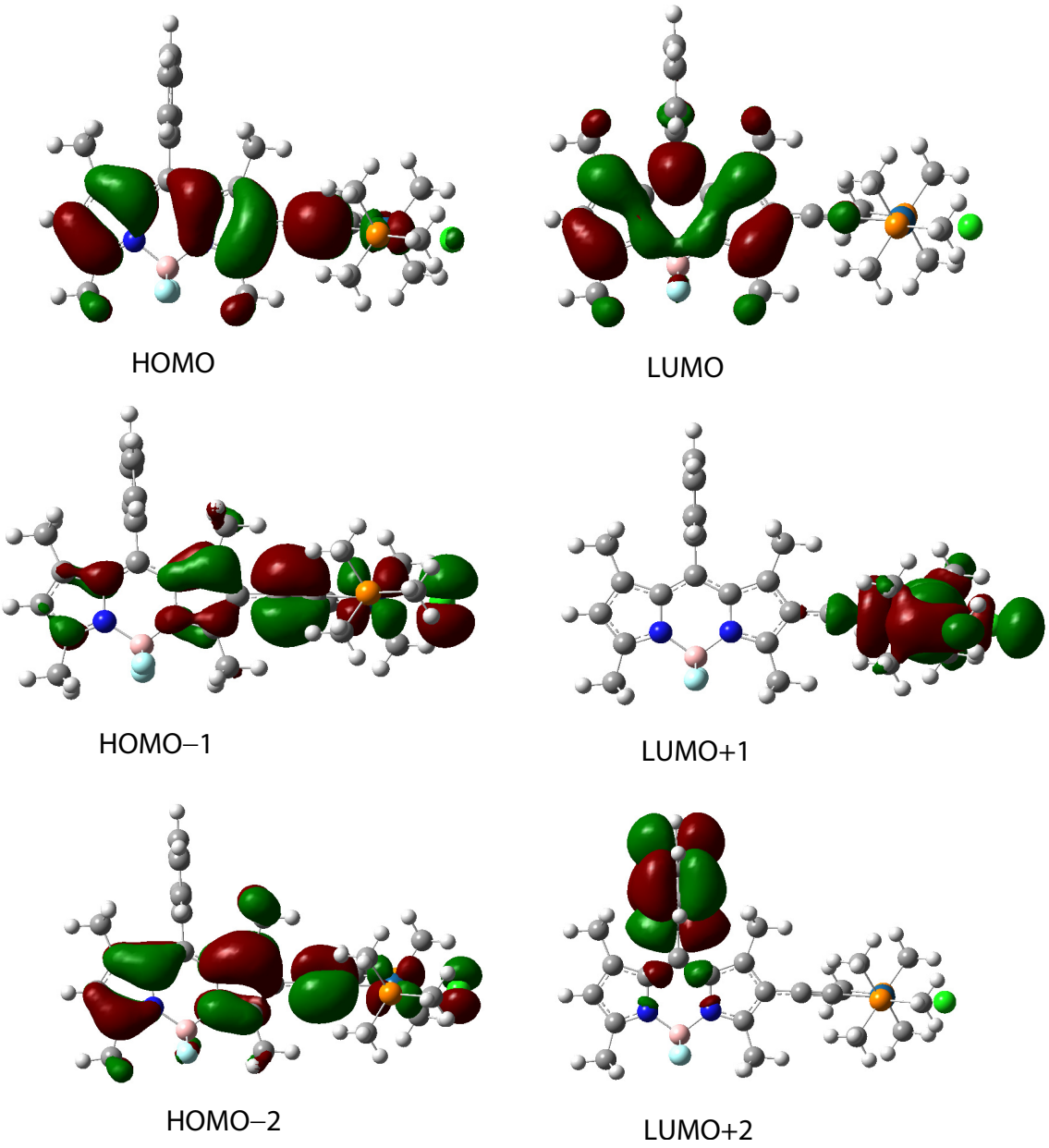


Fig. S22 Electron density maps of the frontier molecular orbitals of complex **Pt-a** based on the optimized ground state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/GENCP/LANL2DZ level with Gaussian 09W.

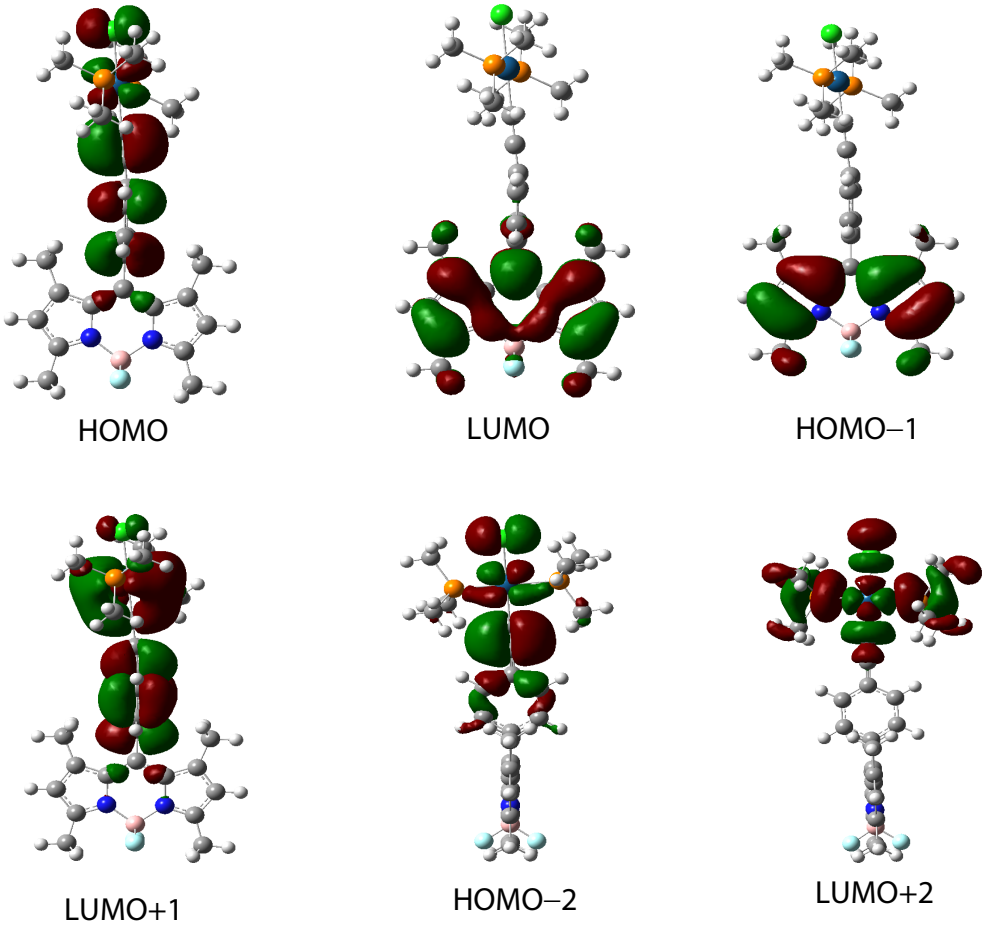
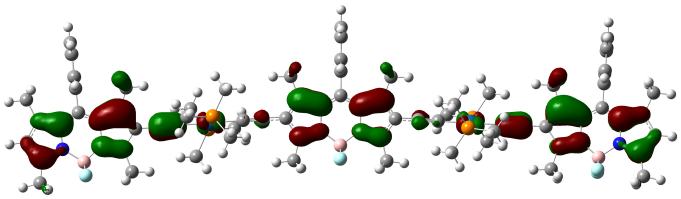


Fig. S23 Electron density maps of the frontier molecular orbitals of complex **Pt-b** based on the optimized ground state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/GENCP/LANL2DZ level with Gaussian 09W.



HOMO–6

Fig. S24 Electron density maps of the frontier molecular orbitals of complex **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 S2: Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-a**, 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	0.4575	H →L	0.68350	MLCT
	$S_0 \rightarrow S_3$	3.06 / 405	0.5386	H-2 →L	0.6273	MLCT
Triplet	$S_0 \rightarrow T_1$	1.42 / 867	0.6677	H →L	0.0000	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.

Table S3: Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-b**, Calculated by TDDFT//B3LYP/LANL2DZ, based on the DFT//B3LYP/LANL2DZ Optimized Ground State Geometries

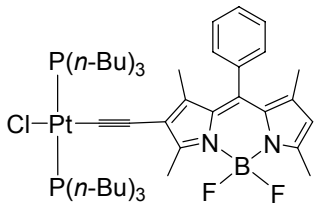
	TDDFT//B3LYP/ LANL2DZ					
	Electronic transition	Energy [eV/nm] [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	2.26 / 548	0.0009	H →L	0.70296	MLCT
	$S_0 \rightarrow S_2$	2.80 / 442	0.5662	H-1 →L	0.69631	ILCT
	$S_0 \rightarrow S_6$	3.61 / 342	1.0131	H →L+1	0.68115	ILCT
Triplet	$S_0 \rightarrow T_1$	1.53 / 809	0.0000	H →L	0.71025	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.

Optimized ground state geometry of Pt-a

0 1

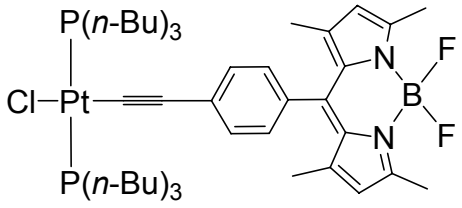
C	2.75414	9.89495	-11.42985
P	0.6833	10.54654	-9.07646
C	-0.0519	12.19226	-8.75219
H	-0.12324	12.3637	-7.66857
H	-1.04555	12.22832	-9.19294
H	0.56765	12.96851	-9.1959
C	-0.33914	9.36561	-8.11622
H	0.09851	8.37027	-8.16805
H	-1.33985	9.34057	-8.5394
H	-0.38963	9.68161	-7.06425
C	2.30514	10.57203	-8.21397
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



Pt-a

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

Optimized ground state geometry of Pt-b



Pt-b

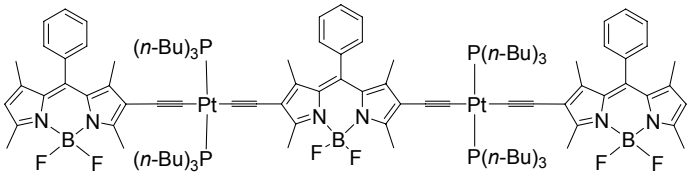
0 1

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

Optimized ground state geometry of Pt-1

0	1		
C	-4.84175	-0.21047	0.04298
C	-6.06742	-0.30014	0.0438
C	-10.09315	-0.64532	-0.00463
Pt	-8.0823	-0.47139	0.02119
P	-7.91367	-0.73491	-2.31114
C	-7.16563	0.72549	-3.14378
H	-7.03472	0.53954	-4.21525
H	-6.19653	0.93284	-2.68306
H	-7.81326	1.59646	-3.00525
C	-6.83072	-2.13883	-2.80204
H	-7.26421	-3.07663	-2.44168
H	-5.85181	-2.00473	-2.33532
H	-6.72052	-2.18669	-3.89074
C	-9.47118	-1.03012	-3.24369
H	-9.94071	-1.94945	-2.8839
H	-10.1648	-0.20417	-3.06753
H	-9.26684	-1.11831	-4.31606
P	-8.23693	-0.2035	2.35298
C	-9.01045	-1.64573	3.19409
H	-9.13335	-1.45355	4.26545
H	-8.37981	-2.52919	3.05654
H	-9.98499	-1.83797	2.73809
C	-6.66981	0.06542	3.2759
H	-6.17926	0.96842	2.9037
H	-5.99609	-0.77795	3.10534
H	-6.86784	0.169	4.3481
C	-9.29151	1.22341	2.84126



Pt-1

H	-8.8346	2.1519	2.48575
H	-10.27025	1.1134	2.36741
H	-9.40785	1.27185	3.92933
C	2.50498	-1.16181	0.07994
C	2.52642	1.11513	-0.026
C	3.35594	-0.02017	0.02007
C	1.18014	0.63664	0.00358
C	-0.05579	1.30675	-0.02259
C	-1.27019	0.59902	0.01349
C	-2.63097	1.03526	-0.01272
C	-2.53794	-1.23916	0.10889
N	1.22129	-0.7641	0.06844
N	-1.26738	-0.8019	0.08723
B	-0.00853	-1.71124	0.13074
F	-0.00503	-2.57703	-0.96736
F	0.01292	-2.44832	1.3184
C	3.04102	2.5211	-0.09226
H	2.73316	3.03134	-1.01198
H	2.68237	3.13426	0.74152
H	4.1346	2.50379	-0.05952
C	-2.90376	-2.68317	0.19032
H	-3.99068	-2.78968	0.21218
H	-2.50084	-3.23385	-0.66677
H	-2.47502	-3.13974	1.08902
C	-3.19024	2.42344	-0.09173
H	-2.87394	2.94557	-1.00156
H	-4.28313	2.36935	-0.09007
H	-2.87563	3.04635	0.75282
C	2.91577	-2.59433	0.1494
H	2.47405	-3.16365	-0.67515
H	4.00449	-2.67046	0.10354
H	2.55884	-3.05396	1.07795
C	-0.07931	2.80084	-0.08271
C	-0.10247	3.55418	1.09928
C	-0.07883	3.4652	-1.31689
C	-0.1243	4.94943	1.04732
C	-0.10157	4.86077	-1.36733
H	-0.06112	2.88638	-2.23629
H	-0.14158	5.52235	1.97044
H	-0.10156	5.36455	-2.33007
C	-0.12411	5.60574	-0.18595
H	-0.14147	6.69134	-0.22601
H	-0.10294	3.04413	2.05869
C	-3.42424	-0.12489	0.04585
C	4.77544	-0.06087	0.0108
C	6.00339	-0.11111	0.00689
C	10.04012	-0.27809	-0.04907
Pt	8.02361	-0.19465	-0.02176
P	8.14459	-0.629	2.28758
C	9.08967	0.6589	3.20108
H	9.18674	0.39844	4.26058
H	8.57485	1.62017	3.11146
H	10.08069	0.75114	2.74937
C	6.55655	-0.75392	3.20443

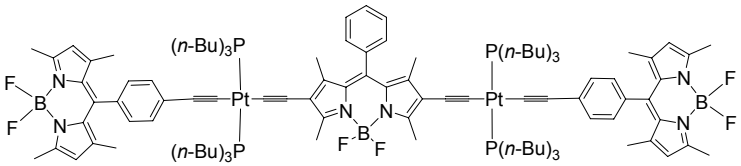
H	5.9563	-1.56511	2.78488
H	5.9948	0.17595	3.08594
H	6.7386	-0.94253	4.26776
C	9.0193	-2.19859	2.68421
H	8.45792	-3.04229	2.27171
H	10.00769	-2.1762	2.21809
H	9.122	-2.32878	3.76693
P	7.8886	0.23498	-2.33151
C	9.46893	0.32868	-3.2667
H	9.27928	0.52357	-4.32756
H	10.01035	-0.61464	-3.15847
H	10.09119	1.12592	-2.85216
C	6.9106	-1.03652	-3.23244
H	5.921	-1.10411	-2.77364
H	7.40499	-2.00831	-3.14095
H	6.81258	-0.77899	-4.29254
C	7.04136	1.82019	-2.72531
H	6.05463	1.81526	-2.25544
H	7.61976	2.65421	-2.31663
H	6.93571	1.95048	-3.80773
C	-11.31824	-0.7417	-0.01019
C	11.3471	-0.3366	-0.11598
C	18.70079	-2.32427	0.05264
C	19.02852	-0.01206	0.08421
C	17.58826	-0.31462	0.03727
C	16.42317	0.54182	0.01393
C	15.09245	-0.01064	-0.02494
C	13.76647	0.62232	-0.05308
C	13.55036	-1.70901	-0.07817
N	17.44023	-1.7456	0.01967
N	14.9024	-1.43986	-0.04227
B	16.06054	-2.54105	-0.03148
F	16.01107	-3.34259	-1.22582
F	15.94906	-3.38558	1.12709
C	19.77205	1.35307	0.12051
H	19.54662	1.97615	-0.79041
H	19.47141	1.96831	1.01477
H	20.88542	1.19357	0.16604
C	12.99463	-3.13432	-0.10873
H	11.87331	-3.09356	-0.1638
H	13.39322	-3.70331	-0.99527
H	13.30456	-3.70712	0.81076
C	13.40834	2.11744	-0.05075
H	13.85929	2.67123	-0.92199
H	12.28876	2.21535	-0.10885
H	13.75931	2.64288	0.88248
C	18.9432	-3.84909	0.04706
H	18.47036	-4.31635	-0.86236
H	20.04162	-4.08732	0.05374
H	18.45909	-4.32502	0.94611
C	16.63093	2.06879	0.02933
C	16.66393	2.78773	1.2782
C	16.77973	2.7965	-1.2061
C	16.84337	4.21253	1.29029

C	16.95831	4.22142	-1.19228
H	16.75481	2.24362	-2.17665
H	16.86762	4.75878	2.26464
H	17.07189	4.77476	-2.15638
C	16.99102	4.93223	0.05574
H	17.12992	6.04078	0.06586
H	16.54941	2.22805	2.23852
C	12.81665	-0.45019	-0.08432
C	19.72185	-1.27921	0.09285
H	20.82285	-1.44207	0.12553
C	-13.67912	-1.86832	-0.11489
C	-13.6259	0.46059	0.05276
C	-15.02092	-0.00719	-0.00363
C	-16.27907	0.70509	0.03111
C	-17.53576	0.00213	-0.03279
C	-18.92738	0.47411	-0.01522
C	-18.86743	-1.8609	-0.17821
N	-14.99943	-1.44212	-0.10578
N	-17.55619	-1.43605	-0.1343
B	-16.27626	-2.39102	-0.19617
F	-16.24635	-3.12142	-1.43593
F	-16.27239	-3.30925	0.91054
C	-13.04809	1.89968	0.16611
H	-13.35718	2.54397	-0.70463
H	-13.40757	2.42151	1.09728
H	-11.92318	1.8708	0.19543
C	-19.25159	-3.33775	-0.29053
H	-20.37051	-3.42695	-0.33643
H	-18.80021	-3.80258	-1.21182
H	-18.86441	-3.92269	0.59126
C	-19.45921	1.91356	0.07851
H	-19.08802	2.56696	-0.76076
H	-20.58319	1.88139	0.033
H	-19.16059	2.42128	1.03935
C	-13.25872	-3.35072	-0.21296
H	-13.68491	-3.81661	-1.14584
H	-12.13988	-3.45713	-0.22703
H	-13.67167	-3.9325	0.65892
C	-16.2526	2.24238	0.13645
C	-16.28843	2.88575	1.4258
C	-16.20664	3.05373	-1.05418
C	-16.27807	4.31859	1.5219
C	-16.19713	4.48649	-0.95635
H	-16.17877	2.55962	-2.05586
H	-16.30578	4.80583	2.52696
H	-16.16208	5.10493	-1.88634
C	-16.2323	5.12181	0.33167
H	-16.22494	6.2365	0.40715
H	-16.32371	2.26113	2.35165
C	-12.78795	-0.71383	-0.0184
C	-19.74445	-0.69967	-0.10482
H	-20.81241	-0.76252	-0.08451

Optimized ground state geometry of Pt-2

0 1

C	4.90307	0.02071	1.2759
C	5.9925	-0.18279	1.81718
C	9.55239	-0.85907	3.5861
Pt	7.77132	-0.51506	2.70099
P	6.69165	-0.20279	4.77169
C	5.95091	1.47246	4.94509
H	5.39914	1.55897	5.88731
H	5.27477	1.64848	4.10445
H	6.74325	2.2266	4.92072
C	5.27774	-1.35221	5.02563
H	5.64501	-2.38271	5.04348
H	4.58146	-1.24459	4.19006
H	4.76245	-1.13603	5.96766
C	7.71216	-0.40504	6.28703
H	8.11527	-1.42045	6.32085
H	8.55429	0.29071	6.25635
H	7.1103	-0.21853	7.1828
P	8.86747	-0.82474	0.63879
C	9.61428	-2.497	0.46761
H	10.171	-2.58064	-0.47194
H	8.82451	-3.25392	0.48749
H	10.28637	-2.66969	1.31203
C	7.85678	-0.62232	-0.88365
H	7.44582	0.39008	-0.91537
H	7.02059	-1.32585	-0.86409
H	8.46616	-0.79903	-1.7763
C	10.27902	0.32997	0.39773
H	9.90773	1.35888	0.37283
H	10.96496	0.2263	1.24224
H	10.8058	0.11345	-0.53785
C	-2.17243	0.09885	-1.95549
C	-1.75096	2.34458	-2.18446
C	-2.71146	1.34054	-2.42937
C	-0.62761	1.69347	-1.5941
C	0.60126	2.21205	-1.09637
C	1.5491	1.32641	-0.51156
C	2.84085	1.56551	0.04463
C	2.31363	-0.66372	0.20508
N	-0.91469	0.31801	-1.50351
N	1.26985	-0.04731	-0.39921
B	-0.0282	-0.75834	-0.83783
F	-0.65702	-1.37021	0.259
F	0.26498	-1.73853	-1.79983
C	-1.94888	3.79484	-2.51322
H	-1.92393	4.4347	-1.62314
H	-1.18224	4.17889	-3.19561
H	-2.92387	3.92354	-2.99474
C	2.34742	-2.1229	0.49502
H	3.29205	-2.3871	0.97646
H	1.51312	-2.40887	1.14657
H	2.23355	-2.7039	-0.42789
C	3.6019	2.85201	0.17281



Pt-2

H	3.0673	3.5975	0.77285
H	4.56273	2.65317	0.65891
H	3.80437	3.31899	-0.79796
C	-2.82792	-1.23702	-1.93851
H	-2.85243	-1.64353	-0.92079
H	-3.84708	-1.15893	-2.32462
H	-2.26253	-1.95435	-2.54573
C	0.9164	3.66658	-1.23677
C	1.58025	4.14951	-2.37566
C	0.55774	4.58332	-0.23593
C	1.87761	5.50762	-2.51179
C	0.8534	5.94228	-0.36835
H	0.0438	4.22332	0.65156
H	2.39194	5.86152	-3.40162
H	0.56777	6.63625	0.41807
C	1.5145	6.40822	-1.50738
H	1.74505	7.46519	-1.61142
H	1.86326	3.45062	-3.15849
C	3.32122	0.31618	0.48995
C	-4.32689	1.61677	-3.16842
C	-5.43526	1.80629	-3.6755
C	-9.05778	2.42573	-5.3328
Pt	-7.24439	2.11565	-4.50318
P	-6.58496	1.20666	-6.57466
C	-6.74178	2.41287	-7.95458
H	-6.49006	1.94672	-8.91324
H	-6.0707	3.25857	-7.7771
H	-7.77014	2.7822	-7.98054
C	-4.85885	0.58914	-6.70725
H	-4.69731	-0.20446	-5.97326
H	-4.16326	1.40219	-6.48421
H	-4.66366	0.20385	-7.7136
C	-7.6204	-0.22086	-7.09783
H	-7.50329	-1.03884	-6.38071
H	-8.66793	0.09099	-7.105
H	-7.33056	-0.57061	-8.09453
P	-7.92243	3.02927	-2.43932
C	-9.65396	3.63293	-2.31962
H	-9.85335	4.03301	-1.31989
H	-10.3413	2.80963	-2.52987
H	-9.82211	4.4112	-3.0682
C	-7.76317	1.83344	-1.05025
H	-6.73055	1.47729	-1.0092
H	-8.42064	0.97754	-1.2297
H	-8.03136	2.30169	-0.09709
C	-6.90292	4.46919	-1.91729
H	-5.85179	4.16971	-1.90107
H	-7.02349	5.28261	-2.63901
H	-7.20221	4.82122	-0.92418
C	-10.16186	2.61452	-5.83791
C	10.63659	-1.06848	4.1249
C	17.93401	0.14024	8.77974
C	15.96895	0.52987	7.65719
C	16.32811	-0.8465	7.55243

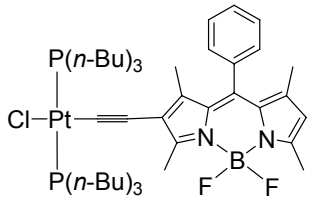
C	15.68747	-1.93567	6.89805
C	16.27521	-3.23027	6.95515
C	15.86259	-4.47577	6.39513
C	17.82207	-4.74625	7.56152
N	17.53301	-1.04054	8.25136
N	17.47538	-3.4404	7.65726
B	18.29242	-2.37409	8.41736
F	19.58421	-2.27176	7.87547
F	18.39414	-2.71207	9.77663
C	14.77863	1.25054	7.09659
H	14.75108	1.22731	6.00069
H	13.82956	0.82527	7.442
H	14.8129	2.29868	7.41166
C	19.04125	-5.3189	8.19402
H	19.10307	-6.38979	7.98596
H	19.94359	-4.82148	7.81893
H	19.02667	-5.15846	9.27862
C	14.65941	-4.79402	5.55741
H	14.63648	-4.22256	4.62225
H	14.67174	-5.85882	5.30231
H	13.71774	-4.58165	6.07665
C	19.17295	0.29701	9.589
H	20.05042	-0.03539	9.02228
H	19.30088	1.34265	9.8791
H	19.12995	-0.32793	10.48931
C	14.40177	-1.72382	6.16539
C	13.16783	-1.94629	6.80172
C	14.39449	-1.35608	4.81061
C	12.0246	-1.69846	6.13503
C	13.12843	-1.11859	4.03137
H	15.3412	-1.22546	4.29287
H	11.10668	-1.7953	6.70918
H	13.04969	-0.82982	2.98635
C	11.97355	-1.32672	4.78931
H	13.15937	-2.22789	7.85148
C	-17.95005	1.60049	-9.07061
C	-15.94176	1.13134	-8.06065
C	-15.99784	2.50996	-8.42209
C	-15.05365	3.56177	-8.25741
C	-15.37454	4.8691	-8.7185
C	-14.62902	6.08507	-8.69135
C	-16.67551	6.43664	-9.67189
N	-17.23992	2.75318	-9.0353
N	-16.61597	5.12841	-9.32606
B	-17.74505	4.1068	-9.57861
F	-18.01743	4.01088	-10.95318
F	-18.91623	4.49554	-8.90824
C	-14.84428	0.36723	-7.38082
H	-13.91815	0.35036	-7.96757
H	-14.58601	0.78559	-6.40144
H	-15.16801	-0.66797	-7.23047
C	-17.85481	7.05604	-10.3352
H	-17.6724	8.11975	-10.50596
H	-18.06543	6.56359	-11.29201

H	-18.75378	6.93456	-9.71926
C	-13.25159	6.34875	-8.15852
H	-12.48593	5.74358	-8.65767
H	-13.00288	7.40368	-8.3143
H	-13.16798	6.13642	-7.08643
C	-19.31709	1.49786	-9.64954
H	-19.32066	1.82711	-10.6951
H	-19.67204	0.46614	-9.59092
H	-20.01498	2.15388	-9.11517
C	-13.73938	3.29792	-7.59576
C	-13.61045	3.37717	-6.1944
C	-12.63608	2.8407	-8.33605
C	-12.36315	3.21678	-5.58618
C	-11.39791	2.63579	-7.7223
H	-12.73785	2.71058	-9.41034
H	-12.25096	3.41458	-4.52322
H	-10.539	2.34626	-8.32238
C	-11.26344	2.80289	-6.34189
H	-14.4648	3.69885	-5.60451
C	-17.16592	0.5611	-8.46919
H	-17.4462	-0.4642	-8.34634
C	-15.44557	7.06741	-9.28981
H	-15.18215	8.09527	-9.42768
C	16.8335	-5.42574	6.77563
H	16.82224	-6.46403	6.51731
C	16.97751	1.14856	8.42574
H	17.01068	2.18494	8.6898

Optimized triplet state geometry of Pt-a

o 3

C	1.90253	-0.07808	-0.03096
P	3.91845	0.41903	-2.36408
C	4.6862	2.01973	-2.84505
H	4.77204	2.09804	-3.93429
H	5.67755	2.08349	-2.38928
H	4.07359	2.84531	-2.4705
C	4.92241	-0.85424	-3.23277
H	4.4621	-1.83689	-3.09272
H	5.92348	-0.8708	-2.79469
H	4.98805	-0.63467	-4.30395
C	2.3081	0.40319	-3.25046
H	1.8164	-0.56064	-3.09614
H	1.65818	1.18198	-2.84357
H	2.45883	0.57126	-4.32206
P	3.76891	-0.22558	2.30827
C	3.03453	-1.84409	2.7823
H	2.93938	-1.92701	3.87027
H	3.66944	-2.65491	2.41283
H	2.04903	-1.93213	2.31798
C	5.36155	-0.16215	3.22373
H	5.83466	0.81045	3.06767
H	6.03663	-0.93	2.83858
H	5.19043	-0.32216	4.29372



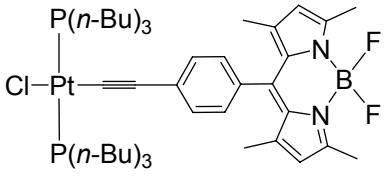
Pt-a

C	2.70959	1.01779	3.15484
H	3.1398	2.01449	3.0179
H	1.7167	1.00074	2.69815
H	2.62973	0.80245	4.22573
C	0.68048	-0.187	-0.03342
C	-1.44428	-1.54651	-0.13041
C	-1.68952	0.71397	0.04691
C	-0.73395	-0.31307	-0.03626
C	-2.97072	0.07968	0.00454
C	-4.27556	0.59665	0.05016
C	-5.39644	-0.25159	-0.01047
C	-6.80433	0.01991	0.02185
C	-6.44939	-2.21904	-0.15503
N	-2.76456	-1.30436	-0.10417
N	-5.23087	-1.63841	-0.11954
B	-3.87569	-2.39018	-0.18892
F	-3.77182	-3.08818	-1.39607
F	-3.75831	-3.27679	0.88543
C	-1.34497	2.16821	0.15549
H	-1.77064	2.75619	-0.66474
H	-1.71585	2.61265	1.08587
H	-0.25699	2.28171	0.13214
C	-6.63933	-3.69715	-0.26785
H	-7.70356	-3.94519	-0.28239
H	-6.17038	-4.07952	-1.18098
H	-6.16318	-4.21411	0.57231
C	-7.52449	1.33241	0.12938
H	-7.29198	2.00048	-0.70684
H	-8.60527	1.15988	0.13406
H	-7.26377	1.87361	1.04519
C	-0.86568	-2.91694	-0.24411
H	-1.23322	-3.41636	-1.14678
H	0.22457	-2.85852	-0.2783
H	-1.17026	-3.53709	0.60626
C	-4.47906	2.07357	0.16697
C	-4.56915	2.67862	1.42813
C	-4.58483	2.86819	-0.98305
C	-4.76201	4.05742	1.53678
C	-4.77704	4.247	-0.87246
H	-4.51559	2.40384	-1.96293
H	-4.83084	4.51549	2.51963
H	-4.85695	4.85298	-1.77077
C	-4.86622	4.84429	0.38719
H	-5.01602	5.91695	0.47257
H	-4.4887	2.06662	2.32229
Cl	6.12978	0.29868	-0.02244
Pt	3.85878	0.09627	-0.02702
C	-7.43563	-1.21788	-0.06951
H	-8.50392	-1.39324	-0.0745

Optimized triplet state geometry of Pt-b

o 3

C	2.50952	0.00691	0.00567



Pt-b

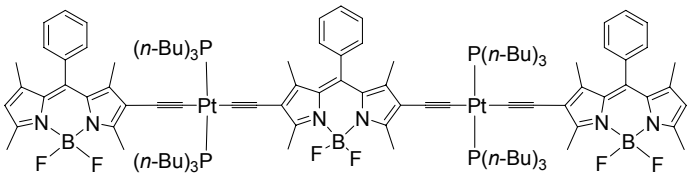
Pt	4.47032	-0.0133	-0.0133
P	4.31963	-1.67937	-1.67782
C	3.40876	-1.11108	-3.17157
H	3.28484	-1.92813	-3.89027
H	3.96261	-0.2947	-3.64468
H	2.42942	-0.73551	-2.86423
C	5.89888	-2.34931	-2.33516
H	6.47816	-2.78649	-1.51829
H	6.48788	-1.53734	-2.76836
H	5.70034	-3.11058	-3.09725
C	3.39364	-3.16565	-1.11414
H	3.93777	-3.64092	-0.29249
H	2.4134	-2.85103	-0.74707
H	3.27157	-3.88508	-1.93083
P	4.60796	1.65341	1.65284
C	3.02528	2.31382	2.31434
H	3.21598	3.07694	3.07621
H	2.44417	1.49758	2.75126
H	2.44193	2.74853	1.49856
C	5.52069	1.08705	3.14551
H	6.50087	0.71633	2.83562
H	4.96963	0.26897	3.61893
H	5.64124	1.90592	3.86291
C	5.51941	3.14661	1.0859
H	6.49948	2.83728	0.71442
H	4.96746	3.61983	0.26832
H	5.6402	3.86395	1.90478
C	1.28276	0.00091	-0.00089
C	-6.98304	-1.9362	1.62229
C	-4.70983	-1.98386	1.65018
C	-5.16859	-0.93045	0.79019
C	-4.47571	0.01373	0.01347
C	-5.16797	0.96134	-0.75963
C	-4.70853	2.01274	-1.62171
C	-6.98177	1.97614	-1.58212
N	-6.56989	-0.94322	0.80784
N	-6.56926	0.98098	-0.76999
B	-7.49925	0.02077	0.02086
F	-8.30646	-0.70338	-0.86237
F	-8.29989	0.74816	0.90741
C	-3.30788	-2.4013	1.98574
H	-2.7403	-2.69304	1.0958
H	-2.742	-1.59723	2.46864
H	-3.33157	-3.25597	2.66899
C	-8.42503	2.28184	-1.82062
H	-8.52873	3.09396	-2.54439
H	-8.9506	1.39708	-2.19477
H	-8.91912	2.57168	-0.88659
C	-3.30631	2.42338	-1.96454
H	-2.74753	1.61709	-2.45204
H	-3.32938	3.27925	-2.64629
H	-2.73205	2.71058	-1.07744
C	-8.42653	-2.235	1.86807
H	-8.92645	-2.52333	0.93667

H	-8.53048	-3.04607	2.59298
H	-8.94619	-1.34752	2.24398
C	-2.98158	0.01018	0.00969
C	-2.2624	0.77796	0.93682
C	-2.27082	-0.76099	-0.92109
C	-0.87025	0.77654	0.93452
C	-0.8787	-0.76591	-0.92575
H	-2.81421	-1.36138	-1.64576
H	-0.32844	1.37672	1.65906
H	-0.3434	-1.36883	-1.65316
C	-0.14429	0.00368	0.00244
H	-2.7993	1.38089	1.66423
Cl	6.93154	-0.02967	-0.02928
C	-5.8551	-2.59236	2.15432
H	-5.88726	-3.4297	2.8398
C	-5.8534	2.62693	-2.11981
H	-5.885	3.46463	-2.80487

Optimized triplet state geometry of Pt-1

o 3

C	-4.81501	-0.21494	0.00301
C	-6.03098	-0.29468	0.01218
C	-10.08621	-0.50106	0.02474
Pt	-8.0533	-0.41344	0.02011
P	-7.93503	-0.75673	-2.30459
C	-7.12781	0.64083	-3.18869
H	-7.02572	0.42276	-4.25731
H	-6.14161	0.80825	-2.74819
H	-7.72685	1.54747	-3.06057
C	-6.92293	-2.223	-2.76427
H	-7.39028	-3.12862	-2.36606
H	-5.93097	-2.11633	-2.31827
H	-6.83423	-2.31134	-3.85255
C	-9.51604	-1.00512	-3.20894
H	-10.03542	-1.87761	-2.80461
H	-10.15976	-0.1337	-3.06586
H	-9.32681	-1.15289	-4.27756
P	-8.1678	-0.08989	2.34728
C	-9.01093	-1.47817	3.21244
H	-9.10706	-1.27258	4.28408
H	-8.43523	-2.39792	3.07142
H	-10.00114	-1.61501	2.77031
C	-6.58172	0.10677	3.25535
H	-6.03445	0.96315	2.85362
H	-5.96511	-0.7839	3.11077
H	-6.76803	0.25601	4.32428
C	-9.14289	1.3954	2.82684
H	-8.64914	2.2951	2.44739
H	-10.13495	1.3234	2.37416
H	-9.2354	1.46668	3.91606
C	2.54238	-1.135	0.05384
C	2.55308	1.14177	-0.06222
C	3.38502	0.01126	-0.00534



Pt-1

C	1.20943	0.65661	-0.03809
C	-0.02983	1.31985	-0.07224
C	-1.24116	0.60671	-0.03551
C	-2.60349	1.03655	-0.06393
C	-2.50064	-1.23667	0.06699
N	1.25733	-0.74375	0.03348
N	-1.23196	-0.7938	0.04424
B	0.03156	-1.69635	0.09178
F	0.04328	-2.56256	-1.00554
F	0.05296	-2.43247	1.28054
C	3.06045	2.55023	-0.13035
H	2.7416	3.06127	-1.04566
H	2.70555	3.15884	0.7084
H	4.15438	2.53856	-0.10632
C	-2.86063	-2.68207	0.14915
H	-3.94672	-2.79122	0.19144
H	-2.47446	-3.22759	-0.71919
H	-2.41234	-3.14214	1.0362
C	-3.16843	2.42205	-0.14801
H	-2.83952	2.9482	-1.05079
H	-4.26092	2.36267	-0.16306
H	-2.87046	3.04358	0.70368
C	2.96111	-2.56509	0.12782
H	2.5557	-3.13142	-0.71765
H	4.05135	-2.63319	0.12111
H	2.57281	-3.03511	1.03804
C	-0.06024	2.81344	-0.1429
C	-0.09415	3.57583	1.03301
C	-0.05517	3.46804	-1.38244
C	-0.12103	4.97066	0.97008
C	-0.08318	4.86292	-1.44384
H	-0.02926	2.88241	-2.29734
H	-0.14704	5.55081	1.88855
H	-0.08021	5.35938	-2.41041
C	-0.11516	5.6171	-0.26844
H	-0.13502	6.7023	-0.31822
H	-0.09857	3.07279	1.99615
C	-3.39092	-0.1267	0.00007
C	4.82302	-0.02537	-0.00324
C	6.02368	-0.07792	0.00344
C	10.0717	-0.32266	-0.02212
Pt	8.05538	-0.19533	-0.0095
P	8.15917	-0.51342	2.31885
C	9.20447	0.74087	3.16737
H	9.29044	0.52129	4.23701
H	8.76032	1.73231	3.03687
H	10.19545	0.73902	2.70654
C	6.57219	-0.47114	3.24635
H	5.89814	-1.23565	2.85233
H	6.0955	0.50231	3.10515
H	6.74501	-0.64437	4.31388
C	8.91514	-2.12293	2.79238
H	8.29051	-2.94331	2.4263
H	9.9007	-2.19819	2.32586

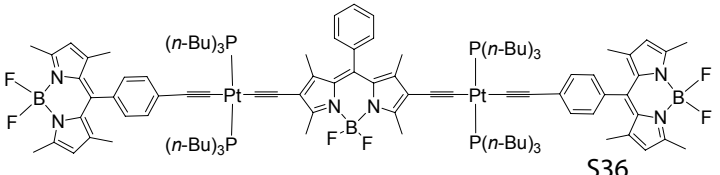
H	9.01391	-2.20262	3.88039
P	7.94743	0.11415	-2.33841
C	9.53521	0.07724	-3.26489
H	9.36162	0.24257	-4.33356
H	10.0184	-0.89204	-3.11748
H	10.20386	0.84887	-2.87536
C	6.9098	-1.14975	-3.18187
H	5.91817	-1.15077	-2.7224
H	7.35843	-2.13843	-3.04582
H	6.82432	-0.93615	-4.2528
C	7.1829	1.71733	-2.82005
H	6.19706	1.78924	-2.35356
H	7.80317	2.54262	-2.45765
H	7.08389	1.79129	-3.90846
C	-11.28786	-0.52498	0.02913
C	11.2984	-0.40234	-0.01365
C	18.48288	-2.24724	0.00023
C	18.77431	0.00746	0.04263
C	17.37549	-0.30452	0.02291
C	16.23053	0.51476	0.02838
C	14.94157	-0.0399	0.01027
C	13.64269	0.5602	0.01346
C	13.45999	-1.71161	-0.02739
N	17.24826	-1.69909	-0.00238
N	14.77335	-1.4333	-0.0158
B	15.91431	-2.49096	-0.02637
F	15.83514	-3.2693	-1.18547
F	15.81689	-3.30921	1.10335
C	19.45788	1.34363	0.07254
H	19.21455	1.95227	-0.8051
H	19.17587	1.93391	0.95099
H	20.54284	1.20079	0.09454
C	12.91929	-3.1016	-0.05582
H	11.82776	-3.07495	-0.08741
H	13.29695	-3.64416	-0.92902
H	13.2449	-3.66057	0.82843
C	13.25841	2.00821	0.03396
H	13.66008	2.55432	-0.82651
H	12.1675	2.0889	0.01431
H	13.62435	2.52084	0.9304
C	18.71312	-3.7238	-0.02307
H	18.25947	-4.17328	-0.91304
H	19.78372	-3.94304	-0.01897
H	18.247	-4.20242	0.84498
C	16.39088	2.00135	0.05399
C	16.43665	2.68901	1.27473
C	16.49463	2.724	-1.14267
C	16.58345	4.07763	1.29734
C	16.64045	4.11267	-1.1182
H	16.45925	2.19595	-2.09165
H	16.61707	4.60021	2.24941
H	16.71872	4.66227	-2.05221
C	16.6853	4.79229	0.10137
H	16.79912	5.8726	0.11952

H	16.35468	2.13382	2.20514
C	12.7148	-0.49458	-0.00858
C	19.44039	-1.21606	0.02826
H	20.51327	-1.36106	0.03783
C	-13.52694	-1.72667	-0.02423
C	-13.59811	0.55084	0.04883
C	-14.92425	0.01553	0.02057
C	-16.1843	0.63313	0.02839
C	-17.36818	-0.12787	-0.01256
C	-18.74995	0.25304	-0.00755
C	-18.56997	-2.01173	-0.09642
N	-14.8247	-1.38437	-0.02509
N	-17.30966	-1.52629	-0.06772
B	-16.01671	-2.38387	-0.0793
F	-15.94896	-3.14504	-1.25048
F	-15.98681	-3.22668	1.03611
C	-13.1448	1.97855	0.09216
H	-13.52322	2.55826	-0.75668
H	-13.48298	2.49268	0.99881
H	-12.0513	2.00872	0.06822
C	-18.87351	-3.474	-0.15389
H	-19.95346	-3.63814	-0.18594
H	-18.41561	-3.93045	-1.03796
H	-18.45947	-3.99043	0.71902
C	-19.36705	1.6206	0.0462
H	-19.08798	2.23558	-0.81626
H	-20.45787	1.53147	0.05802
H	-19.06235	2.17648	0.93932
C	-13.05454	-3.14073	-0.06797
H	-13.41355	-3.63868	-0.97523
H	-11.96282	-3.16904	-0.04528
H	-13.45237	-3.70661	0.78123
C	-16.27203	2.12538	0.07787
C	-16.2923	2.79569	1.30897
C	-16.33417	2.87087	-1.10775
C	-16.37309	4.18937	1.35232
C	-16.4144	4.26436	-1.0627
H	-16.31797	2.35657	-2.06472
H	-16.38794	4.69797	2.31249
H	-16.46241	4.83055	-1.98892
C	-16.43382	4.92667	0.16721
H	-16.49522	6.01095	0.202
H	-16.24329	2.22303	2.23117
C	-12.72593	-0.54824	0.02215
C	-19.47554	-0.93508	-0.06082
H	-20.55427	-1.02678	-0.07231

Optimized triplet state geometry of Pt-2

o 3

C	-4.81004	0.18407	0.15626
C	-6.03707	0.11742	0.14071
C	-10.06821	-0.13768	0.02745
Pt	-8.05463	-0.00921	0.08598



Pt-2

P	-7.89227	0.31895	-2.23858
C	-7.11964	1.92908	-2.68144
H	-6.99274	2.01616	-3.76592
H	-6.14675	1.99792	-2.18831
H	-7.75198	2.74793	-2.32531
C	-6.83417	-0.93437	-3.07186
H	-7.28357	-1.9253	-2.95644
H	-5.85274	-0.93808	-2.59137
H	-6.72559	-0.70898	-4.13822
C	-9.45533	0.29339	-3.20751
H	-9.94046	-0.67892	-3.08782
H	-10.1344	1.05998	-2.82603
H	-9.25332	0.47408	-4.26867
P	-8.20292	-0.33324	2.41105
C	-9.00071	-1.92749	2.8668
H	-9.11949	-2.00863	3.95269
H	-8.38557	-2.75839	2.50856
H	-9.97877	-1.9828	2.38206
C	-6.63072	-0.33086	3.36401
H	-6.12486	0.62842	3.2281
H	-5.97184	-1.11538	2.98366
H	-6.82616	-0.49672	4.42883
C	-9.23228	0.94252	3.24742
H	-8.7596	1.92283	3.13424
H	-10.21311	0.97135	2.76608
H	-9.34698	0.71796	4.31335
C	2.51913	-0.8678	-0.08403
C	2.57995	1.36205	0.38529
C	3.3897	0.23799	0.1405
C	1.2256	0.91388	0.30051
C	0.00144	1.58947	0.44975
C	-1.225	0.91563	0.31303
C	-2.57804	1.36698	0.4041
C	-2.52435	-0.86626	-0.04998
N	1.24252	-0.45872	0.01123
N	-1.24642	-0.45872	0.03247
B	-0.00349	-1.37059	-0.16019
F	-0.01577	-1.93264	-1.44056
F	0.00604	-2.38267	0.80412
C	3.11878	2.73082	0.67173
H	2.81915	3.46081	-0.08878
H	2.77141	3.12069	1.63459
H	4.21192	2.68771	0.69355
C	-2.91507	-2.27814	-0.33205
H	-4.00366	-2.36868	-0.33215
H	-2.52238	-2.60242	-1.302
H	-2.49366	-2.9529	0.42097
C	-3.11324	2.73956	0.67916
H	-2.78858	3.46821	-0.07193
H	-4.20689	2.70493	0.6727
H	-2.78727	3.12499	1.6515
C	2.90509	-2.27842	-0.37872
H	2.45298	-2.61491	-1.3176
H	3.99229	-2.35864	-0.44772

H	2.54091	-2.95062	0.4064
C	0.00378	3.05092	0.76699
C	-0.00548	3.48341	2.10041
C	0.01488	4.00395	-0.26072
C	-0.00317	4.84712	2.40071
C	0.01629	5.36761	0.04113
H	0.0219	3.67449	-1.29612
H	-0.00986	5.16993	3.43822
H	0.02434	6.09704	-0.76418
C	0.00751	5.79213	1.37187
H	0.00893	6.85311	1.60587
H	-0.0141	2.74875	2.90092
C	-3.39125	0.24265	0.17338
C	4.80828	0.17738	0.11414
C	6.03517	0.10936	0.09153
C	10.06835	-0.10515	-0.02495
Pt	8.05362	0.0022	0.03262
P	8.16871	-1.00038	2.15817
C	9.13662	0.00083	3.36111
H	9.22992	-0.51904	4.32071
H	8.63846	0.96219	3.51844
H	10.12876	0.18715	2.94206
C	6.57941	-1.32528	3.02224
H	5.96489	-1.99497	2.41542
H	6.03377	-0.38628	3.14397
H	6.75892	-1.77799	4.00317
C	9.01638	-2.63356	2.14338
H	8.44016	-3.33712	1.53502
H	10.00468	-2.51118	1.69286
H	9.11758	-3.03328	3.15815
P	7.92441	1.00054	-2.09443
C	9.50545	1.29996	-2.98406
H	9.31845	1.75826	-3.96099
H	10.03053	0.35087	-3.119
H	10.14173	1.95704	-2.3857
C	6.92388	0.01258	-3.28092
H	5.93359	-0.15168	-2.84882
H	7.40143	-0.95908	-3.43897
H	6.82958	0.52979	-4.24184
C	7.10449	2.64767	-2.07312
H	6.11815	2.54122	-1.61459
H	7.69754	3.34254	-1.47097
H	7.00033	3.04747	-3.08757
C	11.29497	-0.178	-0.04345
C	-11.29479	-0.20924	0.00404
C	-19.62161	1.90618	-0.82887
C	-17.3535	2.04518	-0.74933
C	-17.7722	0.69694	-0.49153
C	-17.04421	-0.47381	-0.21787
C	-17.70041	-1.69719	0.00032
C	-17.20249	-3.01051	0.29404
C	-19.47374	-3.04436	0.1923
N	-19.17207	0.66468	-0.55161
N	-19.09909	-1.77139	-0.05166

B	-20.06422	-0.58825	-0.33637
F	-20.9177	-0.39047	0.75396
F	-20.8167	-0.84641	-1.48699
C	-15.96953	2.623	-0.80323
H	-15.43459	2.5024	0.14483
H	-15.35324	2.14643	-1.57301
H	-16.02566	3.69275	-1.02768
C	-20.90393	-3.47716	0.21572
H	-20.97533	-4.55031	0.40913
H	-21.45894	-2.93666	0.99031
H	-21.39172	-3.25111	-0.73839
C	-15.78675	-3.48019	0.45883
H	-15.27127	-2.95857	1.27231
H	-15.77762	-4.55144	0.68297
H	-15.19027	-3.31732	-0.44517
C	-21.0741	2.23026	-0.96578
H	-21.61461	1.97932	-0.0468
H	-21.20961	3.29296	-1.18138
H	-21.52771	1.64116	-1.7702
C	-15.55244	-0.41473	-0.15774
C	-14.78057	-0.63339	-1.30792
C	-14.89607	-0.13485	1.04934
C	-13.39094	-0.57009	-1.25489
C	-13.50646	-0.07213	1.10612
H	-15.48043	0.03634	1.94949
H	-12.80799	-0.73994	-2.15502
H	-13.01425	0.14714	2.04894
C	-12.71843	-0.28521	-0.04616
H	-15.27434	-0.85218	-2.25101
C	19.41936	-3.05364	-0.8139
C	17.14698	-3.00341	-0.75293
C	17.67431	-1.69688	-0.48107
C	17.04509	-0.47211	-0.20008
C	17.80004	0.68841	0.04233
C	17.41085	2.03736	0.33953
C	19.67808	1.87841	0.2725
N	19.07258	-1.78133	-0.52894
N	19.20052	0.64396	0.01099
B	20.06497	-0.61149	-0.28621
F	20.8894	-0.89851	0.80703
F	20.84654	-0.39884	-1.42642
C	15.71976	-3.46276	-0.81813
H	15.18452	-3.28181	0.12011
H	15.1564	-2.94855	-1.60413
H	15.6874	-4.53692	-1.02572
C	21.13921	2.18954	0.318
H	21.29746	3.24636	0.54655
H	21.64114	1.57996	1.07712
H	21.61473	1.9553	-0.64053
C	16.03818	2.62683	0.48303
H	15.47634	2.16929	1.30444
H	16.11725	3.69995	0.68318
H	15.43533	2.49252	-0.42127
C	20.8409	-3.49603	-0.94304

H	21.3961	-3.28544	-0.02284
H	20.88994	-4.56713	-1.15402
H	21.34452	-2.94982	-1.74814
C	15.55326	-0.40078	-0.15946
C	14.81751	-0.14609	-1.32577
C	14.86064	-0.58417	1.0459
C	13.42785	-0.0733	-1.28886
C	13.4708	-0.51475	1.0858
H	15.41683	-0.78219	1.95832
H	12.87332	0.12678	-2.20066
H	12.95	-0.6597	2.02762
C	12.71889	-0.25552	-0.08112
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C	18.25002	-3.82686	-0.95661
H	18.22692	-4.88466	-1.18586
C	18.59469	2.75534	0.47886
H	18.68148	3.81027	0.70613
C	-18.32273	-3.82803	0.40823
H	-18.32294	-4.88843	0.62634
C	-18.51996	2.77543	-0.95541
H	-18.58315	3.8333	-1.1767