Supporting Information for:

Naphthalimide-Modified Tridentate Platinum(II) Complexes: Synthesis, Characterization, and Application in Singlet Oxygen Generation

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Table S1. Crystallographic data of **2**.

Complex	**2**
CCDC No.	2206904
empirical formula	C42H41N3O2Pt
formula weight	814.87
space group	$P\bar{1}$
crystal system	Triclinic
a (Å)	8.5185(2)
b (Å)	14.6039(3)
c (Å)	15.4058(3)
α (deg)	63.696(2)
β (deg)	78.345(2)
γ (deg)	82.054(2)
vol (Å^3)	1680.07(7)
Z	2
Density (Mg/m^3)	1.611
temp (K)	170.15
wavelength (Å)	1.54184
final R indices	R_1 = 0.0300, wR_2 = 0.0833
R indices (all data)	R_1 = 0.0309, wR_2 = 0.0839

Table S2. Detailed lifetime data.

Complex[a]	Conditions	τ (μs)[c]
1(PF_6)	$C_2H_4Cl_2$, Air	τ_1 = 0.6 (100%)
	$C_2H_4Cl_2$, N_2	τ_{ave} = 4.84; τ_1 = 1.88, α_1 = 49%; τ_2 = 7.7, α_2 = 51%
	CH_3CN, Air	τ_1 = 0.27 (100%)
	CH_3CN, N_2	τ_1 = 3.21 (100%)
2	$C_2H_4Cl_2$, Air	τ_{ave} = 0.72; τ_1 = 0.47, α_1 = 85%; τ_2 = 2.13, α_2 = 15%
	$C_2H_4Cl_2$, N_2	τ_{ave} = 7.0; τ_1 = 5.08, α_1 = 86%; τ_2 = 18.6, α_2 = 14%
	CH_3CN, Air	τ_1 = 0.24 (100%)
	CH_3CN, N_2	τ_1 = 1.65 (100%)
NI	$C_2H_4Cl_2$, Air	$\tau_{ave} = 3 \times 10^{-4}$; $\tau_1 = 2.4 \times 10^{-4}$, α_1 = 98%; $\tau_2 = 2.9 \times 10^{-3}$, α_2 = 2%

[a]Measured in specific solution of 5×10^{-5} M. [c]Monitored at 620 nm for **1**(PF_6), 640 nm for **2** and 400 nm for **NI**, respectively, under specific condictions, $\tau_{ave} = \alpha_1\tau_1 + \alpha_2\tau_2$.

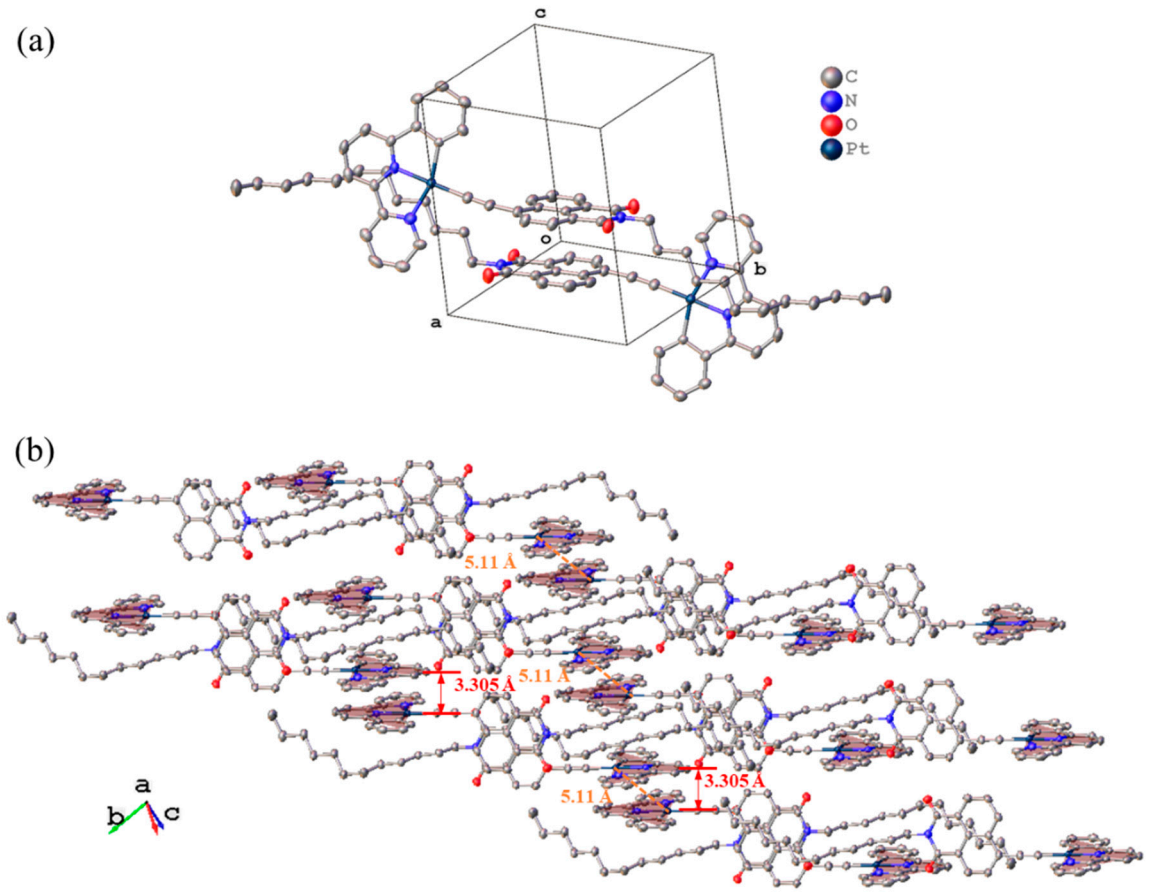

Figure S1. (a) Molecular dimer in one unit cell (b) the stacking model of **2** with thermal ellipsoid plot at 50% probability level.

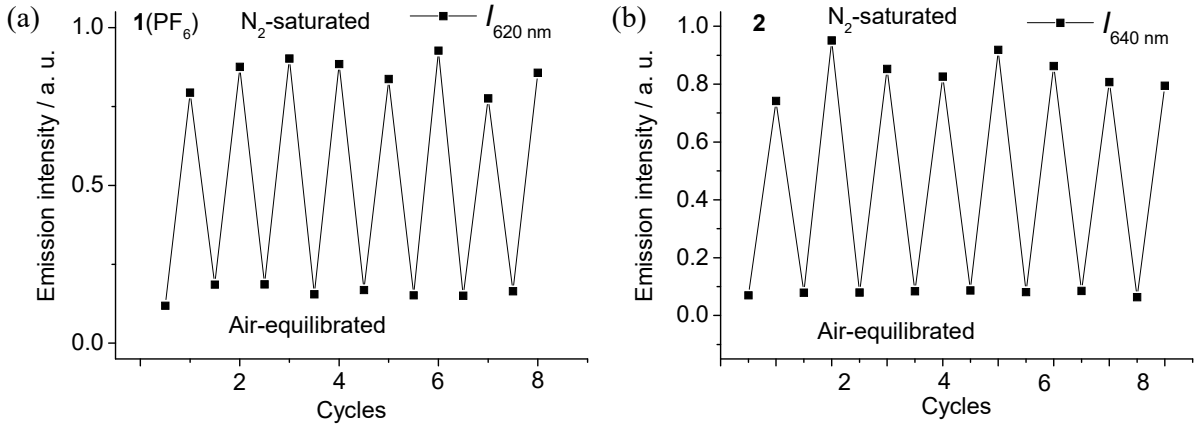

Figure S2. Response of emission intensity of (a) **1**(PF_6) at 620 nm (I_{620} nm) and (b) **2** at 640 nm (I_{640} nm) upon repeated saturated with N_2 and air (containing about 21% O_2) in DCE (5×10^{-5} M). Excitation for **1**(PF_6) and **2** are 450 and 435 nm, respectively.

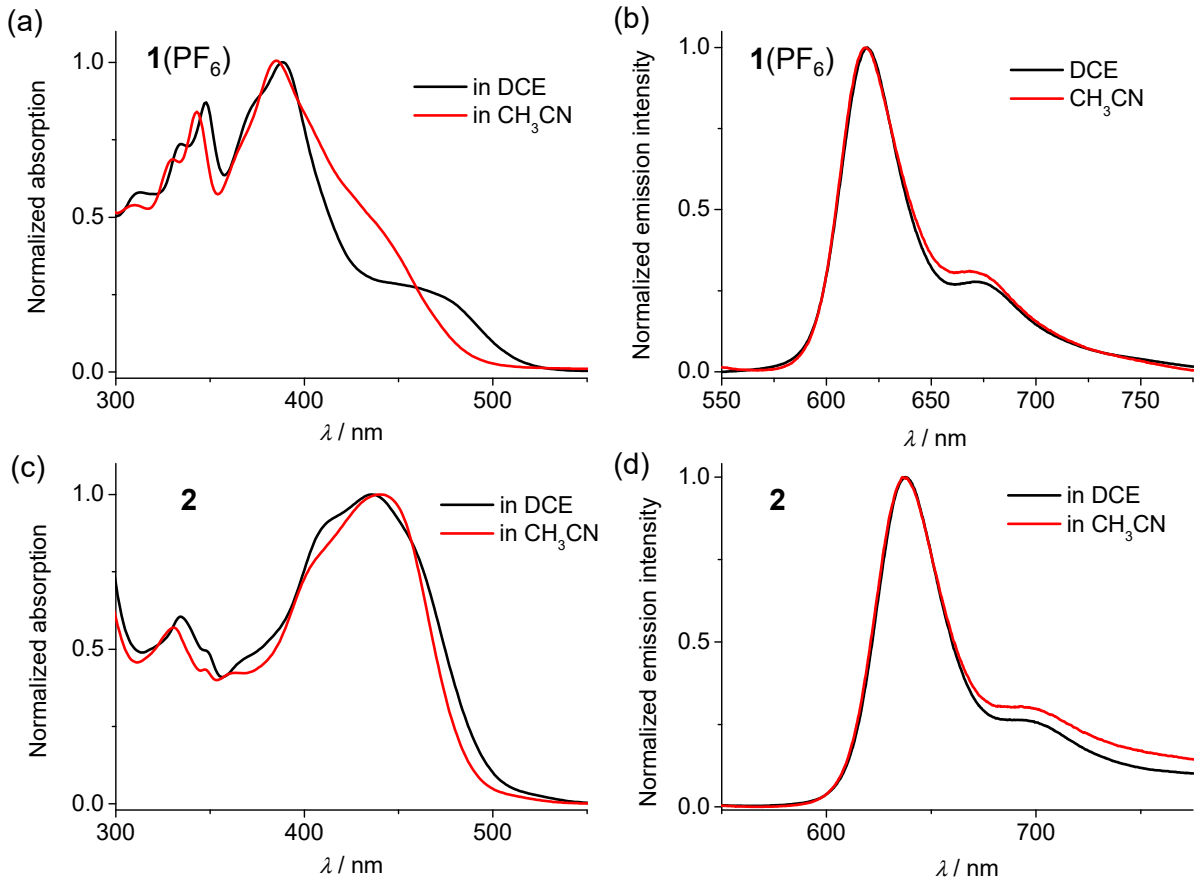

Figure S3. (a,c) Normalized UV-Vis absorption and (b,d) emission spectra of (a,b) **1**(PF_6) and (c,d) **2** in solutions (5×10^{-5} M) of DCE (black) and CH_3CN (red), respectively. Emission spectra were recorded by excitation at 450 nm for **1**(PF_6) and 435 nm for **2** under N_2-saturated condition.

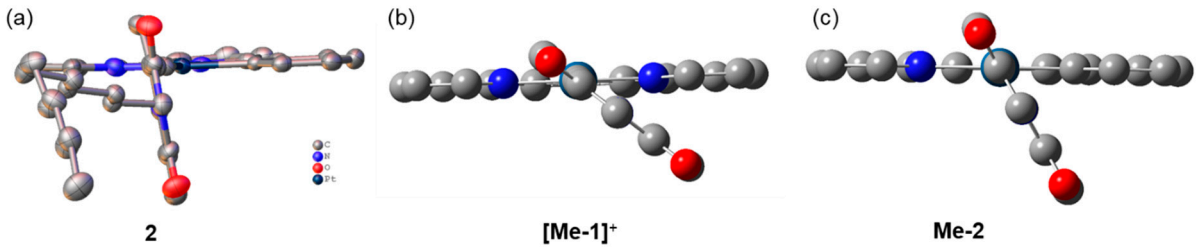

Figure S4. (a) Single crystal structure of **2**, (b,c) optimized structure of (b) [**Me-1**]$^+$ and (c) **Me-2** at ground state by DFT at the PBE1PBE/6-311G*(for C,H,N,O)/SDD(for Pt) level using Gaussian 09.

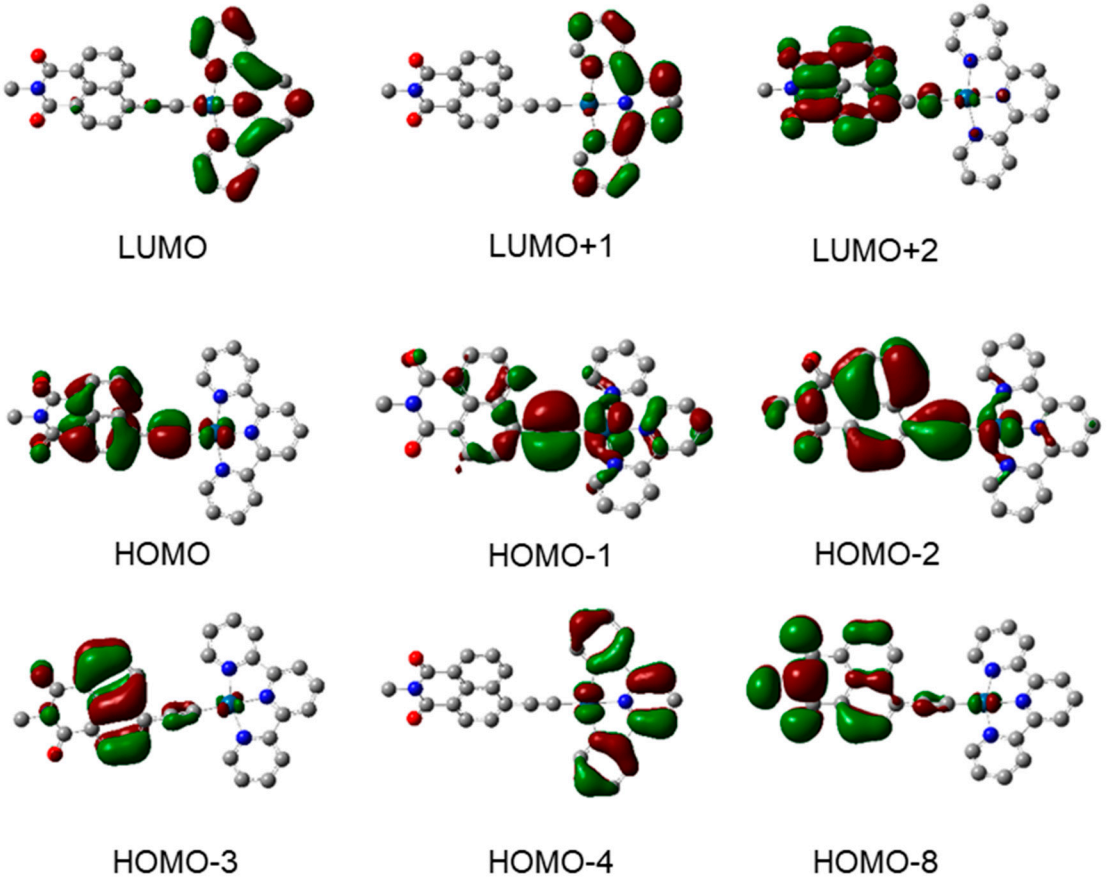

Figure S5. Isodensity plots of frontier molecular orbitals (MOs) of **[Me-1]**$^{+}$ computed based on the optimized ground state geometry (isovalue = 0.03).

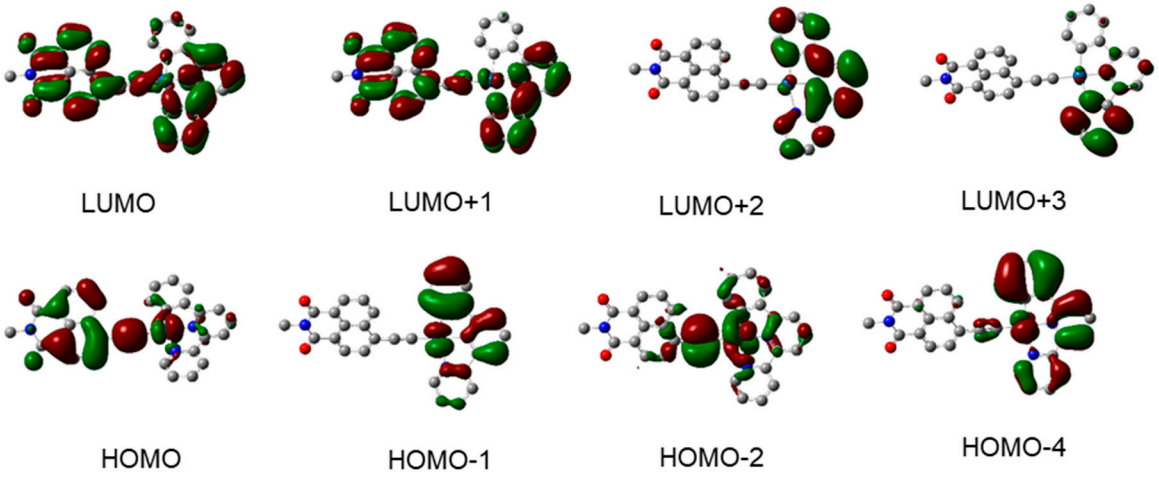

Figure S6. Isodensity plots of frontier molecular orbitals (MOs) of **Me-2** computed based on the optimized ground state geometry (isovalue = 0.03).

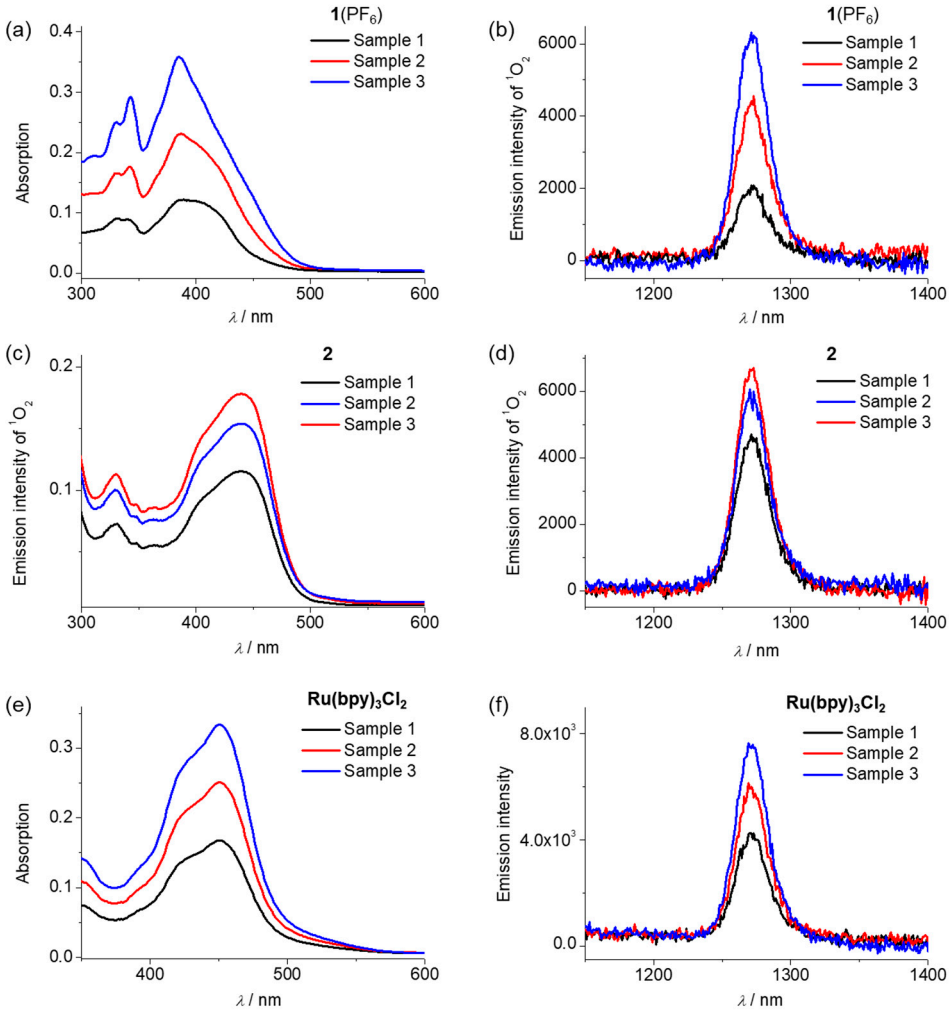

Figure S7. (a,c,e) Absorption and (b,d,f) NIR emission spectra of **1**(PF_6), **2** and $Ru(bpy)_3Cl_2$ in aerated diluted CH_3CN with different concentration under excitation of 435 nm.

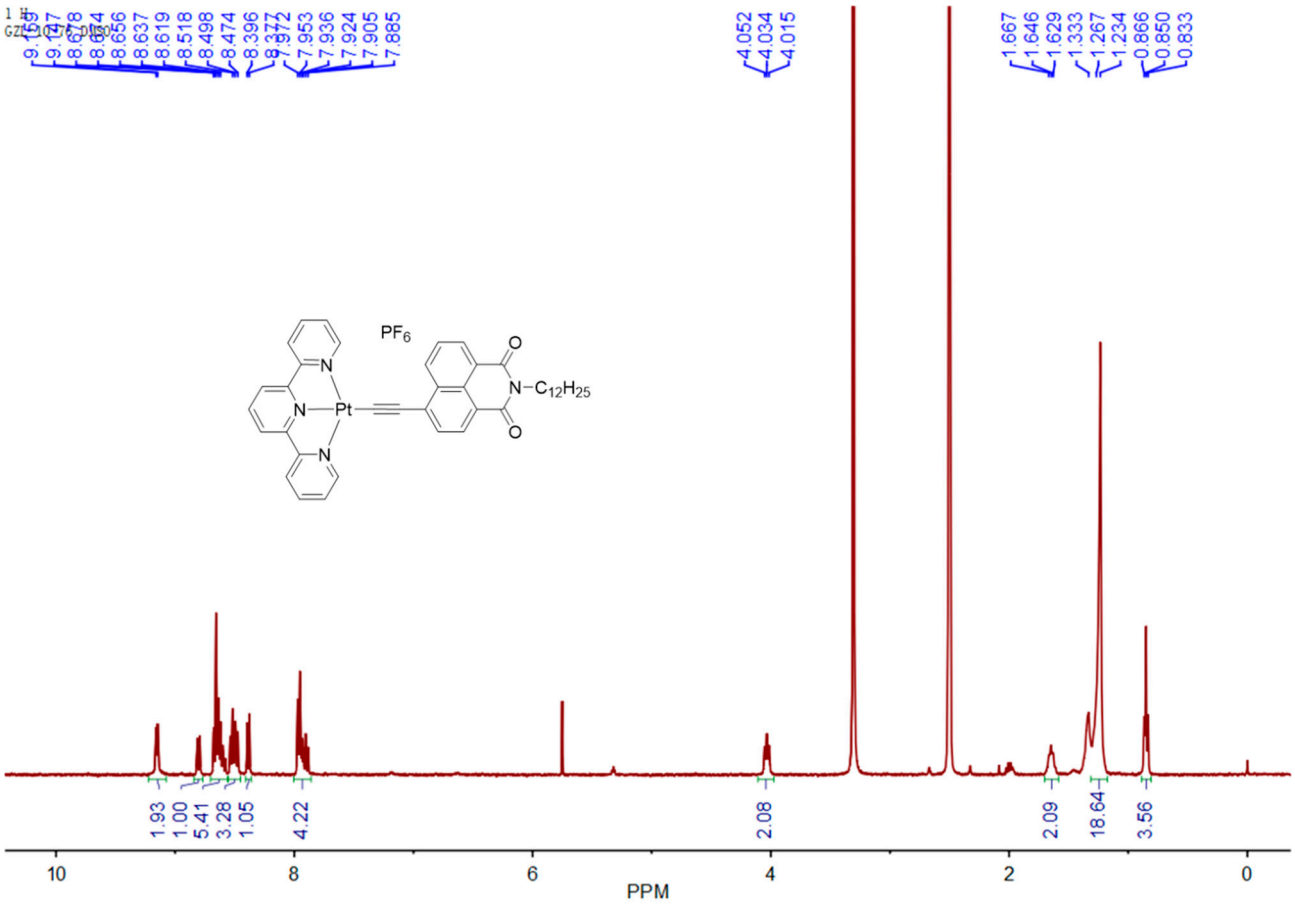

Figure S8. ^{1}H NMR spectrum of **1**(PF_6) in DMSO-d_6.

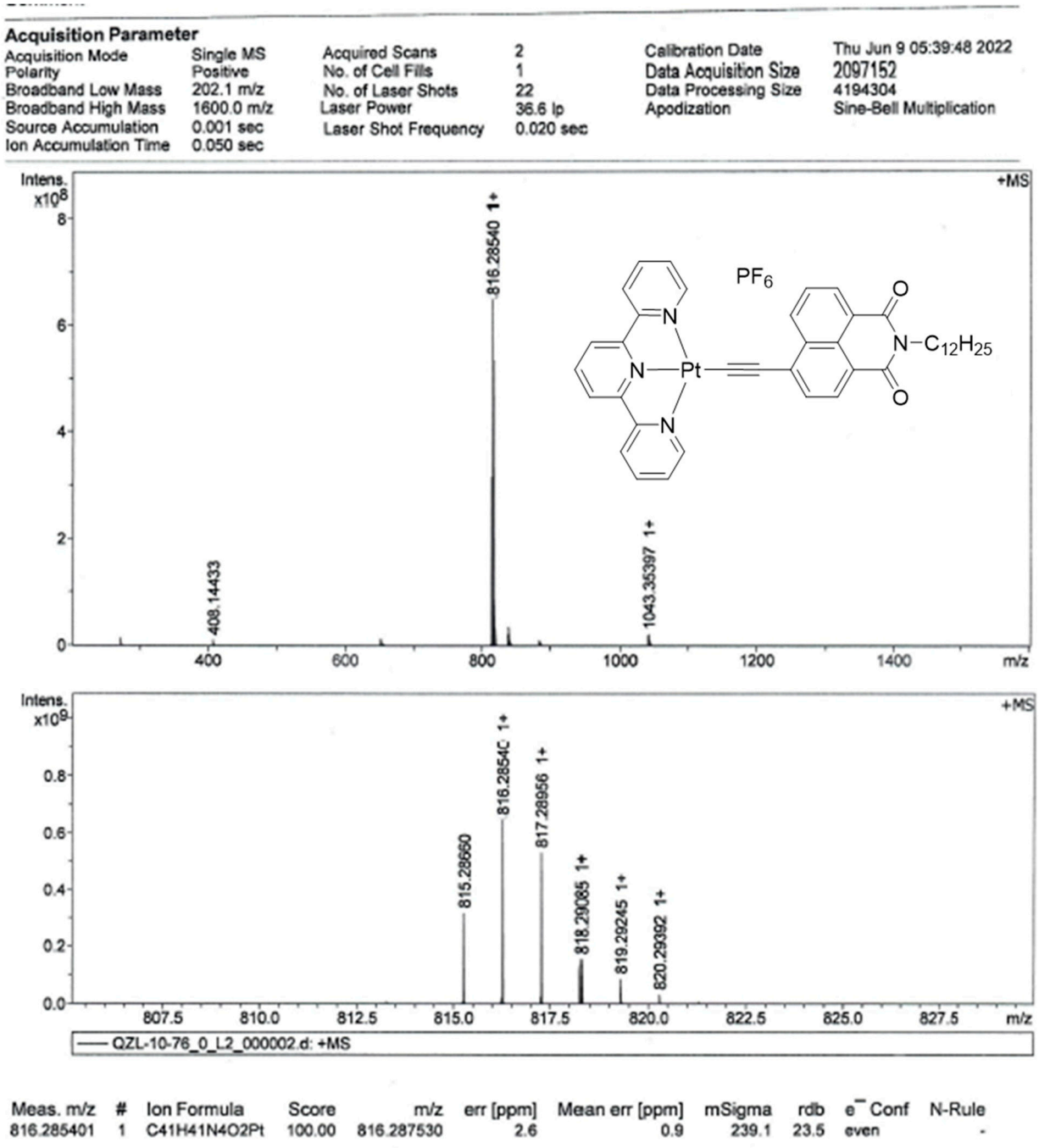

Figure S9. MALDI-TOF-HRMS of **1**(PF_6).

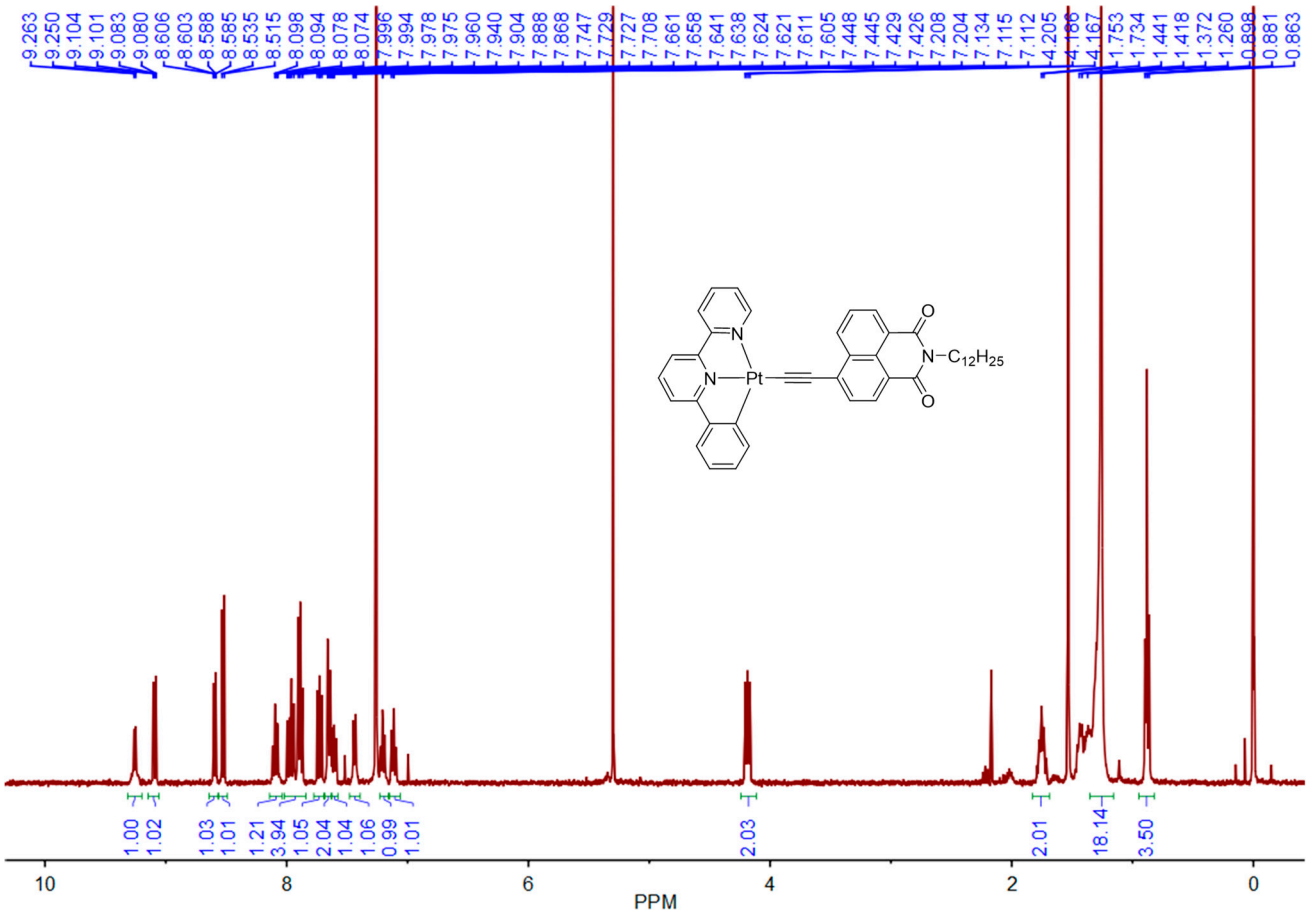

Figure S10. ^{1}H NMR spectrum of **2** in $CDCl_3$.

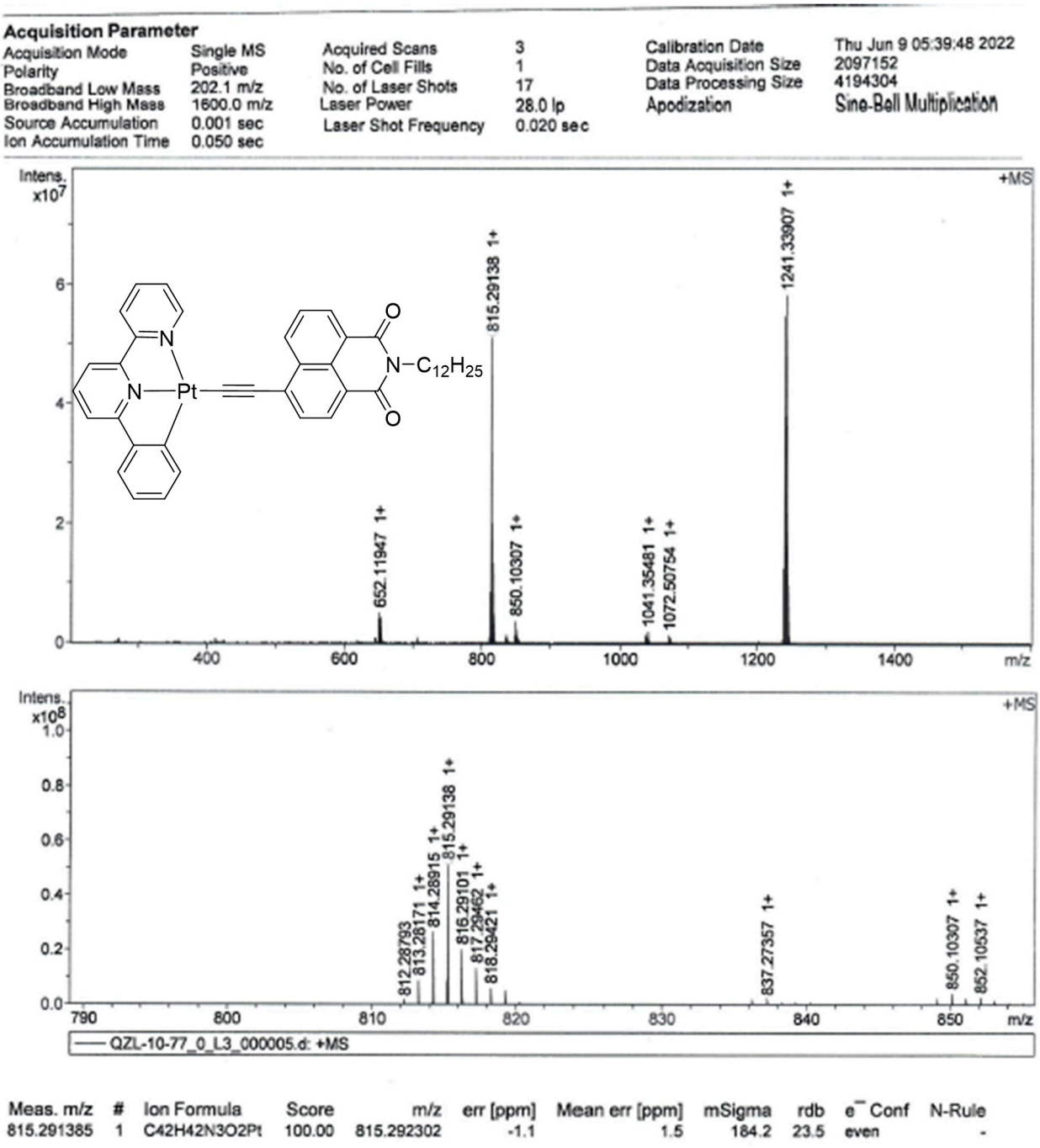

Figure S11. MAIDI-TOF-HRMS of **2**.

Data S1

Cartesian coordinates of DFT-optimized structure of singlet **[Me-1]**$^{+}$:
Charge = 1; multiplicity=1

Pt	2.07135500	-0.10423100	-0.11333500
O	-7.22844200	-2.22287800	-1.20400900
O	-7.85626600	1.60979500	1.13398200
N	4.02387700	0.21001700	0.05758200
N	2.70449100	-2.01616200	0.20529200
N	-7.53582800	-0.31257300	-0.03624300
C	4.46340600	1.47034300	-0.05066800
C	5.82266400	1.71991000	0.08197700
H	6.21829300	2.72445700	0.00081500
C	6.66931400	0.64326900	0.32423200
H	7.73366800	0.81775600	0.43222400
C	6.17565200	-0.65274000	0.43179100
H	6.84525300	-1.48186700	0.62152100
C	4.80853600	-0.84996900	0.29011100
C	3.38262600	2.43982500	-0.30506100
C	1.08154100	2.71973900	-0.61500300
H	0.11347000	2.23858200	-0.66509900
C	1.23684600	4.08600300	-0.78875400
H	0.36436100	4.69823600	-0.98082300
C	2.50731500	4.63187400	-0.71427500
H	2.66160300	5.69667800	-0.84659600
C	3.59123300	3.79770400	-0.46917800
H	4.59420700	4.20095600	-0.40893200
C	4.05873700	-2.11713200	0.36714400
C	4.64955700	-3.34873800	0.58607400
H	5.72262700	-3.41948300	0.71277200
C	3.85633700	-4.48828200	0.64215500
H	4.31121400	-5.45731400	0.81320800
C	2.48693100	-4.36829000	0.47757900
H	1.83141000	-5.22965900	0.51388600
C	1.94413900	-3.11154000	0.25996200
H	0.88151800	-2.95864400	0.12373500
C	-8.97013800	-0.53303100	-0.13561500
H	-9.27390400	-0.55618200	-1.18293200
H	-9.47413100	0.28010900	0.37749700
C	-5.27098900	-1.07135700	-0.54495200
C	-4.74567000	0.05232600	0.12610100
C	-5.61552100	0.99514900	0.71580400
C	-5.10569800	2.09352700	1.37398100

H	-5.79193500	2.80484400	1.81988500
C	-3.71853100	2.28248000	1.46454700
H	-3.32929200	3.14927800	1.98780700
C	-2.85439300	1.37525400	0.89692600
H	-1.78127900	1.51869400	0.97231100
C	-3.34182500	0.24096000	0.21321800
C	-2.47498200	-0.72708500	-0.39169600
C	-3.03188300	-1.82123700	-1.04207000
H	-2.37599900	-2.55342400	-1.49961100
C	-4.41661000	-1.99035500	-1.11795700
H	-4.83427100	-2.85033600	-1.62978800
C	-6.72514100	-1.27118200	-0.63630400
C	-7.07886900	0.81650700	0.63770100
C	-1.06921500	-0.56423000	-0.32578700
C	0.13994000	-0.39861100	-0.25639900
H	-9.23450300	-1.48486800	0.32669300
N	2.12142800	1.91734100	-0.37830700

Cartesian coordinates of DFT-optimized structure of triplet **[Me-1]**$^{+}$:
Charge = 1; multiplicity=3

Pt	11.99450000	-4.03250000	4.63570000
O	9.15730000	4.45130000	1.32680000
O	5.27360000	2.26050000	0.44860000
N	12.63330000	-5.59300000	5.71070000
N	13.18340000	-4.95450000	3.22630000
N	7.23450000	3.34960000	0.84540000
C	12.25850000	-5.67640000	6.99110000
C	12.75300000	-6.70690000	7.78070000
H	12.50230000	-6.78450000	8.69340000
C	13.61970000	-7.61780000	7.20110000
H	13.97090000	-8.32540000	7.72890000
C	13.98430000	-7.51770000	5.87030000
H	14.57310000	-8.15520000	5.48160000
C	13.47220000	-6.46550000	5.10530000
C	11.35940000	-4.58380000	7.41390000
C	10.21760000	-2.63570000	6.75390000
H	10.00280000	-1.98880000	6.09180000
C	9.66160000	-2.51410000	8.02750000
H	9.07550000	-1.79350000	8.22580000
C	9.96610000	-3.44780000	8.99700000
H	9.59400000	-3.37640000	9.86880000
C	10.82680000	-4.49430000	8.68060000

H	11.04610000	-5.14520000	9.33610000
C	13.76180000	-6.12370000	3.70760000
C	14.59310000	-6.88360000	2.90040000
H	14.96640000	-7.69490000	3.22300000
C	14.87460000	-6.44450000	1.61040000
H	15.45050000	-6.95390000	1.05350000
C	14.32480000	-5.27660000	1.13860000
H	14.53470000	-4.97120000	0.26370000
C	13.45620000	-4.53980000	1.94580000
H	13.05250000	-3.74950000	1.60830000
C	6.62070000	4.62890000	0.45000000
H	6.93304771	5.39807469	1.12506237
H	5.55503291	4.53796101	0.48136497
C	9.19640000	2.10600000	1.64310000
C	8.42900000	0.91680000	1.64860000
C	7.07600000	0.93110000	1.23000000
C	6.33710000	-0.23250000	1.23130000
H	5.42730000	-0.22190000	0.95910000
C	6.94080000	-1.43600000	1.64040000
H	6.43140000	-2.23810000	1.63080000
C	8.23870000	-1.47860000	2.04810000
H	8.62020000	-2.30360000	2.32340000
C	9.02420000	-0.30380000	2.06720000
C	10.39930000	-0.30220000	2.49810000
C	11.12250000	0.87010000	2.40810000
H	12.04510000	0.86570000	2.63670000
C	10.52400000	2.06840000	1.98810000
H	11.04410000	2.86180000	1.94170000
C	8.56760000	3.38700000	1.26950000
C	6.43200000	2.19800000	0.81130000
C	10.97460000	-1.49000000	3.06540000
C	11.37440000	-2.46240000	3.62030000
H	6.92814675	4.87996513	-0.54365124
N	11.05880000	-3.65320000	6.43480000

Cartesian coordinates of DFT-optimized structure of singlet **Me-2**:
Charge = 0; multiplicity=1

Pt	2.05074800	-0.05639200	-0.14285300
O	-7.25182500	-1.65369300	-1.85035800
O	-7.86821200	1.14849700	1.65944700
N	4.03971400	0.17138100	0.06658300
N	2.69834400	-2.06860300	0.22872500
N	-7.55026300	-0.26053200	-0.09600400

C	4.52529700	1.42143600	-0.05610300
C	5.89799300	1.61766100	0.07974700
H	6.32474000	2.60852500	-0.01466200
C	6.71051400	0.52291000	0.33724300
H	7.78050600	0.66334600	0.44564600
C	6.17226300	-0.75465400	0.45908700
H	6.81417000	-1.60257100	0.66010400
C	4.80002000	-0.90562900	0.31500100
C	3.47823000	2.41416300	-0.32330900
C	2.14326100	1.91690400	-0.41215300
C	1.12815600	2.84041500	-0.66108900
H	0.10149500	2.49625200	-0.73520000
C	1.40793000	4.19682200	-0.81788400
H	0.59620000	4.89258500	-1.01149700
C	2.71466800	4.66620000	-0.72930200
H	2.92793700	5.72318800	-0.85240400
C	3.74913400	3.77349700	-0.48161500
H	4.76832600	4.14190600	-0.41120600
C	4.04063700	-2.16975800	0.40767800
C	4.63248400	-3.39916500	0.66050600
H	5.70306800	-3.47345900	0.80469100
C	3.83817900	-4.53574700	0.72967700
H	4.28981800	-5.50171200	0.92706100
C	2.46950600	-4.41842400	0.54449800
H	1.81347200	-5.27939900	0.59015000
C	1.93858000	-3.16213400	0.29594700
H	0.87657800	-3.00976000	0.14331200
C	-8.98444900	-0.43378500	-0.26057200
H	-9.29654200	-0.07353000	-1.24203700
H	-9.48552300	0.13426600	0.51718300
C	-5.29021900	-0.79535700	-0.84510100
C	-4.76178100	0.03222900	0.16752600
C	-5.62850700	0.71662100	1.04732600
C	-5.11526400	1.52879300	2.03658900
H	-5.80008500	2.04452200	2.70068800
C	-3.72860300	1.68225200	2.17667000
H	-3.33586400	2.32499200	2.95726100
C	-2.86719700	1.02279800	1.32994400
H	-1.79366000	1.14069300	1.43783200
C	-3.35729100	0.18295100	0.30785700
C	-2.48745800	-0.52177700	-0.59091000
C	-3.05102100	-1.32799700	-1.57575300
H	-2.39668700	-1.86028000	-2.25712700
C	-4.43448900	-1.46050200	-1.70093100

H	-4.85375400	-2.09336200	-2.47564800
C	-6.74149800	-0.95417100	-0.99347600
C	-7.09106100	0.57290100	0.91983600
C	-1.08498000	-0.39337900	-0.47323900
C	0.12665000	-0.24978300	-0.34906300
H	-9.24487500	-1.48951700	-0.17727900

Cartesian coordinates of DFT-optimized structure of triplet **Me-2**:
Charge = 0; multiplicity=3

Pt	11.99450000	-4.03250000	4.63570000
O	9.15730000	4.45130000	1.32680000
O	5.27360000	2.26050000	0.44860000
N	12.63330000	-5.59300000	5.71070000
N	13.18340000	-4.95450000	3.22630000
N	7.23450000	3.34960000	0.84540000
C	12.25850000	-5.67640000	6.99110000
C	12.75300000	-6.70690000	7.78070000
H	12.50230000	-6.78450000	8.69340000
C	13.61970000	-7.61780000	7.20110000
H	13.97090000	-8.32540000	7.72890000
C	13.98430000	-7.51770000	5.87030000
H	14.57310000	-8.15520000	5.48160000
C	13.47220000	-6.46550000	5.10530000
C	11.35940000	-4.58380000	7.41390000
C	11.05880000	-3.65320000	6.43480000
C	10.21760000	-2.63570000	6.75390000
H	10.00280000	-1.98880000	6.09180000
C	9.66160000	-2.51410000	8.02750000
H	9.07550000	-1.79350000	8.22580000
C	9.96610000	-3.44780000	8.99700000
H	9.59400000	-3.37640000	9.86880000
C	10.82680000	-4.49430000	8.68060000
H	11.04610000	-5.14520000	9.33610000
C	13.76180000	-6.12370000	3.70760000
C	14.59310000	-6.88360000	2.90040000
H	14.96640000	-7.69490000	3.22300000
C	14.87460000	-6.44450000	1.61040000
H	15.45050000	-6.95390000	1.05350000
C	14.32480000	-5.27660000	1.13860000
H	14.53470000	-4.97120000	0.26370000
C	13.45620000	-4.53980000	1.94580000

H	13.05250000	-3.74950000	1.60830000
C	6.62070000	4.62890000	0.45000000
H	6.93304771	5.39807469	1.12506237
H	5.55503291	4.53796101	0.48136497
C	9.19640000	2.10600000	1.64310000
C	8.42900000	0.91680000	1.64860000
C	7.07600000	0.93110000	1.23000000
C	6.33710000	-0.23250000	1.23130000
H	5.42730000	-0.22190000	0.95910000
C	6.94080000	-1.43600000	1.64040000
H	6.43140000	-2.23810000	1.63080000
C	8.23870000	-1.47860000	2.04810000
H	8.62020000	-2.30360000	2.32340000
C	9.02420000	-0.30380000	2.06720000
C	10.39930000	-0.30220000	2.49810000
C	11.12250000	0.87010000	2.40810000
H	12.04510000	0.86570000	2.63670000
C	10.52400000	2.06840000	1.98810000
H	11.04410000	2.86180000	1.94170000
C	8.56760000	3.38700000	1.26950000
C	6.43200000	2.19800000	0.81130000
C	10.97460000	-1.49000000	3.06540000
C	11.37440000	-2.46240000	3.62030000
H	6.92814675	4.87996513	-0.54365124