Electronic Supplementary Information

Metal Ions Control Configuration and $^1O_2$ Generation Capacity of Hexaphyrin(2.1.2.1.2.1) with Embedded Benzene

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1. Instrumentation and Materials. The UV-vis absorption spectra were measured with a JASCO UV/VIS/NIR Spectrophotometer V-670. APCI-FT-MS mass spectrum was recorded on a ThermoFisher Scientific spectrometer. ^{1}H NMR spectra were recorded on a JNM-ECX 400 spectrometer (operating as 400 MHz for ^{1}H) using the residual solvent as the internal reference for ^{1}H (δ = 7.26 ppm in $CDCl_3$). X-ray crystallographic data for CCDC: 2392557 (**1Ni**) and 2392559 (**2Pd**) were recorded at 242K for **1Ni** and 193 K for **2Pd** on a Bruker D8 VENTURE Metaljet PHOTON II diffractometer. It using Olex2,[1] the structures were solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimization. All density functional theory calculations were achieved with the Gaussian 09 program package.[4] Frontier molecular orbital and energy levels of **1Ni** and **2Pd** complexes calculated at the B3LYP/6-31G(d, p) (C, H, N, F, Cl, O, Ni) + SDD (Pd) basis set. All solvents and chemicals used without further purification except as noted.

2. Singlet Oxygen Generation Study. A CH_2Cl_2 solution of **MB** or **2Pd** complexes ($1*10^{-4}$ M) in mixture with diphenylisobenzofuran (DPBF) was measured on a UV-vis spectrometer, the solution was irradiated under 570-590 nm yellow laser beam by a time interval of 0, 5, 10, 15, 20, 25, 30, 35 and 40 s, and methylene blue (MB) ($1*10^{-4}$ M) was used as standard photosensitizer, and the decrease of DPBF absorption at 417 nm was monitored, and singlet oxygen generation yield of **2Pd** complex was calculated in comparison with MB by the following formula:

$$\Phi_{\Delta(S)} = \Phi_{\Delta(S0)} \times (S_s/S_{s0}) \times 100\%$$

$\Phi_{\Delta(S)}$ = yield of 2Pd complex, $\Phi_{\Delta(S0)}$ = yield of MB, S_s = slope of 2Pd complex, S_{s0} = slope of MB. The singlet oxygen quantum yield of MB in this work given as 0.52.

3. Synthesis of 1Ni and 2Pd.

1Ni. The $Ni(OAc)_2$•$4H_2O$ (24.9 mg, 0.1 mmol) or $NiCl_2$•$6H_2O$ (23.7 mg, 0.1 mmol) was added to the toluene solution of **Hex** (11.5 mg. 0.01 mmol). The reaction mixture was stirred under N_2 at 90 ^{o}C for 8 hours. After removal of the solvent, the residue was purified by silica gel column chromatography (hexane/CH_2Cl_2 = 4/1) to give **1Ni** in 83% yield (10.0 mg, 0.0083 mmol) when $Ni(OAc)_2$•$4H_2O$ as Ni salt and 79% yield (9.5 mg, 0.0079 mmol) when $NiCl_2$•$6H_2O$ as Ni salt. ^{1}H NMR (400 MHz, $CDCl_3$): 13.02 (s, 1H), 9.41 (d, 2H), 8.92 (d, 2H), 8.16 (d, 2H), 8.11-8.08 (m, 2H), 7.74-7.72 (m, 4H), 7.57-7.55 (m, 3H), 7.38 (d, 2H), 7.33 (d, 2H), 7.22 (d, 1H), 7.12-7.09 (m, 3H), 6.62 (d, 1H) ppm. APCI-HR-MS: 1209.1306 $[M+H]^+$. UV-Vis (in CH_2Cl_2)λ[nm] ($\varepsilon[M^{-1}cm^{-1}]$): 500 (90000), 547 (105000).

2Pd. The $PdCl_2$ (17. 7mg, 0.10 mmol) was added to a mixture solution of **Hex** (23.0 mg. 0.02 mmol) in 25 mL mixture of CH_2Cl_2/MeOH (4/1). The reaction mixture was stirred overnight under nitrogen at room temperature. After removal of the solvent, the crude was purified by silica gel column chromatography (hexane/CH_2Cl_2 = 4/1) to give **2Pd** in 38% yield (10.6 mg, 0.0076 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): 7.98 (d, 1H), 7.80 (d, 1H), 7.67 (d, 1H), 7.53 (d, 1H), 7.48 (d, 1H), 7.42 (d, 1H), 7.37 (d, 1H), 7.35 (d, 1H), 7.25 (d, 1H), 7.23 (d, 1H), 7.15 (d, 1H), 7.09-7.07 (m, 1H), 7.05-7.03 (m, 1H), 7.00 (s, 1H), 6.98 (d, 1H), 6.93-6.92 (m, 1H), 6.89 (d, 1H), 6.77-6.76 (m, 1H), 6.72-6.70 (m, 1H), 6.69 (d, 1H), 6.65 (d, 1H), 6.55 (d, 1H), 6.49-6.47 (m, 1H), 6.41 (d, 1H)

ppm. APCI-HR-MS: 1398.9657 $[M+H]^+$. UV-Vis (in CH_2Cl_2)λ[nm] (ε[$M^{-1}cm^{-1}$]): 603 (157000), 769 (21000).

4. Supporting Figures and Tables

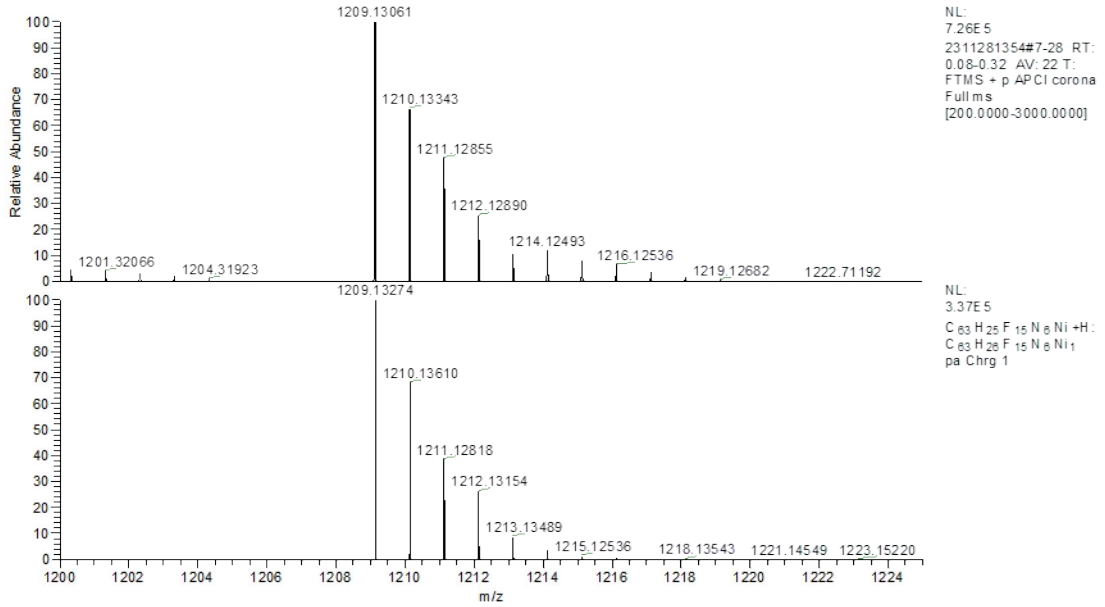

Figure S1. HR-APCI-MS spectrum of **1Ni**.

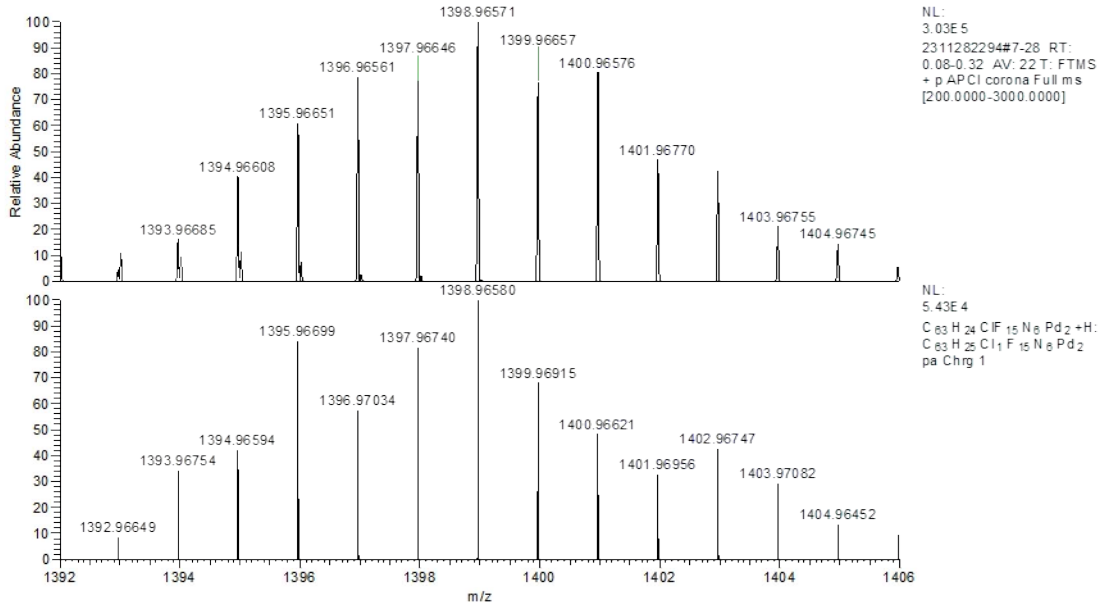

Figure S2. HR-APCI-MS spectrum of **2Pd**.

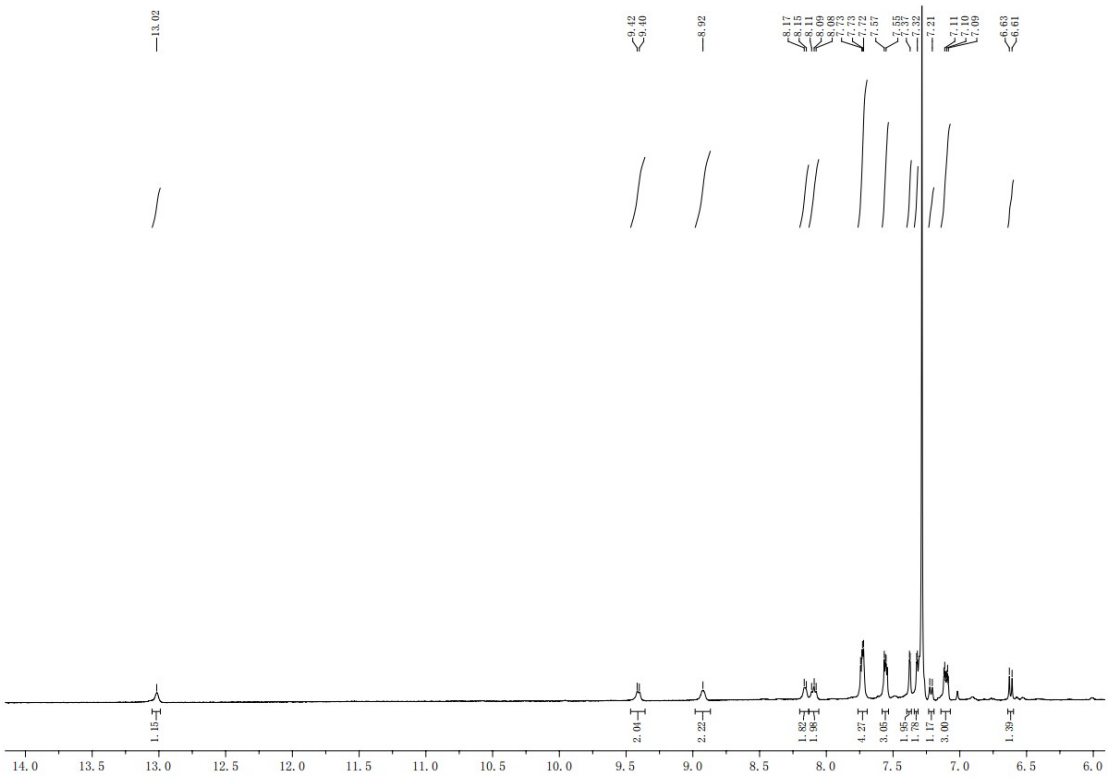

Figure S3. ^{1}H NMR spectrum of **1Ni** recorded at 298 K in $CDCl_3$.

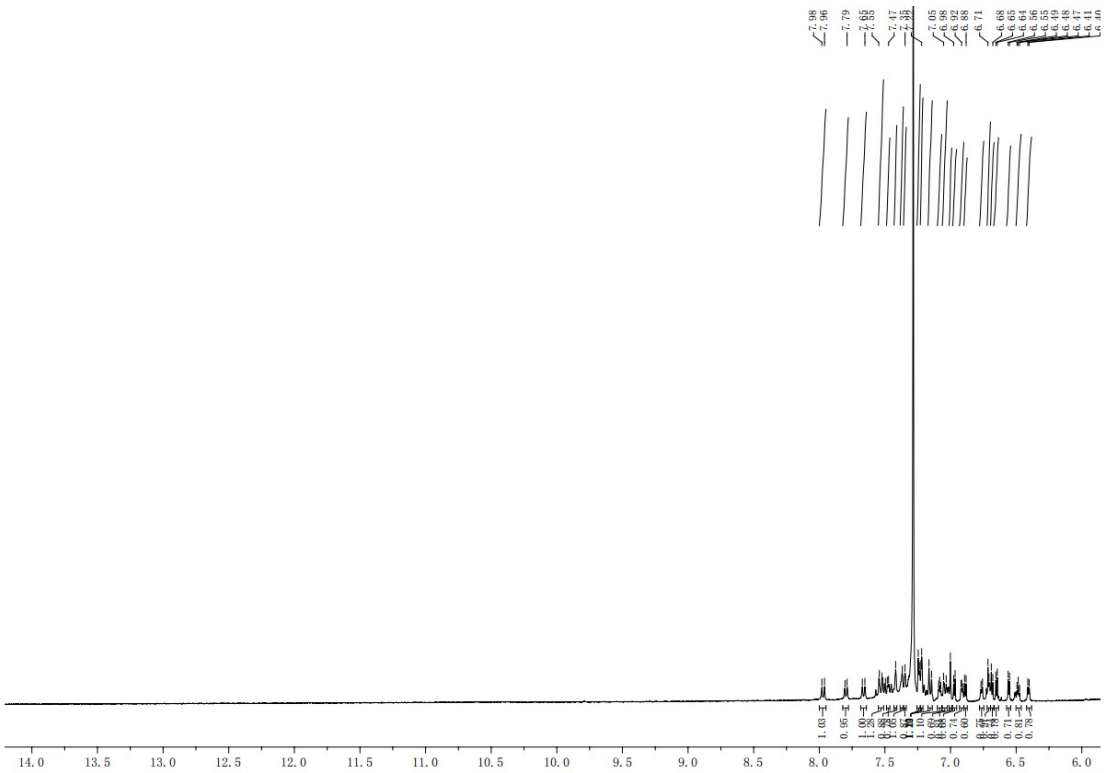

Figure S4. ^{1}H NMR spectrum of **2Pd** recorded at 298 K in $CDCl_3$.

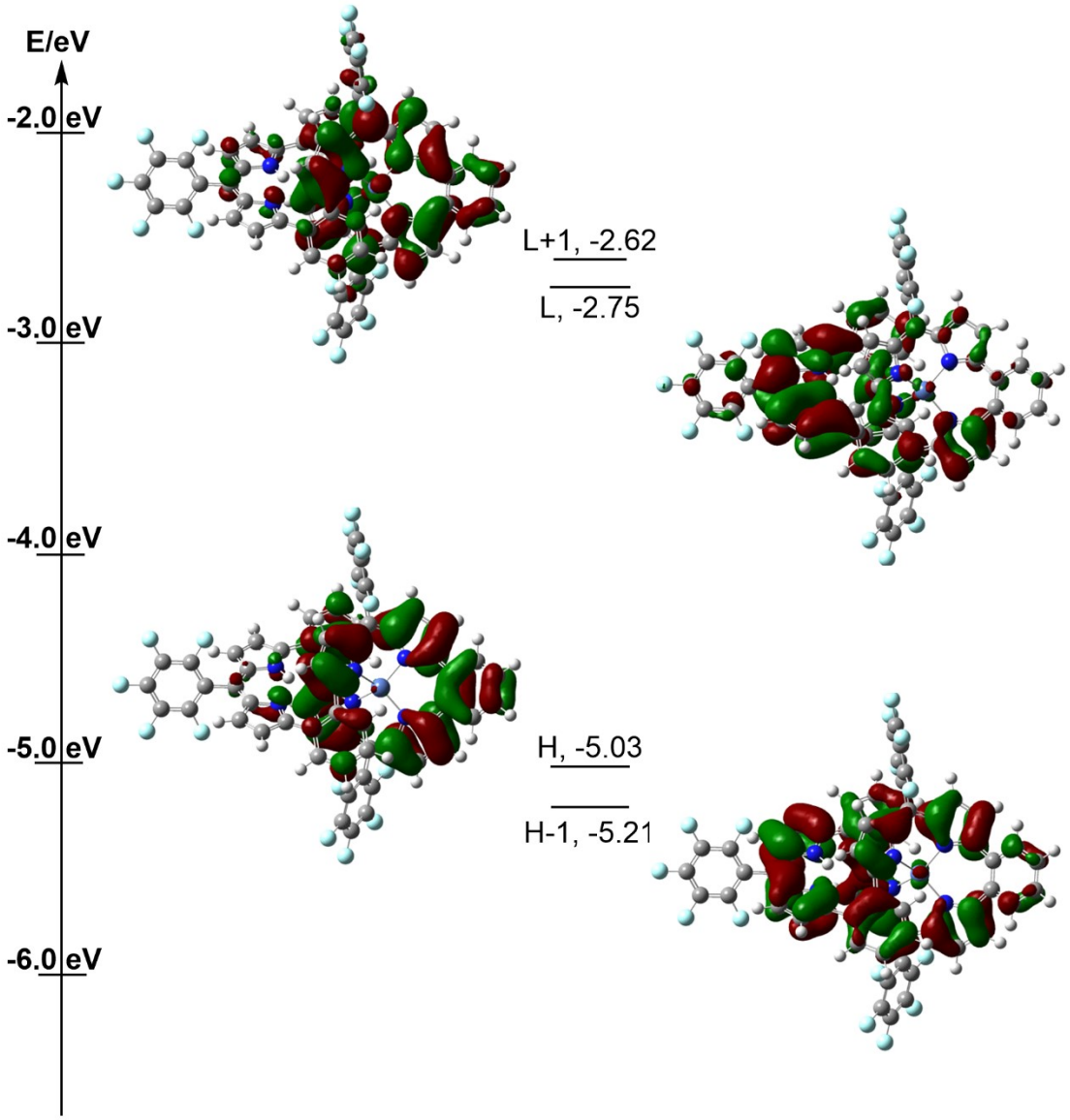

Figure S5. Frontier molecular orbital and energy levels of **1Ni**, calculated at the B3LYP/6-31G(d, p) basis set.

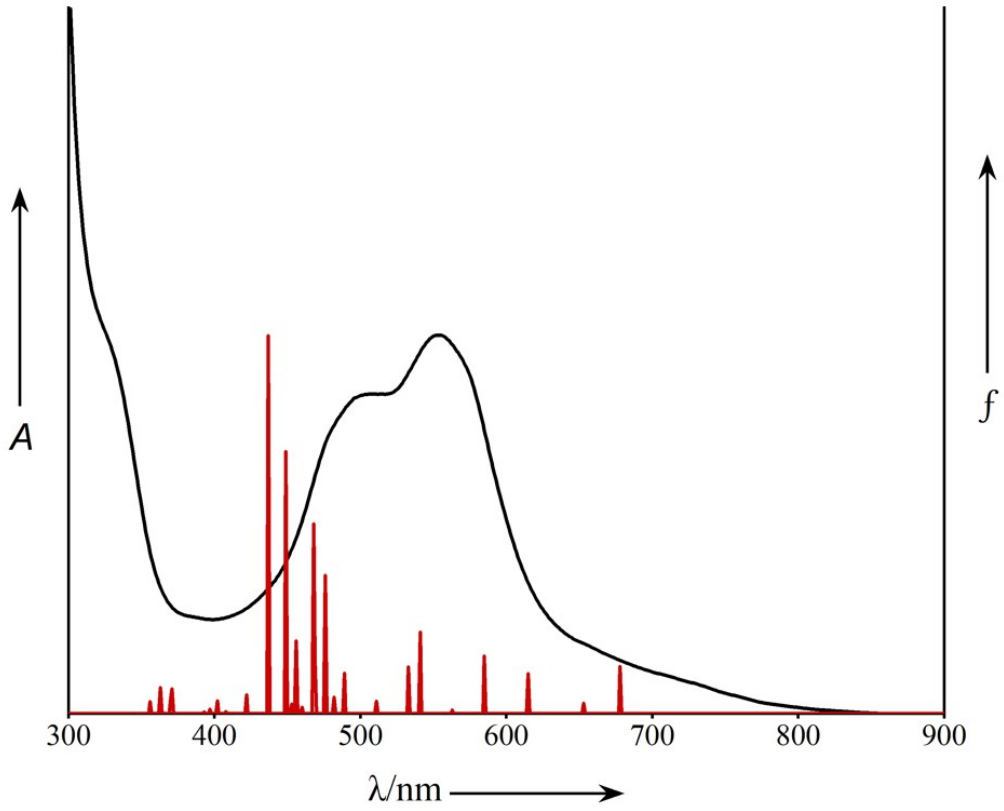

Figure S6. The UV-Vis absorption spectrum (black line, left axis) and oscillator strengths (red bar, right axis), which is calculated at the B3LYP/6-31G(d,p) level of theory of **1Ni**.

Table S1. Major composition, vertical excitation energies (*E*, eV/nm) and oscillator strengths (*f*) for the lowest optically allowed excited states of **1Ni**, calculated at the B3LYP/6-31G(d,p) level of theory.

State	Major Composition	**Exci.** (eV/nm)	***f***
1	H-1 -> L+1 (0.20012) H -> L (0.64055)	1.8280/678.26	0.0411
2	H-1 -> L (0.61752) H -> L+1 (0.24575)	2.0164/614.87	0.0350
3	H-2 -> L (0.28973) H-2 -> L+1 (0.32474) H-1 -> L+1 (-0.29614) H -> L+2 (0.3473)	2.2916/541.04	0.0713
4	H-2 -> L (0.26743) H-2 -> L+2 (0.24239) H-1 -> L+2 (0.31212)	2.6028/476.35	0.1207
5	L-4 -> L+1 (0.32944) H-2 -> L+1 (-0.25867) H -> L+2 (0.22254)	2.6493/467.99	0.1654

*****: H = HOMO, Highest Occupied Molecular Orbital, L = LUMO, Lowest Unoccupied Molecular Orbital.

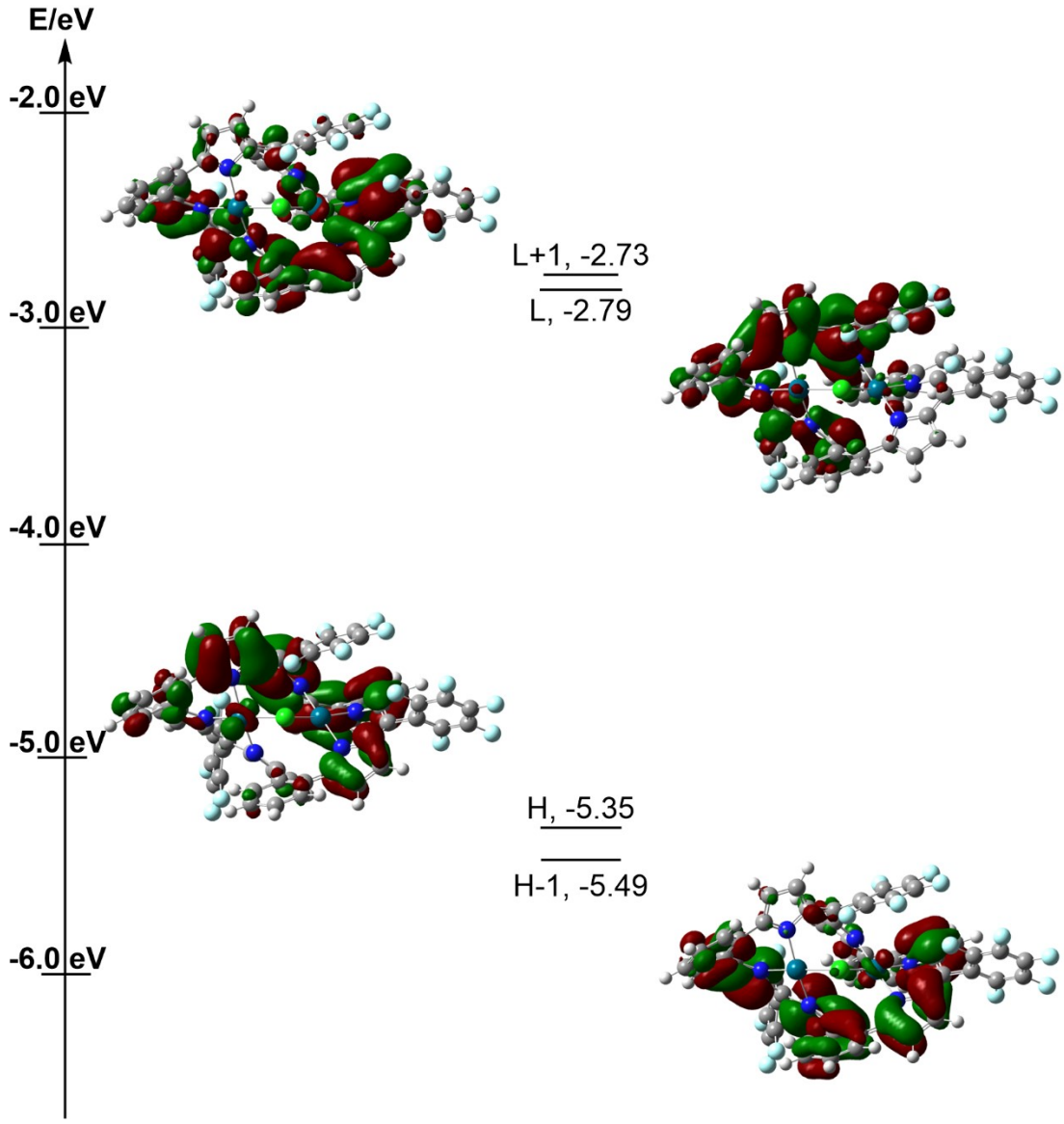

Figure S7. Frontier molecular orbital and energy levels of **2Pd**, calculated at the B3LYP/6-31G(d, p) (C, H, N, F, Cl, O) + SDD (Pd) basis set.

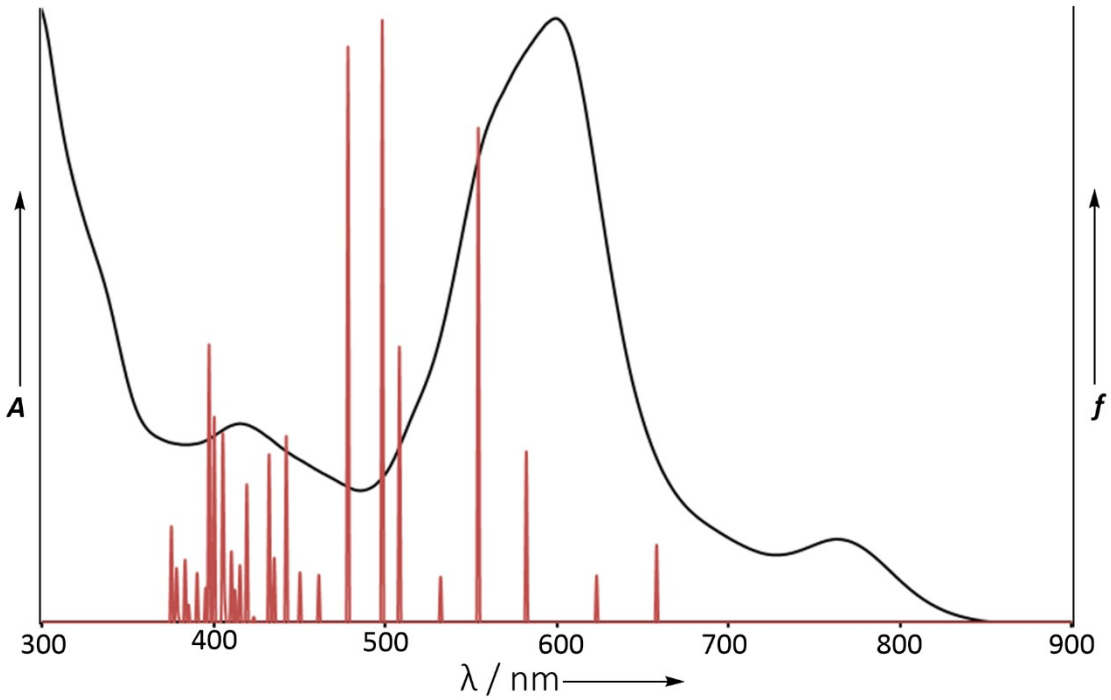

Figure S8. The UV-Vis absorption spectrum (black line, left axis) and oscillator strengths (red bar, right axis), which is calculated at the B3LYP/6-31G(d,p)+SDD level of theory of **2Pd**.

Table S2. Major composition, vertical excitation energies (*E*, eV/nm) and oscillator

strengths (*f*) for the lowest optically allowed excited states of **2Pd**, calculated at the B3LYP/6-31G(d,p)+SDD level of theory.

State	**Major Composition**	**Exci.** (eV/nm)	***f***
1	H-1 -> L+1 (0.16312) H -> L (0.63971)	1.8837/658.19	0.0241
2	H-1-> L (-0.23932) H-1-> L+1 (0.12180) H -> L+1 (0.63861)	1.9901/623.02	0.0146
3	H-1-> L+1 (0.61041)	2.2379/554.02	0.1530
4	H-2 -> L+1 (0.43646) H-1-> L+2 (-0.29988) H -> L+2 (0.30493)	2.4915/497.62	0.1863
5	H-2 -> L+1 (0.34844) H-1 -> L+2 (0.49580)	2.5961/477.57	0.1781

*****: H = HOMO, Highest Occupied Molecular Orbital, L = LUMO, Lowest Unoccupied Molecular Orbital.

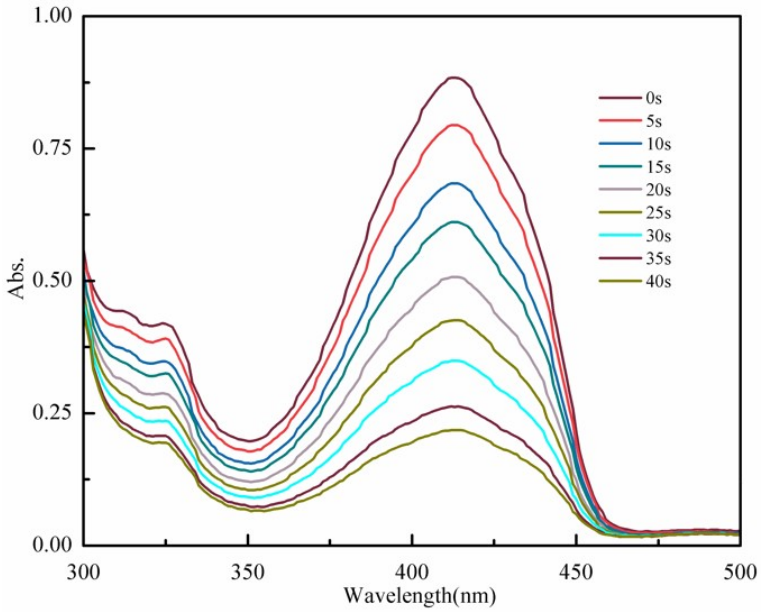

Figure S9. UV-vis absorption spectra of $^1O_2$ generation of MB with DPBF in CH_2Cl_2 upon photoirradiation.

5. Crystal Data

Table S3. Crystal data of **1Ni**.

Empirical formula	$C_{64}H_{27}C_{l2}F_{15}N_6Ni$
Formula weight	1294.52
Temperature/K	242.30
Crystal system	monoclinic
Space group	P21/c
a/Å	12.4402(8)
b/Å	40.906(2)
c/Å	10.2419(5)
α/°	90
β/°	93.779(2)
γ/°	90
Volume/Å^3	5200.5(5)
Z	4
ρcalcg/cm^3	1.653
μ/mm^{-1}	0.582
F(000)	2600.0
Crystal size/mm^3	0.12 × 0.1 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.838 to 55.25
Index ranges	-13≤h≤16, -53≤k≤49, -12≤l≤ 13
Reflections collected	48141
Independent reflections	12039 [R_{int} = 0.0777, R_{sigma} = 0.0758]
Data/restraints/parameters	12039/0/793
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0846, wR_2 = 0.2120
Final R indexes [all data]	R_1 = 0.1324, wR_2 = 0.2455
Largest diff. peak/hole / e Å^{-3}	0.87/-1.58

Figure S10. Crystal structure of **1Ni**. The thermal ellipsoids represent for 40% probability.

Table S4. Crystal data of **2Pd**.

Empirical formula	$C_{63}H_{24}ClF_{15}N_6Pd_2$
Formula weight	1398.13
Temperature/K	193.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	19.170(2)
b/Å	28.916(3)
c/Å	23.167(2)
α/°	90
β/°	112.689(5)
γ/°	90
Volume/Å^3	11848(2)
Z	8
ρcalcg/cm^3	1.568
μ/mm^{-1}	4.127
F(000)	5504.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.346 to 108.302
Index ranges	$-19 \leq_h \leq 23$, $-31 \leq_k \leq 34$, $-26 \leq_l \leq 27$
Reflections collected	60170
Independent reflections	21031 [R_{int} = 0.1211, R_{sigma} = 0.1534]
Data/restraints/parameters	21031/1604/1567
Goodness-of-fit on F^2	0.996
Final R indexes [I>=2σ (I)]	R_1 = 0.0802, wR_2 = 0.2034
Final R indexes [all data]	R_1 = 0.1771, wR_2 = 0.2565
Largest diff. peak/hole / e Å^{-3}	0.67/-1.14

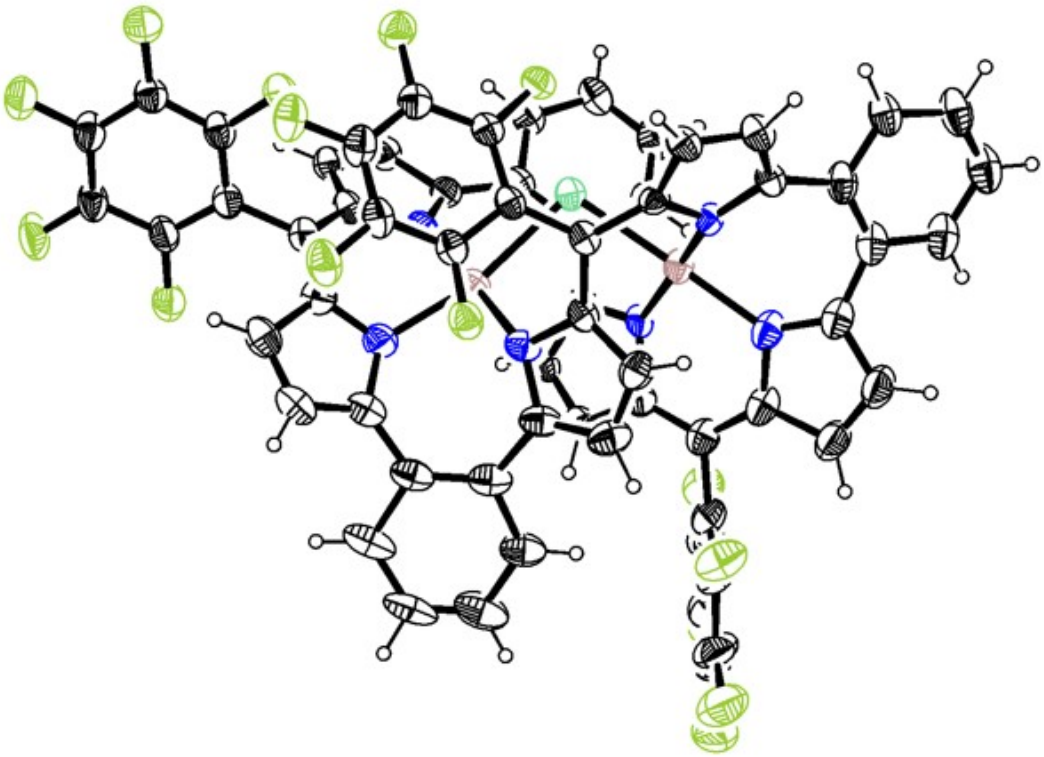

Figure S11. Crystal structure of **2Pd**. The thermal ellipsoids represent for 40% probability.

6.Cartesian Coordinates

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Charge = 0
Spin = Singlet
Total energy: E = -XXX a.u.

Ni	-2.40288700	0.01078400	-0.03410000
N	-1.04925100	0.99950500	-0.90460300
N	-3.57160700	1.53690700	-0.07566000
N	-3.70061900	-1.43109400	0.04808600
N	-1.10372700	-0.96538600	0.99078600
N	2.73418100	0.65252800	1.08813000
N	2.60257300	-0.72751100	-1.25256600
C	-1.71875100	3.19272300	-0.12098700
C	-2.99167200	2.75997000	0.30325200
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C	-5.16002900	2.87678400	0.87947600
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C	-5.94700400	0.89107500	-0.49292100
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C	-7.98020200	-0.16047900	-2.15858200
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C	4.70398200	-0.09949400	-0.19475800
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C	-1.18858700	6.73792000	-1.40262500
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F	6.30529800	2.24529400	-0.45327700
F	-0.70134300	8.76330500	-0.28378500
F	-0.72746100	7.46356400	2.12232100
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C	-1.02329200	-5.36968100	-0.19029300
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H	3.76972000	1.91344200	3.92136000
H	5.75016100	1.06355200	2.31776900
H	5.56357100	-1.36567700	-2.71799600
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2Pd
Charge = 0
Spin = Singlet
Total energy: E = -4952.51207249 a.u.

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Pd	1.08495900	-0.36490500	0.19712900
Cl	0.26695300	1.79294300	0.78834900
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C	2.28132200	3.09295400	-1.66584200
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C	2.24316300	1.15753200	-3.06588600
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C	-1.71596200	0.38805900	-2.80086500
C	-1.85787300	-0.97903000	-2.74319600
C	-0.80662300	-1.47482500	-1.92999000
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H	-2.54559100	-3.29579300	1.46912700

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