Supporting Information

Synergistic meso-β regulation of porphyrin: squeezing the band gap into near-infrared I/II Region

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Contents

1. Materials and methods

All reagents and solvents were commercial reagent grade and used without further purification. HR-ESI-MS data were recorded on a Thermo Scientific Q Exactive MS using a positive ion mode. MALDI-TOF MS data were measured on a Bruker Daltonics autoflex II spectrometer. The NMR spectra were measured on a Bruker AVANCE III HD-400 at 298 K. X-ray diffraction data were collected on a Bruker D8 Venture with GaK\α radiation (λ = 1.34139 Å) at 190(2) K. UV-visible-NIR absorption spectra were measured on a Shimizu UV-2500 spectrophotometer. MCD spectra were measured on a JASCO J-810 spectrometer producing a magnetic field of up to 1.50 T with both parallel and antiparallel fields. Fluorescence spectra were obtained using a FluoroLog-UltraFast (HORIBA Instrument Inc, Edison). Phosphorescence spectra were obtained using FLS 980-STM. The thermal imagines were recorded by an IR-thermal camera (FLIR ONE PRO).

Theoretical calculations: The theoretical calculations were carried out using the Gaussian 09 program[1]. Geometry optimizations and excited-state transitions were performed using density functional theory (DFT) and time-dependent DFT (TD-DFT) at the level of B3LYP/6-31G(d,p) (for C, N, Si, F, O, H) + SDD (for metal ions). The triisopropylsilylethynyl was replaced by trimethylsilylethynyl in the theoretical calculations. NICS values[2] were obtained by GIAO method. The ICSS surface was obtained based on the calculated NICS values of around 125000 points for each molecule and visualized by Multiwfn[2-4]. The hole and electron distributions were obtained by Multiwfn and visualized by VMD program[3, 5, 6].The ESP surface was plotted by VMD program based on the data outputted by Multiwfn[3, 6]. Anisotropy of the induced current density (ACID) plots were calculated using the software package developed by Prof. R. Herges[7]. Magnetically induced current densities were calculated using the GIMIC program[8-10]. The spin–orbit coupling (SOC) matrix elements were obtained using TD-DFT calculations in Orca 5.0.3[11, 12]. The B3LYP functional with the Def2-TZVP basis was used, and the relativistic corrections were performed for the heavy-atom contained system using the Zero-Order Regular Approximation (ZORA).

2. Synthesis procedure and characterization data

Synthesis of **Zn-3**: **3** (24 mg, 0.015 mmol) was added to $CHCl_3$ (20 mL) in a 50 mL round-bottom flask. $Zn(OAc)_2{\cdot}2H_2O$ (32.9 mg, 0.15 mmol) was dissolved in MeOH (10 mL) and poured into the $CHCl_3$ solution of **3**. Then the reaction mixture was stirring for 3 h. The $CHCl_3$ was removed under reduced pressure and reaction mixture was washed by brine to remove excess $Zn(OAc)_2{\cdot}2H_2O$. The residue was purified on silica gel chromatography using CH_2Cl_2/n-hexane (7:3, v/v) as eluents, and the green fraction was collected and subsequent recrystallization from CH_2Cl_2/CH_3OH was to afford pure **Zn-3** (22.5 mg, 0.014 mmol, 93%) as green solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (m, 2H), 7.50–7.45 (m, 2H), 7.43–7.36 (m, 4H), 7.17 (m, 2H), 7.12 (s, 2H), 7.02– 6.95 (m, 8H), 6.92 (s, 4H), 2.73–2.54 (m, 6H), 2.32–2.15 (m, 10H), 1.80–1.67 (m, 12H), 1.59–1.49 (m, 72H). UV-vis (CH_2Cl_2): λ_{max} ($\varepsilon{\cdot}M^{-1}{\cdot}cm^{-1}$) = 482 (219300), 618 (12800), 666 (10000); HR-MS (ESI): m/z calcd. For $C_{104}H_{124}ZnN_4Si_4$: 1604.8189; found: 1604.8138 $[M]^+$. MALDI-TOF MS: m/z calcd for $C_{96}H_{108}ZnN_4Si_4$:1492.694; found: 1492.778 $[M\text{-}4C_2H_4]^+$.

Synthesis of **Zn-TNP**: **Zn-3** (23 mg, 0.014 mmol) was heated at 300 °C under vacuum (2 mm Hg) for 30 min and turned into quantitative **Zn-TNP** (21 mg, 0.014 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.90 (s, 8H), 8.41 (m, 8H), 7.75 (m, 8H), 1.72 (m, 12H), 1.45 (m, 72H). UV-vis (CH_2Cl_2): λ_{max} ($\varepsilon{\cdot}M^{-1}{\cdot}cm^{-1}$)

= 541 (135900), 732 (5940), 807 (34400); HR-MS (ESI): m/z calcd. For $C_{96}H_{108}ZnN_4Si_4$: 1492.6937; found: 1492.6921 $[M]^+$. MALDI-TOF MS: m/z calcd for $C_{96}H_{108}ZnN_4Si_4$:1492.694; found: 1492.845 $[M]^+$.

Synthesis of **Pt-3**: **3** (24 mg, 0.015 mmol), CH_3COONa (123 mg, 1.5 mmol) and $PtCl_2$ (8 mg, 0.03 mmol) were added to acetic acid (30 mL) in a 50 mL round-bottom flask. The mixture was refluxed at 118 ºC for 24 h under nitrogen atmosphere. The reaction was quenched with H_2O (10 mL). Subsequently, the reaction mixture was washed twice with water and three times with saturated $NaHCO_3$ solution, dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified on silica gel chromatography using CH_2Cl_2/n-hexane (1:9, v/v) as eluents. The green fraction was collected and subsequent recrystallization from CH_2Cl_2/CH_3OH was to afford pure **Pt-3** (24.3 mg, 0.014 mmol, 93%) as green solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (m, 2H), 7.52–7.40 (m, 6H), 7.17 (m, 2H), 7.06 (m, 6H), 6.93 (s, 2H), 6.82 (m, 6H), 2.55–2.37 (m, 6H), 2.14 (m, 10H), 1.67 (m, 12H), 1.47 (m, 72H). UV-vis (CH_2Cl_2): λ_{max} ($\varepsilon \cdot M^{-1} \cdot cm^{-1}$) = 464 (201200), 583 (21400); HR-MS (ESI): m/z calcd. For $C_{104}H_{124}PtN_4Si_4$: 1734.8524; found: 1734.8494. $[M]^+$ MALDI-TOF MS: m/z calcd for $C_{96}H_{108}PtN_4Si_4$:1623.730; found: 1623.358 $[M-4C_2H_4]^+$.

Synthesis of **Pt-TNP**: **Pt-3** (24.3 mg, 0.014 mmol) was heated at 300 ℃ under vacuum (2 mm Hg) for 30 min and turned into quantitative **Pt-TNP** (22.7 mg, 0.014 mmol). ^{1}H NMR (400 MHz, Toluene-d_8) : δ 11.17 (s, 8H), 8.66-8.64 (m, 8H), 7.65-7.62 (m, 8H), 1.67-1.61 (m, 12H), 1.46-1.44 (m, 72H). UV-vis (CH_2Cl_2): λ_{max} ($\varepsilon \cdot M^{-1} \cdot cm^{-1}$) = 516 (125500), 717 (15700), 789 (72400); HR-MS (ESI): m/z calcd. For $C_{96}H_{108}PtN_4Si_4$: 1622.7224; found: 1622.7272. $[M]^+$ MALDI-TOF MS: m/z calcd for $C_{96}H_{108}PtN_4Si_4$: 1623.730; found: 1623.290 $[M]^+$.

3. Mass spectra

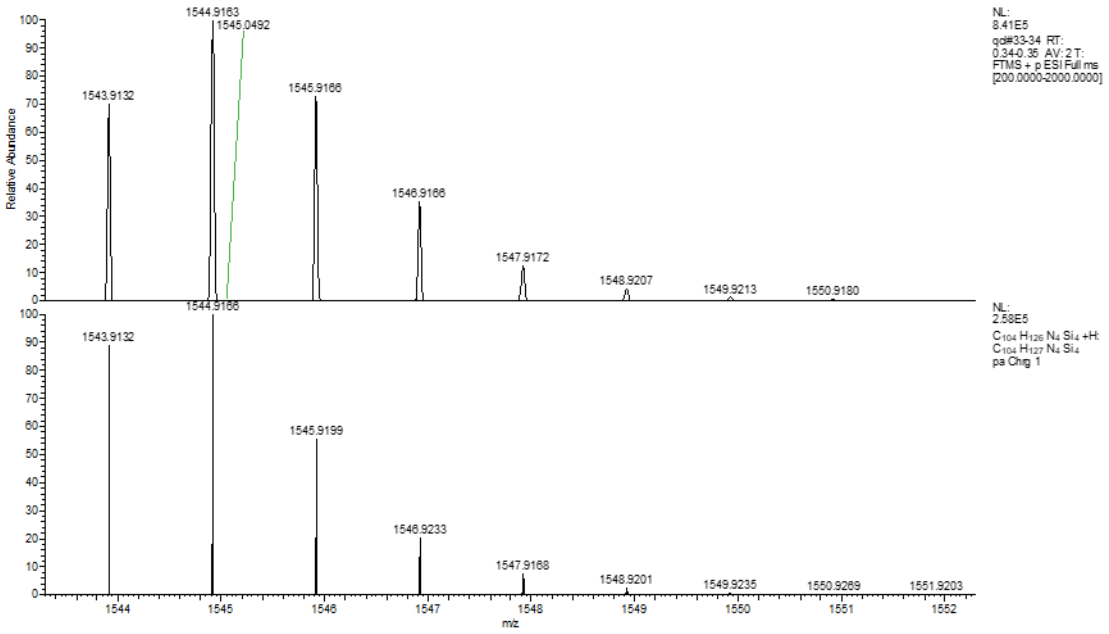

Figure S1. HR-ESI-MS spectrum of **3.**

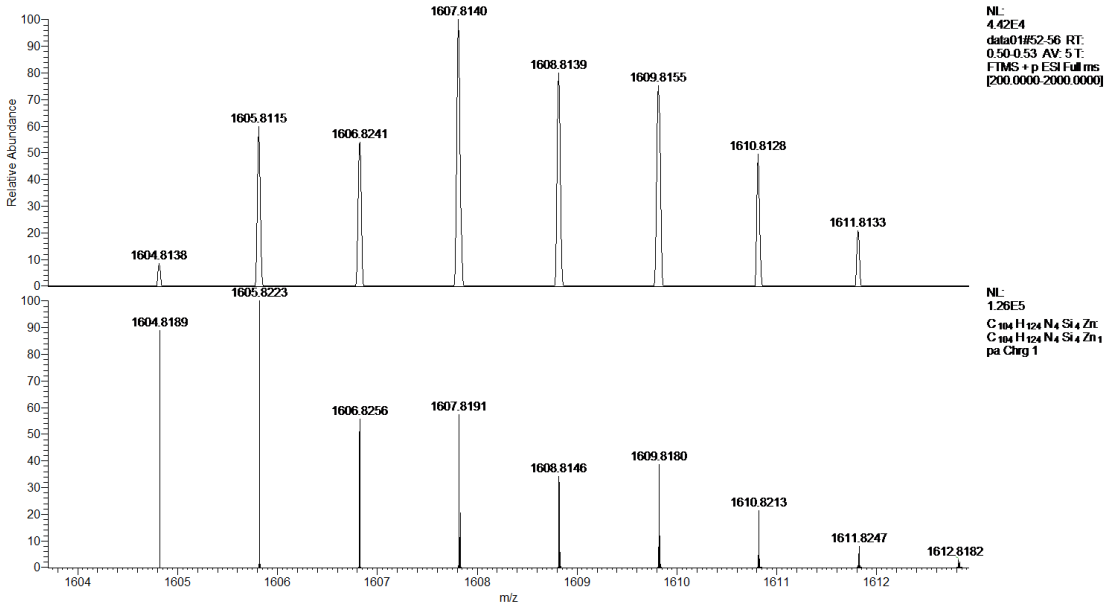

Figure S2. HR-ESI-MS spectrum of **Zn-3.**

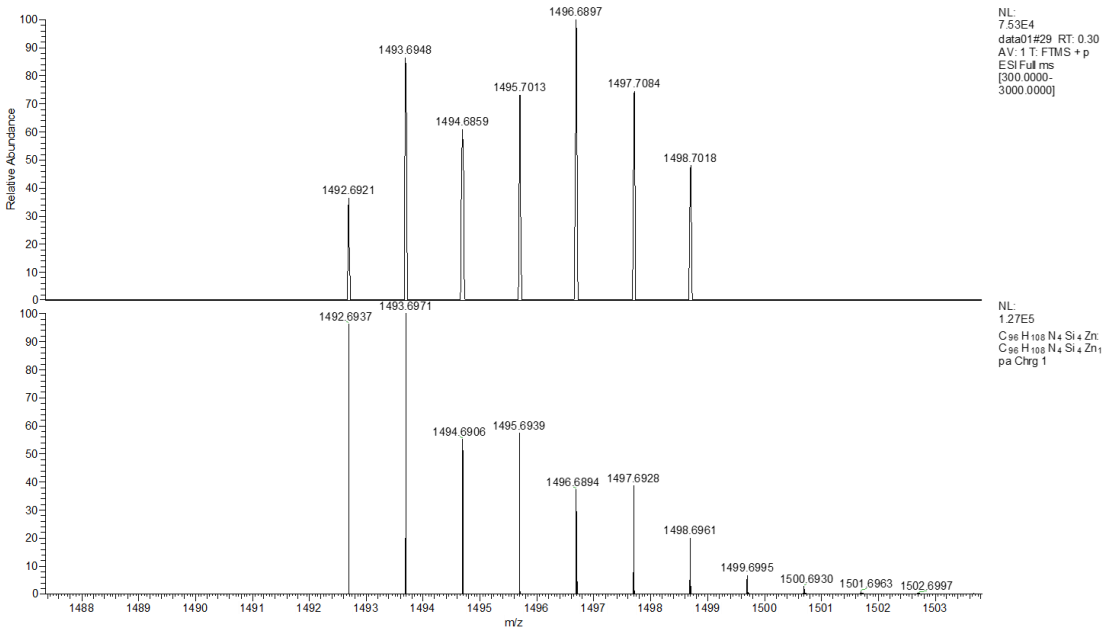

Figure S3. HR-ESI-MS spectrum of **Zn-TNP.**

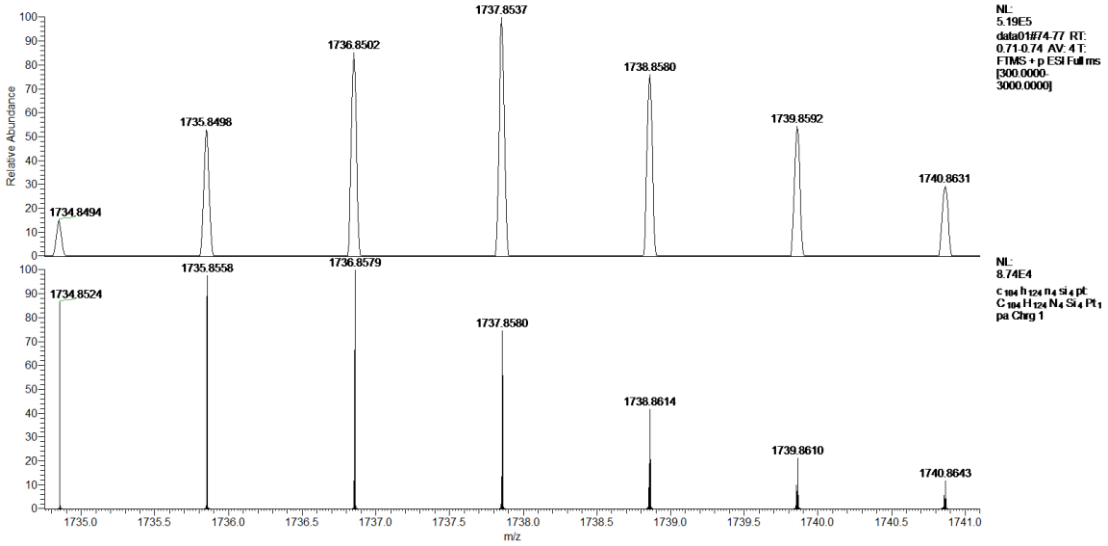

Figure S4. HR-ESI-MS spectrum of **Pt-3.**

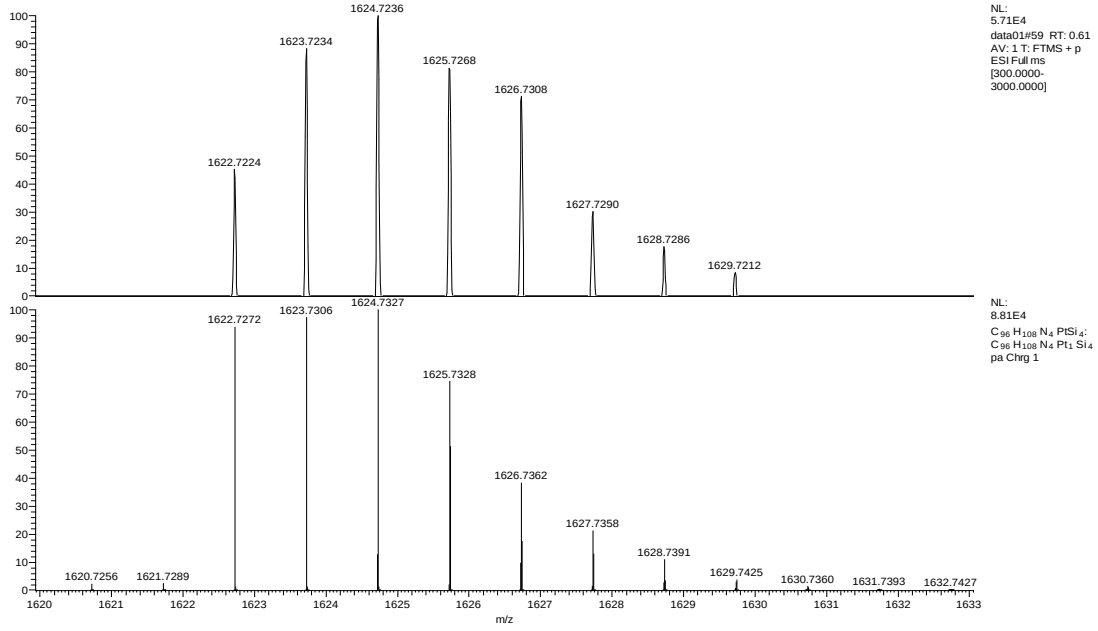

Figure S5. HR-ESI-MS spectrum of **Pt-TNP.**

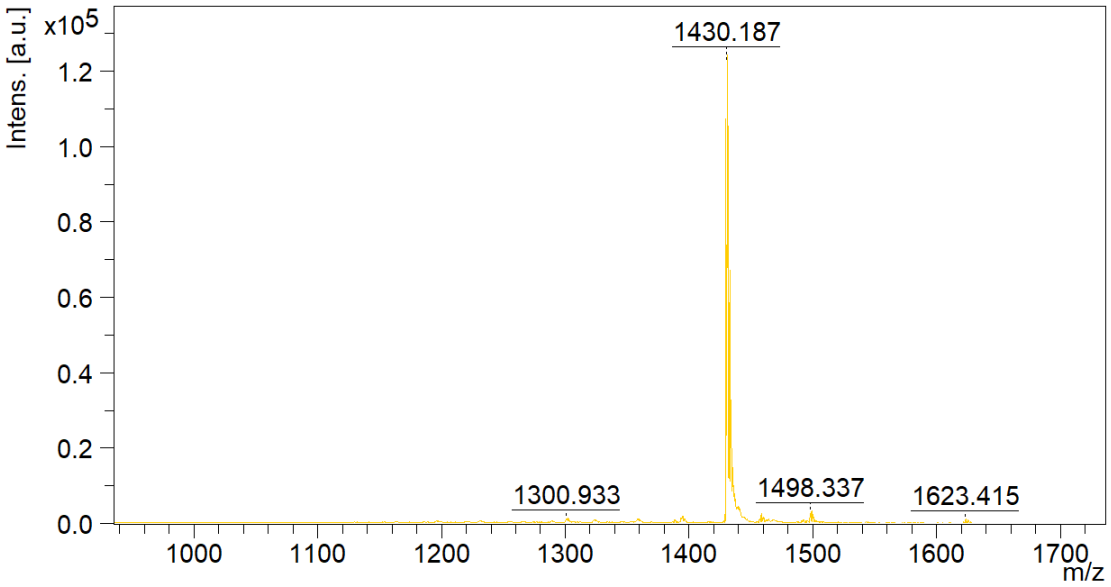

Figure S6. MALDI-TOF mass spectrum of **3**.

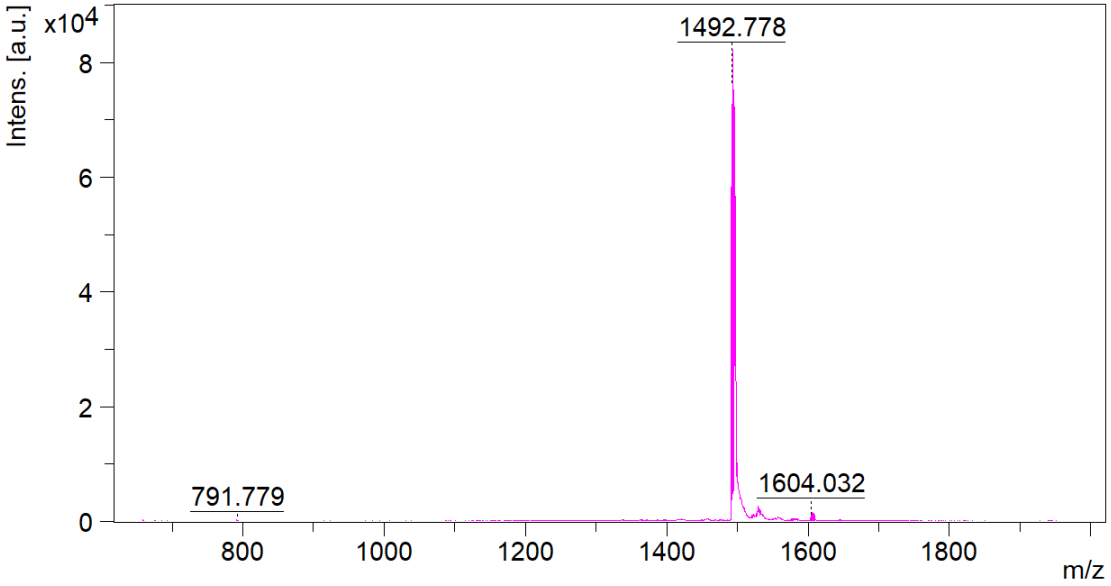

Figure S7. MALDI-TOF mass spectrum of **Zn-3**.

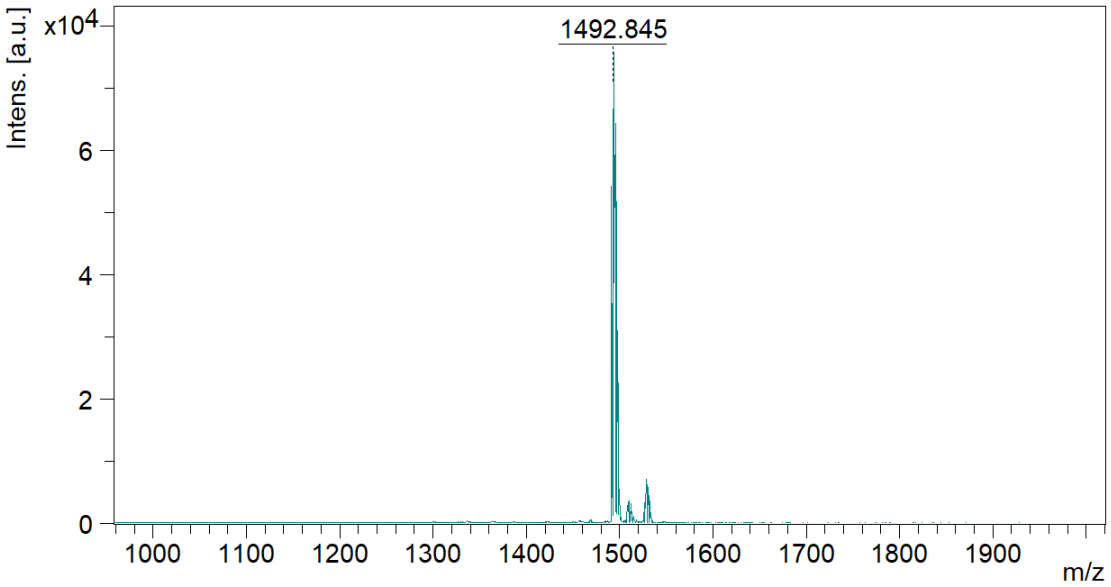

Figure S8. MALDI-TOF mass spectrum of **Zn-TNP**.

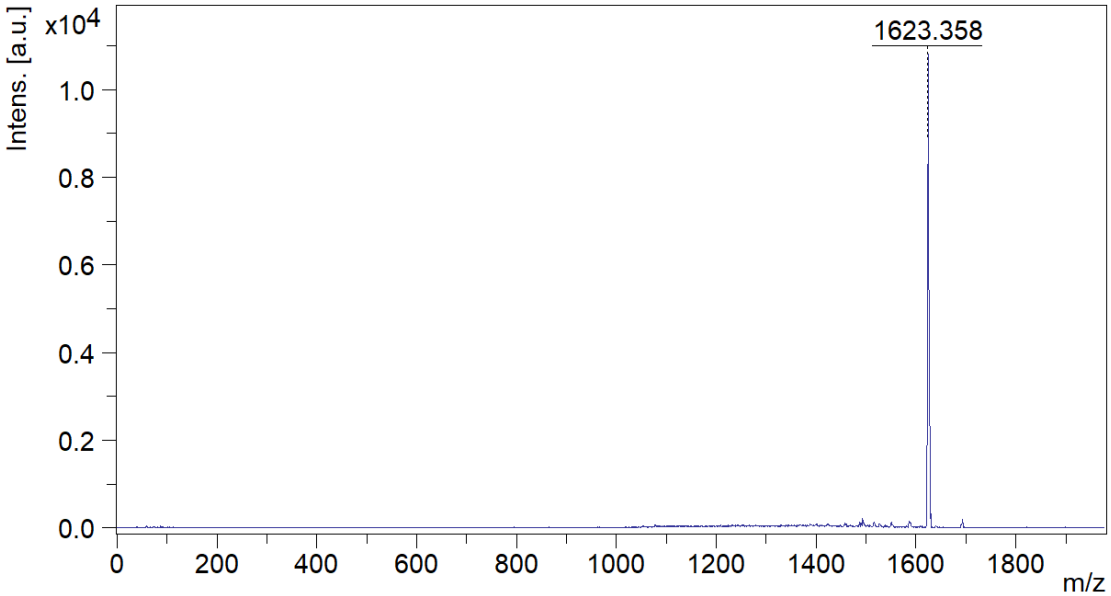

Figure S9. MALDI-TOF mass spectrum of **Pt-3.**

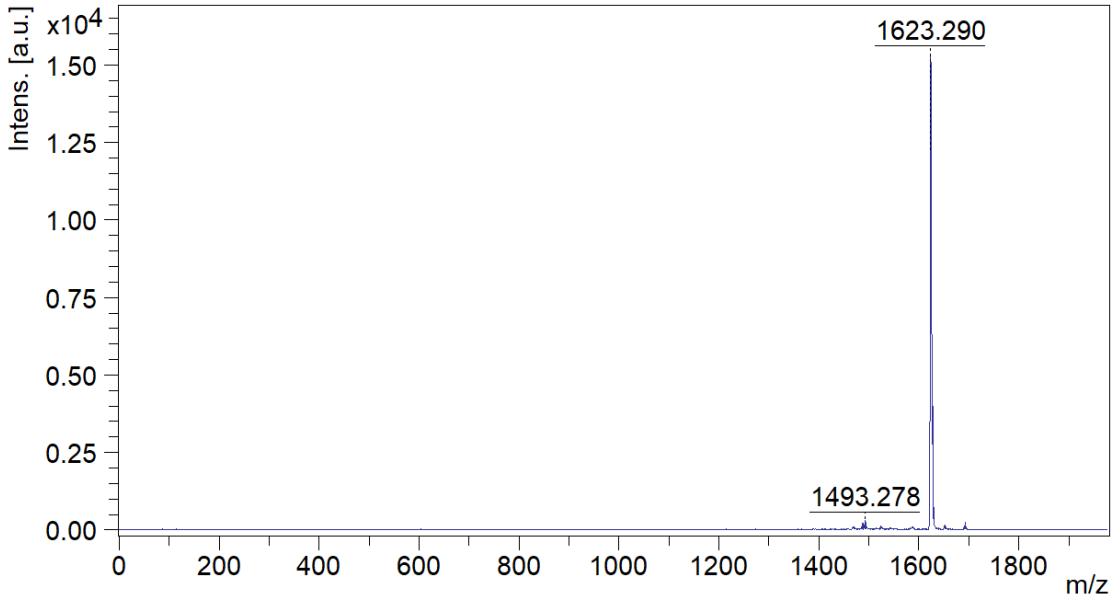

Figure S10. MALDI-TOF mass spectrum of **Pt-TNP.**

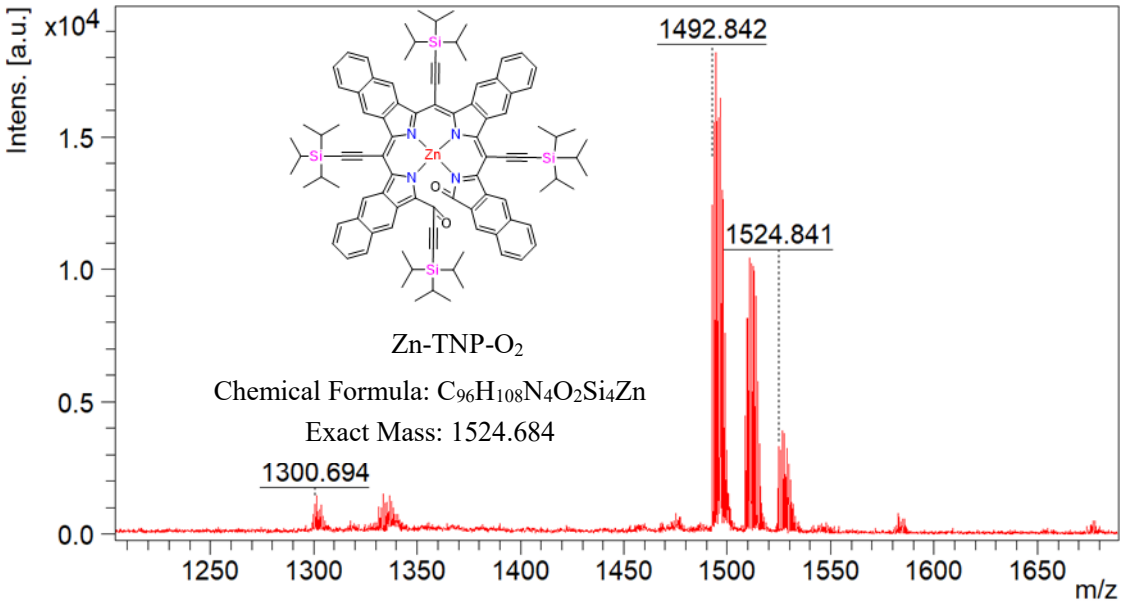

Figure S11. MALDI-TOF mass spectrum of the partially photodegraded **Zn-TNP** under ambient light. Inset: the structure of the proposed product after photo-oxidation.

4. NMR spectra

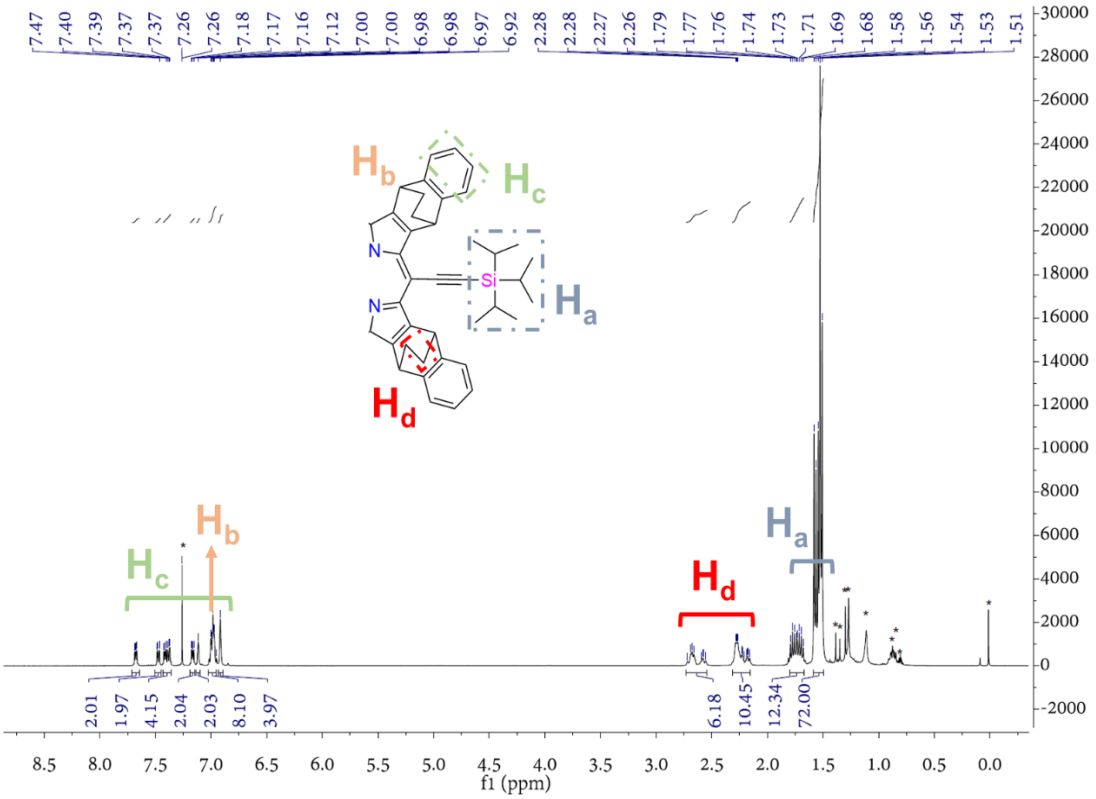

Figure S12. ^{1}H NMR spectrum of **Zn-3** in $CDCl_3$.

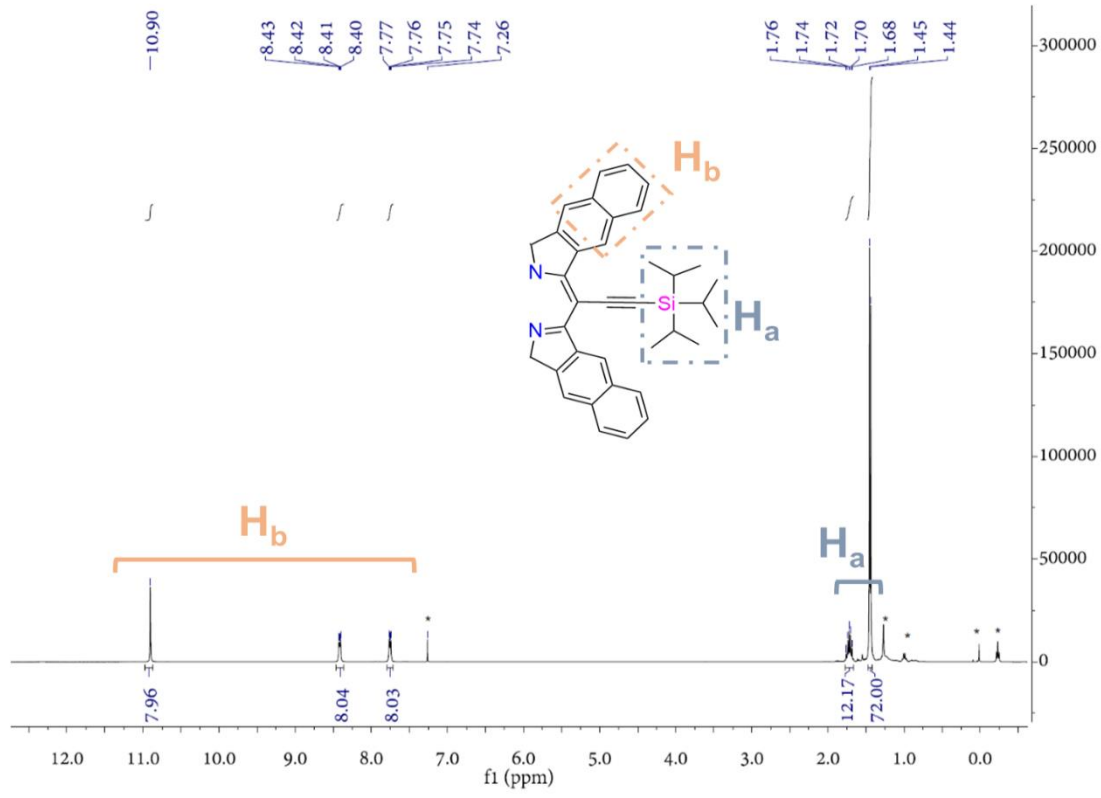

Figure S13. ^{1}H NMR spectrum of **Zn-TNP** in $CDCl_3$.

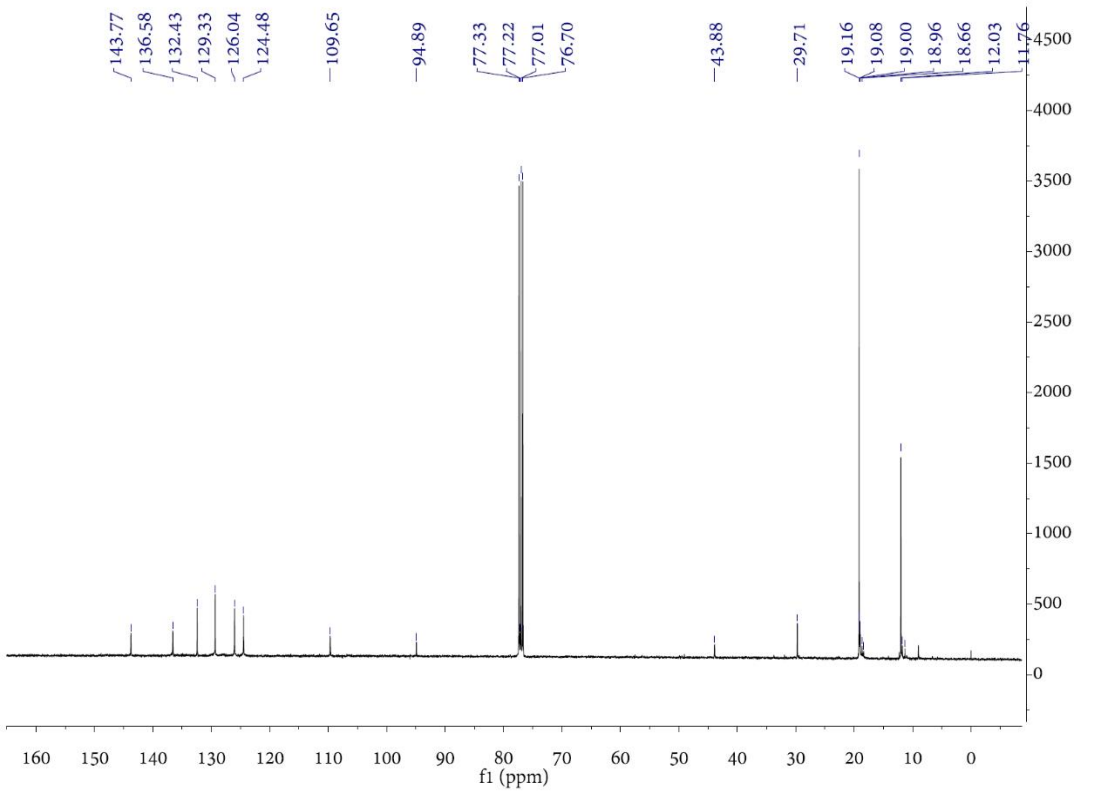

Figure S14. ^{13}C NMR spectrum of **Zn-TNP** in $CDCl_3$.

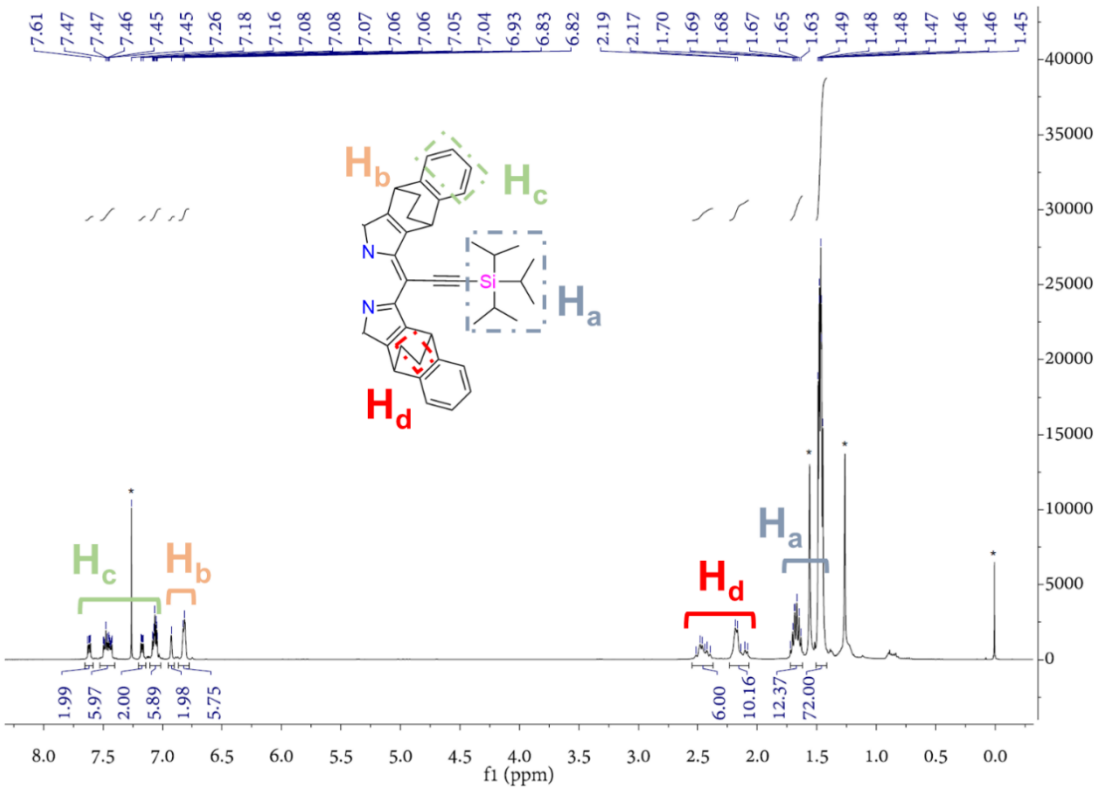

Figure S15. ^{1}H NMR spectrum of **Pt-3** in $CDCl_3$.

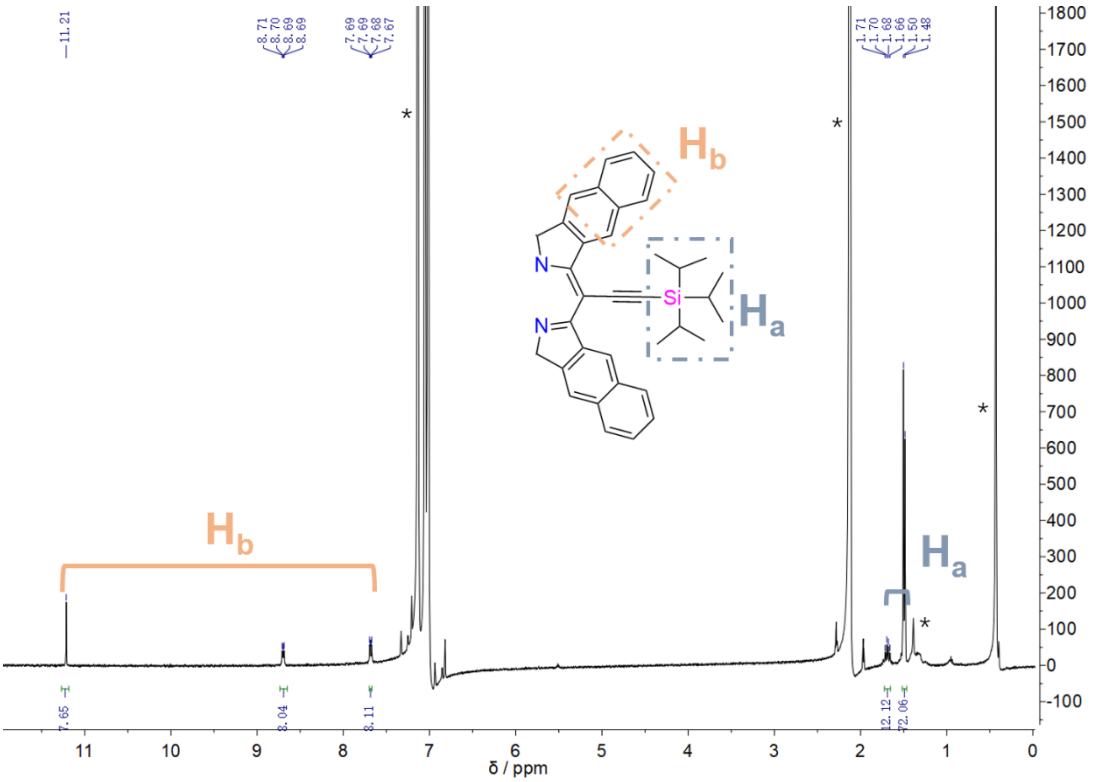

Figure S16. ^{1}H NMR spectrum of **Pt-TNP** in toluene-d_8.

5. Stability monitored by UV-vis absorption spectroscopy

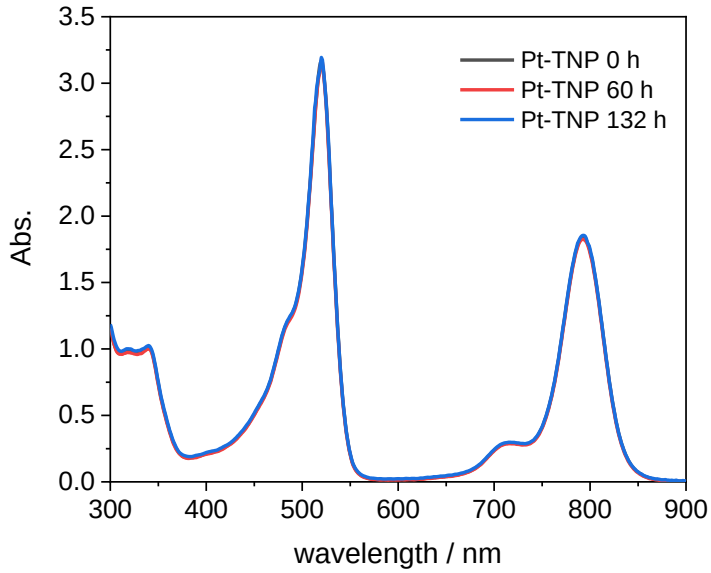

Figure S17. Time course of the absorbance change of **Pt-TNP** in toluene monitored by UV-vis-NIR spectroscopy under ambient conditions.

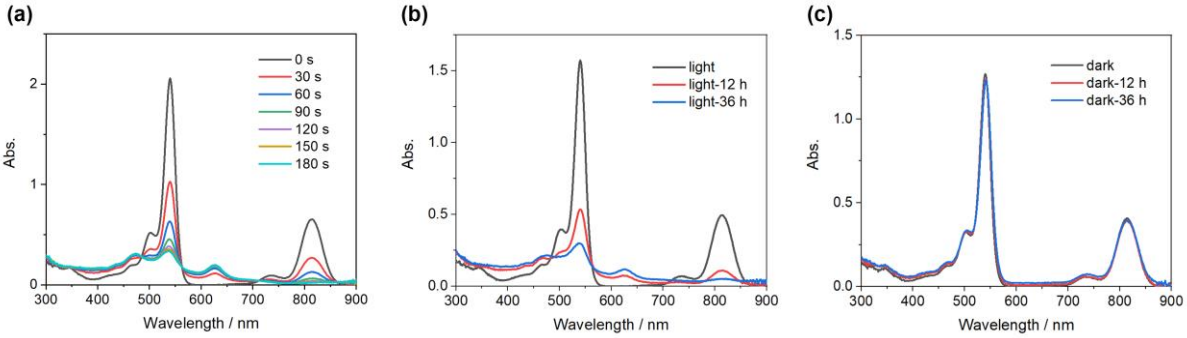

Figure S18. (a) The photothermal stability of **Zn-TNP** in toluene solution under the laser irradiation (808 nm, 0.3 W cm^{-2}). (b) Time course of the absorbance change of **Zn-TNP** in toluene under ambient light monitored by UV-vis-NIR spectroscopy. (c) Time course of the absorbance change of **Zn-TNP** in toluene in a dark environment monitored by UV-vis-NIR spectroscopy.

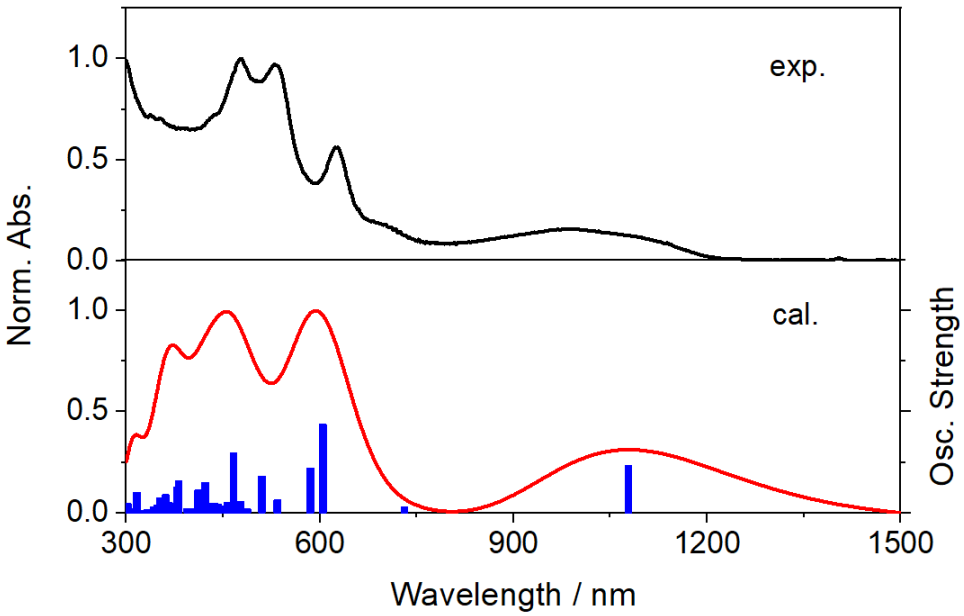

Figure S19. The experimental (up) and simulated (down) absorption spectra of **Zn-TNP-O₂** (FWHM= 3000 cm^{-1}), along with the TD-DFT calculated electronic transitions (blue bars).

6. Additional photophysical data

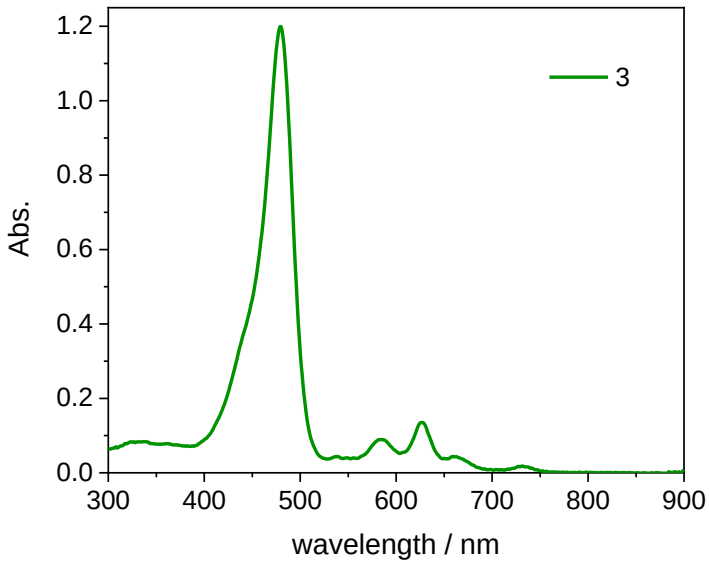

Figure S20. Absorption spectrum of **3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L).

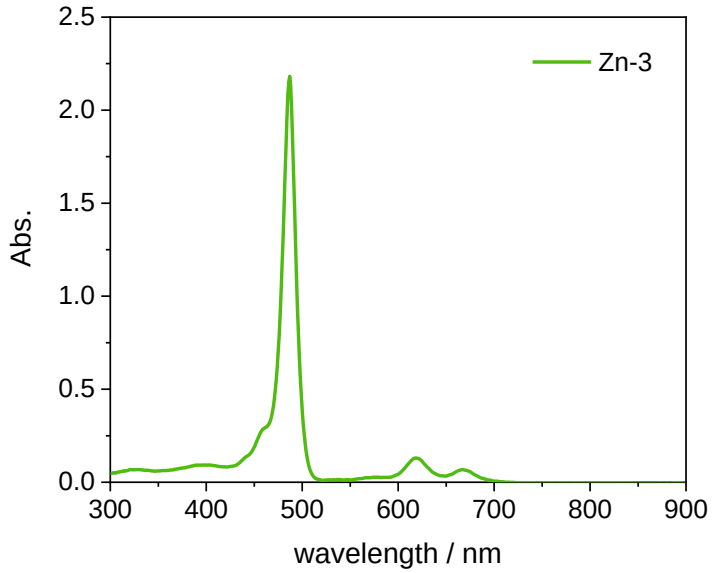

Figure S21. Absorption spectrum of **Zn-3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L).

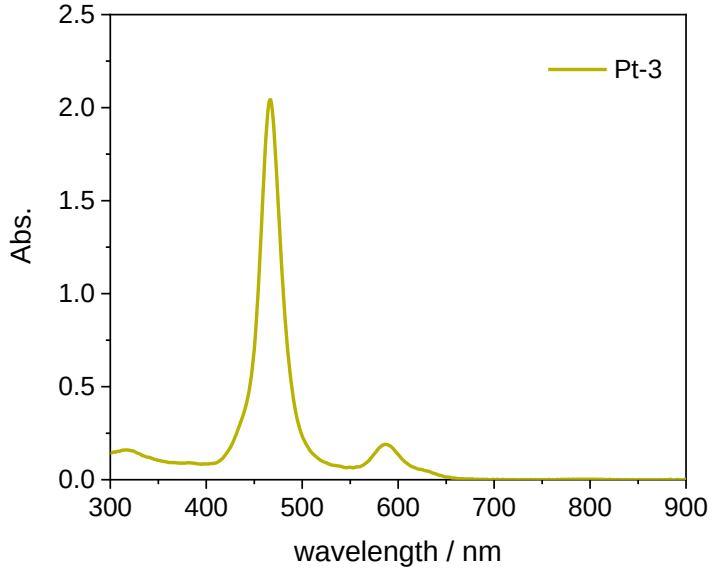

Figure S22. Absorption spectrum of **Pt-3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L)

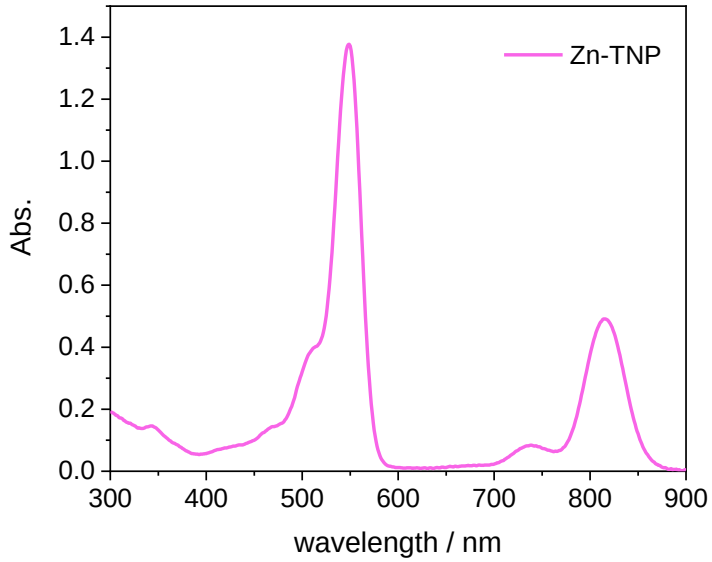

Figure S23. Absorption spectrum of **Zn-TNP** obtained in toluene (3 mL, $1*10^{-5}$ mol/L).

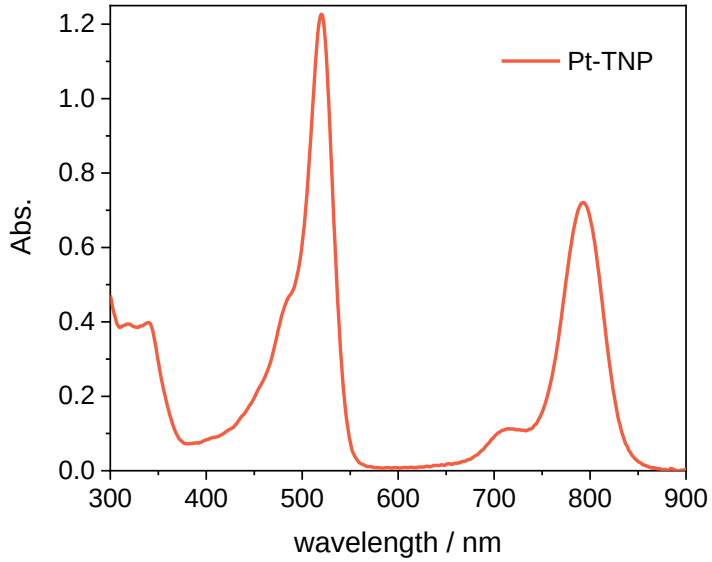

Figure S24. Absorption spectrum of **Pt-TNP** obtained in toluene (3 mL, $1*10^{-5}$ mol/L).

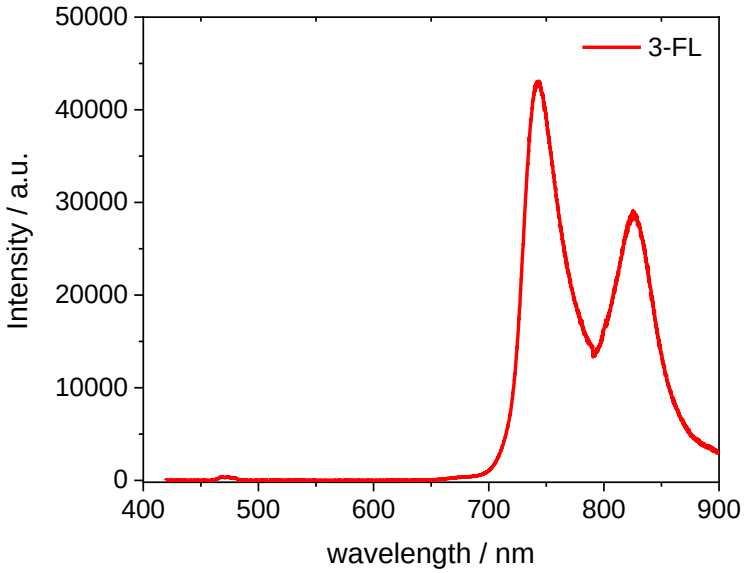

Figure S25. Fluorescent emission spectrum of **3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L) at room temperature with the excitation wavelength of the Soret band (λ_{ex} = 476 nm).

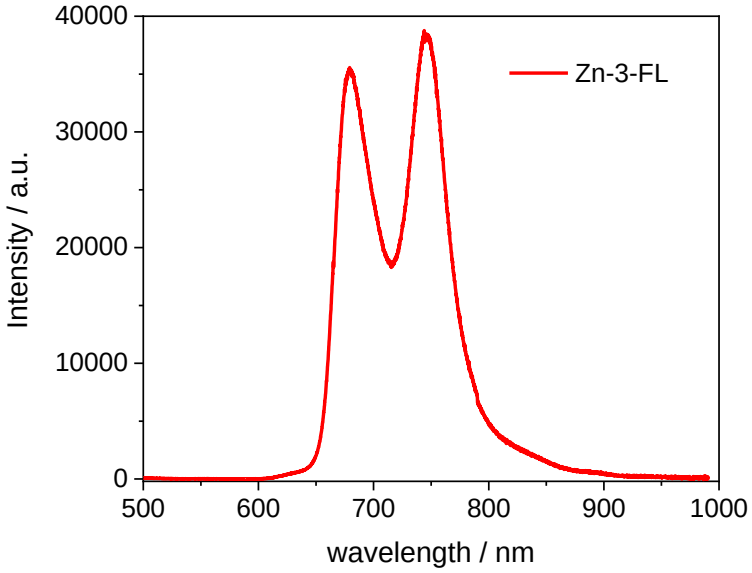

Figure S26. Fluorescent emission spectrum of **Zn-3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L) at room temperature with the excitation wavelength of the Soret band (λ_{ex} = 487 nm).

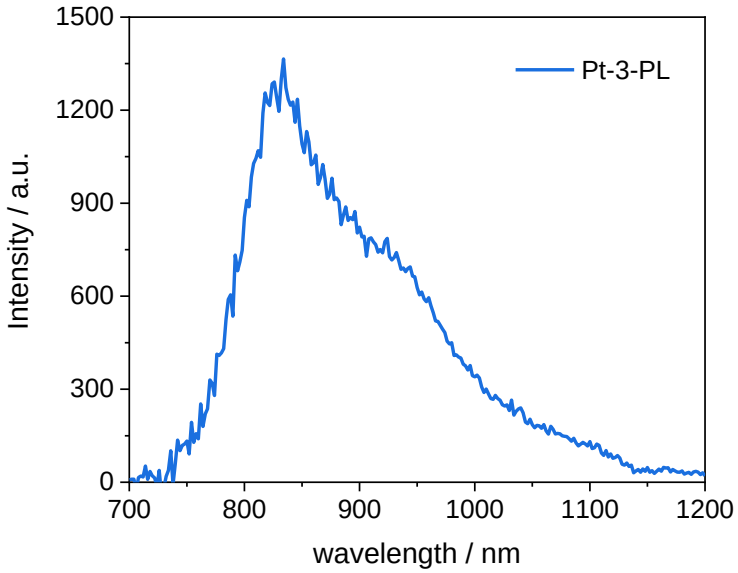

Figure S27. Phosphorescent emission spectrum of **Pt-3** obtained in toluene (3 mL, $1*10^{-5}$ mol/L) at room temperature with the excitation wavelength of the Soret band (λ_{ex} = 466 nm).

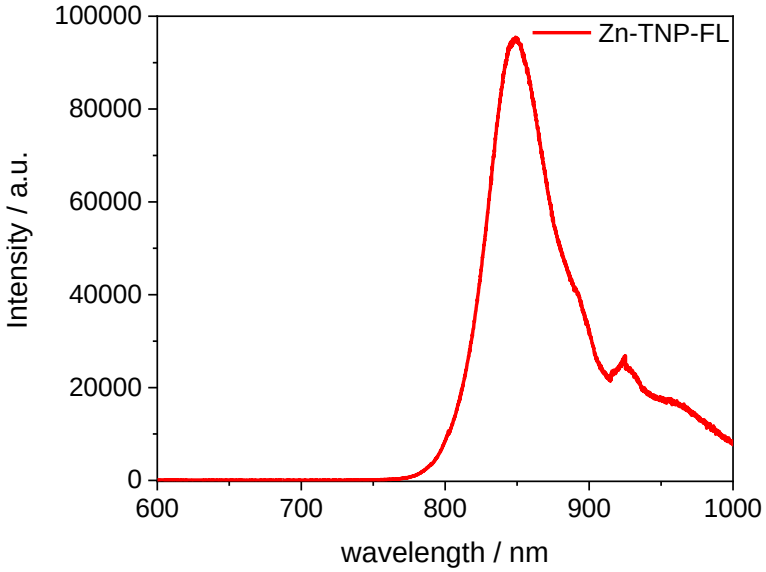

Figure S28. Fluorescent emission spectrum of **Zn-TNP** obtained in toluene (3 mL, $1*10^{-5}$ mol/L) at room temperature with the excitation wavelength of the Soret band (λ_{ex} = 549 nm).

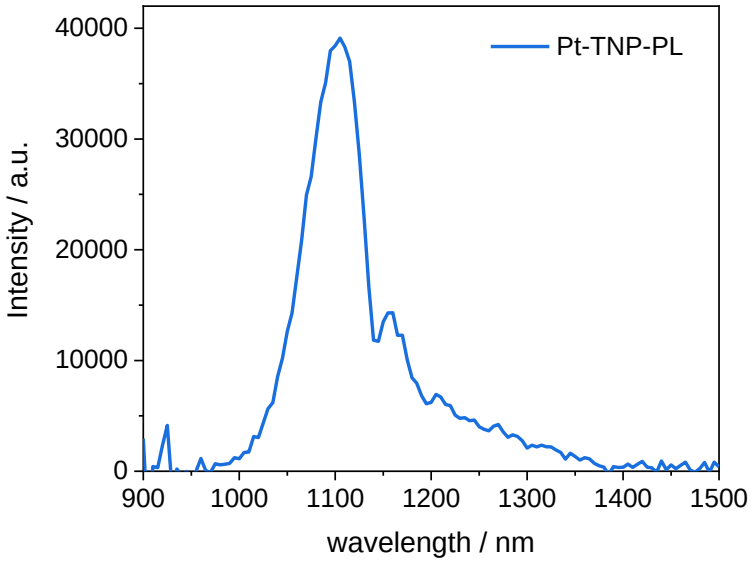

Figure S29. Phosphorescent emission spectrum of **Pt-TNP** obtained in toluene (3 mL, $1*10^{-5}$ mol/L) at room temperature with the excitation wavelength of the Soret band (λ_{ex} = 520 nm).

Table S1. Photophysical properties of compounds in toluene.

Species	**Q1(Soret) [nm]**	**λ_{max}^{em} [nm]**	**Φ_{fl}[c]**	**Φ_{pl}**	**τ**
3[a]	729 (476)	742, 825	0.0245	-	5.54 ns
Zn-3[a]	669 (487)	679, 746	0.0192	-	1.42 ns
Pt-3[b]	628 (466)	823, 930	-	-[d]	1.5 μs*, 11.6 μs*
Zn-TNP[a]	816 (549)	847	0.0093	-	2.03 ns
Pt-TNP[b]	792 (520)	1106	-	-[d]	13.8 μs*

a. in toluene under atmospheric conditions at room temperature. b. in toluene after N_2 deaeration at room temperature. c. Absolute quantum yield. d. Reliable data was not obtained due to the low quantum yield. *. The data is obtained by FLS 980-STM.

7. X-ray diffraction analysis

Table S2. Crystallographic data of **Zn-TNP** and **Pt-TNP.**

Compound	**Zn-TNP**	**Pt-TNP**
CCDC.NO.	2325275	2265412
Formula	$C_{104}H_{128}ClN_5Si_4Zn$	$C_{96}H_{108}N_4PtSi_4$
Formula weight	1661.29	1625.31
Radiation	GaK\α	GaK\α
Temperature[K]	193	193
Crystal System	Triclinic	Tetragonal
Space Group	P -1	$I4_1/a$
a [Å]	16.0410(10)	19.3505(3)
b [Å]	17.7484(11)	19.3505(3)
c [Å]	19.0998(12)	21.7466(5)
α [deg]	107.001(3)	90
β [deg]	106.988(3)	90
γ [deg]	94.445(3)	90
V [$Å^3$]	4893.7(5)	8142.8(3)
Z	2	4
ρ[gcm^{-3}]	1.127	1.326
μ [mm^{-1}]	0.928	2.824
F(000)	1780.0	3384.0
Reflections collected/ unique	53920/17849	51232/4536
R_1	0.1177	0.0207
wR_2	0.3321	0.0546
GOF	1.051	1.054

8. NSD analysis of Zn-TNP and Pt-TNP

Table S3. Summary of the **Zn-TNP** NSD (in Å)**.**

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.29	0.01	-0.02	-0.26	0.06	0.00	0.10	0.00
ext.	0.29	0.01	-0.02	-0.26	0.06	0.00	0.10	0.00
			0.00	-0.04	0.01	0.00	-0.04	-0.01
total	0.34	0.00	-0.02	-0.26	0.06	0.00	0.11	0.00
			0.01	-0.04	0.01	0.00	-0.04	-0.01
			0.00	0.06	0.00	0.01	0.12	0.01
			0.00	-0.02	-0.03	0.00	0.08	0.01
			-0.01	-0.03	-0.04	-0.01	0.01	0.00
			0.02	0.01	-0.01	0.00	-0.04	
					0.01	0.00		
					0.01	-0.01		
					0.01	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.34	0.00	0.03	0.27	0.08	0.02	0.19	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	$E_g(x)$	$E_g(y)$	A_{1u}	A_{2u}
min.	1.92	0.01	-1.89	0.03	-0.10	-0.23	0.00	-0.28
ext.	1.93	0.00	-1.88	0.03	-0.10	-0.23	0.00	-0.27
			0.09	0.01	-0.01	0.04	-0.01	0.20
total	1.93	0.00	-1.88	0.03	-0.10	-0.23	0.00	-0.27
			0.09	0.01	-0.01	0.04	-0.01	0.20
			0.01	-0.01	0.00	-0.03		-0.04
					0.00	0.01		
					-0.01	-0.01		
comp.	1.93	0.00	1.89	0.03	0.10	0.23	0.01	0.34

Table S4. Summary of the **Pt-TNP** NSD (in Å)**.**

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.33	0.02	0.00	0.00	0.00	0.00	-0.33	-0.01
ext.	0.41	0.01	0.00	0.00	0.00	0.00	-0.33	-0.02
			0.00	0.00	0.00	0.00	-0.05	-0.23
total	0.45	0.00	0.00	0.00	0.00	0.00	-0.32	-0.02
			0.00	0.00	0.00	0.00	-0.05	-0.23
			0.00	0.00	0.00	0.00	0.18	0.03
			0.00	0.00	0.00	0.00	0.07	-0.01
			0.00	0.00	0.00	0.00	-0.01	-0.05

			0.00	0.00	0.00	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.45	0.00	0.00	0.00	0.00	0.00	0.38	0.24

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	$E_g(x)$	$E_g(y)$	A_{1u}	A_{2u}
min.	2.83	0.00	2.59	-1.15	0.00	0.00	0.00	0.00
ext.	2.83	0.00	2.59	-1.15	0.00	0.00	0.00	0.00
			-0.02	-0.02	0.00	0.00	0.00	0.00
total	2.83	0.00	2.59	-1.15	0.00	0.00	0.00	0.00
			-0.02	-0.02	0.00	0.00	0.00	0.00
			-0.02	-0.04	0.00	0.00		0.00
					0.00	0.00		
					0.00	0.00		
comp.	2.83	0.00	2.59	1.15	0.00	0.00	0.00	0.00

9. Photothermal studies

Photothermal effect tests: The toluene solution (30 μM, 0.7 mL) of **Pt-TNP** in a polypropylene tube was exposed to 808 nm laser irradiation at 0.35 W·cm^{-2} power densities for total 20 min. An IR-thermal camera was utilized to record the temperature of solutions every 30 s and the thermal images were also monitored and collected during irradiation. The photothermal conversion efficiency (η) of the **Pt-TNP** was calculated according to the reported method[13, 14]. Under continuous laser irradiation, the temperature of the **Pt-TNP** solution was recorded, until the solution had reached a steady-state temperature at 6.5 min. The photothermal conversion efficiency (η) was calculated according to Equation (1):

$$\eta = \frac{hA(T_{Max} - T_{Surr})}{I(1 - 10^{-A_{808}})} - Q_{Dis} \quad (1)$$

Where h represents the heat transfer coefficient, A is the surface area of the container, T_{Max} represents the maximum steady-state temperature, T_{Surr} is the ambient temperature of the environment, Q_{Dis} represents the heat dissipation from the light absorbed by the solvent and tube, I is the incident laser power, and A_{808} is the absorbance of the sample at 808 nm. The value of τ_s is derived from Equation (2)

$$t = -\tau_s \, ln(\theta) = -\tau_s \, ln\left(\frac{T_t - T_{Surr}}{T_{Max} - T_{Surr}}\right) (2)$$

Where t is the cooling time points after continuous irradiation, τ_s is the time constant for heat transfer of the system, Tt is the temperature at the corresponding time points during the cooling process. The value of hA is derived from Equation (3).

$$\tau_s = \frac{m_D c_D}{hA} \quad (3)$$

Where m_D and c_D are the mass (0.61 g) and specific heat capacity (1.68 J/g °C), respectively, of toluene. Q_{Dis} represents the heat dissipation from the light absorbed by the toluene and the container, so Q_{Dis} was calculated according to Equation (4)

$$Q_{Dis} = \frac{m_D c_D}{\tau_s(\text{toluene})}(T_{Max}(\text{toluene}) - T_{Surr}) \quad (4)$$

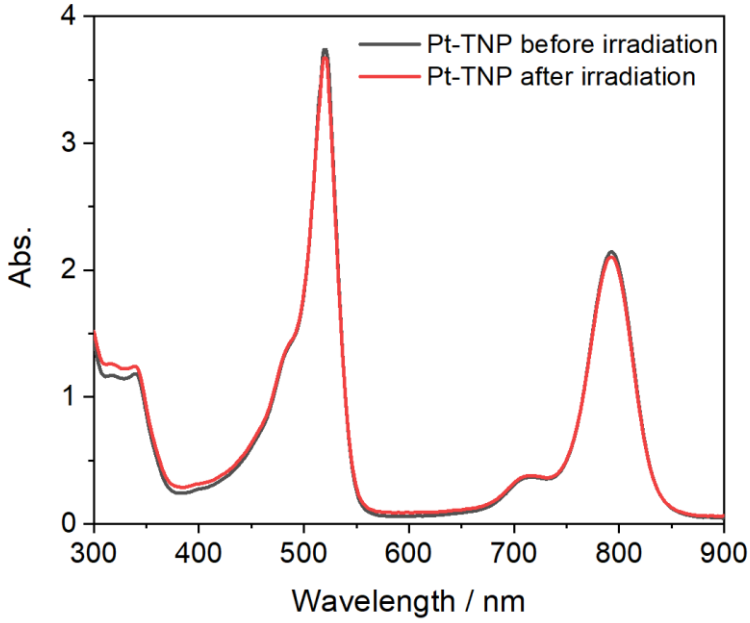

Figure S30. Photothermal stability of **Pt-TNP** (30 μM) in 0.7 mL toluene before and after the irradiation of 808 nm and 0.35 W cm^{-2}.

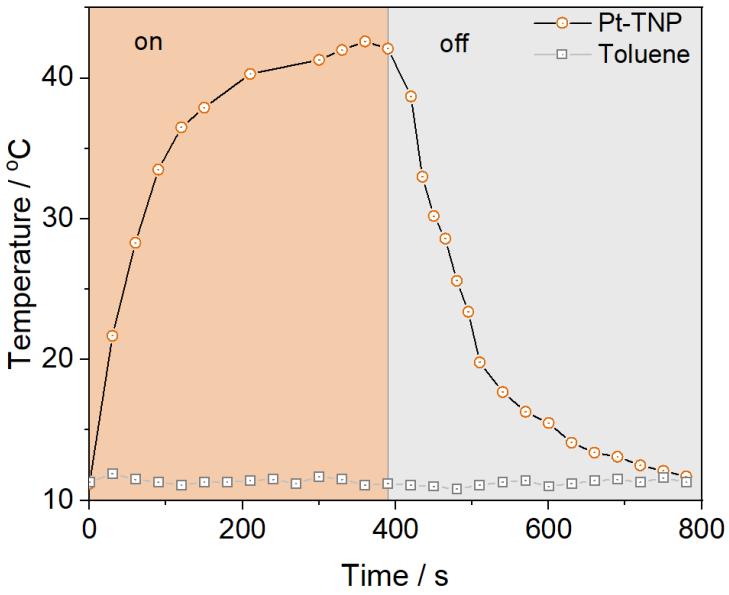

Figure S31. Photothermal conversion behavior of **Pt-TNP** (30 μM) in 0.7 mL toluene and toluene solution (0.7 mL) under the irradiation of 808 nm and 0.35 W cm^{-2}.

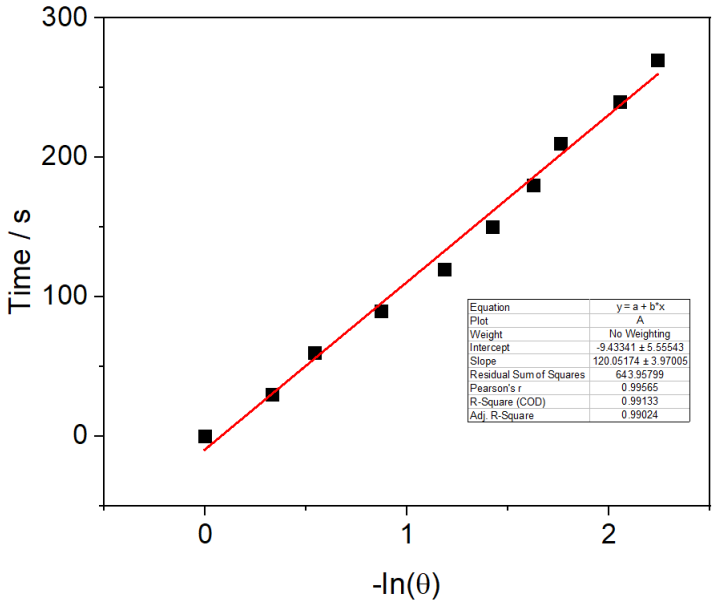

Figure S32. A plot of time versus −ln(θ) during the cooling period for **Pt-TNP** in toluene solution (0.7 mL).

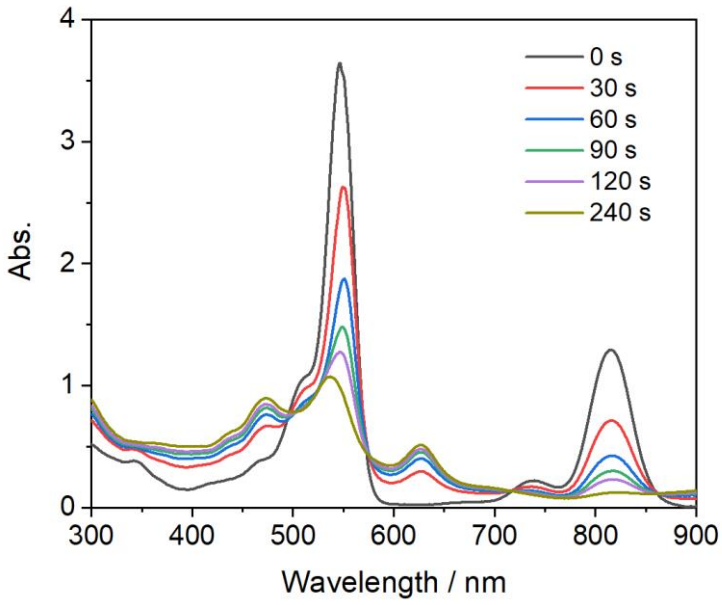

Figure S33. The photothermal stability of **Zn-TNP** in toluene solution (30 μM) under the irradiation of 808 nm and 0.35 W cm^{-2}.

10. Singlet oxygen generation of Zn-TNP and Pt-TNP determined by DPBF

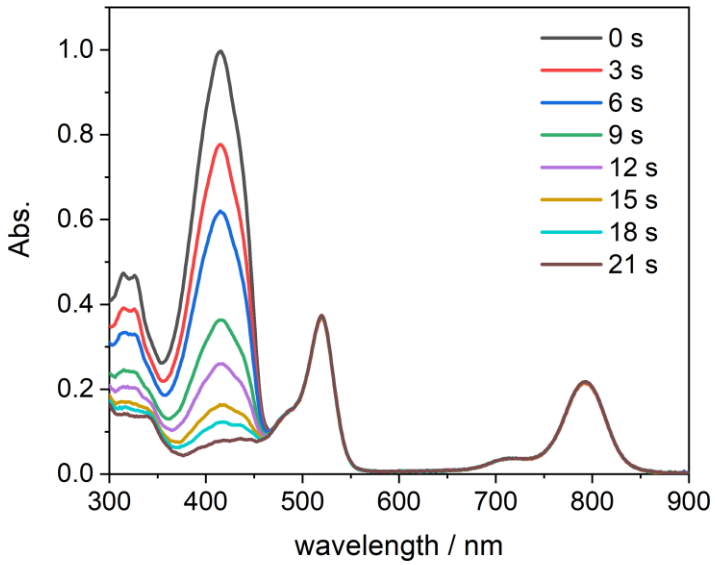

Figure S34. Singlet oxygen generation of **Pt-TNP** obtained in toluene at room temperature under 808 nm (10 mW cm^{-2}) laser irradiation.

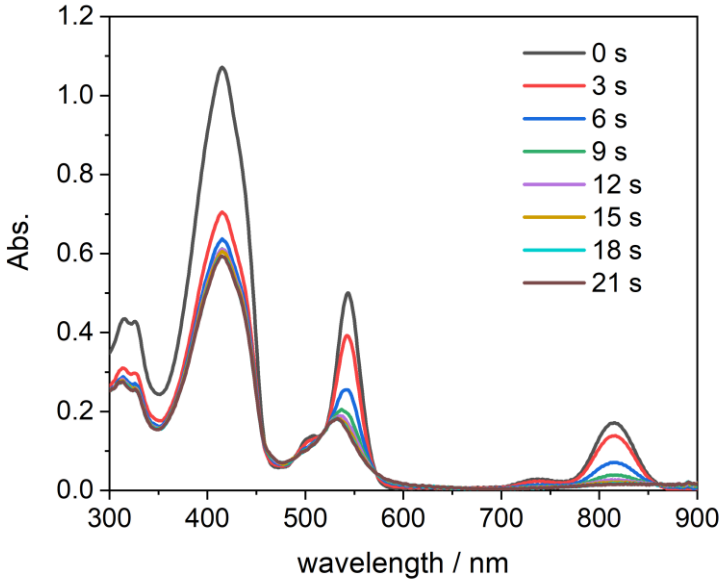

Figure S35. Singlet oxygen generation of **Zn-TNP** obtained in toluene at room temperature under 808 nm (10 mW cm^{-2}) laser irradiation.

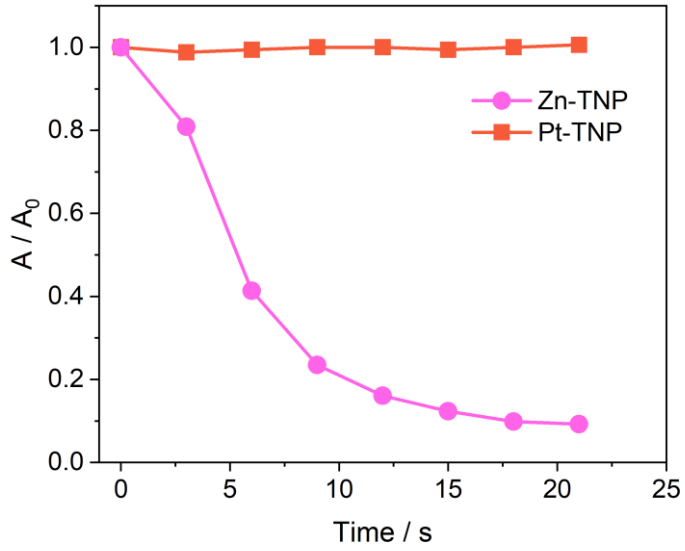

Figure S36. The stability of **Zn-TNP** and **Pt-TNP** measured by the ratio of absorption at 808 nm under 808 nm (10 mW cm^{-2}) laser irradiation.

11. DFT calculations

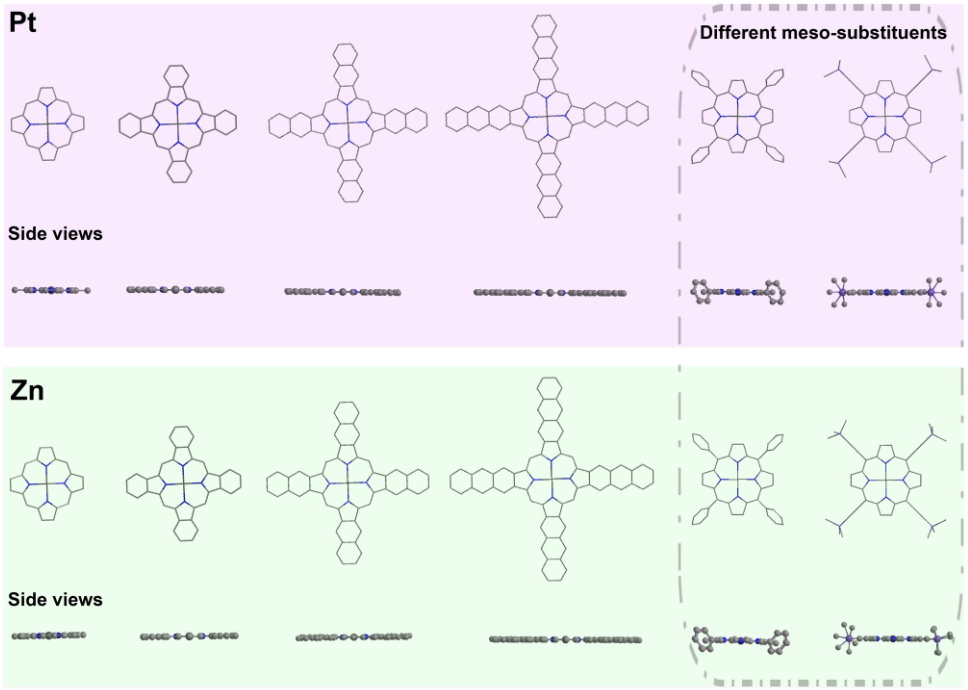

Figure S37. The optimized structures of a series of meso-free or β-free Zn- and Pt-porphyrins with highly planar conformations.

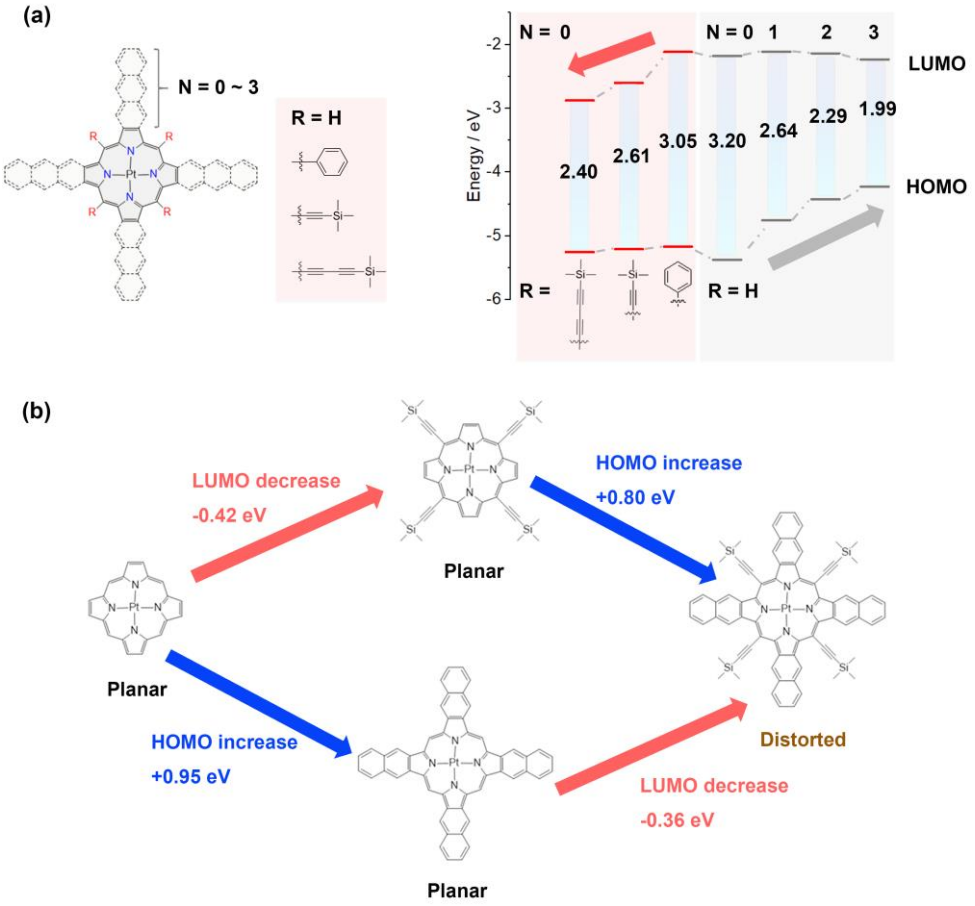

Figure S38. (a) Frontier molecular orbital diagrams of a series of planar Pt-porphyrins with various meso- and β-substituents. The HOMO-lifting effect of aromatic fusion and the LUMO-reducing effect of alkynyl substitution are highlighted with arrows. (b)The HOMO/LUMO energy and conformation changes after the gradual introduction of meso-alkynyl or β-naphthalene into the parent non-fused porphyrin.

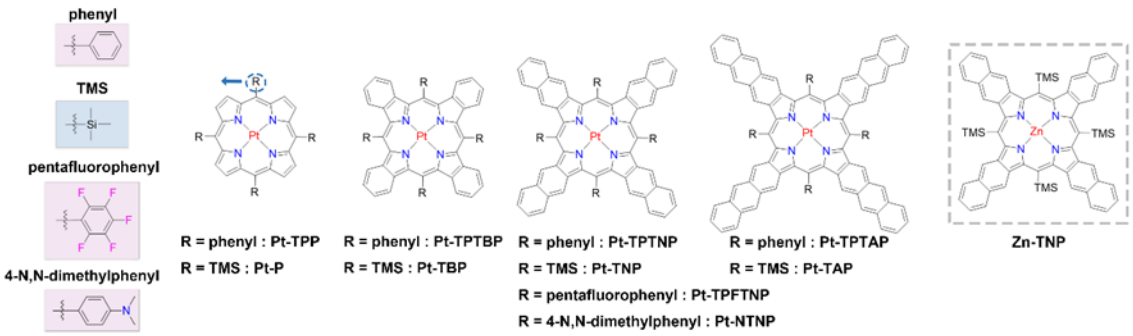

Figure S39. Scheme of the molecular structures for DFT calculations.

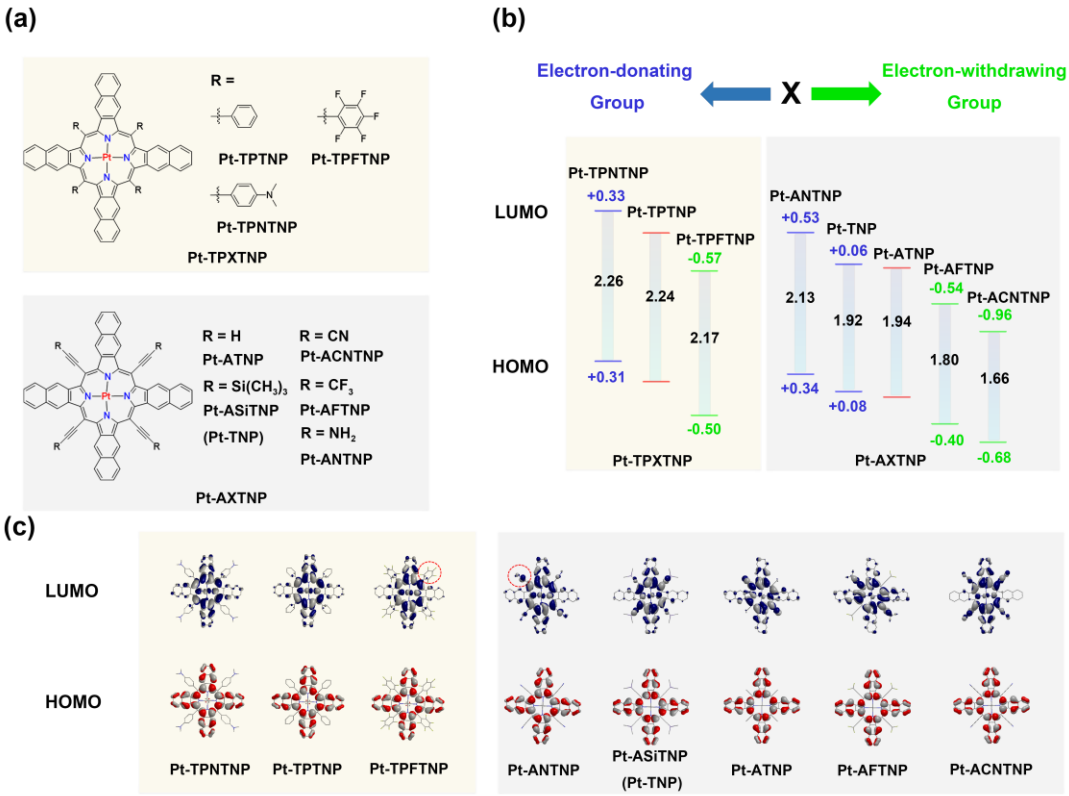

Figure S40. (a) Molecular structures of Pt-porphyrins with meso-phenyl (**Pt-TPXTNP**) or meso-alkynyl (**Pt-AXTNP**) substituents. The electron-donating or electron-withdrawing groups **X** are incorporated into the meso-substituents. (b) Comparison of the HOMO-LUMO energy levels of **Pt-TPXTNP** and **Pt-AXTNP**. (c) The HOMO and LUMO orbital plots of **Pt-TPXTNP** and **Pt-AXTNP**. The π-electron density of the LUMOs in **Pt-AXTNP** extended to the alkynyl units as shown in the red circle.

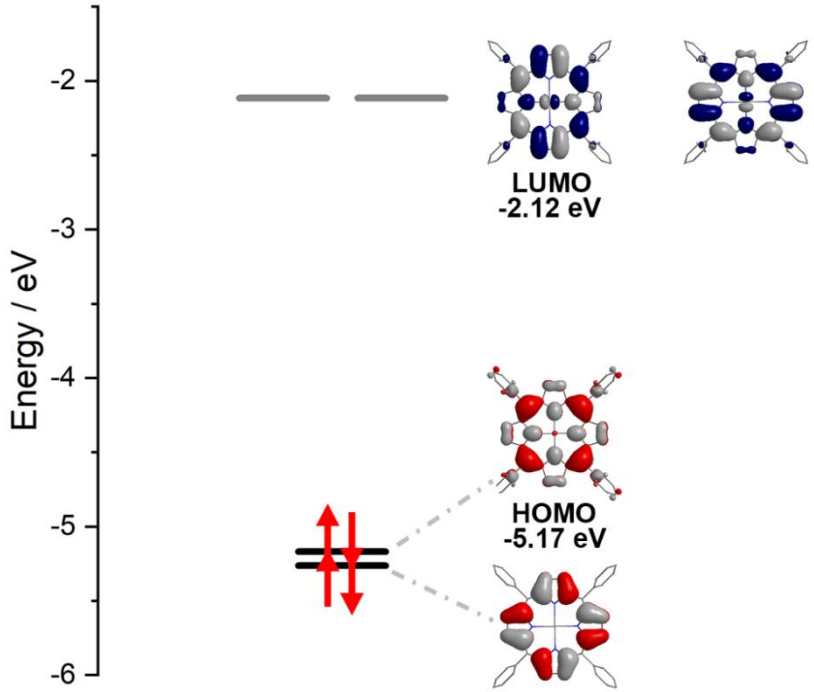

Figure S41. DFT calculated frontier molecular orbital diagrams of **Pt-TPP**.

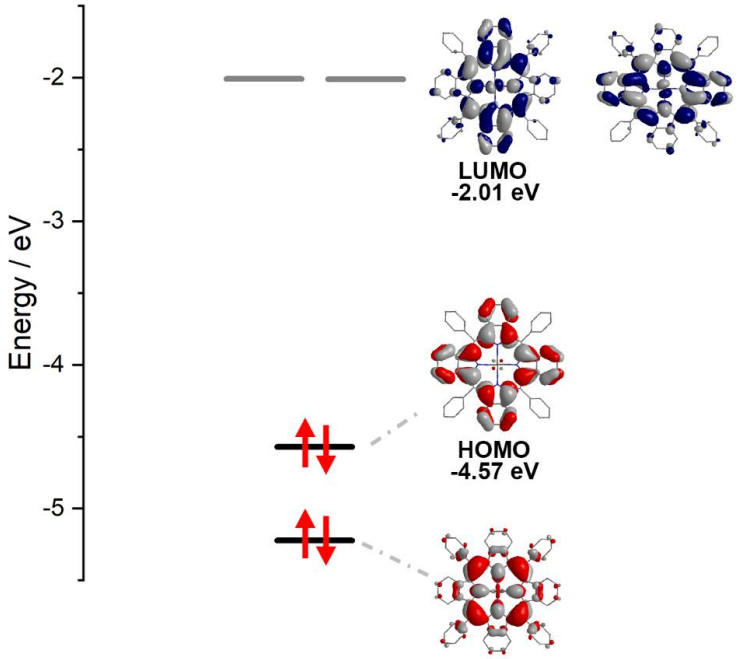

Figure S42. DFT calculated frontier molecular orbital diagrams of **Pt-TPTBP**.

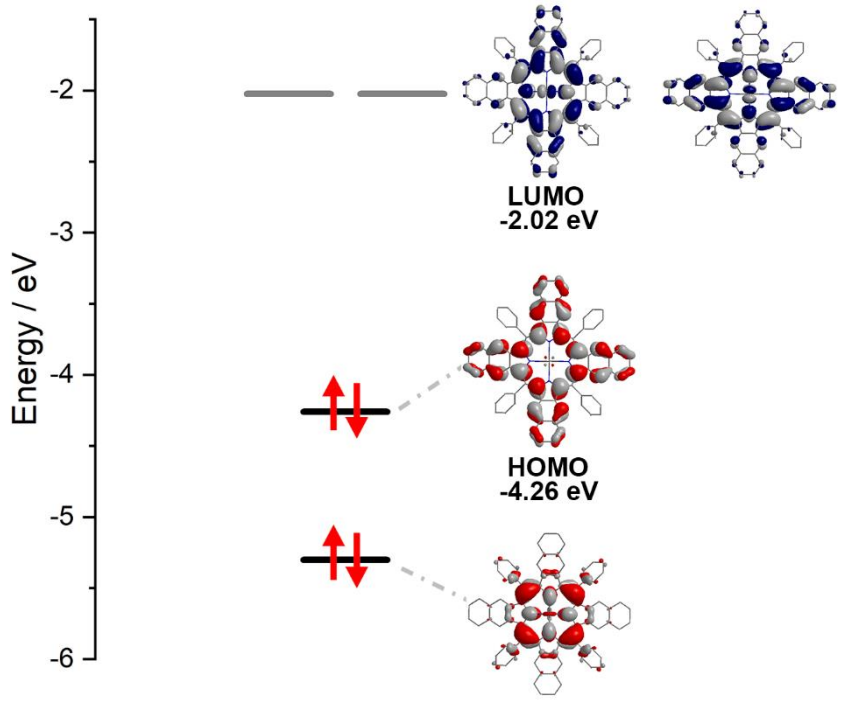

Figure S43. DFT calculated frontier molecular orbital diagrams of **Pt-TPTNP**.

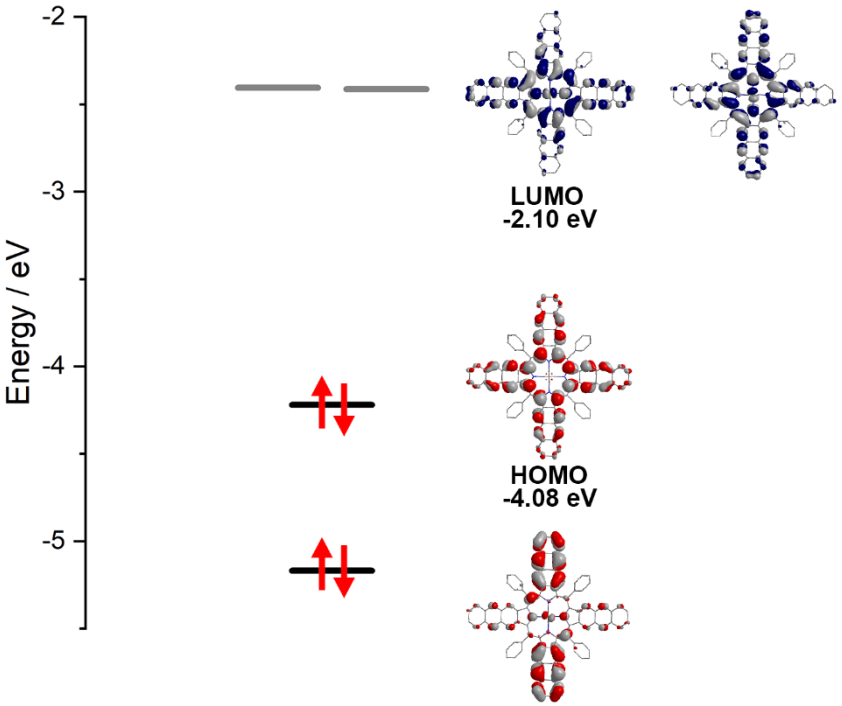

Figure S44. DFT calculated frontier molecular orbital diagrams of **Pt-TPTAP**.

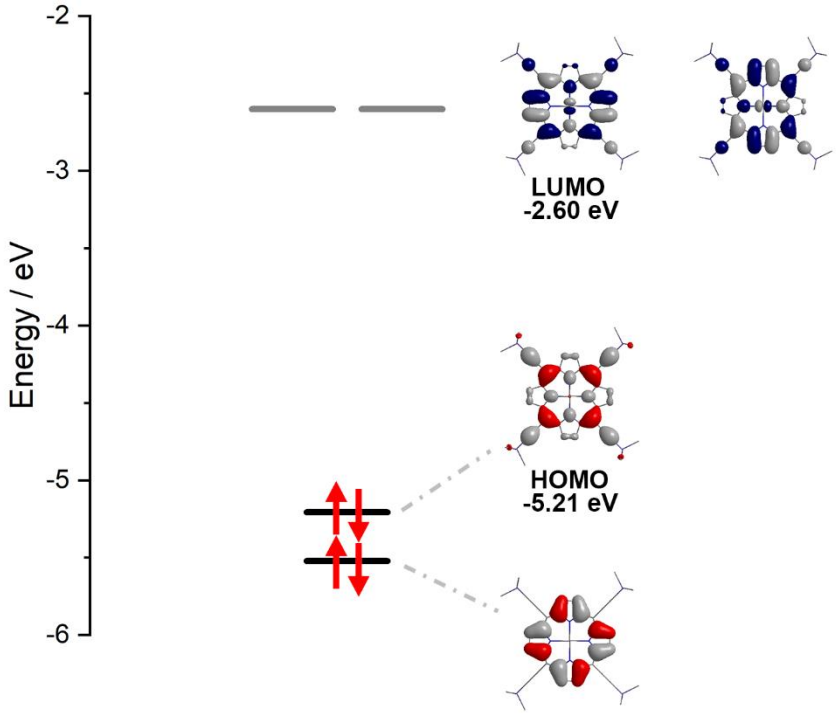

Figure S45. DFT calculated frontier molecular orbital diagrams of **Pt-P**.

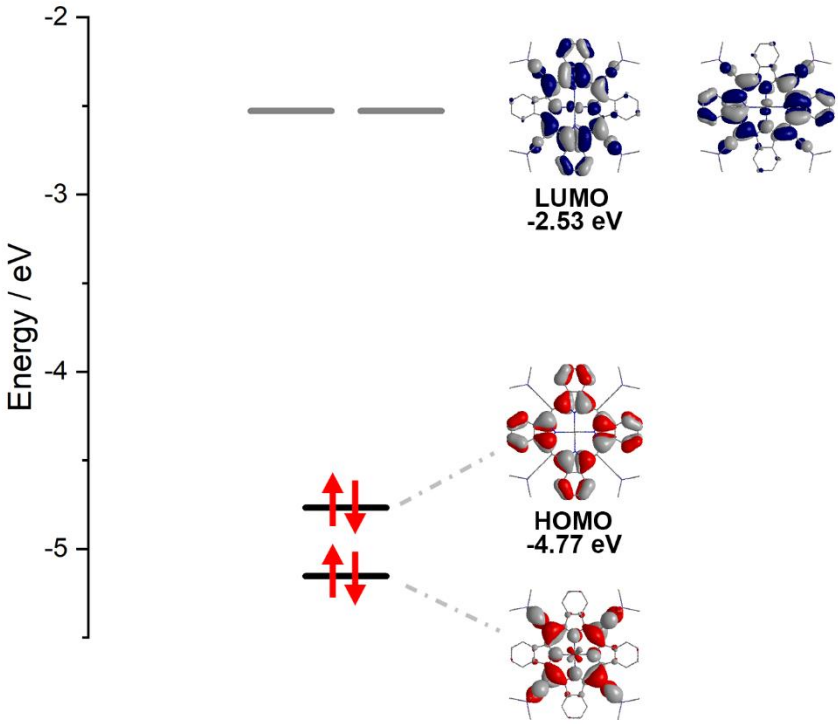

Figure S46. DFT calculated frontier molecular orbital diagrams of **Pt-TBP**.

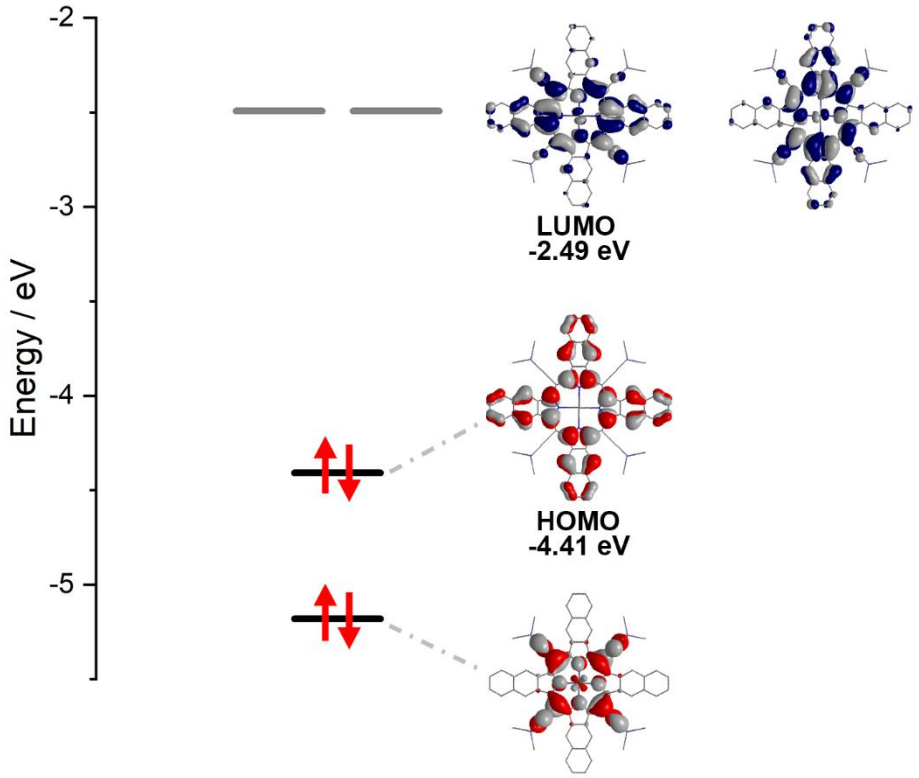

Figure S47. DFT calculated frontier molecular orbital diagrams of **Pt-TNP**.

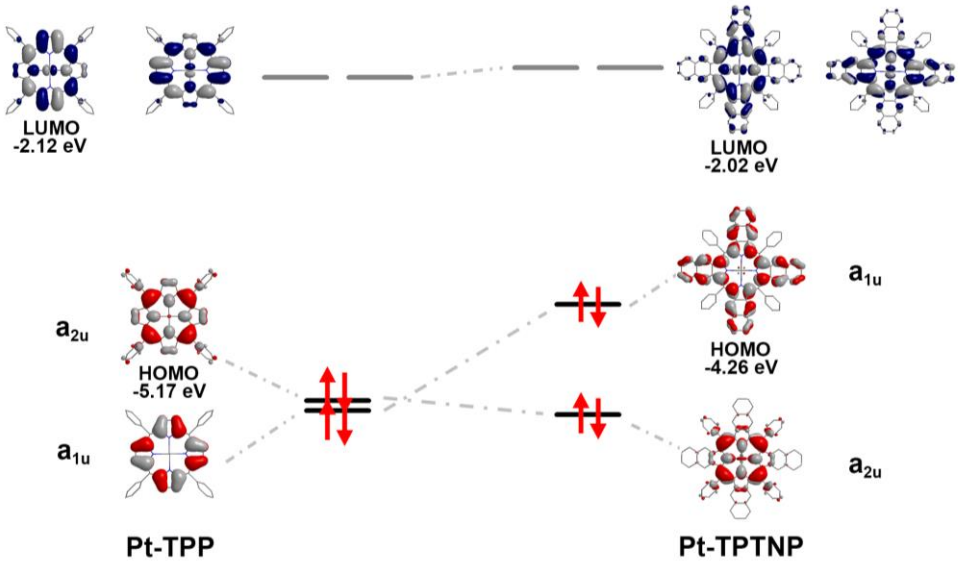

Figure S48. The HOMO/HOMO-1 splitting and a_{1u}/a_{2u} symmetry switching from **Pt-TPP** to **Pt-TPTNP.**

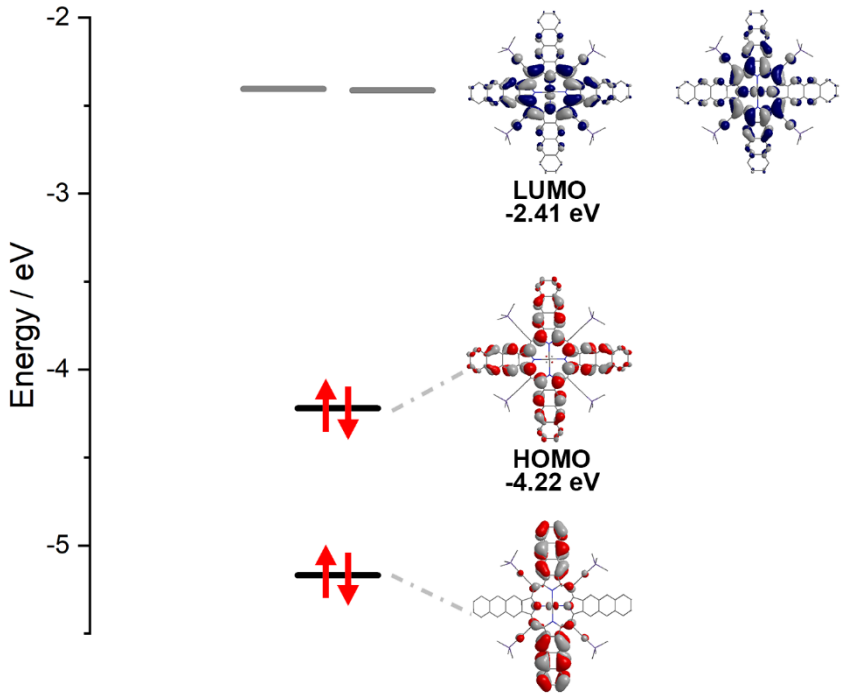

Figure S49. DFT calculated frontier molecular orbital diagrams of **Pt-TAP**.

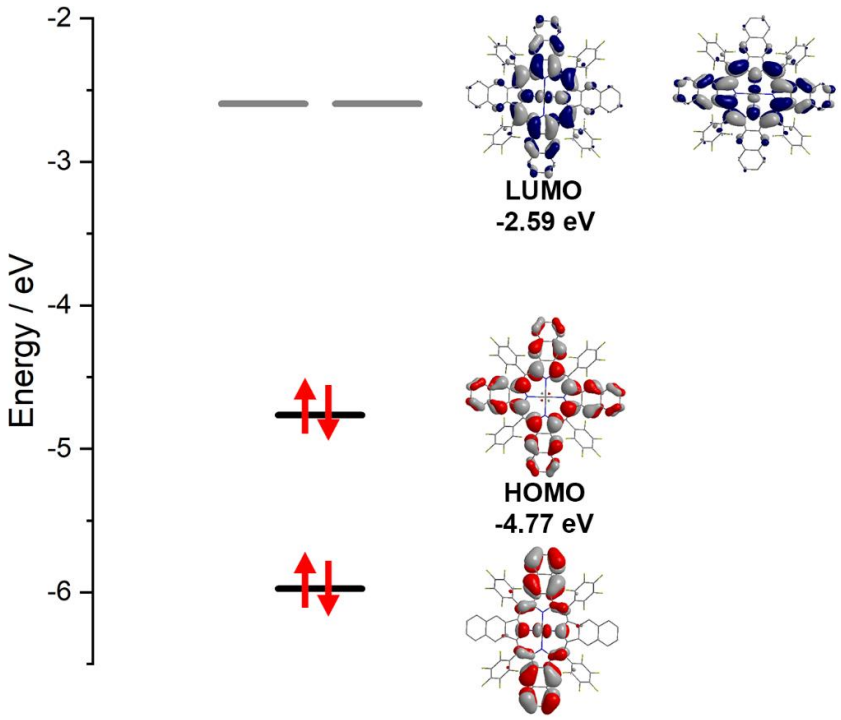

Figure S50. DFT calculated frontier molecular orbital diagrams of **Pt-TPFTNP**.

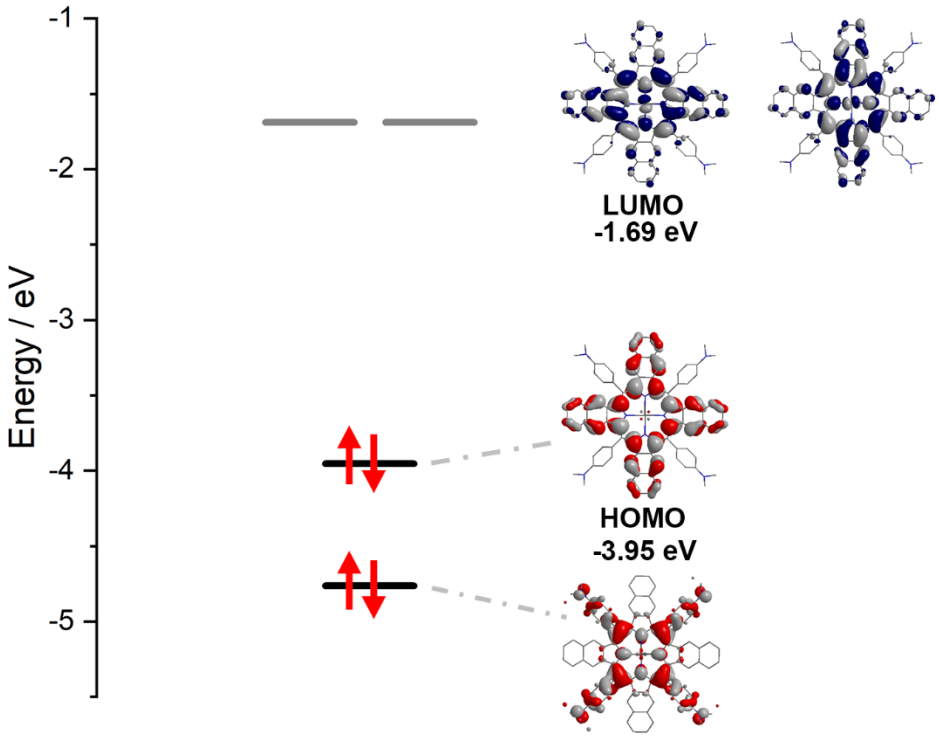

Figure S51. DFT calculated frontier molecular orbital diagrams of **Pt-NTNP**.

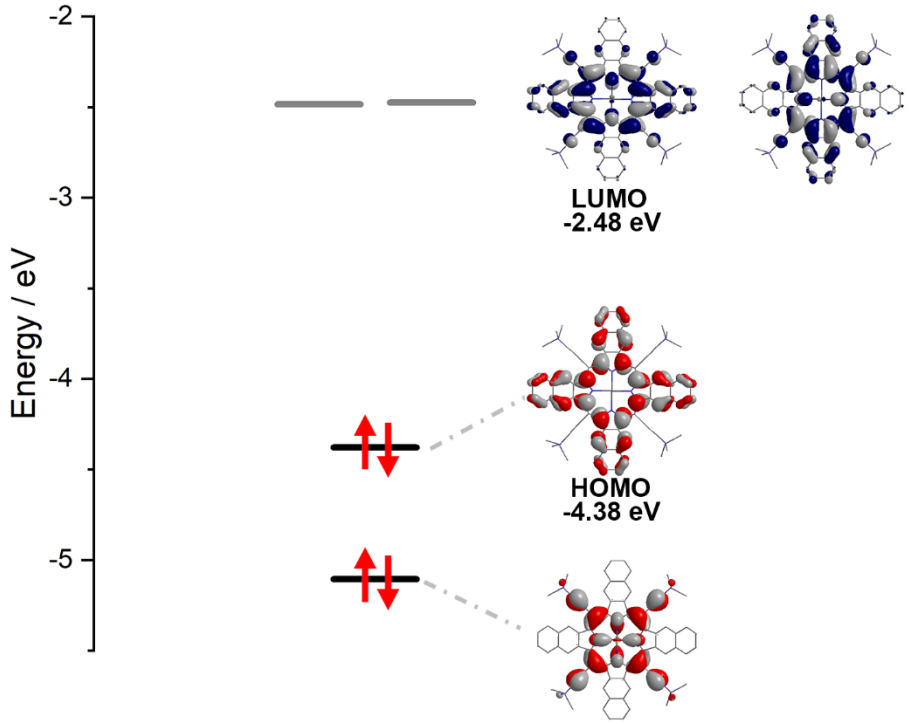

Figure S52. DFT calculated frontier molecular orbital diagrams of **Zn-TNP**.

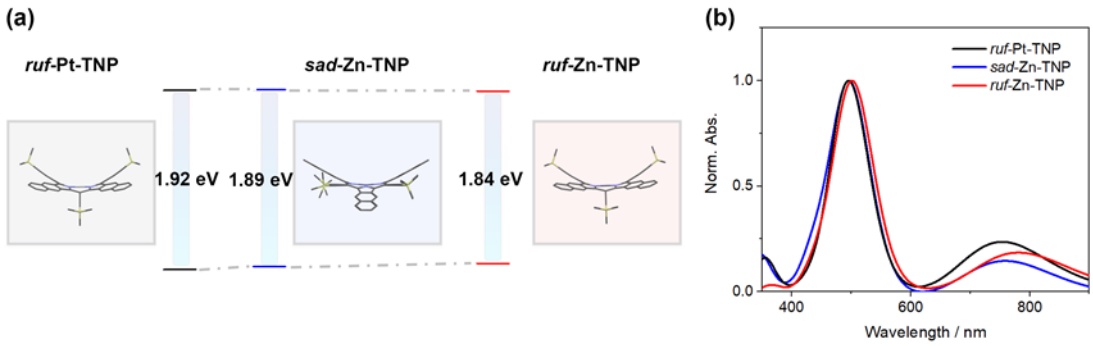

Figure S53. (a) Molecular structures and frontier molecular orbital diagrams of ***ruf*-Pt-TNP**, ***sad*-Zn-TNP** and ***ruf*-Zn-TNP**. (b) TD-DFT simulated absorption spectra of ***ruf*-Pt-TNP** (black line), ***sad*-Zn-TNP** (blue line) and ***ruf*-Zn-TNP** (red line) (FWHM= 3000 cm^{-1}).

12. TD-DFT calculations

Table S5. The calculated wavelengths, oscillation strengths and major contributions of the Q bands of **Pt-AXTNP.**

Compound	Wavelength	Osc. strength	Major contribs.
Pt-ANTNP	688.83	0.1641	HOMO->LUMO (81%)
	688.76	0.1638	HOMO->L+1 (81%)
Pt-TNP	753.42	0.2453	HOMO->LUMO (87%)
	753.42	0.2453	HOMO->L+1 (87%)
Pt-ATNP	738.04	0.2817	HOMO->L+1 (81%)
	738.04	0.2817	HOMO->LUMO (81%)
Pt-AFTNP	779.72	0.3304	HOMO->L+1 (93%)
	779.72	0.3304	HOMO->LUMO (93%)
Pt-ACNTNP	847.69	0.3005	HOMO->LUMO (87%)
	847.69	0.3005	HOMO->L+1 (87%)

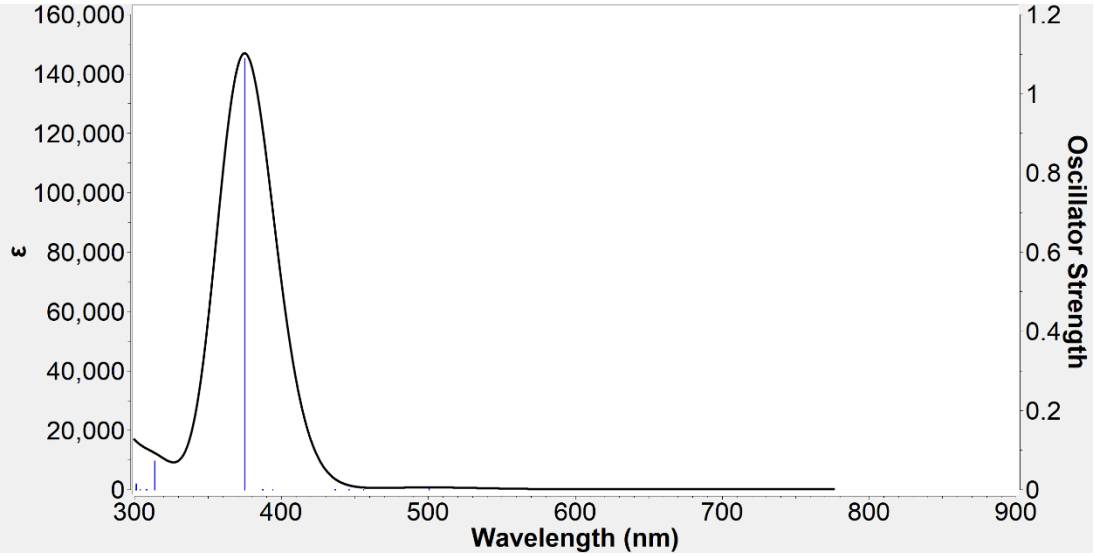

Figure S54. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TPP.**

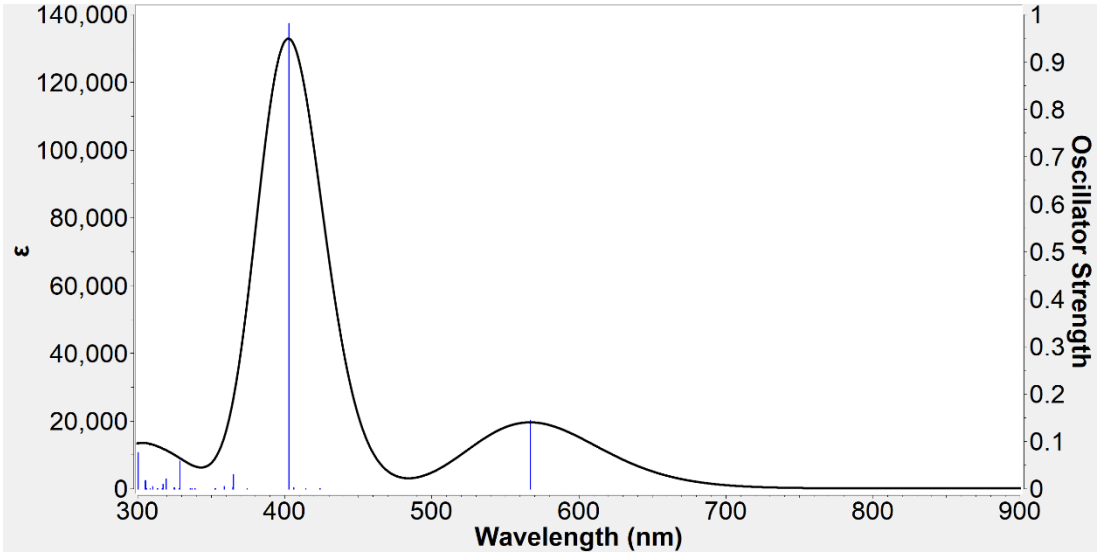

Figure S55. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TPTBP**.

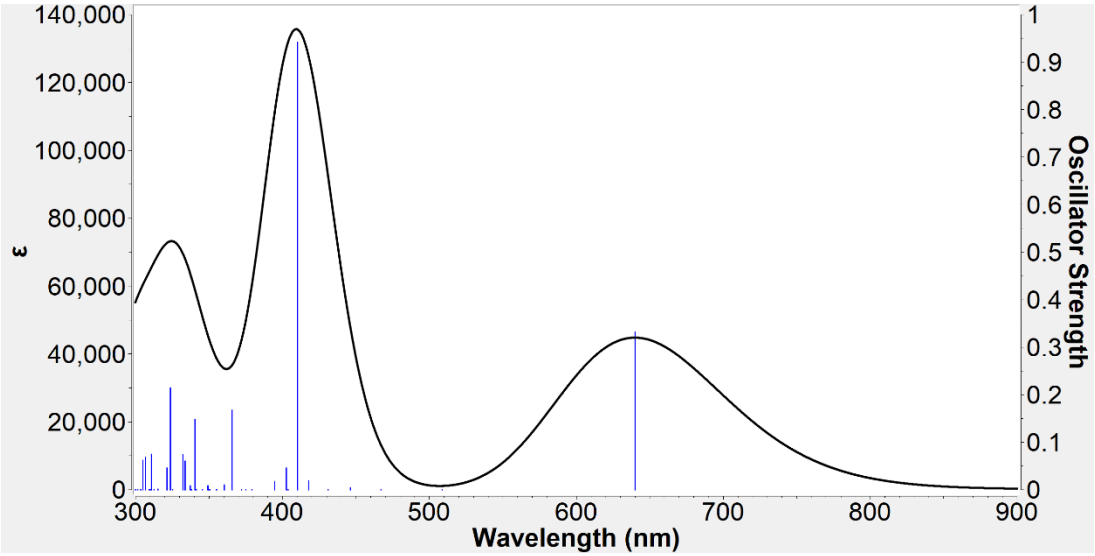

Figure S56. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TPTNP**.

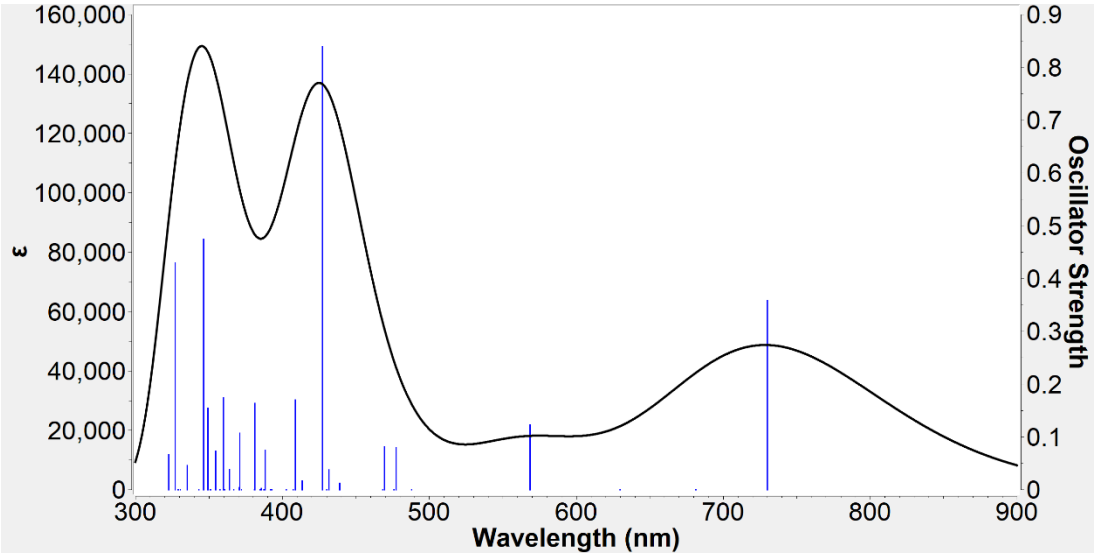

Figure S57. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TPTAP**.

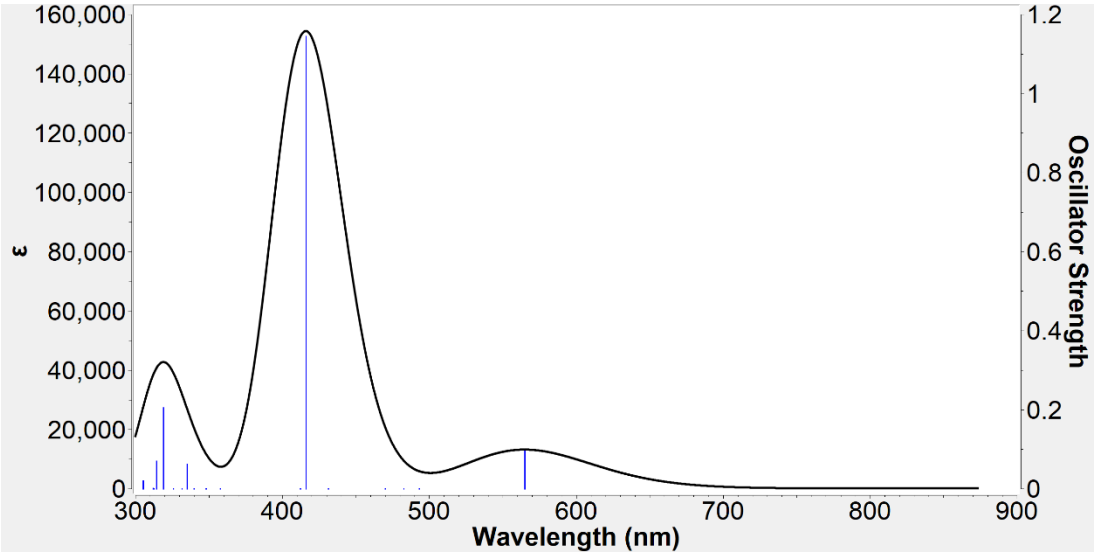

Figure S58. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-P**.

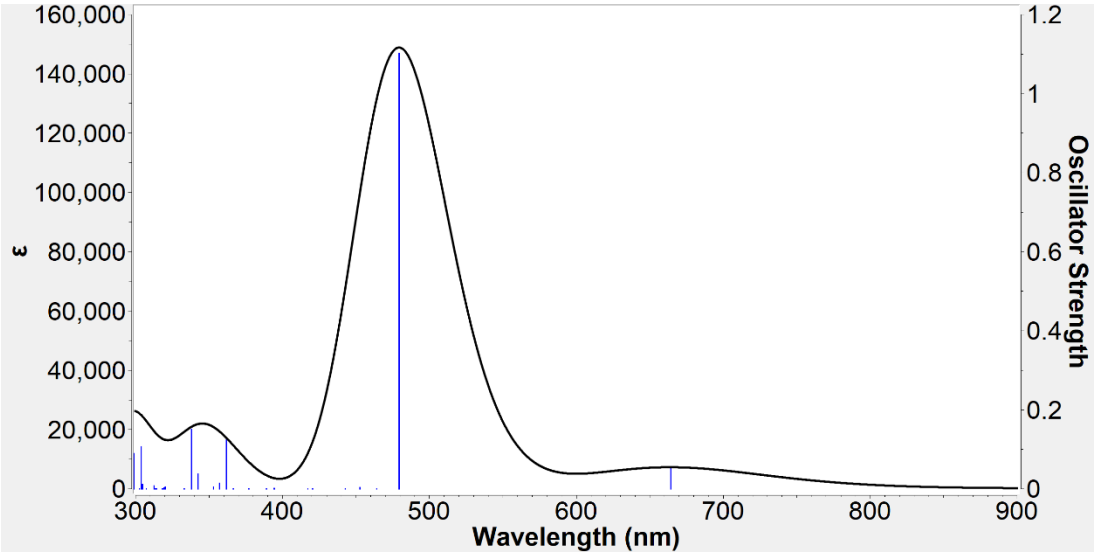

Figure S59. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TBP**.

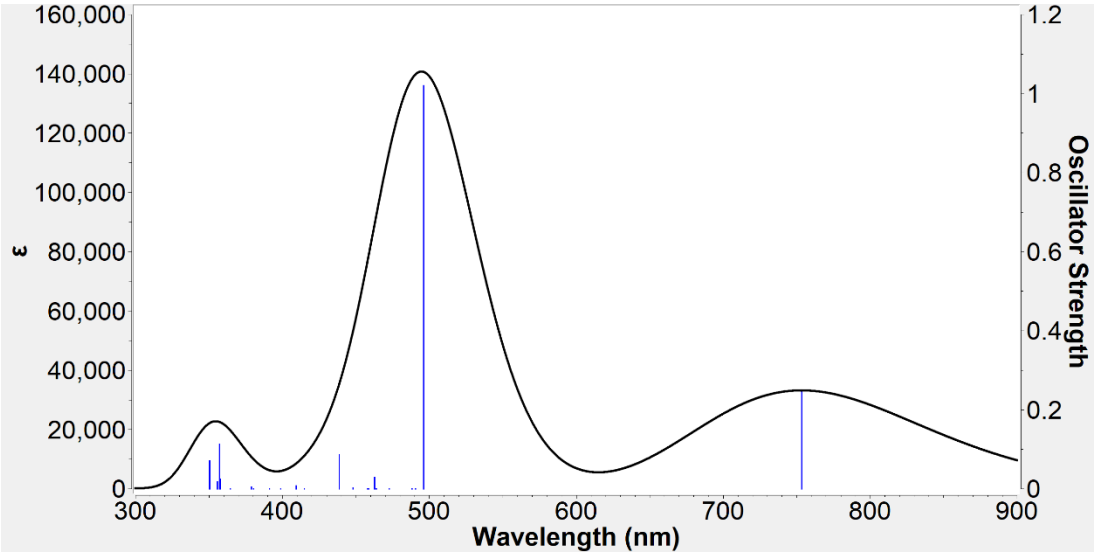

Figure S60. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TNP**.

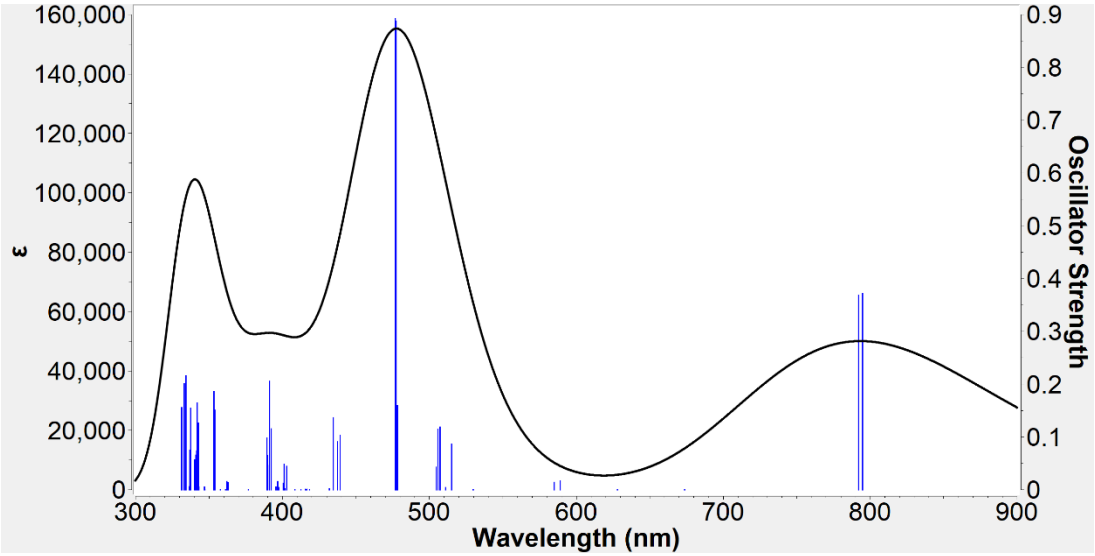

Figure S61. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TAP**.

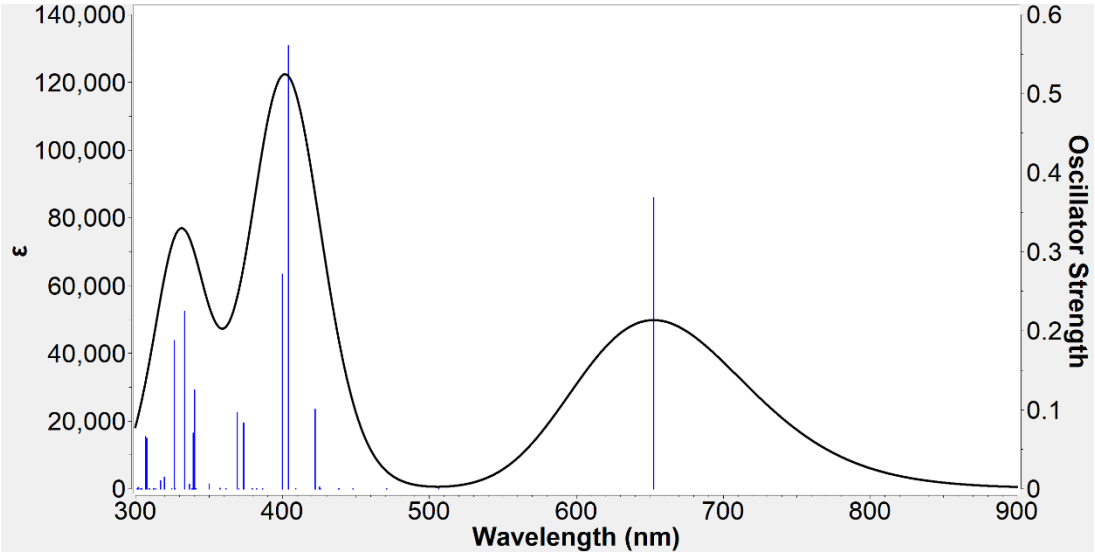

Figure S62. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-TPFTNP**.

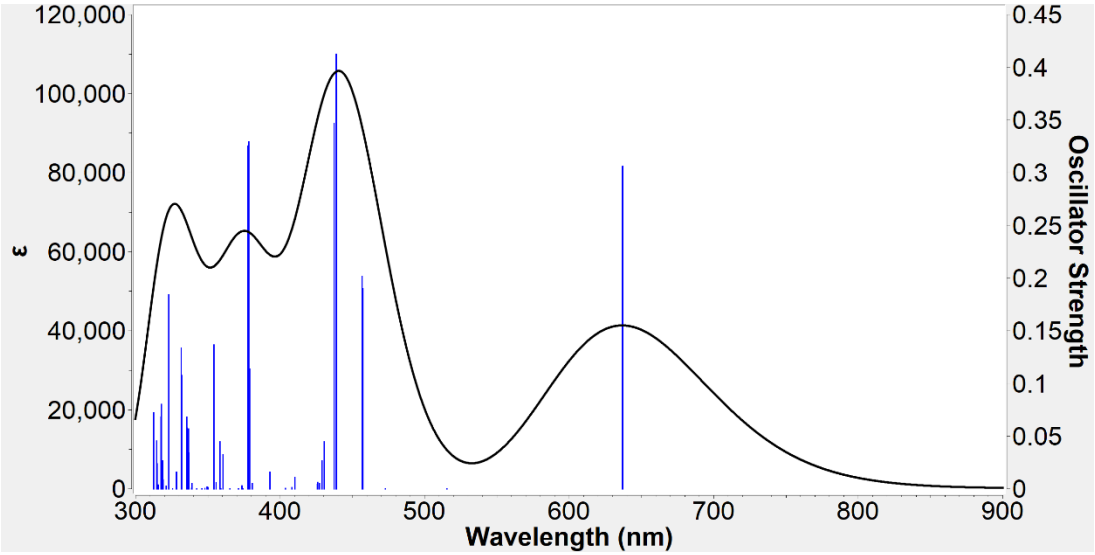

Figure S63. TD-DFT calculated electronic transitions and simulated absorption spectrum of **Pt-NTNP**.

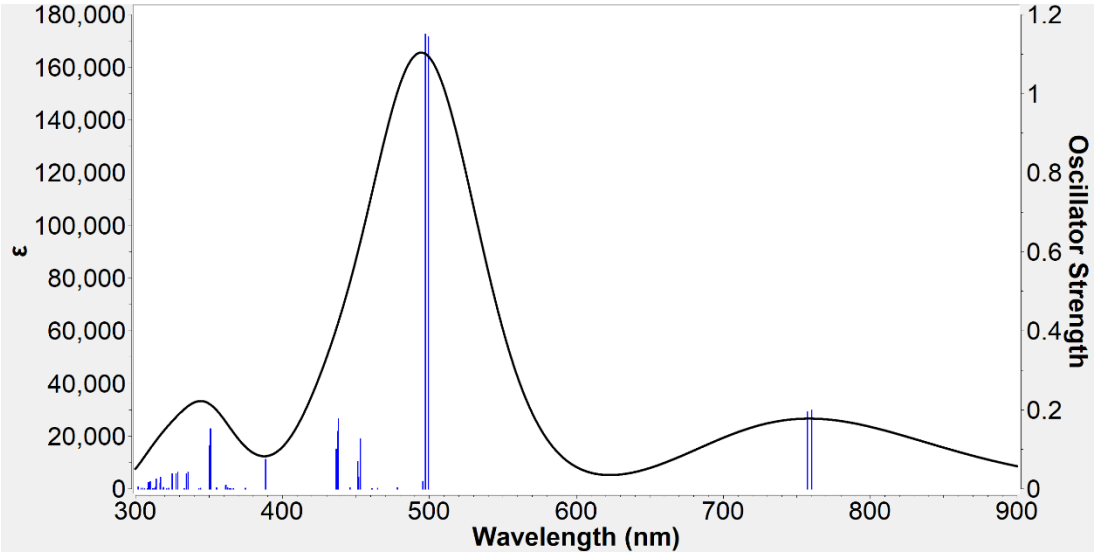

Figure S64 TD-DFT calculated electronic transitions and simulated absorption spectrum of **Zn-TNP**.

Table S6. TD-DFT calculated wavelengths, oscillator strengths and compositions of selected electronic transitions for **Pt-TNP**.

No.	*Wavelength [nm]*	*Osc. Strength*	*Major contributions*
1	753.42	0.2453	HOMO -1-> LUMO +1 (12%), HOMO->LUMO (87%)
2	753.42	0.2453	HOMO -1->LUMO (12%), HOMO-> LUMO +1 (87%)
3	495.93	1.02	HOMO -1->LUMO (85%), HOMO-> LUMO +1 (12%)
4	495.93	1.02	HOMO -1-> LUMO +1 (85%), HOMO->LUMO (12%)

13.. TD-DFT calculations including spin-orbit coupling of excited states

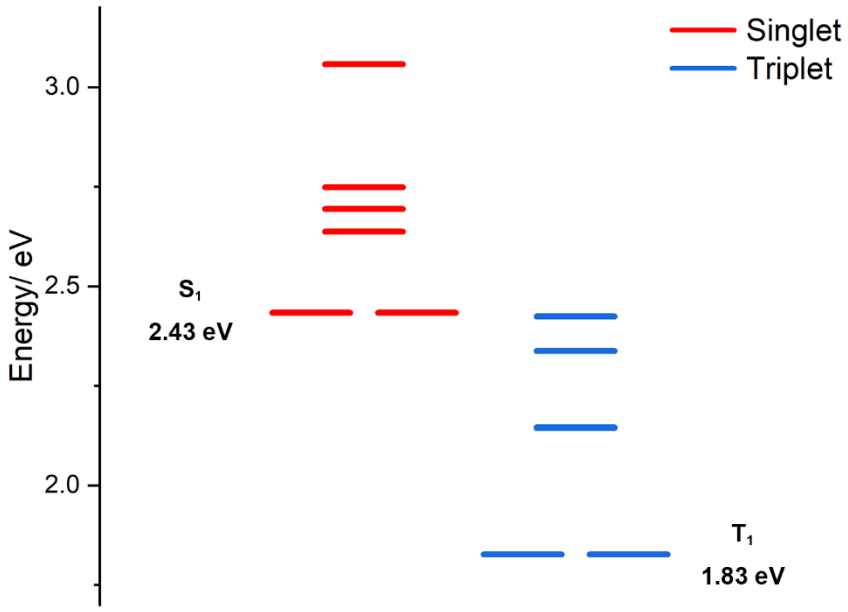

Figure S65. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TPP**.

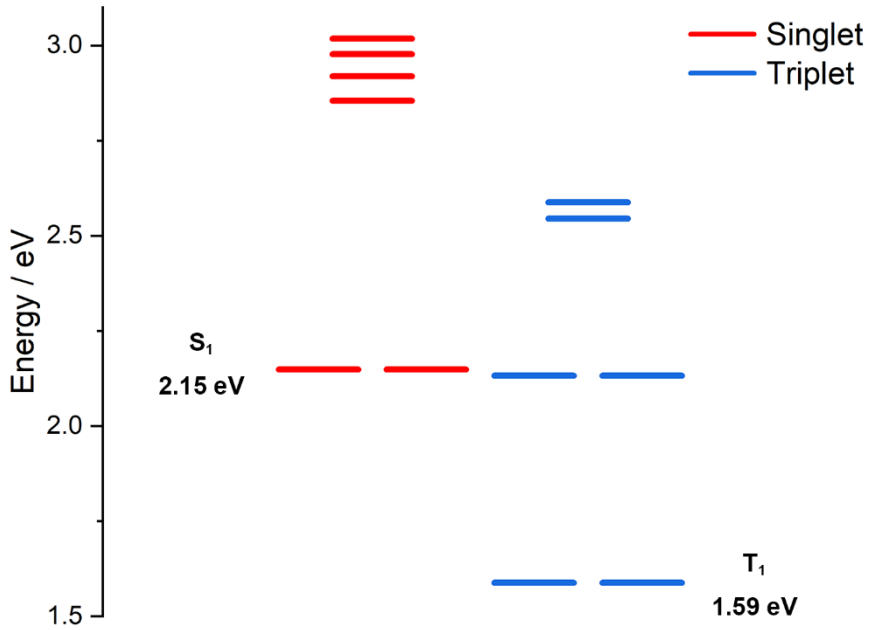

Figure S66. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TPTBP**.

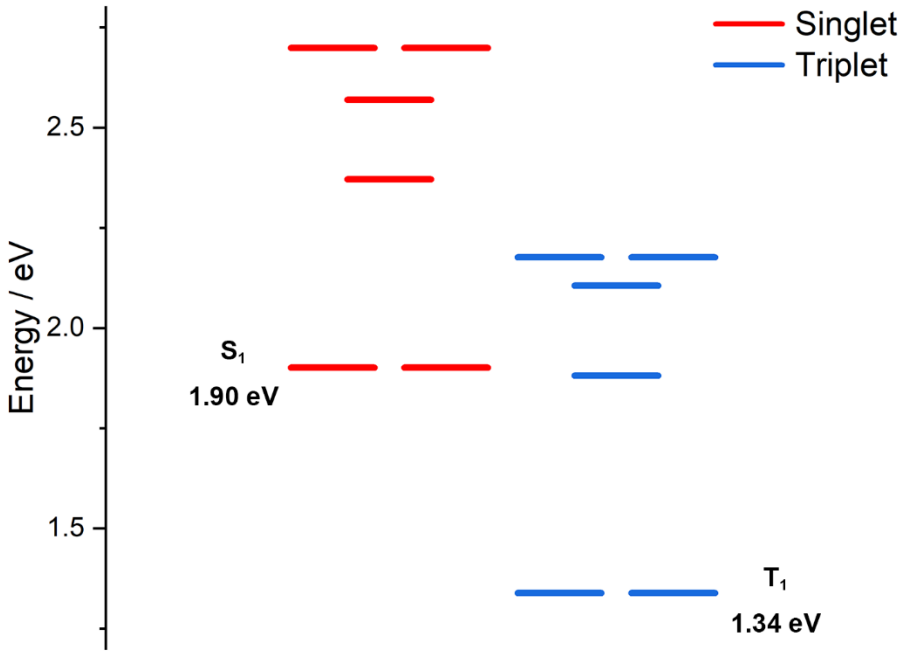

Figure S67. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TPTNP**.

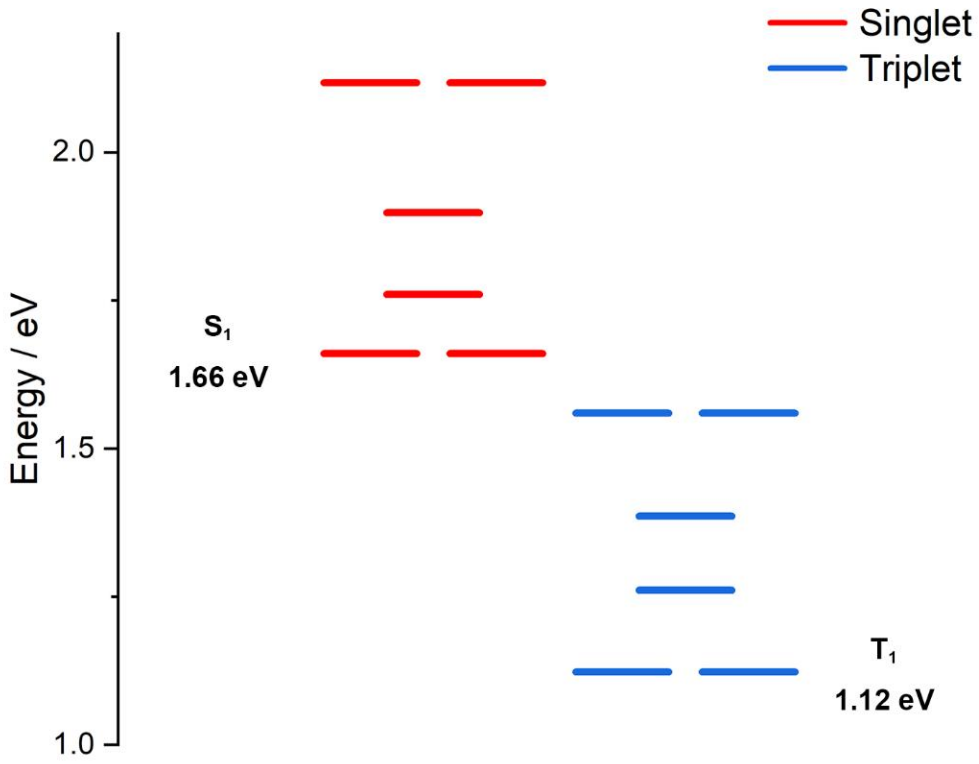

Figure S68. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TPTAP**.

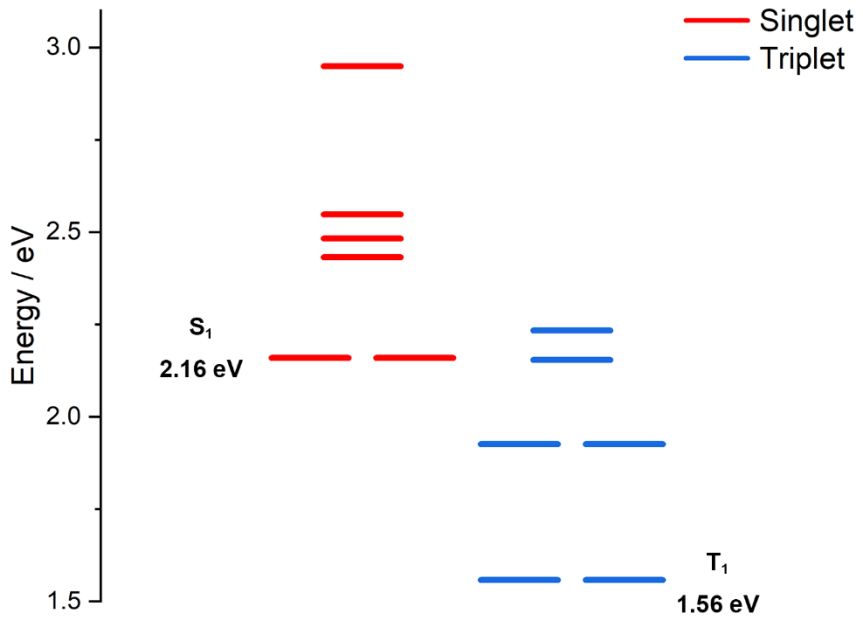

Figure S69. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-P**.

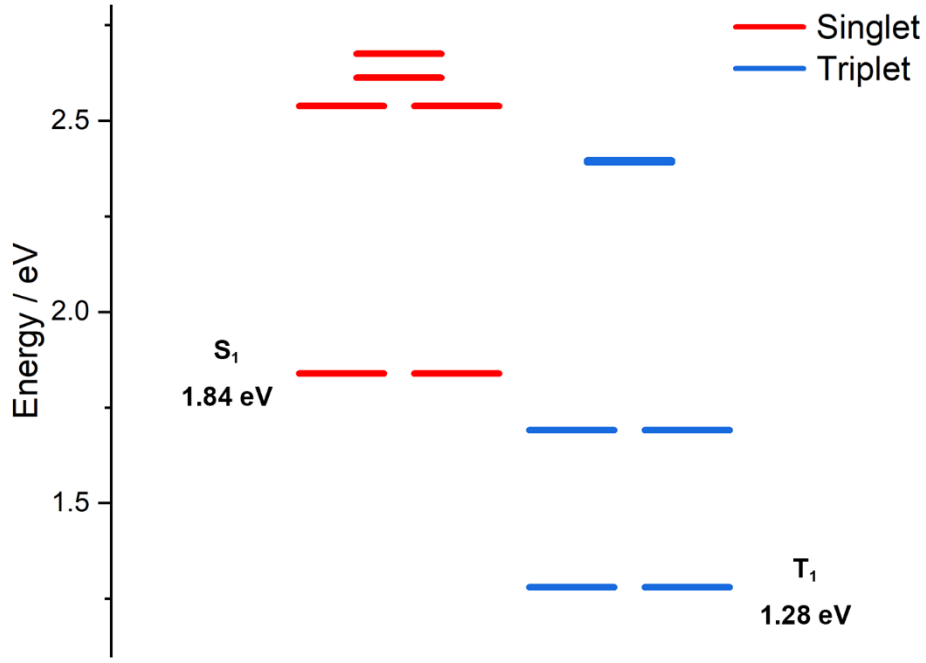

Figure S70. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TBP**.

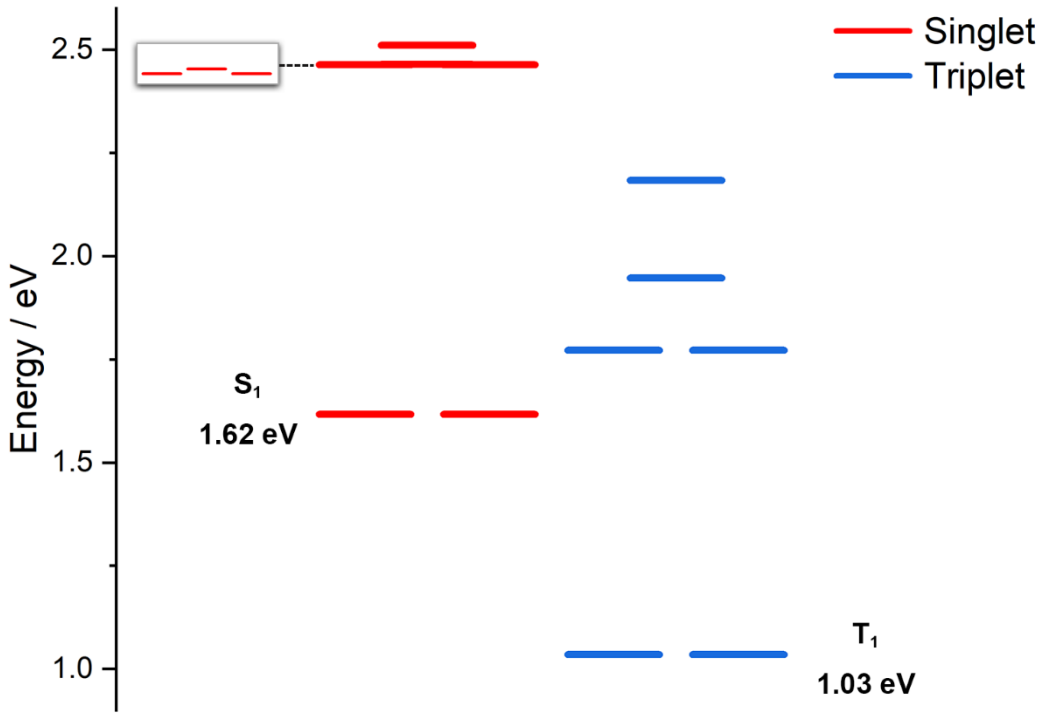

Figure S71. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TNP**.

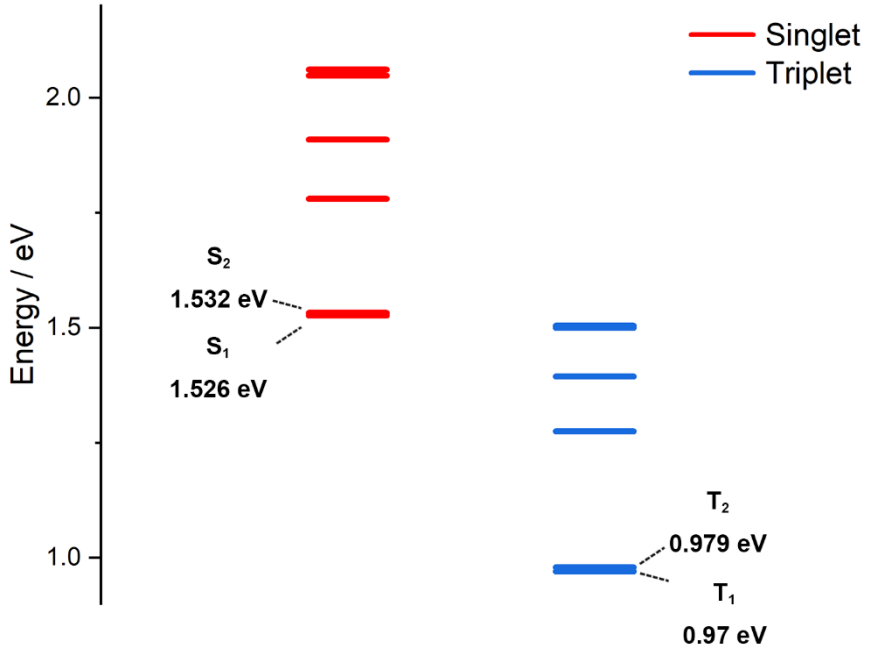

Figure S72. TD-DFT calculated singlet energy levels (from S_6 to S_1) and triplet energy levels (from T_6 to T_1) of **Pt-TAP**.

14. Hole-electron distribution of Zn-TNP and Pt-TNP

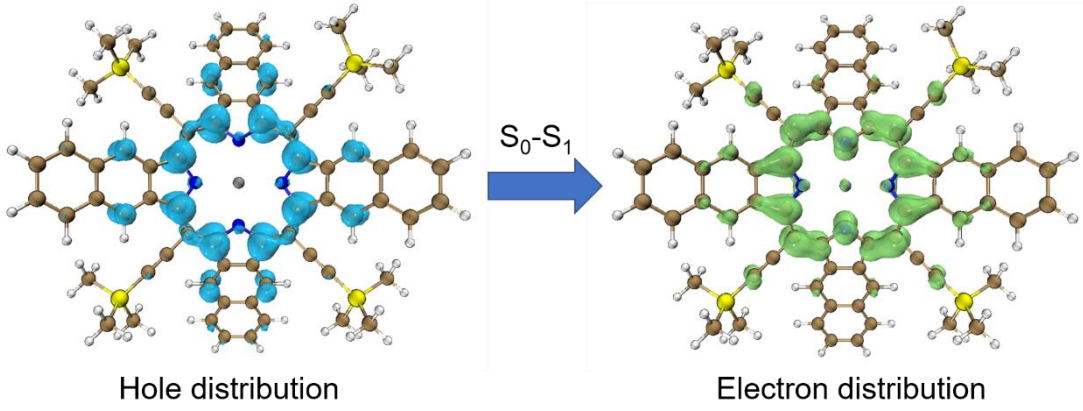

Figure S73. Hole-electron distribution (isovalue = 0.001) of **Zn-TNP** in S_0-S_1 transition.

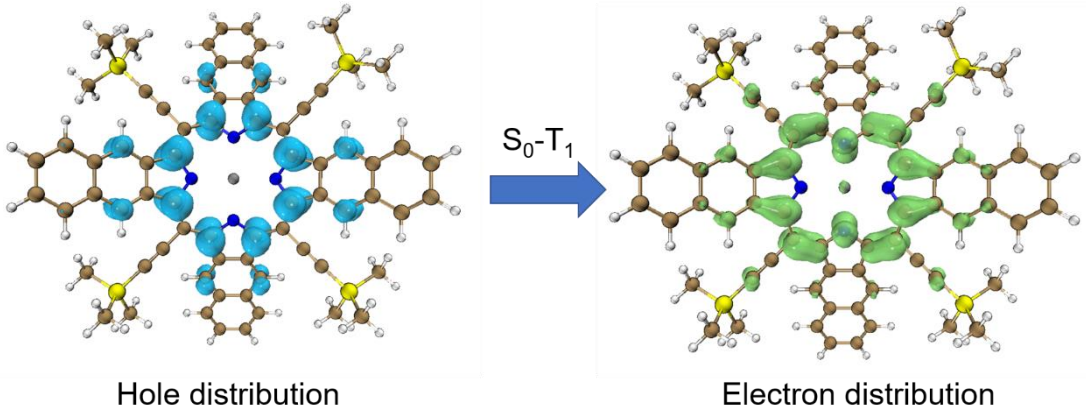

Figure S74. Hole-electron distribution (isovalue = 0.001) of **Zn-TNP** in S_0-T_1 transition.

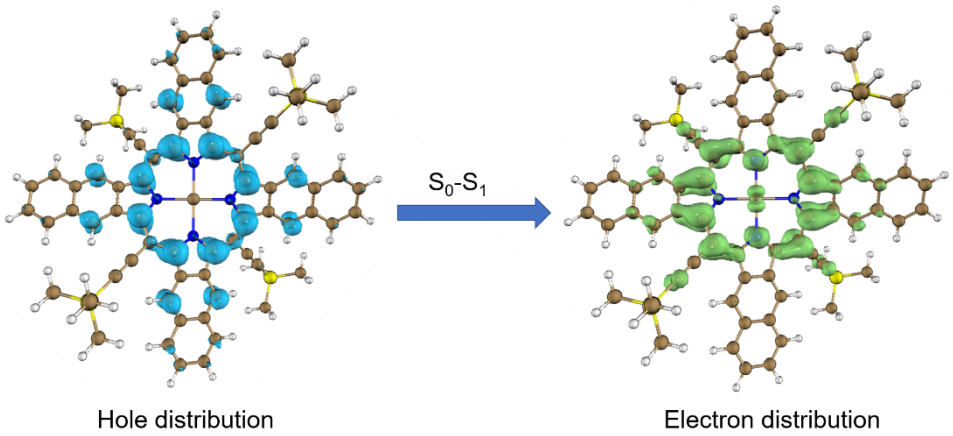

Figure S75. Hole-electron distribution (isovalue = 0.001) of **Pt-TNP** in S_0-S_1 transition.

15. NICS values

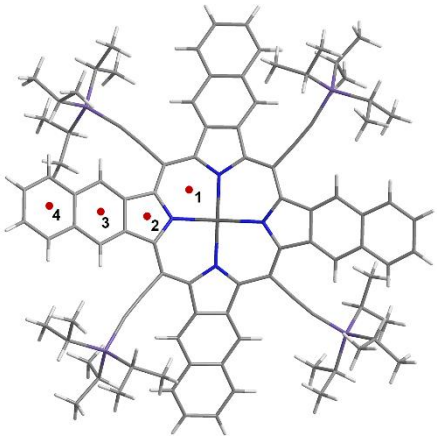

Table S7. NICS values of **Zn-TNP** and **Pt-TNP** at various positions calculated at the GIAO/B3LYP/6-31G(d,p) (for C, N, H, Si) + SDD (for Zn or Pt) levels of theory using the optimized structure.

Positions	**Zn-TNP**	**Pt-TNP**
1	-11.14	-12.52
2	-1.75	-1.69
3	-10.65	-10.14
4	-9.22	-9.01

16. ACID plots

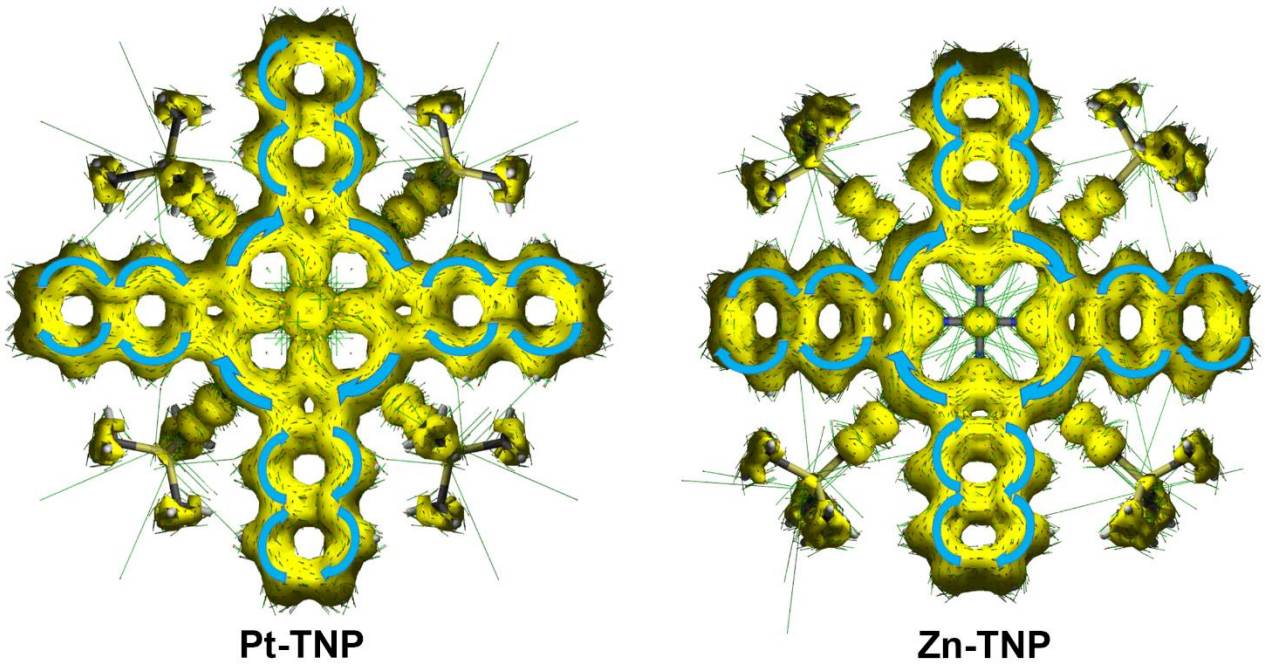

Figure S76. ACID plots (isovalue = 0.03) of **Pt-TNP** and **Zn-TNP**.

17. GIMIC

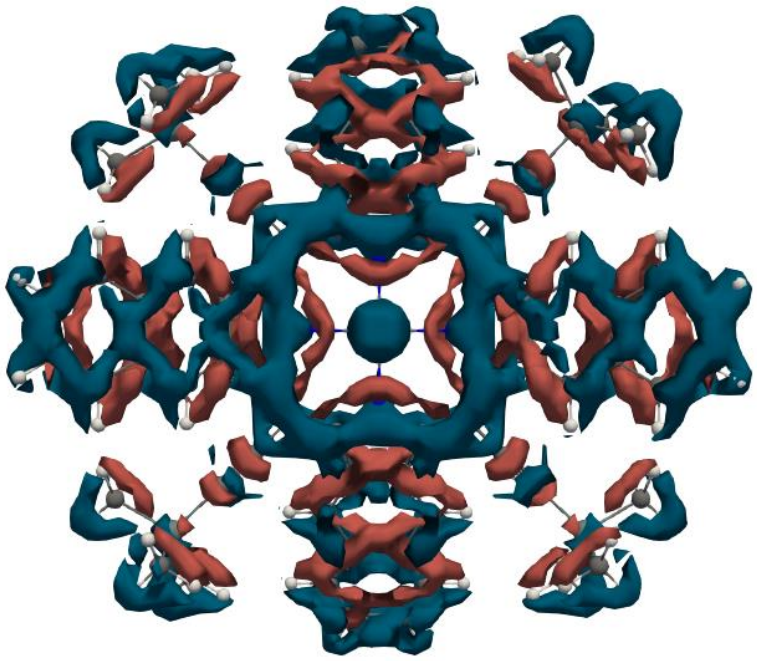

Figure S77. GIMIC of **Zn-TNP** (The signed modulus of the current density shows diatropic ring current (blue, aromaticity) and paratropic ring current (red, antiaromaticity). isovalue = 0.05).

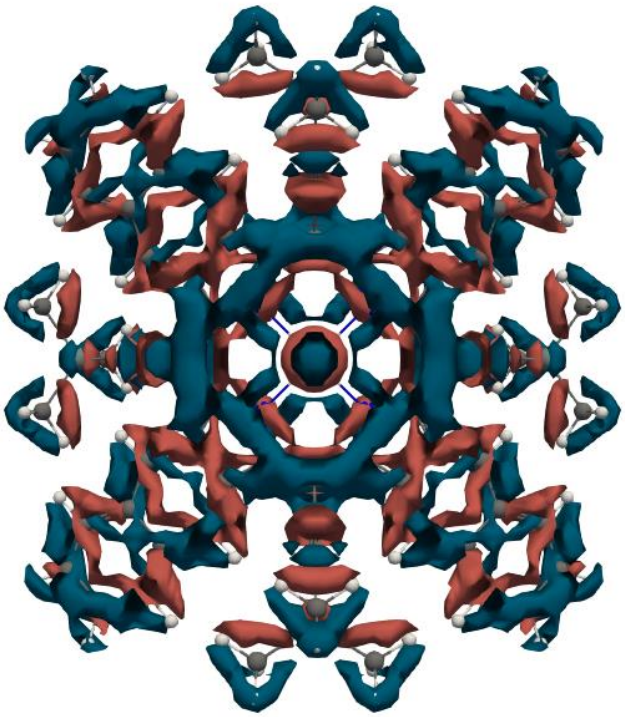

Figure S78. GIMIC of **Pt-TNP** (The signed modulus of the current density shows diatropic ring current (blue, aromaticity) and paratropic ring current (red, antiaromaticity). isovalue = 0.05).

18. Electrostatic potential maps

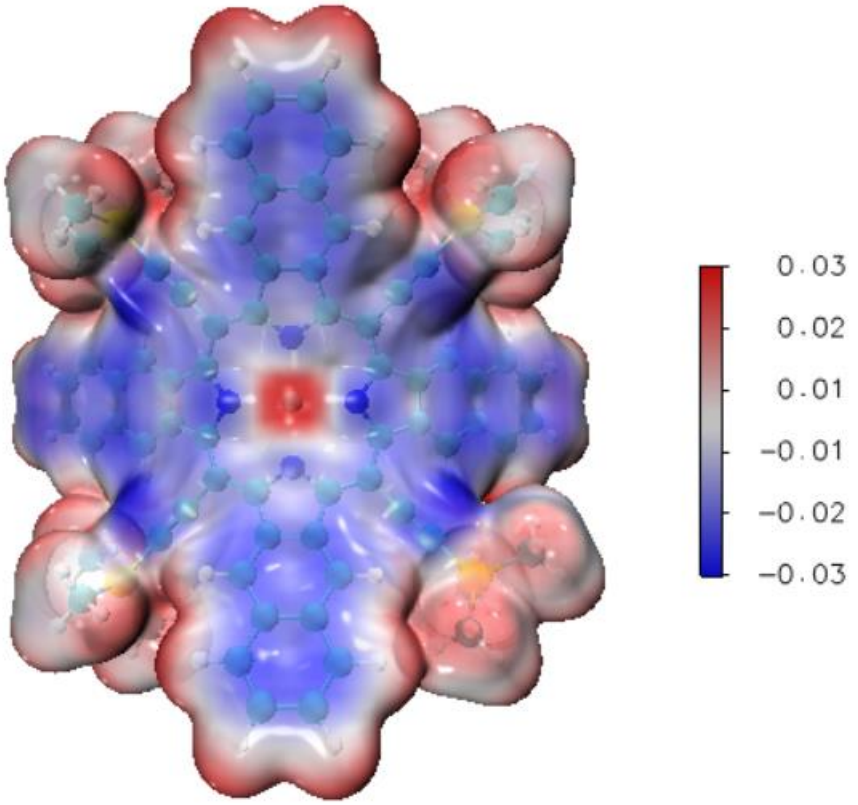

Figure S79. Electrostatic potential map of **Zn-TNP** (isovalue = 0.001).

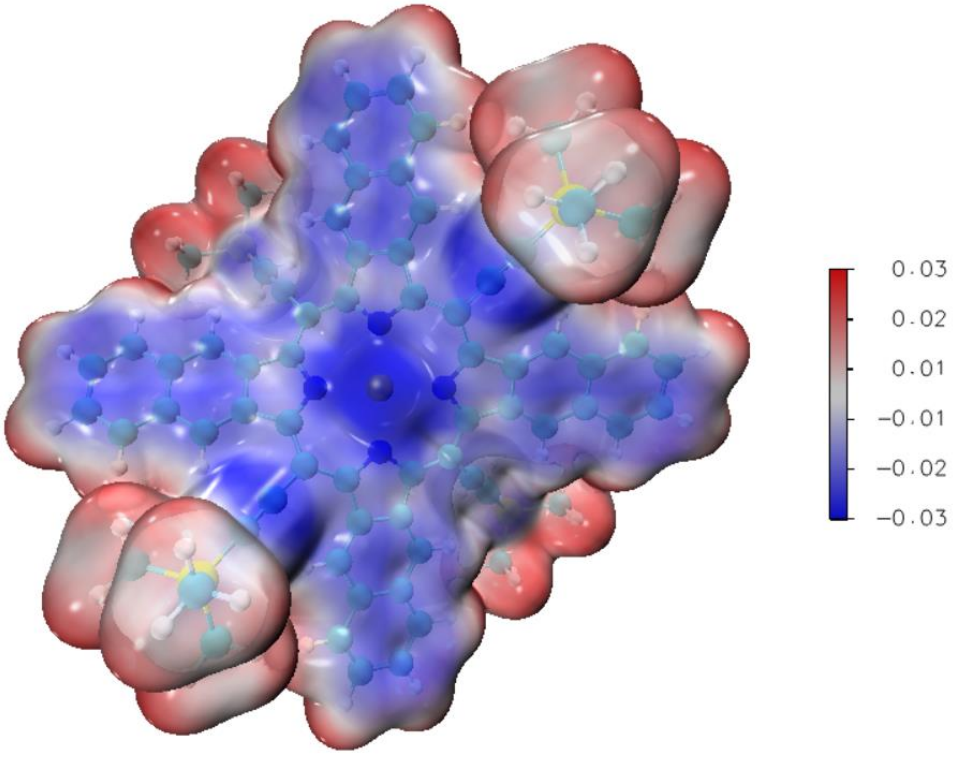

Figure S80. Electrostatic potential map of **Pt-TNP** (isovalue = 0.001).

19. Cartesian Coordinates of optimized structures

Table S8. Coordinates of the optimized structure for **Pt-TPP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2032.068712

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	2.86193173	-1.10730477	0.01638708	C	-3.72875053	-4.28183173	-1.18107959
C	4.23879980	-0.67738015	0.07264249	C	-4.71694770	-5.26735715	-1.19427674
C	4.23823393	0.68093127	0.07251291	C	-5.49721349	-5.49422221	-0.05889231
C	2.86100703	1.10969228	0.01620661	C	-5.28414085	-4.72936840	1.08954421
N	2.04223502	0.00085458	-0.00905215	C	-4.29667462	-3.74312400	1.10239418
C	2.44724290	-2.44527331	0.01769511	C	3.73233097	-4.27879586	1.18102107
C	2.44518894	2.44731241	0.01739812	C	4.72137003	-5.26346905	1.19417391
C	1.10734836	2.86240891	0.00852057	C	5.50185670	-5.48958953	0.05878701
C	0.67739300	4.24035935	-0.00046189	C	5.28815995	-4.72484341	-1.08959799
C	-0.68092011	4.23979833	0.00033735	C	4.29984619	-3.73944139	-1.10240308
C	-1.10973493	2.86149341	-0.00858091	H	5.08876198	-1.34099603	0.11896705
N	-0.00085699	2.04232851	-0.00002428	H	5.08763930	1.34527056	0.11870557
C	-2.44722716	2.44526848	-0.01737921	H	1.34083795	5.09167117	-0.00411662
C	-2.86191553	1.10729954	-0.01607919	H	-1.34506911	5.09056205	0.00396251
C	-4.23879187	0.67739193	-0.07221715	H	-5.08875588	1.34101984	-0.11833702
C	-4.23823316	-0.68091978	-0.07232325	H	-5.08765201	-1.34524059	-0.11854291
C	-2.86100495	-1.10969756	-0.01623801	H	-1.34082730	-5.09166573	0.00370014
N	-2.04222103	-0.00086248	0.00911622	H	1.34509070	-5.09055645	-0.00396036
C	-2.44517975	-2.44731563	-0.01764882	H	3.12593039	4.10359061	2.06602291
C	-1.10733528	-2.86240719	-0.00873427	H	4.87921266	5.85536642	2.09243391
C	-0.67737675	-4.24035742	0.00020975	H	6.26596055	6.26158468	0.06775391
C	0.68093655	-4.23979631	-0.00037720	H	5.88397766	4.90154576	-1.97961646
C	1.10974769	-2.86149313	0.00869496	H	4.12892118	3.15130841	-1.99838446
N	0.00087346	-2.04232722	0.00000748	H	-4.13146440	3.14801149	1.99844690
C	3.50570343	3.50694862	0.03196714	H	-5.88808037	4.89668035	1.97957228
C	3.50864620	-3.50401178	0.03248779	H	-6.27136573	6.25616315	-0.06792402
C	-3.50570870	-3.50693283	-0.03250169	H	-4.88433985	5.85097309	-2.09261993
C	-3.50864397	3.50400087	-0.03196377	H	-3.12950112	4.10075725	-2.06610478
Pt	0.00000626	-0.00000221	0.00001070	H	-3.12557598	-4.10339659	-2.06654945
C	3.72893853	4.28196882	1.18042617	H	-4.87888601	-5.85510861	-2.09346175
C	4.71711494	5.26751437	1.19334360	H	-6.26602818	-6.26150128	-0.06906488
C	5.49717015	5.49427804	0.05779128	H	-5.88435152	-4.90171603	1.97851832
C	5.28392282	4.72929072	-1.09051931	H	-4.12925640	-3.15152137	1.99778891
C	4.29647385	3.74302088	-1.10308969	H	3.12899580	-4.10090585	2.06649290
C	-4.29957410	3.73948899	1.10310088	H	4.88381669	-5.85113597	2.09332212
C	-5.28790272	4.72487665	1.09047060	H	6.27132689	-6.25621194	0.06894095
C	-5.50188316	5.48955132	-0.05791151	H	5.88854499	-4.89659883	-1.97856898

C	-4.72167147	5.26336696	-1.19347207	H	4.13195426	-3.14791400	-1.99775648
C	-3.73261926	4.27870101	-1.18049613				

Table S9. Coordinates of the optimized structure for **Pt-TPTBP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2646.628454

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	2.99711311	-0.34834558	0.37654720	C	-3.83011492	-6.72089572	0.02621371
C	4.11772802	0.38989712	0.95308521	C	-2.84246992	-6.47115438	0.98210385
C	3.74359574	1.75397798	0.95939204	C	-2.14937940	-5.25994684	0.97294900
C	2.40259797	1.82277077	0.38484594	C	5.26041916	-2.14941636	-0.97223990
N	1.96223902	0.53605611	0.15436782	C	6.47154882	-2.84263348	-0.98101851
C	2.97673091	-1.69854321	-0.00721580	C	6.72072723	-3.83059687	-0.02530958
C	1.69858930	2.97676268	0.00708974	C	5.75067897	-4.12460963	0.93593682
C	0.34832154	2.99713831	-0.37644511	C	4.53633320	-3.43712826	0.93818451
C	-0.38994703	4.11768564	-0.95309507	H	5.63449498	-1.04995843	1.54909386
C	-1.75401653	3.74351664	-0.95933833	H	7.11436048	0.65155091	2.52210848
C	-1.82274501	2.40253091	-0.38479389	H	6.45696338	3.04480389	2.53460011
N	-0.53600869	1.96220694	-0.15439125	H	4.31322437	3.76086510	1.57282206
C	-2.97666526	1.69855433	-0.00697346	H	1.04982278	5.63455324	-1.54901939
C	-2.99703214	0.34834264	0.37669614	H	-0.65181440	7.11443314	-2.52185016
C	-4.11761594	-0.38995733	0.95324357	H	-3.04504215	6.45695285	-2.53423404
C	-3.74340891	-1.75401650	0.95952385	H	-3.76097683	4.31312519	-1.57252197
C	-2.40245111	-1.82271817	0.38498643	H	-5.63461188	1.04976160	1.54896449
N	-1.96211179	-0.53599139	0.15461348	H	-7.11446410	-0.65190726	2.52179878
C	-1.69852514	-2.97663645	0.00707750	H	-6.45678970	-3.04510293	2.53445046
C	-0.34833076	-2.99699873	-0.37671011	H	-4.31287313	-3.76096890	1.57291676
C	0.38991087	-4.11753306	-0.95341895	H	-1.04989533	-5.63431459	-1.54951863
C	1.75396988	-3.74330633	-0.95983618	H	0.65164348	-7.11391037	-2.52291498
C	1.82274683	-2.40242204	-0.38510659	H	3.04483094	-6.45622523	-2.53575092
N	0.53605751	-1.96211349	-0.15452705	H	3.76081105	-4.31251078	-1.57380222
C	4.27784024	-2.44003689	-0.01409627	H	-5.06687241	1.37809963	-1.71265926
C	-2.43986534	-4.27784638	0.01427742	H	-7.21995876	2.61029287	-1.73412953
C	-4.27791213	2.43982034	-0.01420603	H	-7.66523622	4.36698606	-0.03060746
C	5.34079780	-0.01041811	1.51836753	H	-5.94009114	4.88898163	1.68334840
C	6.17189559	0.95393060	2.07451497	H	-3.78086764	3.66734512	1.68278645
C	5.80010571	2.30781327	2.08142452	H	-3.66781578	-3.78048618	-1.68231665
C	4.59180722	2.71753077	1.53175273	H	-4.88964136	-5.93960049	-1.68281032
C	0.01029396	5.34080806	-1.51828409	H	-4.36735136	-7.66499016	0.03080151
C	-0.95412632	6.17192147	-2.07430917	H	-2.61009090	-7.22011582	1.73384297
C	-2.30800278	5.80009137	-2.08114424	H	-1.37768384	-5.06715176	1.71227645
C	-2.71764251	4.59174896	-1.53151680	H	5.06808317	-1.37746925	-1.71142315

C	-5.34078468	0.01025043	1.51835123	H	7.22089344	-2.61010762	-1.73233092
C	-6.17188855	-0.95418607	2.07437195	H	7.66476187	-4.36793981	-0.02961481
C	-5.79995543	-2.30804507	2.08134955	H	5.93845805	-4.89060461	1.68297496
C	-4.59156567	-2.71764510	1.53179227	H	3.77950590	-3.66850321	1.68184438
C	-0.01036591	-5.34055253	-1.51882792	C	2.43986754	4.27800163	0.01408634
C	0.95399411	-6.17148363	-2.07522294	C	3.43672523	4.53689109	-0.93832303
C	2.30784828	-5.79954547	-2.08230638	C	2.14937886	5.26023217	0.97262834
C	2.71752007	-4.59128611	-1.53251406	C	4.12403898	5.75132684	-0.93587769
Pt	0.00004291	0.00003684	0.00006483	H	3.66802750	3.78031422	-1.68225967
C	-5.25983931	2.14955417	-0.97312526	C	2.84244011	6.47145368	0.98160737
C	-6.47111612	2.84252484	-0.98222608	H	1.37768226	5.06754128	1.71198077
C	-6.72108347	3.82985217	-0.02606651	C	3.83012125	6.72105526	0.02571962
C	-5.75168949	4.12348214	0.93595952	H	4.88983745	5.93942792	-1.68303606
C	-4.53719666	3.43626315	0.93852922	H	2.61001221	7.22053392	1.73321316
C	-3.43658102	-4.53693368	-0.93822699	H	4.36733945	7.66516018	0.03016932
C	-4.12391154	-5.75136505	-0.93561504				

Table S10. Coordinates of the optimized structure for **Pt-TPTNP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3261.195841

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-1.18994391	-2.77289421	0.37967396	C	-5.15218071	-1.29865804	-1.54922162
C	-0.80785528	-4.05724943	0.96434917	C	7.28686137	-1.57552088	-2.68016421
C	0.62255981	-4.08576841	0.97750517	C	8.34715858	-0.90789895	-3.24507159
C	1.06619714	-2.81965796	0.39662846	C	8.37433638	0.51230582	-3.25969422
N	-0.04462099	-2.03470727	0.16523373	C	7.34063678	1.23146671	-2.70892746
C	-2.47479320	-2.37074261	-0.01442874	C	-1.57625755	-7.28689465	2.67965613
C	2.37072074	-2.47479246	0.01393513	C	-0.90881312	-8.34718260	3.24479009
C	2.77278699	-1.18989431	-0.38009362	C	0.51138679	-8.37441661	3.25974083
C	4.05709569	-0.80768806	-0.96483691	C	1.23071579	-7.34078368	2.70906605
C	4.08555390	0.62271369	-0.97779525	C	-7.28694207	1.57642320	-2.67951299
C	2.81945221	1.06621709	-0.39697046	C	-8.34723060	0.90900513	-3.24467737
N	2.03462593	-0.04460890	-0.16532914	C	-8.37445106	-0.51119415	-3.25972276
C	2.47475614	2.37075476	-0.01438951	C	-7.34080316	-1.23054859	-2.70911016
C	1.18997804	2.77292457	0.38008675	C	1.57576549	7.28642554	2.68145857
C	0.80782724	4.05713777	0.96519710	C	0.90819222	8.34652267	3.24680052
C	-0.62259707	4.08555540	0.97839023	C	-0.51201080	8.37364745	3.26163978
C	-1.06617517	2.81956370	0.39732477	C	-1.23121220	7.34009459	2.71065051
N	0.04463615	2.03471721	0.16565568	H	-2.75867501	-4.45889786	-1.72781896
C	-2.37075007	2.47479900	0.01480081	H	-4.55065746	-6.17398807	-1.75943601
C	-2.77292342	1.18999996	-0.37948831	H	-6.36586139	-6.10842951	-0.05985202
C	-4.05727238	0.80796115	-0.96426095	H	-6.37972562	-4.31261946	1.66138502

C	-4.08576985	-0.62245161	-0.97758323	H	-4.59412406	-2.59050582	1.67240781
C	-2.81964566	-1.06614189	-0.39682310	H	4.45936160	-2.75901314	1.72668686
N	-2.03475043	0.04464441	-0.16512921	H	6.17453947	-4.55092830	1.75737728
C	3.55545299	3.40807814	-0.02680044	H	6.10859816	-6.36570067	0.05734596
C	3.40836310	-3.55519218	0.02520560	H	4.31235875	-6.37916432	-1.66344753
C	-3.40827958	3.55529969	0.02677738	H	2.59016433	-4.59363963	-1.67354109
C	-3.55520680	-3.40836628	-0.02621392	H	-2.59053261	4.59425691	-1.67187362
C	-3.55446643	-4.42805278	-0.98947382	H	-4.31249034	6.38000486	-1.66053202
C	-4.56259221	-5.39287858	-1.00458175	H	-6.10809163	6.36619249	0.06092256
C	-5.58249337	-5.35593587	-0.05049460	H	-6.17360796	4.55088132	1.76039635
C	-5.59041515	-4.34685813	0.91579954	H	-4.45868630	2.75874898	1.72845283
C	-4.58591406	-3.37819281	0.92485231	H	4.59512891	2.58984489	1.67117402
C	4.42834834	-3.55461898	0.98814910	H	6.38133987	4.31132615	1.65904033
C	5.39322281	-4.56270665	1.00273509	H	6.36711898	6.10706334	-0.06226582
C	5.35606356	-5.58236721	0.04839857	H	4.55104682	6.17309428	-1.76090779
C	4.34674613	-5.59006277	-0.91764775	H	2.75847811	4.45863939	-1.72818207
C	3.37803315	-4.58560472	-0.92617594	H	5.08450449	-2.61677909	-1.54935839
C	-3.37812885	4.58606818	-0.92422300	H	5.18100801	2.37913667	-1.59801538
C	-4.34670844	5.59065042	-0.91499217	H	-2.61712509	-5.08450211	1.54860119
C	-5.35567017	5.58275663	0.05142311	H	2.37871047	-5.18132885	1.59838996
C	-5.39258864	4.56279581	1.00544862	H	2.61690084	5.08447008	1.54997777
C	-4.42785699	3.55458447	0.99015565	H	-2.37892464	5.18075836	1.59937747
C	4.58676664	3.37750372	0.92358887	H	-5.08458326	2.61724386	-1.54838158
C	5.59160765	4.34581484	0.91391300	H	-5.18130007	-2.37859169	-1.59852899
C	5.58348118	5.35485703	-0.05241425	H	7.26219456	-2.66222283	-2.66690036
C	4.56309724	5.39206036	-1.00597716	H	9.17044778	-1.46438950	-3.68381052
C	3.55464185	4.42759132	-0.99024706	H	9.21815311	1.02774755	-3.70943871
C	5.09690347	-1.53578409	-1.52162504	H	7.35771423	2.31835632	-2.71773081
C	6.19889644	-0.86359318	-2.09754505	H	-2.66295539	-7.26217318	2.66615026
C	6.22654431	0.57378213	-2.11211860	H	-1.46543977	-9.17041460	3.68346386
C	5.15194809	1.29916310	-1.54912881	H	1.02669093	-9.21822085	3.70966664
C	-1.53612745	-5.09699658	1.52102471	H	2.31760257	-7.35790061	2.71811848
C	-0.86414269	-6.19900825	2.09712038	H	-7.26223457	2.66312038	-2.66593061
C	0.57321558	-6.22670703	2.11202597	H	-9.17047509	1.46565283	-3.68330104
C	1.29877975	-5.15218025	1.54913713	H	-9.21825625	-1.02647699	-3.70967115
C	1.53592637	5.09682626	1.52225648	H	-7.35790844	-2.31743501	-2.71823577
C	0.86378747	6.19862767	2.09859059	H	2.66246607	7.26179122	2.66803230
C	-0.57356894	6.22622241	2.11338599	H	1.46471994	9.16968624	3.68572844
C	-1.29897551	5.15176110	1.55019739	H	-1.02741762	9.21729918	3.71173409
C	-5.09703913	1.53624850	-1.52089433	H	-2.31810127	7.35712108	2.71962203
C	-6.19903895	0.86428256	-2.09703986	Pt	-0.00003525	0.00001246	0.00004176
C	-6.22672666	-0.57307461	-2.11204102				

Table S11. Coordinates of the optimized structure for **Pt-TPTAP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3875.743846

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	0.99898455	2.84453685	-0.39571717	C	3.63934255	-3.31852674	0.00666024
C	0.52944498	4.09777875	-0.98459840	C	3.66700004	-4.34473908	0.96265805
C	-0.90798882	4.03184786	-0.98133209	C	4.69931647	-5.28376828	0.96873560
C	-1.25816059	2.74057477	-0.39151419	C	5.71599172	-5.21396813	0.01297107
N	-0.09425333	2.03329946	-0.17072438	C	5.69607931	-4.19804943	-0.94595845
C	2.30879169	2.53264749	-0.00355368	C	4.66695588	-3.25549992	-0.94617189
C	-2.53264797	2.30879444	0.00356056	C	-4.34470257	-3.66703067	-0.96269681
C	-2.84453909	0.99898861	0.39572754	C	-5.28372656	-4.69935176	-0.96878606
C	-4.09778514	0.52944944	0.98460020	C	-5.21395934	-5.71600315	-0.01299369
C	-4.03185319	-0.90798437	0.98133716	C	-4.19807729	-5.69606343	0.94597409
C	-2.74057705	-1.25815645	0.39152577	C	-3.25553178	-4.66693640	0.94619850
N	-2.03329983	-0.09424939	0.17074274	C	-4.66693444	3.25553263	-0.94620594
C	-2.30879395	-2.53264254	-0.00354997	C	-5.69605899	4.19808099	-0.94599268
C	-0.99898718	-2.84453123	-0.39571341	C	-5.71600114	5.21396883	0.01296897
C	-0.52944733	-4.09777681	-0.98458515	C	-4.69935422	5.28373966	0.96876588
C	0.90798593	-4.03184642	-0.98131729	C	-3.66703556	4.34471279	0.96268799
C	1.25815744	-2.74056872	-0.39151120	C	3.25554797	4.66693178	0.94619984
N	0.09425045	-2.03329356	-0.17072248	C	4.19809703	5.69605565	0.94597142
C	2.53264407	-2.30878877	0.00356330	C	5.21396727	5.71599913	-0.01300886
C	2.84453554	-0.99898339	0.39572957	C	5.28371979	4.69935417	-0.96880915
C	4.09778398	-0.52944299	0.98459569	C	4.34469270	3.66703594	-0.96271573
C	4.03185094	0.90799054	0.98133284	H	-2.26077020	-5.22883902	-1.59501312
C	2.74057389	1.25816156	0.39152360	H	2.73829318	-5.00021972	-1.58274983
N	2.03329647	0.09425423	0.17074329	H	-5.22884794	2.26077316	1.59502603
C	-1.18168783	-5.17232761	-1.55301773	H	-5.00022107	-2.73828940	1.58278694
C	-0.43320415	-6.23561234	-2.12906864	H	5.22885256	-2.26076517	1.59501382
C	1.01290011	-6.16949572	-2.12541057	H	5.00021894	2.73829698	1.58277826
C	1.65836443	-5.04237490	-1.54610232	H	7.39592136	-2.14892052	2.71396972
C	-5.17233579	1.18169076	1.55303315	H	7.16827745	2.83026518	2.70140359
C	-6.23561795	0.43320826	2.12909030	H	-2.14892527	-7.39590596	-2.71397430
C	-6.16949842	-1.01289578	2.12544018	H	2.83026113	-7.16827878	-2.70137567
C	-5.04237823	-1.65836114	1.54613182	H	2.26076811	5.22883523	-1.59503733
C	5.17233835	-1.18168303	1.55302241	H	-2.73829517	5.00021305	-1.58278245
C	6.23562176	-0.43319953	2.12907579	H	2.14892433	7.39589241	-2.71401667
C	6.16950017	1.01290440	2.12542757	H	-2.83026208	7.16826174	-2.70142785
C	5.04237695	1.65836861	1.54612380	H	-7.39591263	2.14893047	2.71399088
C	7.34767447	-1.06226442	2.71249438	H	-7.16827581	-2.83025560	2.70141877
C	8.39252955	-0.33173229	3.28635893	H	-9.57932950	2.04901083	3.88192927

C	8.32641668	1.11450596	3.28268394	H	-11.39858230	0.71374430	4.88114644
C	7.21940100	1.74374683	2.70538193	H	-11.28470706	-1.77725380	4.87482129
C	-1.06226900	-7.34766251	-2.71249205	H	-9.35144286	-2.93588086	3.86927700
C	-0.33173661	-8.39251960	-3.28635270	H	9.57934267	-2.04899910	3.88189945
C	1.11450184	-8.32641160	-3.28266816	H	11.39859764	-0.71373113	4.88111072
C	1.74374268	-7.21939857	-2.70536110	H	11.28471902	1.77726684	4.87478854
C	1.18168574	5.17232456	-1.55304107	H	9.35144910	2.93589228	3.86925322
C	0.43320260	6.23560361	-2.12910323	H	-2.04900352	-9.57932653	-3.88190536
C	-1.01290162	6.16948598	-2.12544810	H	-0.71373509	-11.39858515	-4.88110935
C	-1.65836655	5.04237004	-1.54613071	H	1.77726321	-11.28471484	-4.87477083
C	1.06226807	7.34764843	-2.71253631	H	2.93588854	-9.35144974	-3.86922629
C	0.33173629	8.39249939	-3.28640885	H	2.04900380	9.57930166	-3.88196902
C	-1.11450212	8.32639038	-3.28272720	H	0.71373650	11.39854959	-4.88119396
C	-1.74374360	7.21938254	-2.70541093	H	-1.77726171	11.28467753	-4.87486040
C	-7.34766738	1.06227424	2.71251414	H	-2.93588814	9.35142137	-3.86929991
C	-8.39252119	0.33174295	3.28638214	H	2.87385432	-4.40114876	1.70235004
C	-8.32641033	-1.11449538	3.28270540	H	4.70884511	-6.07035151	1.71792786
C	-7.21939788	-1.74373722	2.70539829	H	6.51832524	-5.94627727	0.01539126
C	-9.53171810	0.96296153	3.88001552	H	6.48273034	-4.13818796	-1.69274492
C	-10.54024606	0.22067216	4.43393010	H	4.65334198	-2.46274503	-1.68830035
C	-10.47504211	-1.20566517	4.43030776	H	-4.40108686	-2.87390337	-1.70241060
C	-9.40312374	-1.85002220	3.87287479	H	-6.07028038	-4.70890233	-1.71800897
C	9.53172974	-0.96294988	3.87998705	H	-5.94626479	-6.51834000	-0.01542281
C	10.54025892	-0.22065971	4.43389834	H	-4.13824097	-6.48269637	1.69278169
C	10.47505301	1.20567754	4.43027771	H	-2.46280546	-4.65330143	1.68835706
C	9.40313152	1.85003367	3.87284970	H	-4.65329750	2.46280168	-1.68835976
C	-0.96295415	-9.53171725	-3.87998583	H	-6.48268795	4.13824235	-1.69280426
C	-0.22066372	-10.54024844	-4.43389308	H	-6.51833593	5.94627659	0.01538927
C	1.20567372	-10.47504729	-4.43026309	H	-4.70890634	6.07029843	1.71798358
C	1.85002980	-9.40312839	-3.87282996	H	-2.87391172	4.40109970	1.70240546
C	0.96295445	9.53169164	-3.88005163	H	2.46283065	4.65329390	1.68836815
C	0.22066466	10.54021690	-4.43397050	H	4.13827252	6.48268324	1.69278563
C	-1.20567273	10.47501475	-4.43034334	H	5.94627537	6.51833360	-0.01544106
C	-1.85002941	9.40310088	-3.87290138	H	6.07026461	4.70890748	-1.71804143
C	-3.31852804	-3.63934452	-0.00665891	H	4.40106554	2.87391374	-1.70243586
C	-3.63934805	3.31853107	0.00665761	Pt	-0.00000172	0.00000302	0.00001800
C	3.31852884	3.63934683	-0.00666636				

Table S12. Coordinates of the optimized structure for **Pt-P** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3047.259662							
Charge = 0, Multiplicity = 1							
Number of Imaginary Frequencies = 0							
Atom	x	y	z	Atom	x	y	z

C	-1.11883612	-2.85979141	0.00026258	H	7.48547720	6.17188850	-1.58197903
C	-0.70420544	-4.23862020	0.00055401	H	7.19247604	4.42630530	-1.57663981
C	0.65539437	-4.24637110	0.00050693	H	5.52870896	8.09736051	-0.00114822
C	1.08596573	-2.87249708	0.00018726	H	4.15681664	7.41543133	-0.88676246
N	-0.01169446	-2.04441274	-0.00001410	H	4.15603524	7.41574556	0.88349564
C	-2.45920676	-2.43114297	0.00028677	C	-5.40552385	6.70246405	1.54978641
C	2.43112591	-2.45921728	0.00012580	C	-5.40556137	6.70246236	-1.55039128
C	2.85977384	-1.11884650	-0.00009425	C	-7.28919678	4.78846599	-0.00027858
C	4.23860272	-0.70421591	-0.00007942	H	-5.50294136	6.10062653	2.45900090
C	4.24635347	0.65538388	-0.00027526	H	-4.42652857	7.19186061	1.57653155
C	2.87247949	1.08595518	-0.00040661	H	-6.17203440	7.48534072	1.58116855
N	2.04439516	-0.01170484	-0.00034761	H	-5.50277118	6.10058203	-2.45959937
C	2.45919969	2.43111519	-0.00054579	H	-6.17221601	7.48519393	-1.58187347
C	1.11882896	2.85976297	-0.00056489	H	-4.42665572	7.19204370	-1.57704793
C	0.70419825	4.23859171	-0.00060550	H	-8.09732601	5.52883919	-0.00010360
C	-0.65540140	4.24634234	-0.00056016	H	-7.41567671	4.15665896	-0.88548726
C	-1.08597243	2.87246847	-0.00049099	H	-7.41552579	4.15640630	0.88477103
N	0.01168747	2.04438445	-0.00053836	C	-6.70198853	-5.40555772	1.55177368
C	-2.43113235	2.45918911	-0.00038167	C	-6.70296031	-5.40557370	-1.54840388
C	-2.85978056	1.11881856	-0.00021732	C	-4.78846853	-7.28921097	0.00110303
C	-4.23860922	0.70418781	0.00000577	H	-6.09986467	-5.50299322	2.46079674
C	-4.24636001	-0.65541184	0.00019761	H	-7.19137228	-4.42656077	1.57868914
C	-2.87248606	-1.08598292	0.00009011	H	-7.48485769	-6.17206636	1.58338975
N	-2.04440203	0.01167709	-0.00021728	H	-6.10136526	-5.50275943	-2.45780331
H	-1.38388223	-5.07755200	0.00078225	H	-7.48569189	-6.17223781	-1.57965247
H	1.32556746	-5.09287528	0.00068851	H	-7.19256383	-4.42667438	-1.57488996
H	5.07753454	-1.38389282	0.00007997	H	-5.52883786	-8.09734369	0.00153302
H	5.09285765	1.32555689	-0.00030777	H	-4.15695658	-7.41569581	-0.88431546
H	1.38387495	5.07752355	-0.00064493	H	-4.15611266	-7.41552923	0.88594268
H	-1.32557448	5.09284639	-0.00055359	C	5.40614034	-6.70152497	1.55177677
H	-5.07754107	1.38386439	0.00003216	C	5.40519158	-6.70332057	-1.54840032
H	-5.09286405	-1.32558499	0.00041314	C	7.28922737	-4.78833493	0.00002170
C	3.47375151	3.43493277	-0.00058068	H	5.50389853	-6.09916261	2.46060729
C	4.34119527	4.29619009	-0.00061083	H	4.42714983	-7.19089497	1.57916313
C	3.43494384	-3.47376905	0.00040741	H	6.17265581	-7.48439022	1.58333090
C	4.29620525	-4.34120884	0.00065189	H	5.50199884	-6.10195503	-2.45799177
C	-3.43494918	3.47374138	-0.00034414	H	6.17191919	-7.48598711	-1.57971250
C	-4.29619673	4.34119471	-0.00031821	H	4.42633004	-7.19302559	-1.57441415
C	-3.47375915	-3.43495995	0.00063840	H	8.09739263	-5.52866874	0.00046365
C	-4.34121124	-4.29620884	0.00093612	H	7.41543837	-4.15710046	-0.88563364
C	6.70204711	5.40605678	1.54974831	H	7.41576386	-4.15569072	0.88462409
C	6.70280362	5.40517771	-1.55042910	Si	-5.64080209	-5.60336491	0.00135284
C	4.78836361	7.28920573	-0.00133198	Si	-5.60334671	5.64079172	-0.00029928
H	6.09999152	5.50378794	2.45878485	Si	5.64074705	5.60338497	-0.00065535

H	7.19142166	4.42706295	1.57693814	Si	5.60341868	-5.64074197	0.00101248
H	7.48492760	6.17256638	1.58106394	Pt	-0.00000342	-0.00001418	-0.00064540
H	6.10113438	5.50203006	-2.45981496				

Table S13. Coordinates of the optimized structure for **Pt-TBP** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3661.819280

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-0.64806356	2.94588461	0.38953989	C	-8.19968593	0.17928110	-2.84935691
C	-1.73854161	3.90291911	0.26680860	C	-6.33018246	1.37922601	-5.01453534
C	-2.84382035	3.18948742	-0.25838650	C	-3.21047710	-7.55628350	2.83014107
C	-2.41903259	1.80267634	-0.38624545	C	-0.17745907	-8.19792012	2.85314129
N	-1.10455562	1.71035595	0.00054534	C	-1.38275308	-6.32784169	5.01487185
C	0.69689719	3.23662887	0.72063067	Pt	-0.00006660	-0.00001909	-0.00017496
C	-3.23676271	0.69690016	-0.72078164	H	-0.99703312	5.83958186	0.89268353
C	-2.94597714	-0.64806159	-0.38972222	H	-3.13194022	6.98947979	0.44128533
C	-3.90298049	-1.73856961	-0.26693012	H	-5.08750526	5.72699839	-0.41893406
C	-3.18949070	-2.84382955	0.25821468	H	-4.91566766	3.30975597	-0.87895847
C	-1.80272619	-2.41897378	0.38607860	H	-5.83970193	-0.99714649	-0.89271652
N	-1.71043137	-1.10452030	-0.00075697	H	-6.98944756	-3.13218036	-0.44142460
C	-0.69695241	-3.23668197	0.72058771	H	-5.72680350	-5.08772879	0.41859107
C	0.64797260	-2.94593302	0.38935167	H	-3.30955674	-4.91574266	0.87862096
C	1.73841987	-3.90297888	0.26643858	H	0.99691305	-5.83964822	0.89230530
C	2.84364458	-3.18955373	-0.25887340	H	3.13172242	-6.98960652	0.44050876
C	2.41886717	-1.80271993	-0.38657848	H	5.08719441	-5.72714212	-0.41994414
N	1.10442846	-1.71039678	0.00034141	H	4.91537812	-3.30988094	-0.87982352
C	3.23658044	-0.69691554	-0.72105881	H	5.83953450	0.99687053	-0.89284327
C	2.94581975	0.64799833	-0.38985204	H	6.98947783	3.13175633	-0.44132079
C	3.90288164	1.73842741	-0.26697861	H	5.72700316	5.08731418	0.41893796
C	3.18946517	2.84368256	0.25826681	H	3.30975723	4.91550546	0.87893506
C	1.80265044	2.41890759	0.38606439	H	7.17485079	-1.55781254	-5.69081987
N	1.71030389	1.10446826	-0.00083498	H	5.55554666	-2.11395644	-5.23638540
C	-4.44360302	0.95757900	-1.43356543	H	5.92540896	-0.38469264	-5.24291489
C	0.95762288	4.44345772	1.43342048	H	9.07824817	-0.32799661	-3.48693834
C	4.44348098	-0.95747461	-1.43377353	H	8.53792804	-0.23509106	-1.80467062
C	-0.95763782	-4.44351475	1.43337598	H	7.82206584	0.82937825	-3.02521955
C	-1.17053284	-5.42757562	2.12832597	H	7.88240157	-3.29483743	-1.79290540
C	-5.42770373	1.17063641	-2.12840774	H	6.79176864	-3.98155970	-3.00707073
C	1.17057478	5.42749439	2.12839087	H	8.41116209	-3.44353772	-3.47484575
C	5.42774607	-1.17045169	-2.12841013	H	1.56218651	7.17194449	5.69165793
C	-1.83899610	5.28197050	0.51042838	H	0.38942659	5.92179325	5.24478268
C	-3.04486585	5.92300348	0.25414027	H	2.11902009	5.55355822	5.23481333

C	-4.15016377	5.20945622	-0.23584734	H	3.44249901	8.41219282	3.47400075
C	-4.06082163	3.84764786	-0.49701529	H	3.29125219	7.88555160	1.79161386
C	-5.28203190	-1.83910033	-0.51052535	H	3.98146719	6.79405701	3.00301823
C	-5.92297464	-3.04503493	-0.25429395	H	0.23117988	8.53713708	1.80907921
C	-5.20933665	-4.15032967	0.23558670	H	-0.83069891	7.81835345	3.03016851
C	-3.84753520	-4.06090354	0.49675032	H	0.32559094	9.07554423	3.49187033
C	1.83884981	-5.28205347	0.50995752	H	-8.41311873	3.44210724	-3.47311003
C	3.04465611	-5.92311540	0.25344709	H	-6.79496524	3.98132547	-3.00244245
C	4.14990206	-5.20957728	-0.23667431	H	-7.88603210	3.29071442	-1.79088300
C	4.06057505	-3.84775076	-0.49774865	H	-7.81808346	-0.83106922	-3.02972383
C	5.28194077	1.83884673	-0.51056791	H	-9.07553381	0.32470903	-3.49196759
C	5.92299554	3.04469128	-0.25420677	H	-8.53751364	0.23080359	-1.80901618
C	5.20945234	4.14998619	0.23580889	H	-5.55444867	2.11957789	-5.23467351
C	3.84763789	4.06066044	0.49695447	H	-5.92215875	0.38987357	-5.24484431
Si	-6.88412446	1.48643823	-3.21271830	H	-7.17273011	1.56231815	-5.69137291
Si	-1.48654147	-6.88341187	3.21335763	H	-3.44100222	-8.41425445	3.47198376
Si	6.88450330	-1.48637251	-3.21222123	H	-3.98120965	-6.79708507	2.99910028
Si	1.48655629	6.88369382	3.21294594	H	-3.28751295	-7.88842197	1.78954733
C	6.33203701	-1.37499997	-5.01423882	H	-0.32326916	-9.07355252	3.49595874
C	8.20170712	-0.18181667	-2.84544195	H	0.83218884	-7.81525649	3.03517546
C	7.55248136	-3.21326966	-2.83386045	H	-0.22672314	-8.53637776	1.81289472
C	1.37893790	6.32954898	5.01467457	H	-2.12405302	-5.55247701	5.23311005
C	3.21199377	7.55413255	2.83226936	H	-1.56633975	-7.16994410	5.69212979
C	0.17973972	8.19957946	2.84951223	H	-0.39409092	-5.91887621	5.24647175
C	-7.55484932	3.21167804	-2.83163313				

Table S14. Coordinates of the optimized structure for **Pt-TNP** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Pt) level of theory.

E(B3LYP) = -4276.386855

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Pt	0.00000000	0.00000000	0.00000000	C	2.89817075	4.75765578	0.53322145
Si	0.00003161	-6.94966327	3.35842422	C	1.25275200	2.73829903	0.40724914
N	-1.44017546	-1.44015312	0.00001917	C	4.65665977	6.50316473	0.51553548
C	-2.73832895	-1.25271292	-0.40716747	C	-0.00001636	5.50727511	2.21212486
C	-2.51702527	-3.45103508	0.27808849	C	6.50331713	4.65648972	-0.51513048
C	-5.16912744	-4.22406981	-0.26542441	C	6.88640230	5.95186777	-0.25971901
C	-0.00001565	-3.29756290	0.75480873	C	5.95206356	6.88621566	0.26020212
C	-3.45110124	-2.51695346	-0.27791327	C	1.54757256	7.98480716	3.03220485
C	-4.75774688	-2.89806264	-0.53297223	C	-1.54762017	7.98480732	3.03213676
C	-4.22420461	-5.16900129	0.26574985	C	-0.00005366	6.31116155	5.13504283
C	0.00000000	-4.51710799	1.49296638	H	-5.47439299	-2.19908438	-0.94032674
C	-2.89817075	-4.75765578	0.53322145	H	-2.19920166	-5.47430816	0.94057892

C	-1.25275200	-2.73829903	0.40724914	H	-3.93966229	-7.21604607	0.91406594
C	-4.65665977	-6.50316473	0.51553548	H	-7.21618869	-3.93948794	-0.91366991
C	0.00001636	-5.50727511	2.21212486	H	-7.90741001	-6.26677062	-0.45523747
C	-6.50331713	-4.65648972	-0.51513048	H	-6.26699367	-7.90720284	0.45578350
C	-6.88640230	-5.95186777	-0.25971901	H	-1.58771726	-8.84375036	3.71175299
C	-5.95206356	-6.88621566	0.26020212	H	-2.45928615	-7.39760229	3.18347083
C	-1.54757256	-7.98480716	3.03220485	H	-1.55847148	-8.37084916	2.00727905
C	1.54762017	-7.98480732	3.03213676	H	2.45934427	-7.39761425	3.18338169
C	0.00005366	-6.31116155	5.13504283	H	1.55847831	-8.37082318	2.00720021
Si	-6.94966327	-0.00003161	-3.35842422	H	1.58777955	-8.84377037	3.71165870
N	-1.44015312	1.44017546	-0.00001917	H	-0.88416996	-5.69740590	5.33450064
C	-1.25271292	2.73832895	0.40716747	H	0.00016403	-7.14414157	5.84753634
C	-3.45103508	2.51702527	-0.27808849	H	0.88417072	-5.69723016	5.33442815
C	-4.22406981	5.16912744	0.26542441	H	-2.19908438	5.47439299	0.94032674
C	-3.29756290	0.00001565	-0.75480873	H	-5.47430816	2.19920166	-0.94057892
C	-2.51695346	3.45110124	0.27791327	H	-7.21604607	3.93966229	-0.91406594
C	-2.89806264	4.75774688	0.53297223	H	-3.93948794	7.21618869	0.91366991
C	-5.16900129	4.22420461	-0.26574985	H	-6.26677062	7.90741001	0.45523747
C	-4.51710799	0.00000000	-1.49296638	H	-7.90720284	6.26699367	-0.45578350
C	-4.75765578	2.89817075	-0.53322145	H	-8.37084916	1.55847148	-2.00727905
C	-2.73829903	1.25275200	-0.40724914	H	-7.39760229	2.45928615	-3.18347083
C	-6.50316473	4.65665977	-0.51553548	H	-8.84375036	1.58771726	-3.71175299
C	-5.50727511	-0.00001636	-2.21212486	H	-8.37082318	-1.55847831	-2.00720021
C	-4.65648972	6.50331713	0.51513048	H	-8.84377037	-1.58777955	-3.71165870
C	-5.95186777	6.88640230	0.25971901	H	-7.39761425	-2.45934427	-3.18338169
C	-6.88621566	5.95206356	-0.26020212	H	-7.14414157	-0.00016403	-5.84753634
C	-7.98480716	1.54757256	-3.03220485	H	-5.69723016	-0.88417072	-5.33442815
C	-7.98480732	-1.54762017	-3.03213676	H	-5.69740590	0.88416996	-5.33450064
C	-6.31116155	-0.00005366	-5.13504283	H	2.19908438	-5.47439299	0.94032674
Si	6.94966327	0.00003161	-3.35842422	H	5.47430816	-2.19920166	-0.94057892
N	1.44015312	-1.44017546	-0.00001917	H	7.21604607	-3.93966229	-0.91406594
C	1.25271292	-2.73832895	0.40716747	H	3.93948794	-7.21618869	0.91366991
C	3.45103508	-2.51702527	-0.27808849	H	6.26677062	-7.90741001	0.45523747
C	4.22406981	-5.16912744	0.26542441	H	7.90720284	-6.26699367	-0.45578350
C	3.29756290	-0.00001565	-0.75480873	H	7.39760229	-2.45928615	-3.18347083
C	2.51695346	-3.45110124	0.27791327	H	8.37084916	-1.55847148	-2.00727905
C	2.89806264	-4.75774688	0.53297223	H	8.84375036	-1.58771726	-3.71175299
C	5.16900129	-4.22420461	-0.26574985	H	8.84377037	1.58777955	-3.71165870
C	4.51710799	0.00000000	-1.49296638	H	8.37082318	1.55847831	-2.00720021
C	4.75765578	-2.89817075	-0.53322145	H	7.39761425	2.45934427	-3.18338169
C	2.73829903	-1.25275200	-0.40724914	H	7.14414157	0.00016403	-5.84753634
C	6.50316473	-4.65665977	-0.51553548	H	5.69723016	0.88417072	-5.33442815
C	5.50727511	0.00001636	-2.21212486	H	5.69740590	-0.88416996	-5.33450064
C	4.65648972	-6.50331713	0.51513048	H	5.47439299	2.19908438	-0.94032674

C	5.95186777	-6.88640230	0.25971901	H	2.19920166	5.47430816	0.94057892
C	6.88621566	-5.95206356	-0.26020212	H	3.93966229	7.21604607	0.91406594
C	7.98480716	-1.54757256	-3.03220485	H	7.21618869	3.93948794	-0.91366991
C	7.98480732	1.54762017	-3.03213676	H	7.90741001	6.26677062	-0.45523747
C	6.31116155	0.00005366	-5.13504283	H	6.26699367	7.90720284	0.45578350
Si	-0.00003161	6.94966327	3.35842422	H	1.55847148	8.37084916	2.00727905
N	1.44017546	1.44015312	0.00001917	H	2.45928615	7.39760229	3.18347083
C	2.73832895	1.25271292	-0.40716747	H	1.58771726	8.84375036	3.71175299
C	2.51702527	3.45103508	0.27808849	H	-1.58777955	8.84377037	3.71165870
C	5.16912744	4.22406981	-0.26542441	H	-1.55847831	8.37082318	2.00720021
C	0.00001565	3.29756290	0.75480873	H	-2.45934427	7.39761425	3.18338169
C	3.45110124	2.51695346	-0.27791327	H	-0.00016403	7.14414157	5.84753634
C	4.75774688	2.89806264	-0.53297223	H	-0.88417072	5.69723016	5.33442815
C	4.22420461	5.16900129	0.26574985	H	0.88416996	5.69740590	5.33450064
C	0.00000000	4.51710799	1.49296638				

Table S15. Coordinates of the optimized structure for **Pt-TAP** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Pt) level of theory.

E(B3LYP) = -4890.932185

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.79656048	-1.14838653	0.39431723	C	-6.84303628	5.25243874	1.46834992
C	-4.05711134	-0.75828894	1.00955188	C	-6.28204966	5.85778963	-1.51187542
C	-4.05907596	0.68059216	1.04758674	C	7.28421405	-4.71104786	-0.23787670
C	-2.79928411	1.10375116	0.45199429	C	5.26643232	-6.90972484	-1.06794844
N	-2.04235753	-0.01666879	0.18502668	C	5.70127615	-6.27686832	1.92879312
C	-2.42408358	-2.43515288	-0.05488321	C	4.31406074	4.25467151	-0.15770319
C	-2.43448936	2.40688532	0.05352466	Pt	-0.00858234	-0.00929312	-0.00251874
C	-1.14806625	2.77920753	-0.39751489	C	-5.27415307	-6.84167905	-1.46664917
C	-0.75838348	4.04007527	-1.01200167	C	-7.29315022	-4.62446955	-0.68242194
C	0.68051344	4.04195277	-1.05111889	C	-5.86556314	-6.28833475	1.51785997
C	1.10396662	2.78184861	-0.45678555	H	5.06370710	2.54065418	1.57734096
N	-0.01627115	2.02466649	-0.18977884	H	5.05958759	-2.46287824	1.72338578
C	2.40727134	2.41716612	-0.05796247	H	-2.55967643	5.06025326	-1.58230386
C	2.77949962	1.13118853	0.39326797	H	2.44573756	5.07568544	-1.70722513
C	4.03957173	0.74085590	1.00900019	H	2.54021518	-5.09575036	-1.56135540
C	4.03854722	-0.69794989	1.05044742	H	-2.46583991	-5.08931115	-1.70521228
C	2.78052689	-1.12097628	0.45159406	H	2.55890899	-7.24830086	-2.74525194
N	2.02454765	-0.00082386	0.18480118	H	-2.42208581	-7.24040495	-2.89039303
C	2.41862542	-2.42453261	0.04712668	H	7.21967888	2.56220385	2.75714049
C	1.13166046	-2.79993620	-0.39582350	H	7.21323323	-2.41900878	2.90624934
C	0.74045308	-4.06271507	-1.00615459	H	-5.07644019	-2.55922491	1.58216208
C	-0.69840453	-4.06126124	-1.04680437	H	-5.09230251	2.44619977	1.70323960

C	-1.12051646	-2.80048086	-0.45278055	H	-7.22880999	-2.58418850	2.76524053
N	-0.00008916	-2.04408385	-0.18700487	H	-7.24687144	2.39766360	2.88514049
C	5.07067326	1.45992867	1.57333521	H	-2.58526605	7.21402213	-2.76277158
C	6.15469193	0.77840074	2.19331732	H	2.39649232	7.23152816	-2.88675571
C	6.15312684	-0.66947147	2.23610749	H	-2.62611757	9.37491801	-3.97397016
C	5.06831255	-1.38439614	1.65617988	H	-1.40985859	11.23138684	-5.05339476
C	-1.47899950	5.07005728	-1.57594255	H	1.08253475	11.23913066	-5.11555819
C	-0.79892924	6.15696417	-2.19208623	H	2.36247251	9.38999215	-4.09839003
C	0.64915635	6.16139904	-2.22796277	H	2.59443570	-9.40543127	-3.96098060
C	1.36659974	5.07767192	-1.64759079	H	1.37416011	-11.25473081	-5.04879254
C	1.45937710	-5.09810961	-1.56268784	H	-1.11794316	-11.25083389	-5.12130663
C	0.77609220	-6.18242209	-2.18147742	H	-2.39360871	-9.39761701	-4.10610205
C	-0.67179090	-6.18038841	-2.22330898	H	9.37897378	2.59905934	3.96964648
C	-1.38682928	-5.09464576	-1.64399536	H	11.22913911	1.38015525	5.05684577
C	1.47189480	-7.25007609	-2.77113158	H	11.22600341	-1.11191051	5.13126457
C	0.80725268	-8.31254938	-3.39249768	H	9.37270605	-2.38886045	4.11858141
C	-0.63908652	-8.31030832	-3.43458680	H	-9.38841647	-2.62433042	3.97880256
C	-1.33540308	-7.24576620	-2.85267411	H	-11.24386600	-1.40743374	5.05929114
C	7.22261158	1.47460852	2.78207054	H	-11.25187907	1.08498939	5.11941614
C	8.28599686	0.81126682	3.40300196	H	-9.40402889	2.36434268	4.09914181
C	8.28418098	-0.63534104	3.44622796	H	7.52182586	3.80271442	-0.00554503
C	7.21910683	-1.33190709	2.86580489	H	8.11565137	5.31104470	-0.71880357
C	-5.08635568	-1.47857216	1.57507504	H	7.18336869	4.16923581	-1.70027064
C	-6.17273751	-0.79815085	2.19192360	H	4.93253277	6.76519272	1.81711867
C	-6.17731696	0.64990939	2.22663354	H	6.66190092	7.00739381	1.52170386
C	-5.09421196	1.36702786	1.64450964	H	6.09066255	5.51000508	2.27247957
C	-7.23720327	-1.49649496	2.78425885	H	6.04453940	7.58210269	-1.51480544
C	-8.30353215	-0.83482760	3.40189668	H	4.32025371	7.34402770	-1.19801109
C	-8.30795639	0.61183679	3.43690835	H	5.12845778	6.40715483	-2.46883012
C	-7.24640349	1.31080752	2.85256650	H	-5.32280990	8.11713788	0.71648110
C	-1.49758335	7.22224882	-2.78271895	H	-3.81648636	7.52110437	0.00079276
C	-0.83629801	8.28912107	-3.39970416	H	-4.18015052	7.18433761	1.69648872
C	0.61037423	8.29338862	-3.43590223	H	-7.35918635	4.32430846	1.20176355
C	1.30965966	7.23114456	-2.85332213	H	-7.59418132	6.04892872	1.51890500
C	-1.53943718	9.38028836	-4.00154499	H	-6.41854839	5.13129534	2.47060022
C	-0.86295793	10.40965707	-4.60019527	H	-7.02519967	6.66348612	-1.51956644
C	0.56403438	10.41406930	-4.63582177	H	-6.78512614	4.93372044	-1.81439440
C	1.27579366	9.38888204	-4.07187486	H	-5.52976334	6.09045506	-2.27285548
C	1.50790332	-9.40592981	-3.99325987	H	8.11145864	-5.42787434	-0.18110561
C	0.82919097	-10.43121602	-4.59648191	H	7.50676505	-3.88682346	0.44761921
C	-0.59762084	-10.42898903	-4.63799827	H	7.26516113	-4.30018362	-1.25247080
C	-1.30704317	-9.40152885	-4.07514851	H	6.04398541	-7.68173840	-1.04345504
C	9.37964806	1.51252722	4.00253160	H	5.22550804	-6.51119928	-2.08724513
C	10.40551266	0.83460540	4.60550732	H	4.30857506	-7.39425614	-0.85237360

C	10.40371118	-0.59219227	4.64813089	H	6.48862823	-7.03553371	2.00612541
C	9.37608257	-1.30230665	4.08662019	H	4.74980009	-6.75240208	2.18776127
C	-9.39389960	-1.53763144	4.00550226	H	5.90347297	-5.50764193	2.68143026
C	-10.42271288	-0.86078840	4.60474392	H	-6.07053942	-7.59306872	-1.51523749
C	-10.42728005	0.56619981	4.63920109	H	-4.34448394	-7.35803983	-1.20594415
C	-9.40279946	1.27764491	4.07352533	H	-5.15806216	-6.41459850	-2.46839176
C	3.42725000	3.41382461	-0.11187985	H	-8.13598897	-5.32503943	-0.69722158
C	-3.43077490	3.42715098	0.10880325	H	-7.20855515	-4.17975188	-1.67922130
C	-3.44409712	-3.43184123	-0.10769233	H	-7.53748045	-3.81987135	0.01879788
C	3.43028652	-3.43057046	0.08078707	H	-6.67074781	-7.03201595	1.52757850
C	-4.33105983	-4.27260014	-0.15242309	H	-6.09506112	-5.53801840	2.28174231
C	7.27325050	4.60999165	-0.70217819	H	-4.93975503	-6.79155305	1.81477989
C	5.85686966	6.26353533	1.51307160	Si	5.67895100	5.49084680	-0.20259309
C	5.24909393	6.82975351	-1.46572006	Si	5.64438478	-5.54724196	0.18642701
C	4.30459744	-4.28499465	0.11480449	Si	-5.69653826	-5.50819238	-0.19531275
C	-4.62269949	7.27396680	0.69916551	Si	-5.50613881	5.68025685	0.20236726
C	-4.27133793	4.31416203	0.15601521				

Table S16. Coordinates of the optimized structure for **Pt-TPFTNP** at the B3LYP/6-31G(d,p) (for C, N, F, H) + SDD (for Pt) level of theory.

E(B3LYP) = -5245.672029

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.74673450	1.23501664	0.39638736	C	-1.21114786	5.17063851	-1.55292742
C	-4.03801440	0.87594840	0.97845730	C	-1.69377986	-7.25022383	-2.70502581
C	-4.09333368	-0.55395959	0.98243908	C	-1.04225846	-8.32261402	-3.26618656
C	-2.83442921	-1.01501182	0.40139822	C	0.37648574	-8.37693771	-3.27110343
N	-2.03090533	0.07998077	0.17454379	C	1.11193837	-7.35769587	-2.71463475
C	-2.31860038	2.50796594	-0.00408967	C	-7.25048414	1.69375517	2.70439514
C	-2.50797102	-2.31859775	0.00392584	C	-8.32291020	1.04222492	3.26547685
C	-1.23501811	-2.74669220	-0.39659278	C	-8.37721849	-0.37652038	3.27039836
C	-0.87595387	-4.03791011	-0.97880543	C	-7.35792611	-1.11196557	2.71401293
C	0.55395473	-4.09323621	-0.98279615	C	1.69405493	7.25045413	-2.70415977
C	1.01501721	-2.83438327	-0.40163732	C	1.04258673	8.32287734	-3.26531948
N	-0.07997832	-2.03089383	-0.17464919	C	-0.37615765	8.37718971	-3.27039045
C	2.31862913	-2.50795912	-0.00417881	C	-1.11166424	7.35790431	-2.71407268
C	2.74672292	-1.23506578	0.39649254	C	7.25024516	-1.69408058	2.70488136
C	4.03793940	-0.87606754	0.97873945	C	8.32264005	-1.04262077	3.26610404
C	4.09326640	0.55383996	0.98288664	C	8.37697068	0.37612324	3.27116425
C	2.83440962	1.01496241	0.40178969	C	7.35773117	1.11163756	2.71477316
N	2.03090867	-0.08000667	0.17473002	H	-2.69773475	-5.02860365	-1.59194642
C	2.50797912	2.31860196	0.00445413	H	2.29049088	-5.22042914	-1.60747487
C	1.23506803	2.74673097	-0.39615164	H	-5.02876948	2.69772623	1.59150478

C	0.87606085	4.03800608	-0.97827103	H	-5.22055437	-2.29050375	1.60704544
C	-0.55384642	4.09332668	-0.98240832	H	5.02861015	-2.69791260	1.59172671
C	-1.01496333	2.83442485	-0.40140850	H	5.22045373	2.29031054	1.60775804
N	0.08000783	2.03090641	-0.17441244	H	2.69790319	5.02874825	-1.59114708
C	3.33091507	-3.60305597	-0.00656736	H	-2.29032301	5.22054382	-1.60720688
C	-3.60309951	-3.33084840	0.00601578	H	-2.77981824	-7.20570860	-2.70236149
C	3.60306864	3.33089506	0.00688060	H	-1.61133521	-9.13410034	-3.70996155
C	-3.33087528	3.60307302	-0.00635857	H	0.87876236	-9.22944512	-3.71858248
C	-4.36505751	3.63628074	-0.94742340	H	2.19818460	-7.39643265	-2.71931620
C	-5.31473852	4.65522406	-0.96096502	H	-7.20597980	2.77979396	2.70172967
C	-5.24182468	5.67341110	-0.01140771	H	-9.13443685	1.61129492	3.70918657
C	-4.22345113	5.66715972	0.94072436	H	-9.22975485	-0.87880319	3.71781524
C	-3.28380157	4.63895572	0.93227479	H	-7.39665146	-2.19821214	2.71869849
C	-3.63638358	-4.36515038	0.94694638	H	2.78009328	7.20594651	-2.70137994
C	-4.65534644	-5.31481345	0.96030377	H	1.61170568	9.13439832	-3.70897680
C	-5.67347270	-5.24176007	0.01069199	H	-0.87839108	9.22972373	-3.71786725
C	-5.66714178	-4.22326740	-0.94131201	H	-2.19791021	7.39663331	-2.71887155
C	-4.63892116	-3.28363824	-0.93267790	H	7.20572437	-2.78011843	2.70210792
C	4.63906666	3.28387517	-0.93162843	H	9.13412511	-1.61174581	3.70981930
C	5.66725677	4.22354168	-0.93991378	H	9.22948168	0.87835006	3.71869234
C	5.67337861	5.24187418	0.01226326	H	7.39647308	2.19788306	2.71956517
C	4.65507775	5.31473016	0.96170276	Pt	0.00000748	-0.00000440	0.00008778
C	3.63615074	4.36503458	0.94799669	F	4.15671029	-6.64491957	1.84934670
C	3.28377872	-4.63908785	0.93189982	F	6.14699362	-6.65410900	-0.01434891
C	4.22341603	-5.66730429	0.94023721	F	6.29236412	-4.66418051	-1.87281596
C	5.24182904	-5.67342682	-0.01185307	F	4.46060528	-2.67270345	-1.87137292
C	5.31478239	-4.65510965	-0.96126869	F	2.31811074	-4.65981513	1.85801989
C	4.36511452	-3.63615585	-0.94761554	F	-4.66460457	-6.29248530	1.87175252
C	-1.61761218	-5.06167251	-1.54452749	F	-2.67311618	-4.46073848	1.87088655
C	-0.96480123	-6.17856376	-2.11539529	F	-6.65416027	-6.14691970	0.01290116
C	0.47111455	-6.23365481	-2.12020114	F	-6.64456359	-4.15648003	-1.85062420
C	1.21131148	-5.17051465	-1.55332249	F	-4.65944197	-2.31789261	-1.85872284
C	-5.06183289	1.61760271	1.54407993	F	-4.46050747	2.67295744	-1.87131924
C	-6.17876950	0.96478445	2.11485331	F	-6.29229405	4.66440758	-1.87253889
C	-6.23384479	-0.47113332	2.11966420	F	-6.14700235	6.65408158	-0.01379272
C	-5.17064904	-1.21132215	1.55287879	F	-4.15679577	6.64464027	1.84998277
C	5.06169152	-1.61778467	1.54439384	F	-2.31817429	4.65955346	1.85844086
C	6.17858789	-0.96503704	2.11532525	F	4.65979169	2.31828681	-1.85783237
C	6.23368624	0.47087910	2.12027627	F	6.64484749	4.15694100	-1.84905820
C	5.17054323	1.21113606	1.55347939	F	6.65403481	6.14706702	0.01480422
C	1.61777505	5.06181491	-1.54383190	F	4.66413818	6.29224532	1.87332111
C	0.96501918	6.17874733	-2.11468464	F	2.67271397	4.46043055	1.87177993
C	-0.47089722	6.23382722	-2.11964601				

Table S17. Coordinates of the optimized structure for **Pt-NTNP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3797.083158

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.77830735	1.16416075	0.37809351	C	7.32221999	1.29215119	2.72344043
C	-4.05830153	0.76843950	0.96262469	H	-2.56708782	-5.09558533	-1.58341639
C	-4.07774865	-0.66236682	0.96328450	H	2.43149491	-5.16438927	-1.58439779
C	-2.80928413	-1.09333232	0.37862079	H	-5.09276376	2.56695950	1.56396352
N	-2.03260295	0.02492675	0.15492682	H	-5.15997270	-2.43170986	1.56649505
C	-2.38883167	2.45603865	-0.00715885	H	5.09579516	-2.57744017	1.56942504
C	-2.45630681	-2.39545494	-0.00731091	H	5.16373114	2.42105899	1.58420111
C	-1.16433069	-2.78391119	-0.39306664	H	2.57745030	5.09370500	-1.56340004
C	-0.76853992	-4.06288557	-0.97983751	H	-2.42107367	5.16139229	-1.57877447
C	0.66221157	-4.08255843	-0.98009460	H	-2.58809440	-7.26436805	-2.72429183
C	1.09311350	-2.81500482	-0.39327183	H	-1.37022138	-9.15872412	-3.74501461
N	-0.02509601	-2.03865428	-0.16812764	H	1.12290506	-9.19341667	-3.74452680
C	2.39510310	-2.46254043	-0.00686649	H	2.39265407	-7.33372626	-2.72377140
C	2.78371932	-1.17161614	0.38245942	H	-7.26268130	2.58786015	2.70167584
C	4.06261826	-0.77740251	0.97051837	H	-9.15795645	1.37008811	3.72108444
C	4.08219257	0.65337590	0.97476359	H	-9.19160127	-1.12302801	3.72251132
C	2.81477041	1.08584313	0.38888875	H	-7.33003673	-2.39270996	2.70468165
N	2.03849487	-0.03185290	0.16059602	H	2.60147908	7.26482812	-2.69862527
C	2.46237435	2.38879818	0.00581636	H	1.38639990	9.16170180	-3.71833396
C	1.17151765	2.77839184	-0.38284209	H	-1.10670608	9.19608097	-3.72503519
C	0.77736971	4.05883324	-0.96753580	H	-2.37918770	7.33369292	-2.71268809
C	-0.65341507	4.07836510	-0.97194027	H	7.26386978	-2.60140611	2.71047070
C	-1.08590619	2.80941919	-0.38947992	H	9.15809017	-1.38624767	3.73502650
N	0.03176103	2.03253504	-0.16316510	H	9.19259226	1.10685168	3.74138094
C	3.43793998	-3.53376488	-0.00928630	H	7.33297604	2.37926119	2.72384580
C	-3.52797164	-3.43771062	-0.00809564	Pt	0.00316904	-0.00326355	-0.00403651
C	3.53350427	3.43172874	0.01139596	H	-4.52696257	2.72981494	-1.68129537
C	-3.43169865	3.52722391	-0.00949502	H	-6.23439365	4.46667163	-1.70055045
C	-4.47506462	3.52701805	-0.94512073	H	-4.32528606	6.33299101	1.70111406
C	-5.45038083	4.51903163	-0.95530661	H	-2.61950125	4.59464086	1.67314395
C	-5.42748190	5.57358996	-0.01229425	H	4.60508522	2.62067299	-1.66914231
C	-4.38365809	5.56201109	0.94284001	H	6.34334331	4.32659956	-1.69177870
C	-3.41103650	4.56725722	0.92954891	H	4.46854385	6.23344542	1.70646966
C	-3.53010405	-4.48198569	0.92689634	H	2.73184755	4.52596384	1.68184314
C	-4.52571905	-5.45338238	0.93861537	H	4.53686166	-2.73277691	-1.67697904
C	-5.57650605	-5.42965428	-0.00948918	H	6.24433879	-4.46956270	-1.69620779
C	-5.57020270	-4.37792099	-0.95683613	H	4.32764291	-6.34333918	1.69709142
C	-4.57124608	-3.40998299	-0.94381009	H	2.62198641	-4.60482858	1.66922117

C	4.57584549	3.41170706	-0.92508377	H	-2.73467209	-4.53413086	1.66501397
C	5.57057328	4.38440292	-0.93529117	H	-4.48165797	-6.23437042	1.68781934
C	5.57977038	5.42759890	0.02053980	H	-6.34911901	-4.31144945	-1.70655382
C	4.52284032	5.44987917	0.96089916	H	-4.60053433	-2.61296805	-1.68148444
C	3.53090567	4.47452223	0.94765033	C	7.56550399	-6.43941660	-0.87019021
C	3.41517702	-4.57582906	0.92745223	H	8.17221248	-5.55832140	-0.60820534
C	4.38774488	-5.57062980	0.94071342	H	8.19187416	-7.32713911	-0.76877240
C	5.43368391	-5.58013811	-0.01213776	H	7.28682776	-6.35412916	-1.92665052
C	5.45864986	-4.52357590	-0.95285043	C	6.43673007	7.55851435	0.88283223
C	4.48332228	-3.53157348	-0.94265039	H	7.32377513	8.18607877	0.78288079
C	-1.48606899	-5.10318496	-1.54984228	H	5.55516412	8.16435800	0.62041605
C	-0.80165678	-6.19624457	-2.12799139	H	6.35066516	7.27882877	1.93895215
C	0.63637568	-6.21615868	-2.12805925	C	-7.55807206	6.43384225	-0.87228368
C	1.35070759	-5.14224196	-1.55019861	H	-8.16438071	5.55165996	-0.61305613
C	-5.09973169	1.48591954	1.53075441	H	-8.18532544	7.32080243	-0.76967498
C	-6.19332203	0.80148451	2.10773430	H	-7.27799172	6.35114317	-1.92858779
C	-6.21272834	-0.63656508	2.10861850	C	-6.54242143	-7.46467873	0.96966529
C	-5.13805319	-1.35089584	1.53228781	H	-7.39465599	-8.12497891	0.80408615
C	5.10297927	-1.49633441	1.53870902	H	-5.62834044	-8.07007973	0.89356617
C	6.19585690	-0.81342681	2.11891019	H	-6.60718553	-7.08400910	1.99893029
C	6.21563717	0.62458531	2.12302200	N	6.38926219	-6.58866760	-0.02982961
C	5.14172963	1.34037106	1.54697943	C	6.45170039	-7.52913459	1.07603149
C	1.49633645	5.10075636	-1.53282945	H	7.23925362	-8.25867464	0.88048930
C	0.81346191	6.19513674	-2.11020960	H	6.66427454	-7.04451539	2.04220024
C	-0.62456383	6.21484944	-2.11451336	H	5.51062956	-8.08152377	1.17635499
C	-1.34038239	5.13938310	-1.54145134	N	-6.56872508	-6.39467413	-0.01025900
C	-1.50107902	-7.28396126	-2.72657645	N	-6.38304144	6.58217682	-0.03005685
C	-0.82252442	-8.33629013	-3.29337283	N	6.58838820	6.38316807	0.04158129
C	0.59811393	-8.35603431	-3.29320255	C	-7.63870687	-6.33593398	-0.98877017
C	1.30554458	-7.32288664	-2.72640793	H	-7.26094851	-6.40877173	-2.01851426
C	-7.28205919	1.50081612	2.70459456	H	-8.32223867	-7.16993431	-0.82465112
C	-8.33484209	0.82240249	3.27066980	H	-8.21841970	-5.40551353	-0.90989285
C	-8.35400560	-0.59827186	3.27152417	C	-6.44772103	7.52056906	1.07742934
C	-7.31992092	-1.30557036	2.70631401	H	-7.23379949	8.25145799	0.88094328
C	1.51444789	7.28444573	-2.70404599	H	-6.66377061	7.03438603	2.04206316
C	0.83750908	8.33810632	-3.27026278	H	-5.50632185	8.07162657	1.18158019
C	-0.58314147	8.35765756	-3.27423400	C	7.52886428	6.44924935	-1.06408809
C	-1.29207646	7.32299867	-2.71210827	H	7.04465879	6.66751782	-2.02923755
C	7.28353178	-1.51437613	2.71576577	H	8.26001372	7.23436561	-0.86471125
C	8.33571761	-0.83739099	3.28467328	H	8.07936880	5.50765172	-1.16893922
C	8.35533961	0.58325418	3.28844740				

Table S18. Coordinates of the optimized structure for **Zn-TNP** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Zn) level of theory.

E(B3LYP) = -4384.108639

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Zn	-0.01255676	0.01282031	-0.00378972	C	0.75196804	8.35112471	-3.33080253
Si	5.65817381	-5.51072974	-0.08068418	C	5.27292240	6.89647519	-1.16851584
Si	5.67311370	5.52067568	0.06432925	C	7.29091169	4.67088861	-0.41475744
Si	-5.68195266	5.53486144	-0.07683757	C	-0.66780785	8.35424813	-3.34525546
Si	-5.53401100	-5.65849100	0.08026021	C	-5.84844330	6.26471275	1.65886660
N	2.03086387	0.00421927	0.18864204	C	-5.25361492	6.90434416	-1.30733511
N	-0.01913021	-2.03248980	-0.19364287	C	-7.28493151	4.67756299	-0.59066508
N	-0.00385376	2.05806002	-0.19250383	C	-4.67734868	-7.25930224	0.60168979
N	-2.05583408	0.01936237	0.18852193	C	-6.26067137	-5.83157080	-1.65611547
C	-1.14504108	-2.78519856	-0.41566796	C	-6.90580993	-5.22547653	1.30659849
C	-2.81654684	-1.09856804	0.43196350	H	5.08916967	-2.51704186	1.60283657
C	4.05388422	-0.72583395	1.01122002	H	5.10017088	2.48150601	1.65554990
C	4.05713472	0.70790918	1.02607571	H	-5.11085742	2.54245339	1.60156322
C	2.78992074	1.12191349	0.43321855	H	2.45741684	-5.12059642	-1.63322816
C	0.68399282	-4.06330921	-1.02369310	H	-7.28073085	2.55472893	2.76664712
C	-4.08658976	-0.68384878	1.01900524	H	9.13985086	1.19652164	3.83440483
C	-1.12162591	2.81828692	-0.43430241	H	7.26132163	-2.52510884	2.76750222
C	2.78395779	-1.12192316	0.41244190	H	-5.14342469	-2.45734874	1.62883407
C	1.09859566	-2.79318628	-0.43725053	H	2.51787767	5.13103773	-1.58003684
C	5.09732830	-1.43637910	1.58028433	H	7.27096229	2.45552096	2.82201345
C	-2.44138272	-2.40255452	0.02007997	H	-9.16190437	1.32928023	3.79811266
C	6.18228006	0.69334620	2.18783334	H	-2.54256053	-5.08836325	-1.60450085
C	6.17930206	-0.74526030	2.17238218	H	9.13501286	-1.29581816	3.80708627
C	2.40245906	-2.41773601	-0.02424378	H	7.51324440	-3.83055856	0.07011686
C	2.41834353	2.42633558	0.01392964	H	8.09665247	-5.36280379	-0.59942650
C	3.43636942	3.42623122	0.01938842	H	7.17325622	-4.24268689	-1.61382065
C	1.12220063	2.81237844	-0.41411193	H	6.63233610	-6.98285533	1.68695629
C	-0.74983665	-4.05685182	-1.01145345	H	6.06880721	-5.46166448	2.39431673
C	5.10354380	1.40160491	1.61020395	H	4.90407013	-6.72311911	1.97413971
C	3.41830927	-3.41946172	-0.05104478	H	-2.48315321	5.14229894	-1.63073590
C	-4.08005983	0.74988144	1.00716828	H	-7.31682756	-2.42579944	2.79193232
C	-6.21716771	-0.66621239	2.17077716	H	-2.55493836	-7.25926811	-2.76763412
C	-2.42610768	2.44201181	-0.02328031	H	2.42560062	-7.29491984	-2.79454768
C	-6.20760347	0.77233922	2.16335765	H	-9.17886588	-1.16313303	3.81119090
C	-5.12226154	1.46194803	1.57580020	H	1.16277598	-9.15789125	-3.81182646
C	1.37701846	-5.11663306	-1.59660640	H	4.29016289	-7.38311358	-1.02790454
C	-2.80849418	1.14540983	0.41093490	H	5.11188684	-6.49058878	-2.32129690
C	0.72585505	4.08651701	-1.00455686	H	6.01425216	-7.64299480	-1.32796066

C	-0.70794937	4.08980347	-1.01890488	H	-1.32967128	-9.14113755	-3.79793827
C	0.66615409	-6.19479891	-2.17372608	H	2.52410520	7.30220692	-2.74439290
C	-7.29458455	1.46760208	2.76713239	H	-2.45608306	7.31310686	-2.79508353
C	8.31299813	0.66701093	3.37001664	H	6.59139149	6.98918350	1.86463362
C	7.26928977	-1.43794957	2.77387819	H	4.85617150	6.72388594	2.10020232
C	-5.13943459	-1.37696720	1.59251256	H	6.01146625	5.46393036	2.54990829
C	1.43699119	5.13504904	-1.56312216	H	1.29476777	9.17626238	-3.78288714
C	7.27482909	1.36846950	2.80443445	H	4.32967400	7.39288663	-0.91834125
C	4.30076377	-4.26655845	-0.07260538	H	6.06151070	7.65760824	-1.16498511
C	-0.77248644	-6.18534733	-2.16585053	H	5.19249493	6.50602567	-2.18856505
C	-3.44183540	3.44389023	-0.04953384	H	7.52727559	3.84299526	0.26162661
C	-8.33942656	0.78487499	3.34321604	H	8.12611235	5.38000470	-0.38261704
C	-1.46201513	-5.09964788	-1.57904663	H	7.23559542	4.26298474	-1.42922541
C	8.31021201	-0.75305992	3.35448593	H	-1.19766774	9.18173799	-3.80825567
C	-3.44325543	-3.41822523	0.04826375	H	-4.92013243	6.75380006	1.97124013
C	7.25931298	-4.65549924	-0.60349738	H	-6.08278580	5.49327477	2.39990253
C	-0.69384852	6.22221913	-2.16622288	H	-6.64961401	7.01214186	1.69015398
C	4.31877169	4.27363730	0.02799332	H	-5.14433067	6.50807544	-2.32243847
C	5.83127076	-6.23527954	1.65657273	H	-6.04458026	7.66268173	-1.32972296
C	-1.40287299	5.14147519	-1.59175666	H	-4.31918385	7.40567753	-1.03480187
C	0.74467113	6.21901607	-2.15163629	H	-8.12250474	5.38458404	-0.58497725
C	-7.31396159	-1.33922568	2.78215035	H	-7.20289343	4.26219059	-1.60027766
C	-1.46780447	-7.27298470	-2.76850583	H	-7.53581032	3.85425969	0.08608542
C	-4.32423642	4.29107490	-0.07046545	H	-4.26367258	-7.17340111	1.61167421
C	1.33902402	-7.29212403	-2.78443509	H	-3.85287347	-7.51241772	-0.07279907
C	-4.29050848	-4.30050468	0.07102333	H	-5.38414752	-8.09707264	0.59790952
C	-8.34889751	-0.63505886	3.35064977	H	-7.00821076	-6.63270002	-1.68567107
C	0.63478954	-8.32757172	-3.35181320	H	-5.48789733	-6.06898353	-2.39477733
C	5.22420622	-6.88371339	-1.30529962	H	-6.74896386	-4.90438657	-1.97304644
C	-0.78519713	-8.31821931	-3.34391589	H	-7.40648342	-4.29199378	1.02958907
C	1.43753243	7.30972034	-2.75159553	H	-6.51148546	-5.11252808	2.32206230
C	-1.36956183	7.31588981	-2.78013053	H	-7.66433038	-6.01622006	1.33044866
C	5.79361334	6.23959948	1.80829061				

Table S19. Coordinates of the optimized structure for **Pt-ATNP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2641.551340							
Charge = 0, Multiplicity = 1							
Number of Imaginary Frequencies = 0							
Atom	x	y	z	Atom	x	y	z
Pt	0.00000000	0.00000000	0.00000000	C	0.65998416	-4.22169019	0.27936911
N	-0.00002601	2.03712948	-0.00005087	C	-0.66533923	-6.64443590	-0.27164207
C	1.05057872	2.82274502	-0.40663404	C	2.33187117	-2.33183632	0.74846886
C	-0.65998416	4.22169019	0.27936911	C	-0.65967011	-4.22169019	-0.28009943

C	0.66533923	6.64443590	-0.27164207
C	-2.33187117	2.33183632	0.74846886
C	0.65967011	4.22169019	-0.28009943
C	1.31062372	5.41591578	-0.54085943
C	-0.66612525	6.64443352	0.26978687
C	-3.20274378	3.20282184	1.47053580
C	-1.31116558	5.41591626	0.53958676
C	-1.05069748	2.82272089	0.40635227
C	-1.30151395	7.89319213	0.52587294
C	1.30045860	7.89319022	-0.52838504
C	0.65759709	9.07999784	-0.26771913
C	-0.65891177	9.07999784	0.26457421
N	2.03712948	0.00002601	0.00005087
C	2.82274502	-1.05057872	0.40663404
C	4.22169019	0.65998416	-0.27936911
C	6.64443590	-0.66533923	0.27164207
C	2.33183632	2.33187117	-0.74846886
C	4.22169019	-0.65967011	0.28009943
C	5.41591578	-1.31062372	0.54085943
C	6.64443352	0.66612525	-0.26978687
C	3.20282184	3.20274378	-1.47053580
C	5.41591626	1.31116558	-0.53958676
C	2.82272089	1.05069748	-0.40635227
C	7.89319213	1.30151395	-0.52587294
C	7.89319022	-1.30045860	0.52838504
C	9.07999784	-0.65759709	0.26771913
C	9.07999784	0.65891177	-0.26457421
N	-2.03712948	-0.00002601	0.00005087
C	-2.82274502	1.05057872	0.40663404
C	-4.22169019	-0.65998416	-0.27936911
C	-6.64443590	0.66533923	0.27164207
C	-2.33183632	-2.33187117	-0.74846886
C	-4.22169019	0.65967011	0.28009943
C	-5.41591578	1.31062372	0.54085943
C	-6.64443352	-0.66612525	-0.26978687
C	-3.20282184	-3.20274378	-1.47053580
C	-5.41591626	-1.31116558	-0.53958676
C	-2.82272089	-1.05069748	-0.40635227
C	-7.89319213	-1.30151395	-0.52587294
C	-7.89319022	1.30045860	0.52838504
C	-9.07999784	0.65759709	0.26771913
C	-9.07999784	-0.65891177	-0.26457421
N	0.00002601	-2.03712948	-0.00005087
C	-1.05057872	-2.82274502	-0.40663404
C	-1.31062372	-5.41591578	-0.54085943
C	0.66612525	-6.64443352	0.26978687
C	3.20274378	-3.20282184	1.47053580
C	1.31116558	-5.41591626	0.53958676
C	1.05069748	-2.82272089	0.40635227
C	1.30151395	-7.89319213	0.52587294
C	-1.30045860	-7.89319022	-0.52838504
C	-0.65759709	-9.07999784	-0.26771913
C	0.65891177	-9.07999784	0.26457421
H	2.30909932	5.43120842	-0.95361043
H	-2.30965789	5.43120974	0.95230391
H	-2.30927772	7.89010179	0.93320784
H	2.30822006	7.89009491	-0.93572556
H	1.15468366	10.02466110	-0.46831619
H	-1.15619818	10.02466284	0.46466525
H	5.43120842	-2.30909932	0.95361043
H	5.43120974	2.30965789	-0.95230391
H	7.89010179	2.30927772	-0.93320784
H	7.89009491	-2.30822006	0.93572556
H	10.02466110	-1.15468366	0.46831619
H	10.02466284	1.15619818	-0.46466525
H	-5.43120842	2.30909932	0.95361043
H	-5.43120974	-2.30965789	-0.95230391
H	-7.89010179	-2.30927772	-0.93320784
H	-7.89009491	2.30822006	0.93572556
H	-10.02466110	1.15468366	0.46831619
H	-10.02466284	-1.15619818	-0.46466525
H	-2.30909932	-5.43120842	-0.95361043
H	2.30965789	-5.43120974	0.95230391
H	2.30927772	-7.89010179	0.93320784
H	-2.30822006	-7.89009491	-0.93572556
H	-1.15468366	-10.02466110	-0.46831619
H	1.15619818	-10.02466284	0.46466525
C	-3.91000105	-3.90977841	-2.15533805
H	-4.52534238	-4.52498872	-2.77022824
C	3.90977841	-3.91000105	2.15533805
H	4.52498872	-4.52534238	2.77022824
C	-3.90977841	3.91000105	2.15533805
H	-4.52498872	4.52534238	2.77022824
C	3.91000105	3.90977841	-2.15533805
H	4.52534238	4.52498872	-2.77022824

Table S20. Coordinates of the optimized structure for **Pt-ACNTNP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3010.531770

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Pt	0.00000250	-0.00000886	-0.00005192	C	-5.47408876	3.83367698	-0.23008668
N	1.33337424	1.54371452	-0.00319900	C	-4.49683751	-0.32319577	-1.47864055
C	2.64040608	1.45421454	-0.41124435	C	-4.96502985	2.54324770	-0.50502123
C	2.25910040	3.63271158	0.25886996	C	-2.82607180	1.05459749	-0.39633008
C	4.84274941	4.60125111	-0.30426507	C	-6.83653116	4.16412183	-0.47577921
C	-0.23875237	3.28478472	0.75024242	C	-5.12970368	6.13725988	0.57074451
C	3.25915554	2.76736243	-0.29409907	C	-6.45178802	6.42195571	0.32111422
C	4.53078177	3.24574113	-0.55989470	C	-7.31363329	5.42563920	-0.20709384
C	3.83363911	5.47409088	0.23066521	N	-1.33336880	-1.54372931	-0.00346245
C	-0.32332238	4.49672741	1.47882777	C	-2.64038740	-1.45417063	-0.41154387
C	2.54319583	4.96499862	0.50547234	C	-2.25910004	-3.63276687	0.25824912
C	1.05457323	2.82603902	0.39652242	C	-4.84273427	-4.60121849	-0.30511087
C	4.16405135	6.83652015	0.47647285	C	0.23872879	-3.28490360	0.74981148
C	6.13728036	5.12978497	-0.57002903	C	-3.25914057	-2.76733242	-0.29461186
C	6.42194433	6.45185597	-0.32029020	C	-4.53076178	-3.24566759	-0.56051256
C	5.42558226	7.31365451	0.20790716	C	-3.83363385	-5.47414623	0.22969577
N	1.54372722	-1.33337673	0.00322765	C	0.32323898	-4.49693561	1.47825701
C	1.45419013	-2.64042171	0.41123464	C	-2.54319892	-4.96509701	0.50462025
C	3.63276301	-2.25907571	-0.25861100	C	-1.05458049	-2.82611197	0.39607354
C	4.60126910	-4.84272339	0.30458229	C	-4.16404936	-6.83661794	0.47526607
C	3.28487296	0.23878563	-0.74997269	C	-6.13725935	-5.12970976	-0.57098972
C	2.76735849	-3.25915474	0.29422838	C	-6.42192650	-6.45182279	-0.32147895
C	3.24572307	-4.53078102	0.56005135	C	-5.42557363	-7.31370896	0.20659373
C	5.47416232	-3.83358769	-0.23021272	H	5.30276546	2.60944862	-0.96806618
C	4.49687611	0.32336373	-1.47845620	H	1.80173265	5.63761612	0.91213503
C	4.96508571	-2.54314536	-0.50505224	H	3.40025473	7.49432573	0.88233757
C	2.82609515	-1.05455327	-0.39632749	H	6.89827773	4.46872900	-0.97587342
C	6.83662794	-4.16397420	-0.47585440	H	7.41349989	6.84294526	-0.52738070
C	5.12978768	-6.13725348	0.57038079	H	5.66517271	8.35515297	0.39999375
C	6.45189433	-6.42189252	0.32080275	H	2.60939210	-5.30278440	0.96812479
C	7.31374611	-5.42550500	-0.20725980	H	5.63774418	-1.80166061	-0.91160791
N	-1.54372078	1.33335966	0.00333611	H	7.49447422	-3.40015795	-0.88161607
C	-1.45419345	2.64035347	0.41149084	H	4.46869112	-6.89827048	0.97612231
C	-3.63272883	2.25911882	-0.25852929	H	6.84297130	-7.41344776	0.52791805
C	-4.60120207	4.84274107	0.30485628	H	8.35527246	-5.66507598	-0.39921966
C	-3.28483974	-0.23869733	-0.75013665	H	-2.60934865	5.30268502	0.96856161
C	-2.76733761	3.25912418	0.29446224	H	-5.63768365	1.80182213	-0.91169191
C	-3.24568045	4.53073881	0.56037708	H	-7.49437267	3.40036079	-0.88165272

C	-5.49113425	-0.39100905	-2.18276013	H	-4.46861201	6.89822179	0.97659727
C	0.39104003	-5.49127194	2.18232039	H	-6.84285255	7.41350126	0.52829934
C	-0.39123540	5.49097052	2.18301413	H	-8.35514217	5.66525436	-0.39909332
C	5.49117743	0.39123140	-2.18256252	H	-5.30273720	-2.60930800	-0.96859665
C	-6.61761937	-0.46838662	-2.95127520	H	-1.80174369	-5.63778170	0.91118556
C	0.46841004	-6.61777113	2.95080834	H	-3.40026029	-7.49449062	0.88103621
C	6.61764683	0.46872632	-2.95108199	H	-6.89824926	-4.46858684	-0.97673910
C	-0.46873706	6.61737811	2.95162774	H	-7.41347718	-6.84287885	-0.52865538
N	-7.58679522	-0.53519136	-3.60194108	H	-5.66516662	-8.35524023	0.39849967
N	0.53519218	-7.58697191	3.60143941	N	-0.53563887	7.58649317	3.60237414
N	7.58682401	0.53561091	-3.60173787				

Table S21. Coordinates of the optimized structure for **Pt-AFTNP** at the B3LYP/6-31G(d,p) (for C, N, F, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3989.677076

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Pt	-0.00001013	-0.00001683	0.00004580	H	-3.16591916	-7.58275453	-0.99471949
N	-1.58982284	1.28146545	0.00329544	H	-5.41086420	-8.51998390	-0.53857655
C	-2.86273283	0.95665855	0.40169038	H	-7.20573712	-7.07609414	0.40770736
C	-2.87585722	3.17347693	-0.25543910	H	1.62733532	5.69168661	-0.97110438
C	-5.59112033	3.66419253	0.30795909	H	5.22950232	2.79389684	0.91416575
C	-0.35413950	3.28425886	-0.72247116	H	6.75969007	4.69181164	0.89898368
C	-3.70627574	2.14105511	0.29163093	H	3.16503352	7.58329821	-0.99303643
C	-5.04247358	2.38625529	0.56177016	H	5.40991226	8.52067273	-0.53677332
C	-4.75725726	4.70072465	-0.23290766	H	7.20508560	7.07665962	0.40871102
C	-0.49194358	4.53464602	-1.38448652	H	5.69156479	-1.62758208	0.97153915
C	-3.39642743	4.43235392	-0.50599643	H	2.79362572	-5.22975789	-0.91347019
C	-1.54308963	2.59658888	-0.38638719	H	4.69138910	-6.76018231	-0.89772058
C	-5.32688758	5.98078931	-0.48524505	H	7.58299239	-3.16546028	0.99400487
C	-6.95838068	3.95267504	0.58006881	H	8.52018287	-5.41054082	0.53834430
C	-7.47592444	5.20116431	0.32626594	H	7.07610616	-7.20574257	-0.40699858
C	-6.65244119	6.22485708	-0.21265389	C	5.55693892	0.60603168	2.02484691
N	-1.28152169	-1.58980143	-0.00301877	C	0.60615931	-5.55645790	-2.02571765
C	-0.95673396	-2.86273592	-0.40147549	C	-0.60620975	5.55641070	-2.02581509
C	-3.17362445	-2.87573785	0.25541672	C	-5.55622549	-0.60617848	2.02638951
C	-3.66455281	-5.59086379	-0.30841630	C	-0.75128768	6.88010023	-2.61041335
C	-3.28426897	-0.35405328	0.72274921	C	-6.87992443	-0.75157793	2.61090479
C	-2.14121012	-3.70618289	-0.29163101	C	0.75176470	-6.87999428	-2.61056375
C	-2.38652695	-5.04232157	-0.56198117	C	6.88063734	0.75143164	2.60932644
C	-4.70107460	-4.75697056	0.23242588	F	0.77089810	-6.85348758	-3.95561323
C	-4.53459103	-0.49187841	1.38486532	F	-0.26893163	-7.68916318	-2.23670940
C	-4.43258960	-3.39621741	0.50574509	F	1.90316205	-7.46584456	-2.20150730

C	-2.59663085	-1.54303392	0.38658328	F	7.68961383	-0.26926861	2.23506222
C	-5.98123864	-5.32649911	0.48448312	F	6.85454096	0.77032524	3.95438482
C	-3.95313970	-6.95805364	-0.58077874	F	7.46647735	1.90284084	2.20019887
C	-5.20172468	-7.47549861	-0.32724333	F	0.26916019	7.68913890	-2.23557334
C	-6.22540885	-6.65198445	0.21165104	F	-0.76948738	6.85399226	-3.95547973
N	1.28147946	1.58980141	-0.00324529	F	-1.90294000	7.46590711	-2.20194340
C	0.95660564	2.86274679	-0.40141902	F	-7.68906507	0.26882624	2.23619813
C	3.17352496	2.87581348	0.25535430	F	-7.46553722	-1.90325196	2.20228764
C	3.66402313	5.59121670	-0.30756002	F	-6.85386954	-0.76989997	3.95597988
C	3.28433412	0.35406471	0.72224023	C	3.70622113	-2.14110667	0.29157322
C	2.14097138	3.70630726	-0.29134802	C	5.04244072	-2.38628104	0.56165425
C	2.38603955	5.04259133	-0.56119104	C	4.75695418	-4.70108381	-0.23197881
C	4.70072636	4.75724793	0.23282126	C	0.49178717	-4.53472237	-1.38436774
C	4.53489238	0.49186559	1.38395823	C	3.39614166	-4.43271059	-0.50509690
C	4.43245931	3.39635806	0.50569264	C	1.54298521	-2.59670278	-0.38622558
C	2.59666842	1.54304216	0.38625316	C	5.32646133	-5.98131796	-0.48374612
C	5.98084530	5.32686155	0.48494149	C	6.95822753	-3.95283350	0.58045483
C	3.95239121	6.95855880	-0.57941850	C	7.47564281	-5.20148185	0.32720095
C	5.20093101	7.47607568	-0.32583434	C	6.65201568	-6.22536186	-0.21115885
C	6.22479379	6.65248569	0.21260703	H	-5.69147160	1.62769449	0.97209223
N	1.58977805	-1.28152813	0.00317518	H	-2.79403784	5.22927500	-0.91480156
C	2.86275191	-0.95667580	0.40140591	H	-4.69190783	6.75949549	-0.89965517
C	2.87569555	-3.17366759	-0.25507281	H	-7.58306325	3.16545487	0.99403579
C	5.59095740	-3.66436706	0.30832768	H	-8.52046826	5.41021834	0.53739549
C	0.35397868	-3.28432121	-0.72236248	H	-7.07663046	7.20510872	-0.40892211
H	-5.22950647	-2.79378675	0.91449538	H	-1.62799535	-5.69136381	-0.97228269
H	-6.75993979	-4.69149721	0.89887306				

Table S22. Coordinates of the optimized structure for **Pt-ANTNP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2862.979998

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Pt	0.00012474	0.00009290	0.00048584	C	4.33886891	2.05711306	0.60854331
N	-1.90268905	0.72665968	0.15240065	C	5.23806217	-0.66072380	1.66861849
C	-2.23231646	2.05923503	0.18655828	C	2.98320092	0.03237776	0.55451216
C	-4.02550570	0.86683441	1.03053822	C	7.27354340	-1.60048414	2.72732330
C	-5.55929620	3.10173480	1.79387680	C	6.36692837	-4.20319192	2.20042568
C	-3.09519802	-1.41926687	0.33172397	C	7.56792291	-4.00393516	2.83839949
C	-3.55961723	2.19604532	0.77027735	C	8.02654305	-2.68631647	3.10577908
C	-4.31721829	3.29310524	1.14766674	H	-3.96849000	4.30170506	0.97435657
C	-6.02511087	1.76716635	2.06084863	H	-5.58458759	-0.33732753	1.89592562
C	-4.33802504	-2.05754275	0.60948498	H	-7.62108125	0.59105232	2.93372019

C	-5.23789337	0.66076244	1.66837834
C	-2.98297272	-0.03224716	0.55444856
C	-7.27318441	1.60051153	2.72745448
C	-6.36584435	4.20327624	2.20204665
C	-7.56689895	4.00398279	2.83988981
C	-8.02589375	2.68633862	3.10650169
N	0.72671383	1.90278300	-0.15148814
C	2.05922597	2.23252650	-0.18551214
C	0.86683701	4.02515800	-1.03053004
C	3.10155621	5.55895858	-1.79416711
C	-1.41923766	3.09539954	-0.33101995
C	2.19605506	3.55974088	-0.76945830
C	3.29303233	4.31745660	-1.14688236
C	1.76696735	6.02403336	-2.06238161
C	-2.05693511	4.33877686	-0.60759653
C	0.66063922	5.23680359	-1.66973735
C	-0.03221972	2.98288955	-0.55387032
C	1.60024532	7.27138568	-2.73031534
C	4.20302262	6.36553277	-2.20247480
C	4.00366666	7.56591151	-2.84156806
C	2.68601137	8.02414895	-3.10943296
N	-0.72646611	-1.90250841	-0.15198802
C	-2.05903094	-2.23199645	-0.18629025
C	-0.86687638	-4.02513737	-1.03048167
C	-3.10228464	-5.55767003	-1.79526957
C	1.41934057	-3.09545698	-0.33036695
C	-2.19599456	-3.55909000	-0.77019600
C	-3.29330299	-4.31595589	-1.14828320
C	-1.76779688	-6.02364913	-2.06243187
C	2.05615677	-4.33957743	-0.60599180
C	-0.66114981	-5.23707122	-1.66930402
C	0.03238251	-2.98291135	-0.55377430
C	-1.60138888	-7.27128059	-2.72994799
C	-4.20398357	-6.36360407	-2.20422281
C	-4.00492286	-7.56424830	-2.84291205
C	-2.68737182	-8.02341196	-3.10969605
N	1.90278512	-0.72657647	0.15280931
C	2.23252739	-2.05912285	0.18665400
C	4.02577722	-0.86675344	1.03052975
C	5.56010340	-3.10164234	1.79284285
C	3.09546956	1.41946861	0.33188566
H	-6.00929249	5.20972234	1.99765721
H	-8.17053530	4.85405728	3.14483514
H	-8.97577755	2.54160994	3.61338055
H	4.30167627	3.96907456	-0.97314823
H	-0.33748554	5.58278521	-1.89825755
H	0.59077498	7.61865619	-2.93757934
H	5.20950094	6.00954682	-1.99724134
H	4.85370469	8.16955627	-3.14659675
H	2.54123329	8.97347171	-3.61734611
H	-4.30180291	-3.96673985	-0.97514978
H	0.33683042	-5.58386727	-1.89715881
H	-0.59198895	-7.61925591	-2.93635611
H	-5.21038095	-6.00694268	-1.99977645
H	-4.85512576	-8.16742099	-3.14841579
H	-2.54284713	-8.97295306	-3.61727548
H	3.96939194	-4.30157707	0.97325710
H	5.58444556	0.33730435	1.89682137
H	7.62112956	-0.59103959	2.93419179
H	6.01063994	-5.20963007	1.99552724
H	8.17178014	-4.85401683	3.14288356
H	8.97636404	-2.54161441	3.61278434
C	2.62914571	-5.38176035	-0.85583520
C	5.38037147	2.63132309	0.85843653
C	-5.37860180	-2.63294318	0.86057308
C	-2.63114589	5.38037274	-0.85718644
N	-3.30294745	6.53422961	-1.05720030
H	-2.74179966	7.37763384	-1.04279534
H	-3.97059931	6.52883284	-1.81956862
N	6.53421368	3.30297677	1.05919928
H	6.52846295	3.97041496	1.82177047
H	7.37752028	2.74163248	1.04516151
N	3.29942727	-6.53652581	-1.05640431
H	2.73732002	-7.37928985	-1.03976695
H	3.96498661	-6.53256698	-1.82062542
N	-6.53160002	-3.30575991	1.06229468
H	-6.52424234	-3.97395938	1.82417442
H	-7.37542939	-2.74517740	1.04990381
C	3.56005950	-2.19593407	0.76989739
C	4.31799747	-3.29297614	1.14668941
C	6.02554422	-1.76711446	2.06057400

Table S23. Coordinates of the optimized structure for **Pt-THP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -1107.862808

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.91425876	0.95173279	0.00013353	C	2.29406790	2.55318590	0.00014036
C	-4.26922776	0.45319596	0.00025273	C	0.95173521	2.91425421	0.00035016
C	-4.19658943	-0.90584931	0.00023799	C	0.45319666	4.26922521	0.00015369
C	-2.79622036	-1.25702504	0.00011467	C	-0.90584837	4.19658766	-0.00031112
N	-2.03918289	-0.10902675	-0.00049691	C	-1.25702710	2.79621668	-0.00042933
C	-2.55318822	2.29406666	-0.00021267	N	-0.10902668	2.03917674	-0.00000632
C	-2.29406733	-2.55318635	-0.00024544	Pt	-0.00000007	0.00000008	0.00008478
C	-0.95173454	-2.91425393	-0.00044732	H	-5.15197510	1.07874149	0.00033827
C	-0.45319585	-4.26922482	-0.00032064	H	-5.00760559	-1.62196545	0.00031313
C	0.90584882	-4.19658694	0.00016813	H	-1.07873804	-5.15197427	-0.00070795
C	1.25702726	-2.79621620	0.00036782	H	1.62196133	-5.00760606	0.00051279
N	0.10902701	-2.03917663	-0.00000761	H	5.15197391	-1.07874244	-0.00044652
C	2.55318771	-2.29406638	0.00016593	H	5.00760574	1.62196406	-0.00047030
C	2.91425796	-0.95173282	-0.00017036	H	1.07873907	5.15197459	0.00047432
C	4.26922691	-0.45319679	-0.00033808	H	-1.62196094	5.00760695	-0.00069690
C	4.19658923	0.90584835	-0.00034677	H	-3.36064498	3.01951018	-0.00044765
C	2.79622057	1.25702456	-0.00018713	H	-3.01951239	-3.36064148	-0.00050842
N	2.03918285	0.10902636	0.00049263	H	3.36064447	-3.01950944	0.00036398
				H	3.01951306	3.36064102	0.00033315

Table S24. Coordinates of the optimized structure for **Pt-THTBP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -1722.466631

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.81479140	1.23851640	-0.00001180	C	3.43529111	-0.00135528	-0.00007749
C	-3.50747319	2.51435382	0.00006283	C	2.81479252	-1.23851572	0.00000222
C	-2.51194646	3.50935322	0.00017155	C	3.50747086	-2.51435901	0.00011017
C	-1.23628403	2.81588752	0.00006359	C	2.51194168	-3.50935330	0.00017098
N	-1.45552756	1.45686593	0.00004915	C	1.23628106	-2.81588142	0.00007069
C	-3.43529610	0.00135844	-0.00008085	N	1.45553358	-1.45685974	0.00006584
C	0.00135540	3.43530419	0.00007574	C	-0.00135713	-3.43529206	0.00007352
C	1.23851418	2.81479984	0.00000701	C	-1.23851559	-2.81478974	0.00000926
C	2.51435533	3.50747444	-0.00007086	C	-2.51435427	-3.50747237	-0.00006521
C	3.50935082	2.51194374	-0.00017577	C	-3.50935298	-2.51194468	-0.00017086
C	2.81587803	1.23628451	-0.00006913	C	-2.81588499	-1.23628191	-0.00006776
N	1.45685628	1.45553629	-0.00004617	N	-1.45686483	-1.45552797	-0.00004132

H	-5.64103418	2.09862095	-0.00037853	C	-4.86476746	2.85850349	-0.00039565
H	-6.24776167	4.50069413	-0.00112865	C	-5.20196137	4.20787054	-0.00075470
H	-4.49825365	6.24968983	-0.00105820	C	-4.20562069	5.20382023	-0.00069058
H	-2.09647166	5.64300436	-0.00019402	C	-2.85617113	4.86662365	-0.00023286
H	2.09863050	5.64103741	0.00036830	C	2.85850976	4.86476732	0.00038070
H	4.50070487	6.24775559	0.00110441	C	4.20787805	5.20195618	0.00073487
H	6.24969449	4.49824186	0.00104114	C	5.20382410	4.20561199	0.00067491
H	5.64299965	2.09646081	0.00019422	C	4.86662225	2.85616359	0.00022560
H	6.24776987	-4.50068574	-0.00117829	C	4.86477559	-2.85849916	-0.00033763
H	4.49826657	-6.24967438	-0.00114109	C	5.20196804	-4.20786050	-0.00076031
H	2.09649174	-5.64301733	-0.00021858	C	4.20563055	-5.20380558	-0.00074191
H	-2.09862253	-5.64103249	0.00038003	C	2.85617458	-4.86662064	-0.00026637
H	-4.50069702	-6.24775860	0.00111640	C	-2.85850476	-4.86476532	0.00039074
H	-6.24969105	-4.49824913	0.00104672	C	-4.20787290	-5.20195851	0.00074531
H	-5.64300219	-2.09646671	0.00019382	C	-5.20382111	-4.20561748	0.00068203
H	-0.00151815	-4.51983294	0.00019036	C	-4.86662267	-2.85616754	0.00022991
H	-4.51983653	0.00152125	-0.00020114	Pt	-0.00000108	-0.00000664	0.00000573
H	0.00151368	4.51984457	0.00020082				
H	4.51983189	-0.00150295	-0.00020105				
H	5.64099328	-2.09855140	-0.00024716				

Table S25. Coordinates of the optimized structure for **Pt-THTNP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2337.032319

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	2.23696413	2.11358761	-0.00029447	C	-3.25432765	-8.54191417	0.00019461
C	2.46602590	3.54911861	-0.00056516	C	-2.12036409	-7.76568751	0.00009449
C	1.17968030	4.15760585	-0.00082058	H	-3.86195103	4.60375597	-0.00045842
C	0.21536448	3.06992660	-0.00058852	H	-6.00824218	0.06484088	0.00093120
N	0.88264881	1.86547932	-0.00030511	H	4.60375630	3.86195250	-0.00047526
C	3.23582199	1.15740876	-0.00002937	H	0.06483961	6.00824007	-0.00140632
C	-1.15740794	3.23582569	-0.00054201	H	-4.60375556	-3.86194925	0.00066195
C	-2.11358755	2.23696627	-0.00020578	H	-0.06484071	-6.00824187	-0.00004462
C	-3.54911983	2.46602632	-0.00006798	H	3.86195239	-4.60375653	0.00032405
C	-4.15760589	1.17967957	0.00032077	H	6.00824007	-0.06483911	0.00050723
C	-3.06992309	0.21536558	0.00029876	H	-6.09977757	5.63983560	-0.00023040
N	-1.86547790	0.88265564	0.00000370	H	-8.55918567	5.42665501	0.00035556
C	-3.23582273	-1.15740594	0.00044941	H	-9.62497394	3.17321737	0.00107771
C	-2.23696559	-2.11358785	0.00033267	H	-8.22891302	1.13689392	0.00119937
C	-2.46602581	-3.54911863	0.00038971	H	5.63983443	6.09977868	-0.00099111
C	-1.17967891	-4.15760524	0.00019491	H	5.42665273	8.55918673	-0.00170984
C	-0.21536555	-3.06992395	0.00012657	H	3.17321478	9.62497426	-0.00220550

N	-0.88265415	-1.86547643	0.00018216	H	1.13689179	8.22891265	-0.00196503
C	1.15740611	-3.23582045	0.00011835	H	6.09977926	-5.63983438	0.00062033
C	2.11358674	-2.23696321	0.00016165	H	8.55918731	-5.42665247	0.00095234
C	3.54911826	-2.46602649	0.00025055	H	9.62497479	-3.17321453	0.00106299
C	4.15760597	-1.17967947	0.00029981	H	8.22891292	-1.13689160	0.00083297
C	3.06992477	-0.21536456	0.00013911	H	-5.63983602	-6.09977625	0.00068133
N	1.86548020	-0.88264970	0.00008114	H	-5.42665596	-8.55918456	0.00048819
C	-4.31480088	3.61567896	-0.00016238	H	-3.17321875	-9.62497341	0.00011284
C	-5.72593835	3.50690249	0.00015274	H	-1.13689480	-8.22891318	-0.00005638
C	-6.34337511	2.20156124	0.00056808	Pt	0.00000157	-0.00000388	-0.00001915
C	-5.53203642	1.04191775	0.00064331	H	4.25680919	1.52288209	0.00000486
C	3.61567851	4.31480130	-0.00067602	H	-1.52287990	4.25681296	-0.00073911
C	3.50690105	5.72593861	-0.00107160	H	1.52287848	-4.25680842	0.00012528
C	2.20155954	6.34337532	-0.00135374	H	-4.25681128	-1.52287542	0.00063328
C	1.04191697	5.53203605	-0.00121944	C	-8.54191470	3.25432647	0.00082368
C	-3.61567869	-4.31479972	0.00050755	C	-7.76568767	2.12036329	0.00089725
C	-3.50690279	-5.72593776	0.00041263	C	4.65765986	6.56575460	-0.00121685
C	-2.20156165	-6.34337495	0.00019809	C	4.53798751	7.93476218	-0.00161251
C	-1.04191774	-5.53203611	0.00009209	C	3.25432406	8.54191507	-0.00189151
C	4.31480109	-3.61567842	0.00036162	C	2.12036125	7.76568772	-0.00176436
C	5.72593935	-3.50690103	0.00054171	C	6.56575508	-4.65765969	0.00067811
C	6.34337580	-2.20155972	0.00060535	C	7.93476302	-4.53798719	0.00085809
C	5.53203579	-1.04191656	0.00048132	C	8.54191565	-3.25432413	0.00091886
C	-6.56575375	4.65766135	0.00009197	C	7.76568804	-2.12036116	0.00079630
C	-7.93476149	4.53798963	0.00041431	C	-4.65766183	-6.56575275	0.00050791
				C	-4.53799038	-7.93476070	0.00040515

Table S26. Coordinates of the optimized structure for **Pt-THTAP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Pt) level of theory.

E(B3LYP) = -2951.579844

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.96544935	-0.82761543	-0.00000299	C	2.18614461	7.73244025	-0.00024865
C	-4.31505143	-0.28641313	0.00004083	C	-0.36484490	10.47868073	-0.00015435
C	-4.17232734	1.13728394	0.00010630	C	0.44371552	11.58358367	-0.00022773
C	-2.74214826	1.39981488	0.00008028	C	1.86448061	11.44115625	-0.00031178
N	-2.05565300	0.20608475	0.00002058	C	2.43763114	10.19774137	-0.00031990
C	-2.66080436	-2.17591264	-0.00005127	C	0.36484796	-10.47867951	-0.00006013
C	-2.17591366	2.66080473	0.00008497	C	-0.44371192	-11.58358288	-0.00011095
C	-0.82761677	2.96545040	0.00002215	C	-1.86447705	-11.44115619	-0.00017600
C	-0.28641346	4.31505176	-0.00002390	C	-2.43762819	-10.19774153	-0.00018820
C	1.13728357	4.17232711	-0.00010610	C	10.47867994	0.36484492	0.00002253
C	1.39981337	2.74214749	-0.00008703	C	11.58358288	-0.44371551	0.00007839

N	0.20608360	2.05565313	-0.00001494
C	2.66080368	2.17591349	-0.00010859
C	2.96544922	0.82761692	-0.00005363
C	4.31505101	0.28641349	-0.00002647
C	4.17232636	-1.13728346	0.00005282
C	2.74214629	-1.39981330	0.00005126
N	2.05565191	-0.20608348	-0.00000805
C	2.17591248	-2.66080330	0.00007583
C	0.82761559	-2.96544814	0.00003620
C	0.28641317	-4.31505067	0.00001079
C	-1.13728385	-4.17232658	-0.00005223
C	-1.39981481	-2.74214703	-0.00004291
N	-0.20608463	-2.05565179	0.00000593
C	5.55651368	0.87739724	-0.00004586
C	6.72055307	0.05696695	0.00000588
C	6.57550808	-1.38989809	0.00008885
C	5.27177370	-1.96293854	0.00011502
C	-0.87739714	5.55651458	-0.00001894
C	-0.05696694	6.72055376	-0.00008869
C	1.38989819	6.57550876	-0.00017467
C	1.96293860	5.27177465	-0.00018571
C	0.87739770	-5.55651288	0.00001946
C	0.05696811	-6.72055281	-0.00002714
C	-1.38989700	-6.57550850	-0.00009373
C	-1.96293824	-5.27177453	-0.00010919
C	0.60772182	-8.01251673	-0.00001677
C	-0.19098966	-9.15974104	-0.00006872
C	-1.63104647	-9.01538027	-0.00013485
C	-2.18614287	-7.73244031	-0.00014491
C	8.01251726	0.60772002	-0.00001499
C	9.15974120	-0.19099204	0.00004178
C	9.01537969	-1.63104878	0.00012418
C	7.73243946	-2.18614454	0.00014475
C	-5.55651384	-0.87739760	0.00004595
C	-6.72055355	-0.05696810	0.00010953
C	-6.57550919	1.38989710	0.00017860
C	-5.27177547	1.96293829	0.00017945
C	-8.01251752	-0.60772178	0.00011369
C	-9.15974184	0.19098967	0.00018249
C	-9.01538101	1.63104655	0.00025109
C	-7.73244115	2.18614295	0.00024666
C	-0.60771997	8.01251811	-0.00008313
C	0.19099205	9.15974194	-0.00015789
C	1.63104886	9.01538049	-0.00024327
C	11.44115551	-1.86448056	0.00015949
C	10.19774058	-2.43763109	0.00018226
C	-10.47868031	-0.36484793	0.00018884
C	-11.58358367	0.44371194	0.00025602
C	-11.44115699	1.86447709	0.00032351
C	-10.19774238	2.43762825	0.00032173
H	5.67713693	1.95749144	-0.00010523
H	5.17559558	-3.04548325	0.00017623
H	-1.95749131	5.67713788	0.00004221
H	3.04548330	5.17559658	-0.00024953
H	1.95749199	-5.67713534	0.00006646
H	-3.04548301	-5.17559717	-0.00015826
H	1.68997494	-8.12209352	0.00003086
H	-3.26861131	-7.62501103	-0.00019619
H	8.12209463	1.68997308	-0.00007490
H	7.62500960	-3.26861294	0.00020823
H	-5.67713635	-1.95749185	-0.00000273
H	-5.17559819	3.04548306	0.00023068
H	-8.12209436	-1.68997489	0.00006418
H	-7.62501193	3.26861138	0.00029977
H	-1.68997302	8.12209547	-0.00002103
H	3.26861300	7.62501050	-0.00031442
H	-1.44664463	10.58504250	-0.00009120
H	0.00808658	12.57852088	-0.00022334
H	2.48893459	12.32982355	-0.00036946
H	3.51901712	10.08725181	-0.00038408
H	1.44664776	-10.58504070	-0.00001146
H	-0.00808252	-12.57851987	-0.00010297
H	-2.48893056	-12.32982376	-0.00021593
H	-3.51901422	-10.08725245	-0.00023795
H	10.58504170	1.44664466	-0.00003835
H	12.57852014	-0.00808660	0.00006220
H	12.32982276	-2.48893452	0.00020316
H	10.08725096	-3.51901706	0.00024422
H	-10.58504155	-1.44664772	0.00013829
H	-12.57852067	0.00808250	0.00025928
H	-12.32982456	2.48893063	0.00037648
H	-10.08725329	3.51901427	0.00037329
Pt	-0.00000025	0.00000032	0.00000148
H	2.86235621	-3.50021676	0.00011439
H	-3.50021819	-2.86235596	-0.00008280
H	3.50021677	2.86235771	-0.00015835
H	-2.86235744	3.50021823	0.00012644

Table S27. Coordinates of the optimized structure for **Pt-P-2alkynyl** (meso-substituents are bialkynyl groups) at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Pt) level of theory.

E(B3LYP) = -3351.888697

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.87531668	1.10564892	-0.00006300	C	7.27411492	8.48243825	1.55165233
C	-4.25116702	0.68331922	-0.00006168	H	6.29766250	8.97668678	1.57532124
C	-4.25015124	-0.67665700	0.00001385	H	7.36653810	7.87925312	2.46041029
C	-2.87371165	-1.09691487	0.00004859	H	8.04513659	9.26077178	1.58512726
N	-2.05226553	0.00497497	0.00000249	C	9.14566429	6.55169404	0.00051599
C	-2.45365795	2.45020373	-0.00009433	H	9.26425313	5.91802196	0.88521007
C	-2.45017658	-2.44077841	0.00010314	H	9.26431912	5.91810472	-0.88422973
C	-1.10563661	-2.86244837	0.00006598	H	9.96104007	7.28414939	0.00057878
C	-0.68332687	-4.23829104	0.00006036	C	7.27425853	-8.46752550	-1.55168131
C	0.67665200	-4.23727511	-0.00001804	H	6.29704776	-8.96027287	-1.57540298
C	1.09688979	-2.86084294	-0.00005365	H	7.36764848	-7.86446818	-2.46042332
N	-0.00498152	-2.03937655	-0.00000264	H	8.04408152	-9.24704577	-1.58513162
C	2.44073793	-2.43729508	-0.00011392	C	9.14874596	-6.53982804	-0.00030132
C	2.86235868	-1.09276523	-0.00009024	H	9.26842061	-5.90630513	-0.88495732
C	4.23818532	-0.67048689	-0.00010331	H	9.26835759	-5.90648034	0.88448669
C	4.23720531	0.68947330	-0.00003069	H	9.96293617	-7.27360003	-0.00034849
C	2.86075957	1.10978592	0.00001944	C	7.27411746	-8.46783068	1.55054918
N	2.03930428	0.00791903	-0.00001849	H	7.36741897	-7.86494348	2.45941301
C	2.43720236	2.45373750	0.00008349	H	6.29690054	-8.96057640	1.57408111
C	1.09275229	2.87538580	0.00006053	H	8.04393049	-9.24736322	1.58392939
C	0.67049748	4.25122132	0.00006278	C	-9.16161454	6.55284670	-0.00050801
C	-0.68949614	4.25024167	-0.00000957	H	-9.28122146	5.91938877	-0.88522078
C	-1.10978524	2.87378711	-0.00004474	H	-9.28132227	5.91944264	0.88422579
N	-0.00792511	2.05232412	-0.00000321	H	-9.97578676	7.28663858	-0.00058409
H	-5.09637502	1.35540600	-0.00010841	C	-7.28704383	8.48067709	1.55064208
H	-5.09433120	-1.35006317	0.00004192	H	-7.38041223	7.87771946	2.45945121
H	-1.35542170	-5.08349226	0.00010807	H	-6.30981665	8.97339969	1.57427215
H	1.35006627	-5.08144819	-0.00004861	H	-8.05683892	9.26022683	1.58403868
H	5.08338568	-1.34258272	-0.00015750	C	-8.48050876	-7.27438104	-1.55067947
H	5.08145242	1.36275736	-0.00001375	H	-8.97323459	-6.29715968	-1.57442027
H	1.34271364	5.09635506	0.00010941	H	-7.87752102	-7.36783639	-2.45946113
H	-1.36290107	5.09442212	-0.00003438	H	-9.26005077	-8.04418640	-1.58402888
C	3.44585501	-3.44016557	-0.00019260	C	-8.48057665	-7.27411910	1.55155100
C	-3.45305995	-3.44587880	0.00018352	H	-7.87762416	-7.36736695	2.46037702
C	3.44111406	3.45780829	0.00016075	H	-8.97334603	-6.29691425	1.57507586
C	-3.45877121	3.45306965	-0.00016951	H	-9.26008723	-8.04395108	1.58501992
Pt	-0.00647095	0.00646400	-0.00000878	C	-6.55268667	-9.14879840	0.00063284

C	-4.31441175	-4.31312365	0.00025280	H	-5.91921864	-9.26850401	-0.88405755
C	-4.32600945	4.31442898	-0.00024459	H	-5.91928654	-9.26837584	0.88538898
C	4.30830084	4.31921793	0.00022818	H	-7.28645792	-9.96298935	0.00066355
C	4.31309050	-4.30152570	-0.00026293	C	7.27425594	8.48257334	-1.55060642
C	-5.29291271	5.27131910	-0.00032093	H	7.36678639	7.87946956	-2.45940798
C	-6.16619524	6.13272833	-0.00038053	H	6.29779961	8.97680971	-1.57433679
C	5.27562216	5.27568600	0.00030110	H	8.04527111	9.26092005	-1.58393092
C	6.14968311	6.13630578	0.00037420	Si	-7.42191200	-7.47260427	0.00047578
C	5.27999915	-5.25841082	-0.00033459	Si	7.47255046	-7.40904797	-0.00045415
C	6.15331004	-6.11979047	-0.00037263	C	-7.28697196	8.48063174	-1.55158305
C	-5.27129321	-5.28003502	0.00032961	H	-6.30973494	8.97333084	-1.57521209
C	-6.13265673	-6.15336227	0.00039075	H	-7.38034947	7.87766702	-2.46038785
Si	-7.48539629	7.42202530	-0.00046167	H	-8.05675336	9.26019460	-1.58499447
Si	7.47085291	7.42359188	0.00048558				

Table S28. Coordinates of the optimized structure for **Zn-TNP-O$_2$** at the B3LYP/6-31G(d,p) (for C, N, Si, O, H) + SDD (for Zn) level of theory.

E(B3LYP) = -4534.551665							
Charge = 0, Multiplicity = 1							
Number of Imaginary Frequencies = 0							
Atom	x	y	z	Atom	x	y	z
C	-2.94500246	-1.23565869	0.76401952	H	7.58651814	1.99090226	-1.05037693
C	-3.57976145	-2.48501938	1.18747640	H	8.68837673	4.20409937	-1.09289013
C	-2.56679278	-3.21632658	1.90214865	H	7.33899258	6.28044202	-0.82309836
C	-1.39745186	-2.38875762	1.88164301	H	4.89142245	6.14427894	-0.51395710
N	-1.63974558	-1.24946936	1.20378498	H	-0.31180852	-5.49132026	-2.69556491
C	-3.52090135	-0.12231224	0.07359896	H	4.29301803	-3.70051386	-1.82552459
C	-0.13050639	-2.66305913	2.55546257	H	0.71878780	-7.58315173	-3.62856685
C	-0.11288347	-2.88422278	-1.50444013	H	2.72676711	-8.89609462	-4.23206165
C	0.88356002	-3.89843935	-1.92452144	H	4.99987131	-7.97418636	-3.80521749
C	2.17428787	-3.36145182	-1.65713659	H	5.26580549	-5.74489443	-2.77307675
C	1.94240884	-2.01336692	-1.06709982	H	-5.62623707	-2.53390044	0.51180914
N	0.60917718	-1.79560649	-0.97661399	H	-2.01845060	-4.98002297	2.99294845
C	2.92809086	-1.05588643	-0.71126647	H	-7.16414040	-4.39300006	0.91280483
C	2.63466158	0.33556423	-0.50783158	H	-7.64176250	-6.60847778	1.88770863
C	3.58278069	1.45592041	-0.53986606	H	-5.87264443	-7.84053592	3.14025707
C	2.79891841	2.65258124	-0.40038948	H	-3.62382686	-6.84916188	3.41173287
C	1.40111664	2.21558039	-0.31071119	H	-1.67067610	5.27146639	-1.28248601
N	1.38746217	0.83161802	-0.34234581	H	-5.54697250	2.12657517	-0.94966713
C	0.23694120	3.00177593	-0.30173077	H	-3.19009596	7.04475907	-2.06745890
C	-1.12551494	2.51513051	-0.41927624	H	-5.47117728	7.81674576	-2.62168125
C	-2.31369148	3.28044557	-0.77532862	H	-7.40649845	6.25927593	-2.41325533
C	-3.42221216	2.36268683	-0.70150935	H	-7.05846344	3.93388574	-1.66194149

C	-2.85881412	1.08361182	-0.28393729	H	8.22149057	-3.28409458	2.09266773
N	-1.49340693	1.23774131	-0.18537305	H	7.00503950	-2.04715566	2.45281260
C	4.95006887	1.52326192	-0.72303138	H	6.50014540	-3.70357127	2.09579736
C	5.59577773	2.78570207	-0.74994933	H	8.46778337	-4.41451291	-0.85226412
C	4.81660572	3.98243319	-0.59708851	H	7.39616679	-3.80651398	-2.12233147
C	3.41033238	3.89127956	-0.43058480	H	6.74979223	-4.83141351	-0.82682479
C	7.00174850	2.89887202	-0.93006149	H	8.31102334	-0.86326239	-1.48685523
C	7.61363488	4.13178101	-0.95442116	H	8.17819779	-0.23187139	0.16505483
C	6.84548182	5.31314485	-0.80094273	H	9.38329869	-1.46829016	-0.21583177
C	5.48168695	5.23909361	-0.62746094	H	2.46596202	9.03361768	0.57288371
C	0.69163501	-5.12239774	-2.50226956	H	3.08090408	7.41221859	0.91894414
C	1.83154999	-5.90214606	-2.84904933	H	2.65268171	7.86477637	-0.74180699
C	3.14301655	-5.36909825	-2.59724098	H	-0.55569703	9.43535963	-0.22126133
C	3.29631052	-4.08340200	-1.99800693	H	-1.63701068	8.03877609	-0.31785536
C	1.71259786	-7.18490669	-3.44243641	H	-0.36713754	8.26335871	-1.53381622
C	2.83266123	-7.91510716	-3.77833963	H	-0.87617217	7.20562626	2.61947424
C	4.12415983	-7.39124168	-3.53530283	H	0.82101825	6.98656111	3.06554584
C	4.27407556	-6.14806044	-2.95907174	H	0.19463324	8.61138117	2.74054418
C	-4.83977258	-3.04605565	1.04679206	H	2.73506936	3.01622270	4.16828345
C	-5.11132486	-4.31992524	1.60085173	H	2.14435834	2.54067674	2.57024960
C	-4.08779907	-5.03641355	2.32248015	H	1.07333027	2.43704683	3.97514288
C	-2.80911466	-4.45957357	2.46444993	H	5.14548568	0.92887286	3.81529776
C	-6.39309687	-4.92757781	1.46235373	H	4.49998313	0.43958265	2.24037090
C	-6.65794971	-6.16266367	2.00374779	H	4.76314689	-0.77373414	3.50130876
C	-5.64962945	-6.86534015	2.71707917	H	2.92854639	-0.85741813	6.04141387
C	-4.40010785	-6.31561648	2.86942016	H	1.60903182	0.30701655	6.22038029
C	-2.50351077	4.58646473	-1.19666198	H	3.28903324	0.84477506	6.37807279
C	-3.80017842	5.03706194	-1.52900329	H	-9.60409875	1.08328190	-1.82784396
C	-4.91550388	4.13423510	-1.41753452	H	-8.47875792	1.92519997	-0.75431048
C	-4.70224272	2.79831063	-1.00534741	H	-8.00127923	1.54291487	-2.41928380
C	-4.03711463	6.37002950	-1.97451828	H	-9.06459704	-1.92162798	-2.63465636
C	-5.30577394	6.79767187	-2.28421193	H	-7.60997837	-2.74197150	-2.04450387
C	-6.40809947	5.90954639	-2.16658144	H	-7.46856194	-1.44967763	-3.24149230
C	-6.21611491	4.61487416	-1.74686404	H	-8.73395259	-0.32646048	1.37672054
C	4.27623732	-1.49374299	-0.57389017	H	-9.87429840	-1.20761312	0.34784344
C	0.38232431	4.40613747	-0.10336738	H	-8.42026537	-2.01341573	0.95625457
C	0.77768597	-1.54212818	2.77648008	C	2.10441585	2.29504471	3.63546659
C	-4.90765693	-0.21233578	-0.24368183	C	4.43866353	0.25537664	3.31680134
C	-6.09310491	-0.30273280	-0.53190582	C	2.62177909	0.17123366	5.82784333
C	1.54528381	-0.67172575	3.16309657	C	-8.54861287	1.17225429	-1.54646798
C	5.42096858	-1.88554488	-0.38477819	C	-8.01649191	-1.77271937	-2.35057531
C	0.48258844	5.60059382	0.14457818	C	-8.81099149	-1.06540218	0.57259795
Si	7.11537587	-2.49408680	-0.00445971	Zn	-0.24142102	-0.30494681	0.04167179
Si	2.69349672	0.53621966	3.97540862	O	-1.32881060	-2.92429128	-1.59351812

Si	-7.87611886	-0.49566321	-0.96683312	O	0.14622477	-3.77397358	3.01607853
Si	0.59495130	7.38158261	0.60524644	H	5.53948274	0.62615132	-0.85461174
C	7.22020440	-2.92248836	1.83141790	H	2.83360615	4.80069084	-0.33797560
C	7.46120442	-4.02985796	-1.05209934				
C	8.36084130	-1.13493832	-0.42704716				
C	2.36565597	7.97457679	0.30940116				
C	-0.60431553	8.36905191	-0.46994917				
C	0.14121579	7.56183716	2.42893990				

Table S29. Coordinates of the optimized structure for **Zn-THP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Zn) level of theory.

E(B3LYP) = -1215.585252

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	1.80396954	2.49031031	-0.00014465	H	-3.91524031	3.54329250	0.00016719
C	3.00763834	0.63985226	-0.00009067	C	-3.93714519	-1.74750509	-0.00024084
N	1.72117501	1.11975477	-0.00013024	H	-5.01528756	-1.65215788	-0.00035365
C	0.71156983	3.36081737	-0.00003515	C	-3.19331398	-2.89103761	-0.00011075
C	3.36081462	-0.71157172	0.00005224	H	-3.54329202	-3.91523828	-0.00012849
C	2.49030643	-1.80397017	0.00016710	H	-4.42332125	0.93653122	0.00001967
C	0.63985011	-3.00764165	0.00009165	H	-0.93653514	-4.42331811	-0.00003894
N	1.11975018	-1.72117796	0.00014525	H	4.42331687	-0.93653029	0.00005794
C	-0.71157458	-3.36081636	-0.00005624	H	0.93652634	4.42331997	-0.00005532
C	-1.80397162	-2.49030614	-0.00017469	N	-1.11975573	1.72117645	0.00014031
C	-3.00764201	-0.63985155	-0.00011458	Zn	0.00001010	-0.00000214	0.00000579
N	-1.72117945	-1.11975112	-0.00014827	C	1.74750364	-3.93714335	0.00026703
C	-3.36081915	0.71157269	0.00002527	H	1.65215754	-5.01528586	0.00040722
C	-2.49031007	1.80397100	0.00014724	C	2.89103650	-3.19331191	0.00007770
C	-0.63985370	3.00763867	0.00010155	H	3.91523684	-3.54329104	0.00007835
H	3.54329139	3.91523893	-0.00025354	C	3.93714133	1.74750517	-0.00012765
C	-1.74750657	3.93714315	0.00017636	H	5.01528381	1.65215783	-0.00017254
H	-1.65215822	5.01528550	0.00025454	C	3.19331138	2.89103897	-0.00016960
C	-2.89104008	3.19331343	0.00012442				

Table S30. Coordinates of the optimized structure for **Zn-THTBP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Zn) level of theory.

E(B3LYP) = -1830.188252

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z
C	2.75611906	-1.39364894	0.00024087
C	4.18595871	-1.12384038	0.00003036
C	4.32511084	0.28022632	-0.00038126
C	2.97602936	0.82552038	-0.00052842
N	2.06662481	-0.20484353	-0.00017746
C	2.18057457	-2.66036437	0.00046336
C	2.66031509	2.18057859	-0.00091878
C	1.39359056	2.75610756	-0.00079231
C	1.12380030	4.18595312	-0.00085698
C	-0.28026454	4.32512337	-0.00045747
C	-0.82557542	2.97605132	-0.00004074
N	0.20476379	2.06663227	-0.00022641
C	-2.18062798	2.66032095	0.00042493
C	-2.75612167	1.39357860	0.00055119
C	-4.18598204	1.12380146	0.00068461
C	-4.32515144	-0.28025980	0.00056252
C	-2.97606172	-0.82555955	0.00023781
N	-2.06664354	0.20476592	0.00021033
C	-2.66036932	-2.18062260	0.00003172
C	-1.39363598	-2.75613151	0.00000105
C	-1.12384134	-4.18598612	0.00014221
C	0.28022164	-4.32513822	0.00027640
C	0.82550555	-2.97603954	0.00033235
N	-0.20484407	-2.06663500	0.00019311
C	1.95380369	5.31431025	-0.00139785
C	-0.87255522	5.59448331	-0.00058708
C	5.31432232	-1.95383479	0.00034478
C	5.59446622	0.87252702	-0.00049055
C	-5.31433412	1.95380508	0.00107512
C	-5.59450601	-0.87255243	0.00082240

Atom	x	y	z
H	1.98241781	7.46123316	-0.00199003
C	6.71052109	0.04287196	-0.00018187
H	7.70521572	0.47905586	-0.00025848
C	6.57154205	-1.35945372	0.00024675
H	7.46124638	-1.98242752	0.00052324
C	0.04286690	-6.71054691	0.00009664
H	0.47905216	-7.70524107	0.00007613
C	-1.35945499	-6.57156793	-0.00005463
H	-1.98243052	-7.46127120	-0.00021851
C	-6.71055686	-0.04288585	0.00120440
H	-7.70525546	-0.47906078	0.00141238
C	-6.57156311	1.35943455	0.00134336
H	-7.46125998	1.98241926	0.00168530
H	-2.86861140	3.49977448	0.00060384
H	-3.49983871	-2.86858670	-0.00000366
H	2.86851886	-3.49984993	0.00065483
H	3.49978432	2.86854275	-0.00125387
C	-1.95383654	-5.31434428	-0.00002218
C	0.87252370	-5.59448865	0.00025526
H	3.03599537	5.21901030	-0.00175007
H	-1.95238605	5.71351834	-0.00024347
H	5.21902869	-3.03602692	0.00070420
H	5.71349495	1.95235867	-0.00084533
H	-5.21903694	3.03599727	0.00121429
H	-5.71354327	-1.95238330	0.00069193
H	-3.03602915	-5.21905296	-0.00016841
H	1.95235532	-5.71352009	0.00039733
Zn	0.00015902	0.00012927	-0.00000064
C	-0.04288983	6.71053024	-0.00111910
H	-0.47906286	7.70522959	-0.00122971
C	1.35943432	6.57153560	-0.00153553

Table S31. Coordinates of the optimized structure for **Zn-THTNP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Zn) level of theory.

E(B3LYP) = -2444.753697

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-1.12500797	2.88019823	-0.00019674	C	-4.90854325	-6.40757585	-0.00033405
C	-2.36960653	3.63830472	-0.00045858	C	-4.33935454	6.80603869	-0.00076438
C	-3.42086192	2.67385699	-0.00056820	C	-5.65221554	7.21156516	-0.00092804
C	-2.77261770	1.36867481	-0.00040136	C	-6.69877510	6.25139336	-0.00103970
N	-1.40843400	1.53540203	-0.00017748	C	-6.40756426	4.90853644	-0.00098534
C	0.14823778	3.43841702	-0.00000906	C	6.80605298	4.33936894	0.00088680
C	-3.43838808	0.14820737	-0.00043443	C	7.21158072	5.65223115	0.00091741
C	-2.88015516	-1.12503401	-0.00030402	C	6.25141030	6.69878928	0.00079134
C	-3.63827675	-2.36962539	-0.00027261	C	4.90855206	6.40757733	0.00063791
C	-2.67384067	-3.42089147	-0.00014333	C	4.33936333	-6.80604097	0.00047034
C	-1.36865258	-2.77266288	-0.00006846	C	5.65222189	-7.21158045	0.00062967
N	-1.53535597	-1.40848423	-0.00017302	C	6.69878881	-6.25141961	0.00073669
C	-0.14817957	-3.43841955	0.00005942	C	6.40758886	-4.90855872	0.00068146
C	1.12505004	-2.88015381	0.00015683	H	-5.73634070	-1.85566898	-0.00051923
C	2.36964197	-3.63829325	0.00021324	H	-2.34209418	-5.55533652	-0.00005064
C	3.42090644	-2.67385856	0.00032318	H	-1.85566282	5.73637065	-0.00043823
C	2.77266002	-1.36866843	0.00029676	H	-5.55530609	2.34209768	-0.00083833
N	1.40848991	-1.53536233	0.00020258	H	1.85568335	-5.73635652	0.00017634
C	3.43844826	-0.14820996	0.00038410	H	5.55535097	-2.34210971	0.00054850
C	2.88019673	1.12502405	0.00034395	H	5.73638637	1.85567712	0.00078110
C	3.63832116	2.36962314	0.00051796	H	2.34211334	5.55532070	0.00034051
C	2.67387490	3.42087700	0.00038837	H	-7.53981465	-3.53722250	-0.00069134
C	1.36869064	2.77261500	0.00017310	H	-8.27008111	-5.89549785	-0.00074331
N	1.53540827	1.40843984	0.00014799	H	-6.58478535	-7.73245835	-0.00051386
C	-4.99170812	-2.64768540	-0.00043659	H	-4.17243869	-7.20757453	-0.00023243
C	-5.42331013	-3.99538502	-0.00044325	H	-3.53723467	7.53983376	-0.00068025
C	-4.44700839	-5.05955559	-0.00031219	H	-5.89551695	8.27007910	-0.00096976
C	-3.06719158	-4.74539522	-0.00017971	H	-7.73246195	6.58476646	-0.00116577
C	-2.64767541	4.99173409	-0.00050381	H	-7.20755643	4.17242483	-0.00107212
C	-3.99537847	5.42332527	-0.00069437	H	7.53984820	3.53724912	0.00098452
C	-5.05953987	4.44701356	-0.00080579	H	8.27009497	5.89553135	0.00103534
C	-4.74536845	3.06719924	-0.00072179	H	6.58478228	7.73247650	0.00081416
C	2.64769796	-4.99172177	0.00027526	H	4.17244057	7.20756971	0.00054284
C	3.99540101	-5.42332585	0.00041691	H	3.53723710	-7.53982915	0.00038701
C	5.05956995	-4.44702555	0.00052772	H	5.89551245	-8.27009693	0.00067766
C	4.74540770	-3.06720516	0.00049531	H	7.73247301	-6.58480096	0.00086541
C	4.99174766	2.64768795	0.00066513	H	7.20758770	-4.17245422	0.00076170
C	5.42334104	3.99539441	0.00072070	Zn	-0.00019414	0.00000833	0.00000000

C	4.44703079	5.05955427	0.00059026	H	-4.52264452	0.19499196	-0.00056731
C	3.06721289	4.74538103	0.00040619	H	-0.19494229	-4.52267687	0.00007425
C	-6.80602668	-4.33934883	-0.00059281	H	4.52270457	-0.19499453	0.00050925
C	-7.21156495	-5.65220617	-0.00061910	H	0.19504422	4.52267245	-0.00001618
C	-6.25140283	-6.69877452	-0.00048838				

Table S32. Coordinates of the optimized structure for **Zn-THTAP** (meso-substituents are H) at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Zn) level of theory.

E(B3LYP) = -3059.301002

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	1.28802092	-2.81303261	-0.00007924	C	-8.59235492	-7.81472377	0.00035899
C	2.57313481	-3.50155012	-0.00006947	C	-7.56841965	-8.81009982	0.00029619
C	3.57305880	-2.47290162	-0.00012911	C	-6.24810151	-8.44794647	0.00021103
C	2.84839770	-1.20780856	-0.00012621	C	-6.48467337	8.26767923	0.00054146
N	1.49619201	-1.45439894	-0.00009732	C	-7.81470244	8.59236805	0.00059778
C	0.04876276	-3.44226856	-0.00006292	C	-8.81008728	7.56844129	0.00063314
C	3.44223932	0.04879047	-0.00018439	C	-8.44794504	6.24812008	0.00061039
C	2.81299019	1.28804407	-0.00018006	C	6.48467702	-8.26766340	-0.00041733
C	3.50152192	2.57315197	-0.00029658	C	7.81470821	-8.59234037	-0.00052087
C	2.47288368	3.57308652	-0.00020969	C	8.81008506	-7.56840430	-0.00057451
C	1.20778424	2.84843946	-0.00008914	C	8.44793229	-6.24808680	-0.00052402
N	1.45435227	1.49623739	-0.00007440	H	-2.17440755	5.61972295	0.00032939
C	-0.04881897	3.44226777	0.00003158	H	-5.67918199	2.01441962	0.00045712
C	-1.28805991	2.81298810	0.00014413	H	5.61970834	2.17439297	-0.00042949
C	-2.57316864	3.50153695	0.00032064	H	2.01440559	5.67916707	-0.00014624
C	-3.57310194	2.47289993	0.00035126	H	-5.61975237	-2.17440151	0.00016834
C	-2.84843767	1.20780018	0.00023687	H	-2.01442648	-5.67915278	-0.00005564
N	-1.49624351	1.45435834	0.00011479	H	-7.31794688	-3.95332212	0.00027119
C	-3.44229684	-0.04879127	0.00021577	H	-3.74461247	-7.42701375	0.00005270
C	-2.81303040	-1.28803678	0.00011520	H	-3.95331204	7.31792804	0.00042559
C	-3.50156511	-2.57315147	0.00004538	H	-7.42703285	3.74462200	0.00054864
C	-2.47291789	-3.57307428	-0.00001240	H	2.17438704	-5.61973776	-0.00006835
C	-1.20782448	-2.84839603	-0.00002150	H	5.67913780	-2.01441233	-0.00025513
N	-1.45440489	-1.49619824	0.00005693	H	3.95330770	-7.31793338	-0.00021978
C	-2.92296218	4.83156766	0.00035605	H	7.42699989	-3.74459828	-0.00040773
C	-4.30008646	5.19394572	0.00042292	H	7.31791455	3.95329744	-0.00047711
C	-5.31367667	4.15127731	0.00045610	H	3.74460802	7.42701899	-0.00019350
C	-4.91250116	2.78495259	0.00041659	H	9.04563715	5.72545658	-0.00051767
C	4.83155506	2.92294951	-0.00036758	H	9.63407881	8.12209902	-0.00048012
C	5.19393107	4.30007045	-0.00035369	H	7.84627252	9.86007036	-0.00033894
C	4.15126182	5.31366159	-0.00026801	H	5.46723147	9.20414780	-0.00023347

C	2.78494035	4.91248827	-0.00019463	H	-9.04565535	-5.72549664	0.00038394
C	-4.83159361	-2.92295260	0.00011960	H	-9.63407754	-8.12214432	0.00042678
C	-5.19396165	-4.30007965	0.00014034	H	-7.84625644	-9.86010047	0.00031669
C	-4.15128457	-5.31366095	0.00007942	H	-5.46722110	-9.20415706	0.00016533
C	-2.78496289	-4.91247548	0.00000488	H	-5.72547172	9.04565096	0.00051226
C	-6.53724433	-4.71084265	0.00022763	H	-8.12211421	9.63409331	0.00061617
C	-6.90059584	-6.06050368	0.00025243	H	-9.86008554	7.84628697	0.00067835
C	-5.86273765	-7.06940995	0.00018845	H	-9.20416214	5.46724587	0.00063508
C	-4.52389529	-6.66803234	0.00010336	H	5.72548177	-9.04564143	-0.00037865
C	-4.71083873	6.53723163	0.00044828	H	8.12212939	-9.63406283	-0.00056288
C	-6.06049658	6.90059436	0.00050885	H	9.86008549	-7.84624167	-0.00065604
C	-7.06941169	5.86274474	0.00054503	H	9.20414277	-5.46720639	-0.00056684
C	-6.66804509	4.52389885	0.00051869	Zn	0.00019298	0.00000272	-0.00000002
C	2.92294000	-4.83158105	-0.00010815	H	-0.06424726	4.52738786	0.00005025
C	4.30006372	-5.19394696	-0.00020960	H	-4.52741714	-0.06419895	0.00027478
C	5.31364587	-4.15126898	-0.00026747	H	0.06414984	-4.52738923	-0.00007362
C	4.91246256	-2.78495057	-0.00022676	H	4.52735978	0.06419815	-0.00025136
C	4.71082843	-6.53723115	-0.00026484	C	5.86272934	7.06939666	-0.00031129
C	6.06048785	-6.90058129	-0.00036804	C	4.52388504	6.66803154	-0.00025227
C	7.06939508	-5.86272209	-0.00042217	C	8.26766552	6.48465829	-0.00045822
C	6.66801879	-4.52388131	-0.00036972	C	8.59235376	7.81468667	-0.00043593
C	6.53721856	4.71082435	-0.00041113	C	7.56842626	8.81007231	-0.00035478
C	6.90057991	6.06048055	-0.00039327	C	6.24810564	8.44793076	-0.00029734
				C	-8.26767727	-6.48469189	0.00033402

Table S33. Coordinates of the optimized structure for **Zn-TPP** at the B3LYP/6-31G(d,p) (for C, N, H) + SDD (for Zn) level of theory.

E(B3LYP) = -2139.791147

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
C	-2.87583488	-1.09739757	-0.02328899	H	6.24741294	-6.28842466	-0.01234106
C	-2.86919750	1.11475788	-0.02563822	H	4.73541898	-6.02208906	-1.96984266
N	-2.05444061	0.00625834	0.02464443	H	2.99070848	-4.26308055	-1.96104031
C	-2.45651980	-2.44178592	0.00222789	H	3.02315772	4.25005663	-1.95103119
C	-2.44178351	2.45652695	-0.00221875	H	4.78003423	5.99698955	-1.95003083
C	-1.09739541	2.87583940	0.02332577	H	6.28845482	6.24738230	0.01225996
C	1.11474981	2.86920975	0.02562458	H	6.02208001	4.73545058	1.96980548
N	0.00625704	2.05444095	-0.02458504	H	4.26305194	2.99076088	1.96103765
C	2.45651293	2.44179707	0.00219114	Zn	0.00000740	-0.00000450	0.00005468
C	2.87583141	1.09741297	-0.02331818	C	0.69343047	4.24796360	0.12915287
C	2.86920474	-1.11474367	-0.02561871	H	1.35500671	5.09742316	0.20892305
N	2.05444188	-0.00624862	0.02464162	C	-0.66802520	4.25206453	0.12747778

C	2.44179139	-2.45651503	-0.00219783	H	-1.32481293	5.10535179	0.20587217
C	1.09740397	-2.87583567	0.02333006	C	-4.24794977	0.69343320	-0.12903959
C	-1.11475323	-2.86920206	0.02565809	H	-5.09743466	1.35500749	-0.20855803
N	-0.00625524	-2.05444233	-0.02457518	C	-4.25204848	-0.66802481	-0.12748655
C	3.51930901	3.49772434	0.00476669	H	-5.10534411	-1.32479833	-0.20590434
C	-3.49771860	3.51931754	-0.00480122	C	-0.69342836	-4.24795102	0.12909071
C	3.49772628	-3.51930542	-0.00479520	H	-1.35500099	-5.09742927	0.20868867
C	-3.51931029	-3.49771976	0.00478613	C	0.66803122	-4.25205378	0.12748498
C	-4.37985694	-3.64767039	1.10415150	H	1.32480665	-5.10535197	0.20586376
C	-5.36945851	-4.63152459	1.10747709	C	4.24795223	-0.69341492	-0.12907870
C	-5.51761470	-5.48205944	0.01020304	H	5.09742711	-1.35498432	-0.20874062
C	-4.66902054	-5.34286672	-1.08973127	C	4.25205062	0.66804412	-0.12746134
C	-3.67821494	-4.36017310	-1.09182734	H	5.10534546	1.32482262	-0.20585383
C	-3.64767851	4.37983271	-1.10419150	C	5.36944513	4.63151293	1.10748970
C	-4.63155004	5.36941687	-1.10754854	C	4.37983213	3.64767098	1.10414976
C	-5.48209543	5.51758528	-0.01028428	H	-4.26309672	-2.99076095	1.96104210
C	-5.34290318	4.66901455	1.08966804	H	-6.02210578	-4.73547047	1.96978248
C	-4.36019496	3.67822348	1.09179513	H	-6.28842836	-6.24740882	0.01223608
C	4.36021134	-3.67821647	1.09179280	H	-4.77997644	-5.99700288	-1.95002769
C	5.34290392	-4.66902320	1.08966237	H	-3.02311918	-4.25005173	-1.95100052
C	5.48206431	-5.51761047	-0.01028141	H	-2.99076395	4.26305965	-1.96107636
C	4.63149882	-5.36944661	-1.10753057	H	-4.73550115	6.02204048	-1.96987111
C	3.64764473	-4.37984497	-1.10417049	H	-6.24745702	6.28838661	-0.01234141
C	3.67824150	4.36017214	-1.09184667	H	-5.99705183	4.77997662	1.94995416
C	4.66905793	5.34285524	-1.08973563	H	-4.25007678	3.02314276	1.95098034
C	5.51763264	5.48204166	0.01021482	H	4.25011392	-3.02312633	1.95097380
				H	5.99706464	-4.77998493	1.94993930

Table S34. Coordinates of the optimized structure for **Zn-P** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Zn) level of theory.

E(B3LYP) = -3154.984956							
Charge = 0, Multiplicity = 1							
Number of Imaginary Frequencies = 0							
Atom	x	y	z	Atom	x	y	z
C	1.10211775	-2.87784347	0.00287049	C	5.25556359	6.85875872	1.36902089
C	0.68553868	-4.25800871	0.00357116	H	4.28467017	7.34261284	1.22067363
C	-0.67723251	-4.25992557	0.00238291	H	5.23934299	6.37087301	2.34888876
C	-1.09773740	-2.88096047	0.00099161	H	6.01967998	7.64408199	1.39733929
N	0.00102322	-2.05752950	0.00144165	C	5.62312381	6.48404027	-1.68685860
C	2.44882662	-2.44570477	0.00347965	H	4.65803085	6.95965382	-1.88934782
C	-2.44565795	-2.45262989	-0.00051326	H	6.39422142	7.26229558	-1.72187620
C	-2.87776051	-1.10587015	-0.00051082	H	5.82320070	5.77665046	-2.49805136
C	-4.25799804	-0.68933085	-0.00090893	C	-4.85594711	7.23406466	-0.60217254

C	-4.25985600	0.67344976	-0.00025147
C	-2.88088377	1.09397032	0.00035358
N	-2.05743523	-0.00478593	0.00020231
C	-2.45259558	2.44190178	0.00071773
C	-1.10585018	2.87403734	-0.00013997
C	-0.68931949	4.25425456	-0.00137295
C	0.67346081	4.25612730	-0.00202116
C	1.09398597	2.87717084	-0.00100893
N	-0.00476603	2.05372524	-0.00005119
C	2.44190271	2.44884135	-0.00050342
C	2.87400269	1.10208509	0.00152796
C	4.25423003	0.68553093	0.00352871
C	4.25613195	-0.67725908	0.00478234
C	2.87710960	-1.09773460	0.00341395
N	2.05366229	0.00101107	0.00173551
Zn	-0.00188721	-0.00190161	0.00070636
C	-3.45371628	-3.46264997	-0.00237337
C	-4.31885838	-4.32694700	-0.00441228
Si	-5.62880225	-5.62215388	-0.00738512
C	-7.29699453	-4.78619574	0.28913603
H	-7.31432397	-4.26280282	1.25060621
H	-7.52128969	-4.05563732	-0.49500707
H	-8.10516911	-5.52651478	0.29655445
C	-5.26287455	-6.85897753	1.37318113
H	-4.29158008	-7.34315450	1.22855555
H	-5.24916516	-6.36859824	2.35184104
H	-6.02702496	-7.64426525	1.40155133
C	-5.62273571	-6.49213567	-1.68455876
H	-4.65718849	-6.96835540	-1.88342053
H	-6.39381316	-7.27041729	-1.71947637
H	-5.82073891	-5.78683395	-2.49807514
C	-3.46281938	3.44975904	0.00242356
C	-4.32781713	4.31419941	0.00440935
C	3.45959932	-3.45301324	0.00350531
C	4.32666967	-4.31537700	0.00305532
C	3.44996223	3.45886372	-0.00239835
C	4.31510133	4.32316136	-0.00445871
Si	5.62501615	5.61840138	-0.00743226
Si	-5.62697352	5.62023530	0.00663934
Si	5.63695703	-5.61024639	0.00327601
C	7.29246768	4.78329582	0.29556858
H	7.30728295	4.26237903	1.25842471
H	7.51889263	4.05072589	-0.48607895
H	8.10057511	5.52368680	0.30322268
H	-4.03564639	7.55435766	0.04856828
H	-4.45726597	7.12646494	-1.61608797
H	-5.60158196	8.03721407	-0.61874474
C	-7.02331670	5.08628206	-1.14863069
H	-6.66010177	4.94492549	-2.17163409
H	-7.47457985	4.14408141	-0.82081036
H	-7.81467043	5.84419290	-1.17499768
C	-6.27868732	5.83045609	1.76758982
H	-7.05534320	6.60316172	1.80309951
H	-6.71456374	4.89967363	2.14470582
H	-5.47913039	6.12662067	2.45423703
C	5.10502343	-7.00872787	1.15688966
H	4.96016810	-6.64627019	2.17967037
H	4.16506685	-7.46303924	0.82684055
H	5.86550530	-7.79756017	1.18474104
C	5.85326665	-6.26051844	-1.75747285
H	6.62863525	-7.03457384	-1.79162662
H	4.92478464	-6.69930094	-2.13688504
H	6.14829900	-5.45964519	-2.44307429
C	7.24690182	-4.83422423	0.61599908
H	7.56601380	-4.01260510	-0.03365722
H	7.13576232	-4.43632647	1.62983809
H	8.05241262	-5.57727626	0.63404269
H	5.10315661	-1.34736445	0.00702613
H	5.09941007	1.35797733	0.00437963
H	1.34367288	5.10304167	-0.00282073
H	-1.36183573	5.09936831	-0.00220903
H	-5.10679033	1.34364608	-0.00066332
H	-5.10317089	-1.36178468	-0.00129915
H	-1.34745360	-5.10683152	0.00283529
H	1.35814068	-5.10303167	0.00535049

Table S35. Coordinates of the optimized structure for ***ruf*-Zn-TNP** at the B3LYP/6-31G(d,p) (for C, N, Si, H) + SDD (for Zn) level of theory.

E(B3LYP) = -4384.108908

Charge = 0, Multiplicity = 1

Number of Imaginary Frequencies = 0

Atom	x	y	z	Atom	x	y	z
Zn	0.00000000	0.00000000	0.00000000	H	-2.35147822	5.45395415	0.84700466
Si	-4.96314010	4.96298313	3.23979396	H	-2.35337749	7.91572645	0.81556080
N	-0.00000366	2.05604324	-0.00002762	H	2.35360536	7.91569857	-0.81492099
C	1.05976840	2.84399057	-0.37036826	H	1.17849411	10.04998429	-0.40533554
C	-0.67103933	4.24611724	0.25311297	H	-1.17817148	10.04998895	0.40619265
C	0.67879090	6.66906683	-0.23747176	H	-5.18542399	7.42790721	3.57007017
C	-2.35060946	2.35061671	0.69823615	H	-3.54122020	7.01906450	3.06034427
C	0.67112119	4.24612643	-0.25286485	H	-4.85550375	7.05851710	1.87174636
C	1.33487267	5.44083304	-0.48025890	H	-7.01913356	3.54098570	3.06013464
C	-0.67861695	6.66906683	0.23797091	H	-7.05889377	4.85564011	1.87195375
C	-3.22347662	3.22346025	1.41229446	H	-7.42797590	5.18500229	3.57045684
C	-1.33474606	5.44083288	0.48062689	H	-3.47373185	4.72392296	5.23517017
C	-1.05975145	2.84398421	0.37041433	H	-5.12730657	5.12720820	5.72615224
C	-1.32643635	7.91865460	0.45997561	H	-4.72444597	3.47354371	5.23515096
C	-3.93229836	3.93222583	2.11498471	H	5.45395547	-2.35160206	0.84664027
C	1.32666166	7.91864720	-0.45934531	H	5.45395415	2.35147822	-0.84700466
C	0.67145208	9.10526304	-0.23129399	H	7.91572645	2.35337749	-0.81556080
C	-0.67116692	9.10526452	0.23204942	H	7.91569857	-2.35360536	0.81492099
C	-4.59940576	6.78698085	2.90147998	H	10.04998429	-1.17849411	0.40533554
C	-6.78714675	4.59923542	2.90155358	H	10.04998895	1.17817148	-0.40619265
C	-4.53080077	4.53056233	5.02634877	H	7.05851710	4.85550375	-1.87174636
Si	4.96298313	4.96314010	-3.23979396	H	7.01906450	3.54122020	-3.06034427
N	2.05604324	0.00000366	0.00002762	H	7.42790721	5.18542399	-3.57007017
C	2.84399057	-1.05976840	0.37036826	H	4.85564011	7.05889377	-1.87195375
C	4.24611724	0.67103933	-0.25311297	H	5.18500229	7.42797590	-3.57045684
C	6.66906683	-0.67879090	0.23747176	H	3.54098570	7.01913356	-3.06013464
C	2.35061671	2.35060946	-0.69823615	H	5.12720820	5.12730657	-5.72615224
C	4.24612643	-0.67112119	0.25286485	H	3.47354371	4.72444597	-5.23515096
C	5.44083304	-1.33487267	0.48025890	H	4.72392296	3.47373185	-5.23517017
C	6.66906683	0.67861695	-0.23797091	H	-5.45395547	2.35160206	0.84664027
C	3.22346025	3.22347662	-1.41229446	H	-5.45395415	-2.35147822	-0.84700466
C	5.44083288	1.33474606	-0.48062689	H	-7.91572645	-2.35337749	-0.81556080
C	2.84398421	1.05975145	-0.37041433	H	-7.91569857	2.35360536	0.81492099
C	7.91865460	1.32643635	-0.45997561	H	-10.04998429	1.17849411	0.40533554
C	3.93222583	3.93229836	-2.11498471	H	-10.04998895	-1.17817148	-0.40619265
C	7.91864720	-1.32666166	0.45934531	H	-7.01906450	-3.54122020	-3.06034427
C	9.10526304	-0.67145208	0.23129399	H	-7.05851710	-4.85550375	-1.87174636
C	9.10526452	0.67116692	-0.23204942	H	-7.42790721	-5.18542399	-3.57007017

C	6.78698085	4.59940576	-2.90147998	H	-5.18500229	-7.42797590	-3.57045684
C	4.59923542	6.78714675	-2.90155358	H	-4.85564011	-7.05889377	-1.87195375
C	4.53056233	4.53080077	-5.02634877	H	-3.54098570	-7.01913356	-3.06013464
Si	-4.96298313	-4.96314010	-3.23979396	H	-5.12720820	-5.12730657	-5.72615224
N	-2.05604324	-0.00000366	0.00002762	H	-3.47354371	-4.72444597	-5.23515096
C	-2.84399057	1.05976840	0.37036826	H	-4.72392296	-3.47373185	-5.23517017
C	-4.24611724	-0.67103933	-0.25311297	H	-2.35160206	-5.45395547	-0.84664027
C	-6.66906683	0.67879090	0.23747176	H	2.35147822	-5.45395415	0.84700466
C	-2.35061671	-2.35060946	-0.69823615	H	2.35337749	-7.91572645	0.81556080
C	-4.24612643	0.67112119	0.25286485	H	-2.35360536	-7.91569857	-0.81492099
C	-5.44083304	1.33487267	0.48025890	H	-1.17849411	-10.04998429	-0.40533554
C	-6.66906683	-0.67861695	-0.23797091	H	1.17817148	-10.04998895	0.40619265
C	-3.22346025	-3.22347662	-1.41229446	H	4.85550375	-7.05851710	1.87174636
C	-5.44083288	-1.33474606	-0.48062689	H	3.54122020	-7.01906450	3.06034427
C	-2.84398421	-1.05975145	-0.37041433	H	5.18542399	-7.42790721	3.57007017
C	-7.91865460	-1.32643635	-0.45997561	H	7.42797590	-5.18500229	3.57045684
C	-3.93222583	-3.93229836	-2.11498471	H	7.05889377	-4.85564011	1.87195375
C	-7.91864720	1.32666166	0.45934531	H	7.01913356	-3.54098570	3.06013464
C	-9.10526304	0.67145208	0.23129399	H	5.12730657	-5.12720820	5.72615224
C	-9.10526452	-0.67116692	-0.23204942	H	4.72444597	-3.47354371	5.23515096
C	-6.78698085	-4.59940576	-2.90147998	H	3.47373185	-4.72392296	5.23517017
C	-4.59923542	-6.78714675	-2.90155358	C	1.33474606	-5.44083288	0.48062689
C	-4.53056233	-4.53080077	-5.02634877	C	1.05975145	-2.84398421	0.37041433
Si	4.96314010	-4.96298313	3.23979396	C	1.32643635	-7.91865460	0.45997561
N	0.00000366	-2.05604324	-0.00002762	C	3.93229836	-3.93222583	2.11498471
C	-1.05976840	-2.84399057	-0.37036826	C	-1.32666166	-7.91864720	-0.45934531
C	0.67103933	-4.24611724	0.25311297	C	-0.67145208	-9.10526304	-0.23129399
C	-0.67879090	-6.66906683	-0.23747176	C	0.67116692	-9.10526452	0.23204942
C	2.35060946	-2.35061671	0.69823615	C	4.59940576	-6.78698085	2.90147998
C	-0.67112119	-4.24612643	-0.25286485	C	6.78714675	-4.59923542	2.90155358
C	-1.33487267	-5.44083304	-0.48025890	C	4.53080077	-4.53056233	5.02634877
C	0.67861695	-6.66906683	0.23797091	H	2.35160206	5.45395547	-0.84664027
C	3.22347662	-3.22346025	1.41229446				

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