Electronic Supplementary Information for

γ-Cyclodextrin-based [2]rotaxane stoppered with gold(I)-ethynyl complexation: phosphorescent sensing for nitroaromatics

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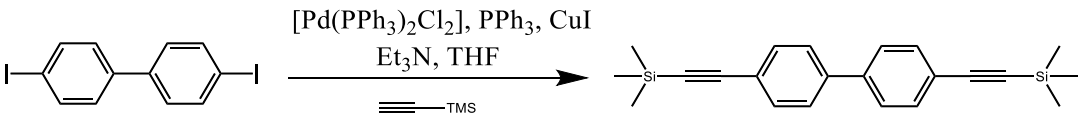
Content

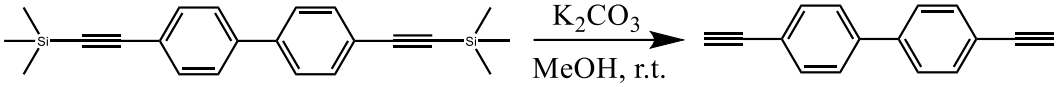
1. Materials and methods

All reagents were purchased commercially and used without further purification unless otherwise noted. The solvents used for synthesis were of analytical grade. 4,4'-bis[(trimethylsilyl)ethynyl]-1,1'-biphenyl, [1] (tppts)AuCl (tppts = sodium triphenylphosphine-3,3',3''-trisulfonate,[2] and **Au-Axle**[3] were prepared according to literature procedures. ^{1}H and ^{13}C NMR spectra were recorded at room temperature on a Bruker AMX-400 (operating at 400 MHz for ^{1}H NMR and 101 MHz for ^{13}C NMR). HRMS data were measured with a Waters-Q-TOF Premiers (ESI) or a MALDI-TOF-MS spectrometer. UV-vis spectra were recorded by using a JASCO V650 spectrometer. Circular dichroism spectra were measured on a JASCO J-1500 spectrometer. Emission spectra were taken on a JASCO FP-8500 spectrofluorometer, and the bandwidth for the measurement was not fixed. Fluorescence and phosphorescence lifetime decay were taken on the Fluoromax-4 spectrofluorometer. The phosphorescence spectra were measured by bubbling Ar gas over 10 min in an ice bath to remove dissolved oxygen. The density functional theory (DFT) calculations were used for optimization of the ground state geometries at the B3LYP[4] functional and the SDD basis set. All the calculations were performed with Gaussian 09W.[5,6]

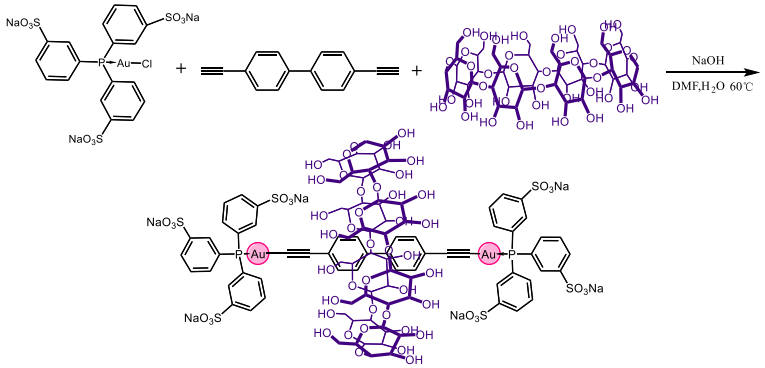
2. Synthesis and characterizations of Au-γ-Rot:



4,4'-Bis(2-trimethylsilylethynyl)biphenyl: 4,4'-diiodo-1,1'-biphenyl (2.5 g, 6.2 mmol), [Pd $(PPh_3)_2Cl_2$] (0.22 g, 0.31 mmol), CuI (0.06g, 0.31 mmol), PPh_3 (0.05 g, 0.19 mmol), and a solvent mixture of Et_3N/THF (50/100 mL) were added to a two-necked round-bottom flask (500 mL) in the atmosphere of nitrogen. After the mixture were completely dissolved, (trimethylsilyl)acetylene (2.61 mL, 18.5 mmol) was injected into the flask and the mixture was stirred at 70 ℃ for 15 h. After filtrating and washing with diethyl ether, the solvent was removed under reduced pressure and the crude product was purified by column chromatography to give a offwhite solid (1.9 g, yield: 89%). ^{1}H NMR (400 MHz, DMSO-d_6) δ= 7.71 (d, J = 8.4 Hz, 4H), 7.54 (d, J = 8.5 Hz, 4H), 0.24 (s, 18H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 139.6, 132.8, 127.2, 122.1, 105.3, 95.8, 0.4. HRMS (ESI): calcd for $[M + H]^+$, m/z =203.0855, found m/z =203.0869.



4,4'-diethynyl-1,1'-biphenyl: 4,4'-bis[(trimethylsilyl)ethynyl]-1,1'-biphenyl (300 mg, 0.87 mmol) was dissolved 15.0 mL in MeOH, and potassium carbonate (607 mg, 5 eq) was added. The reaction mixture was stirred at room temperature for 5 h and then added with 50 mL dichloromethane. The solutions was filtered and the volume of the filtrate was reduced in vacuum, and the crude product was purified by column chromatography to give a white solid (165 mg, yield: 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ= 7.58-7.54 (m, 8H), 3.15 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.5, 132.7, 126.9, 121.5, 83.4, 78.1. HRMS (ESI): calcd for $[M + H]^+$, m/z =347.1646, found m/z = 347.1639.



Au-γ-Rot: 4,4'-diethynyl-1,1'-biphenyl (6 mg, 0.03 mmol) was dissolved in DMF (3.0 mL). γ-CD (194 mg, 5 eq) was added under stirring. After the mixture was stirred at 50 ℃ for 2 h, (tppts)AuCl (48 mg, 2 eq) and a mixture of 0.5 mL H_2O and NaOH (10 mg) were then added. The reaction mixture was stirred at 60 ℃ for additional 24 h. The crude product was subjected to reversed-phase flash column chromatography(cosmosil 75C_{18}-PREP) with a gradient elution from 0% aqueous ethanol to 35% aqueous ethanol to afford **Au-γ-Rot** (35 mg, yield: 39 %) as a white solid. ^{1}H NMR (400 MHz, D_2O) δ = 7.78 (dd, J = 15.3, 9.7 Hz, 12H), 7.57 (dd, J = 13.5, 7.8 Hz, 6H), 7.39 (t, J = 7.7 Hz, 6H), 7.12 (d, J = 8.0 Hz, 4H), 6.97 (d, J = 8.2 Hz, 4H), 4.88 (s, 8H), 3.92 (dd, J = 21.2, 10.4 Hz, 16H), 3.73 (d, J = 11.2 Hz, 8H), 3.48 (ddd, J = 42.0, 21.0, 11.2 Hz, 26H). ^{13}C NMR (101 MHz,

D_2O : DMSO-d_6 =1:1) δ 147.5, 145.7, 145.6, 136.3, 133.8, 133.7, 132.7, 131.3, 130.8, 130.7, 130.6, 130.5, 130.4, 130.23 130.2, 130.1, 128.4, 128.2, 126.9, 101.9, 80.9, 72.9, 72.4, 72.0, 60.2, 60.1. ^{31}P NMR (D_2O) : δ =36.04, 27.07. MALDI-TOF-HRMS: calcd for $[M - 5Na^+ + K^+]^{4-}$, m/z =737.5625, found m/z =737.1051.

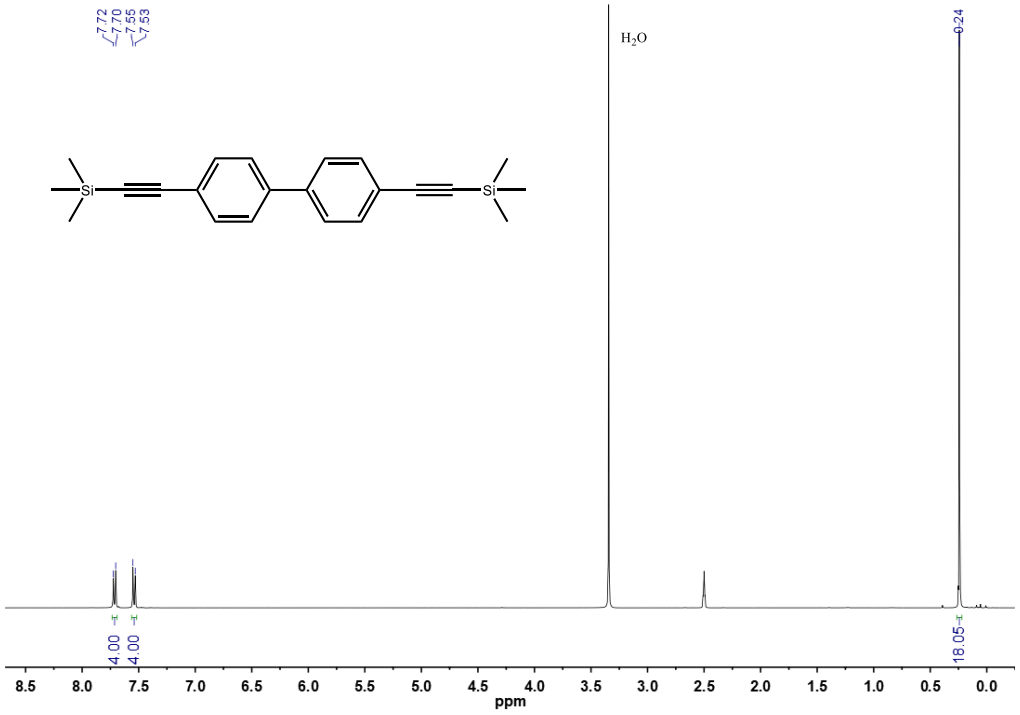


Figure S1. ^{1}H NMR spectrum of 4,4'-Bis(2-trimethylsilylethynyl)biphenyl measured in DMSO-d_6 at 25 °C.

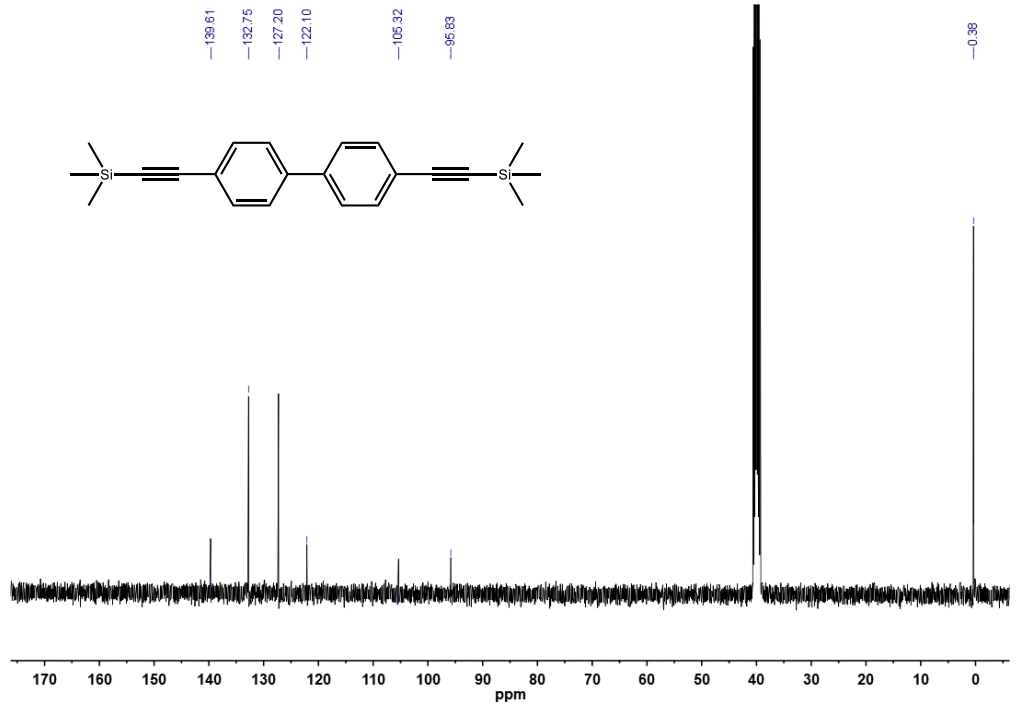


Figure S2. ^{13}C NMR spectrum of 4,4'-Bis(2-trimethylsilylethynyl)biphenyl measured in DMSO-d_6 at 25 °C

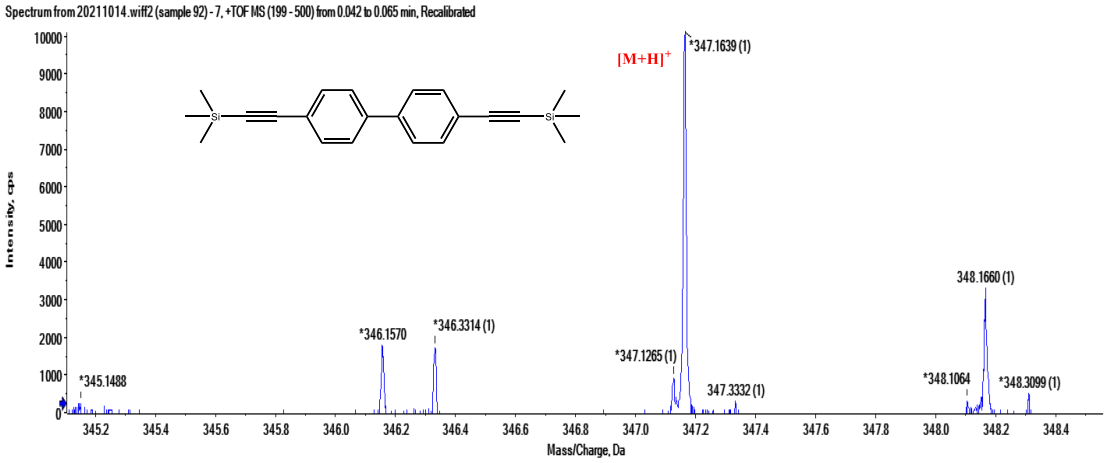


Figure S3. HRMS spectrum of 4,4'-Bis(2-trimethylsilylethynyl)biphenyl.

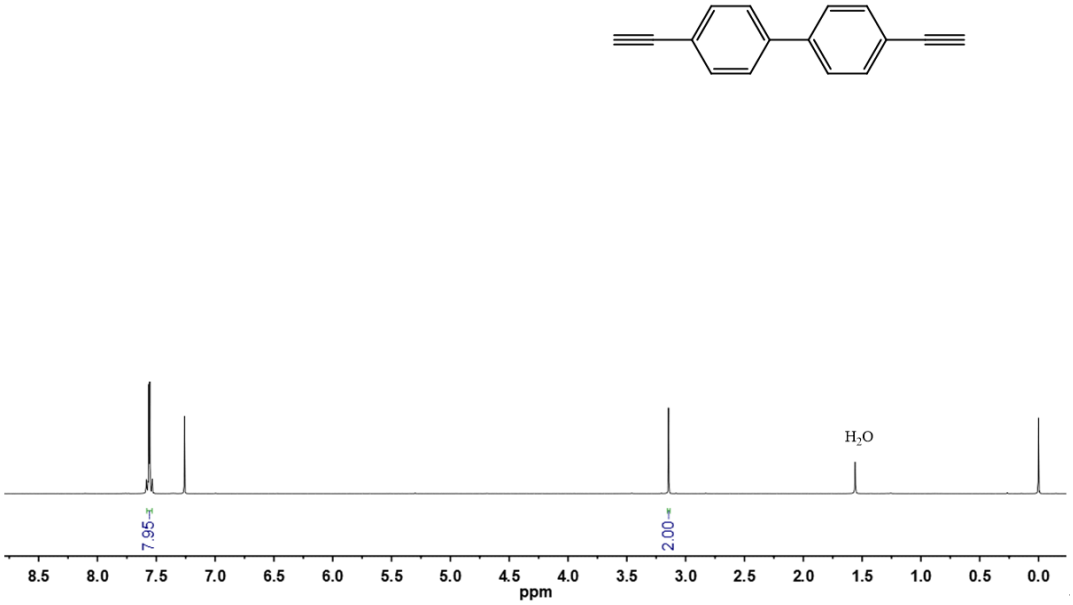


Figure S4. ^{1}H NMR spectrum of 4,4'-diethynyl-1,1'-biphenyl measured in $CDCl_3$ at 25 °C.

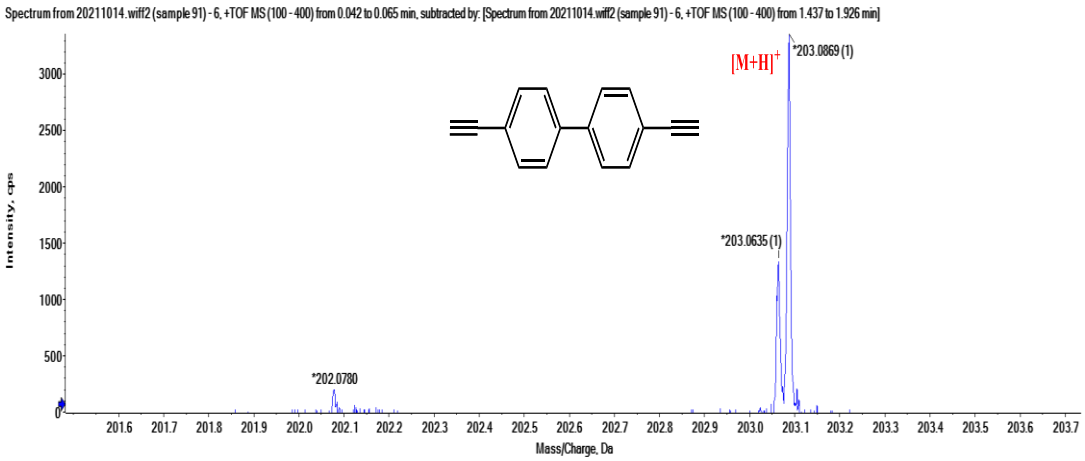


Figure S5. HRMS spectrum of 4,4'-diethynyl-1,1'-biphenyl.

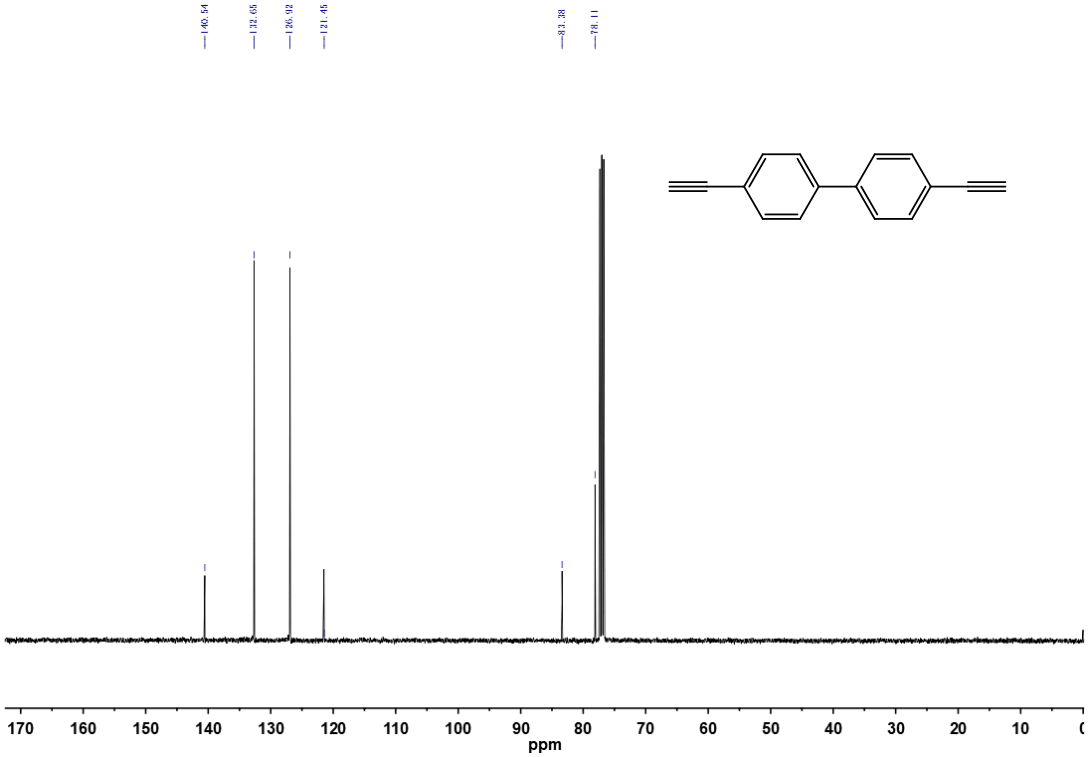


Figure S6. ^{13}C NMR spectrum of 4,4'-diethynyl-1,1'-biphenyl measured in $CDCl_3$ at 25 °C..

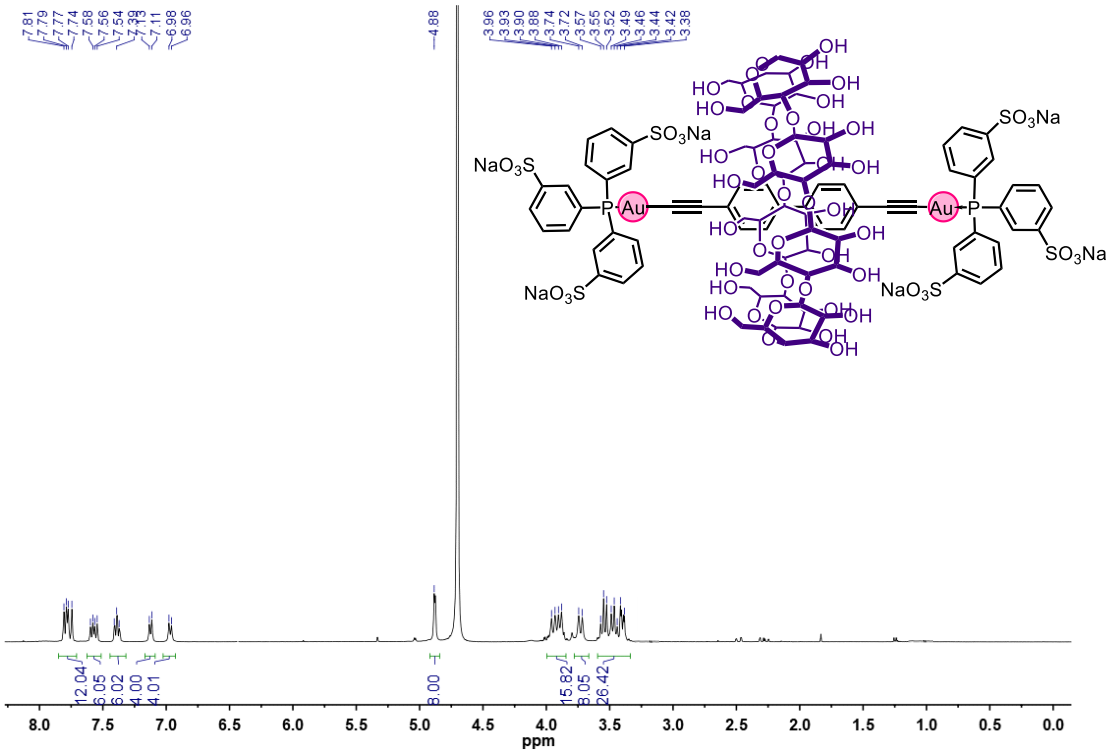


Figure S7. ^{1}H NMR spectrum of **Au-λ-Rot** measured in D_2O at 25 °C.

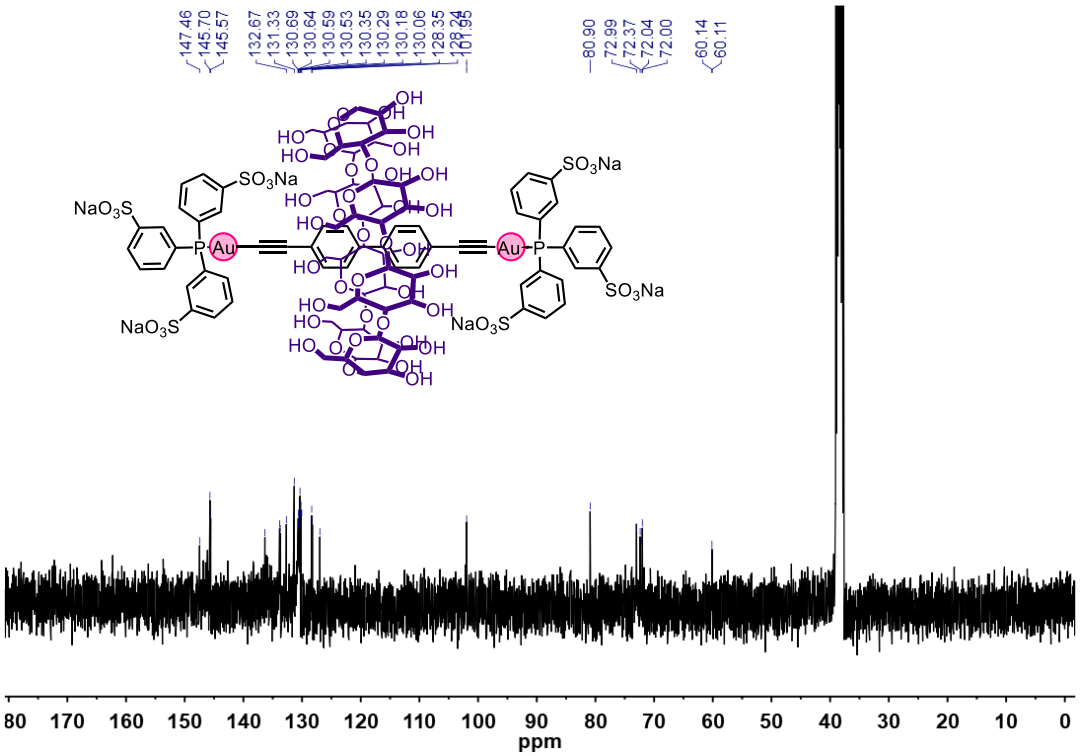


Figure S8. ^{13}C NMR spectrum of **Au-γ-Rot** measured in D_2O : DMSO-d_6 =1:1 at 25 °C.

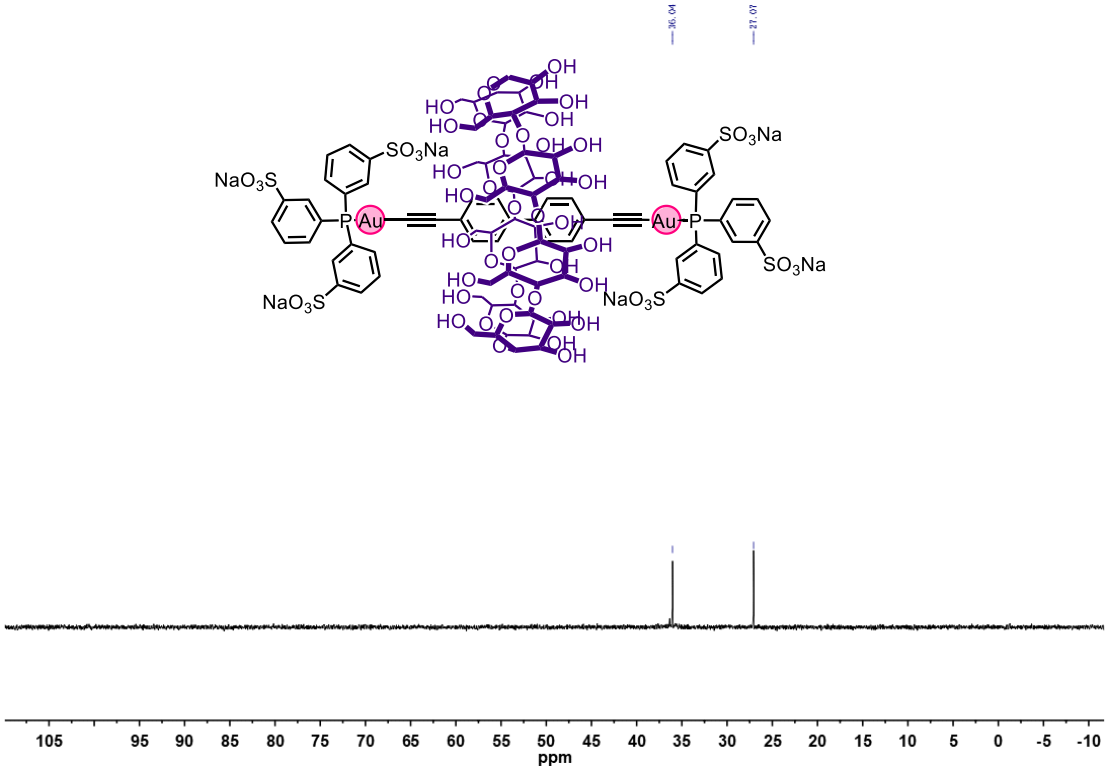


Figure S9. ^{31}P NMR spectrum of **Au-γ-Rot** measured in D_2O at 25 °C.

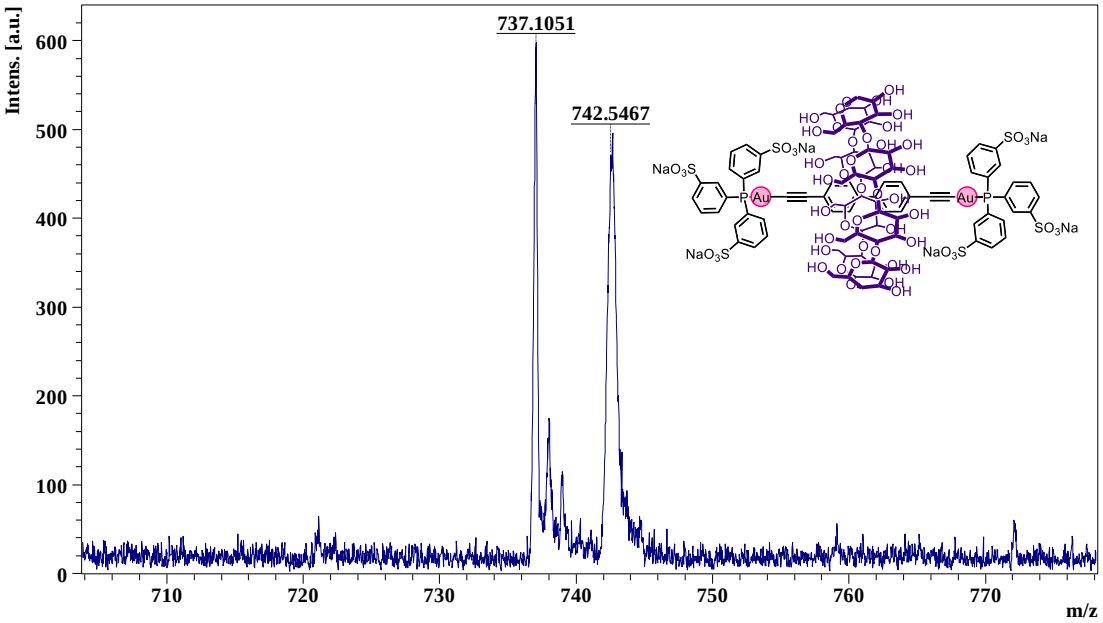


Figure S10. MALDI-TOF-HRMS spectrum of **Au-γ-Rot**.

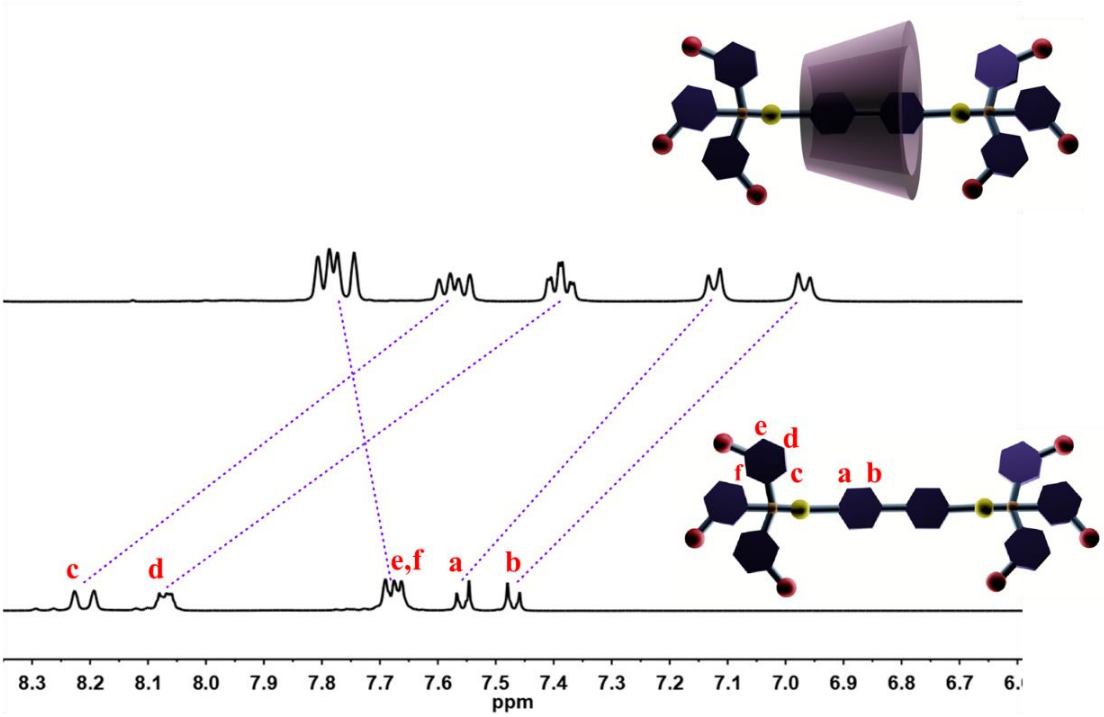


Figure S11. The partial ^{1}H NMR spectra (400 MHz) of **Au-Axle** and **Au-γ-Rot** measured in D_2O solution at 298 K.

3. Photophysical properties of Au-Axle and Au-γ-Rot

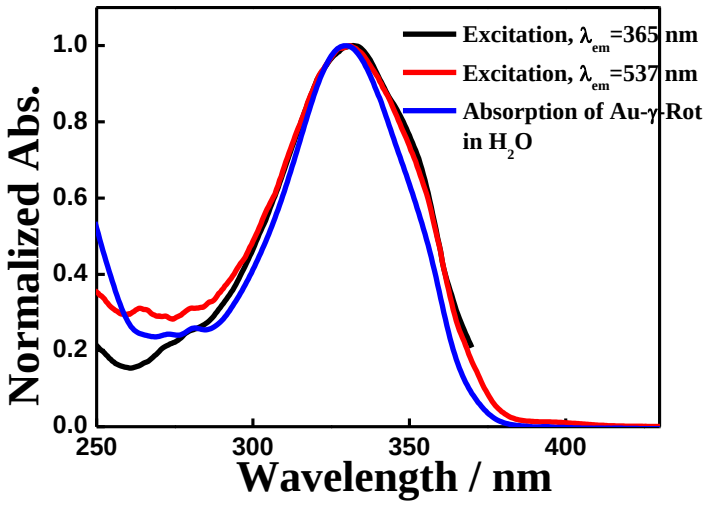


Figure S12. Normalized excited and absorption spectra of **Au-γ-Rot** in H_2O at 25 °C.

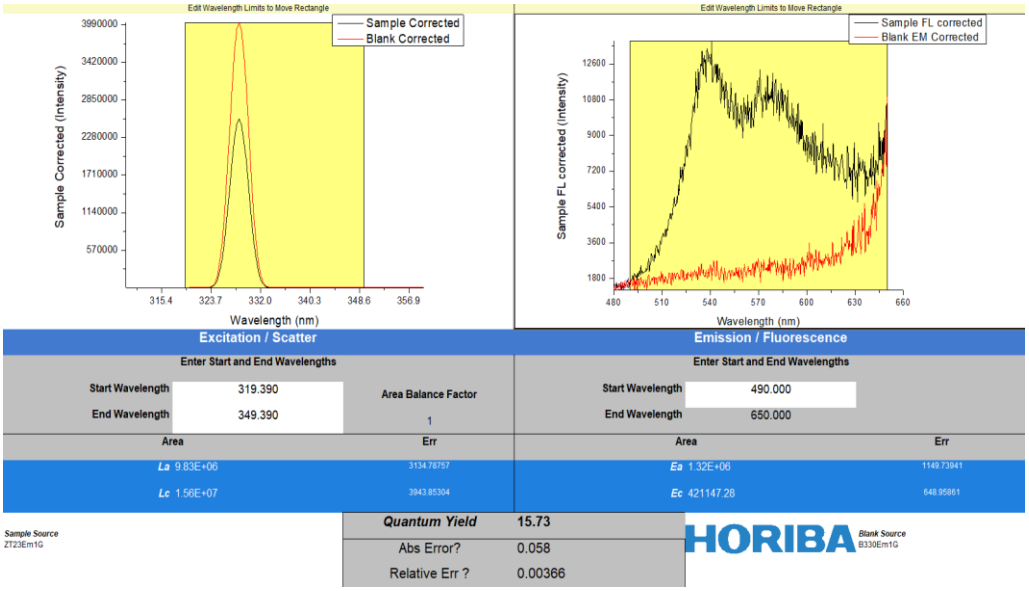


Figure S13. The absolute quantum efficiency of **Au-γ-Rot** in solid, the quantum efficiency is 15.7%.

Table S1. Photophysical properties of the axle and rotaxanes[a]

Comp.	λ_{Abs}/nm	λ_{FL}/nm	$\lambda_P{}^b$/nm	$\lambda_P{}^c$/nm	$\Phi_P{}^c$ /%	Φ_{FL} /%	$\Phi_P{}^d$ /%	τ_{FL}/ns	$\tau_P{}^b$/μs	$\tau_P{}^c$/μs
Au-Axle	341	364 380		541 571	2.90	2.08	7.88	0.22		260.7
Au-γ-Rot	330	366 384	537 571	537 570	5.12	2.40	15.7	0.96	22.7	318.5

[a]All photophysical data were measured in water at 25 °C. [b]Data were measured under aerated conditions. [c]Data were measured under deaerated conditions. [d]RTP quantum yields were measured in solid state.

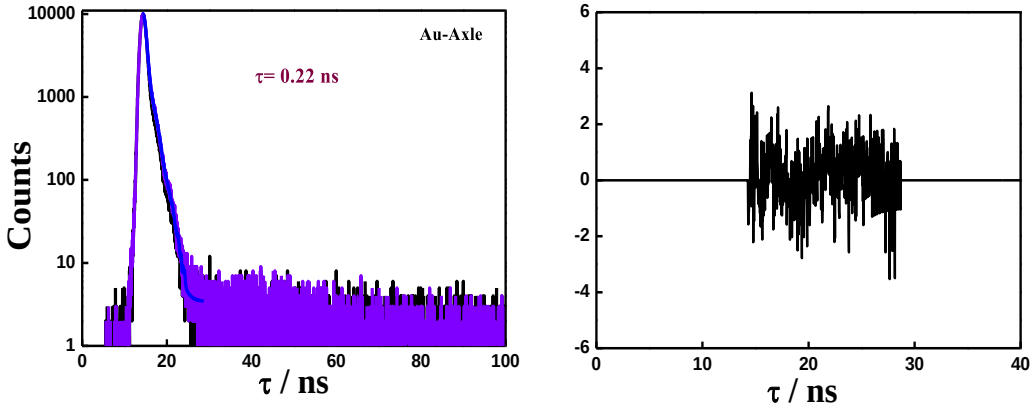


Figure S14. The fluorescence lifetime decay curves of **Au-Axle** in H_2O at 25 ℃, λ_{ex} = 280 nm (Nano LED), λ_{em} =380 nm.

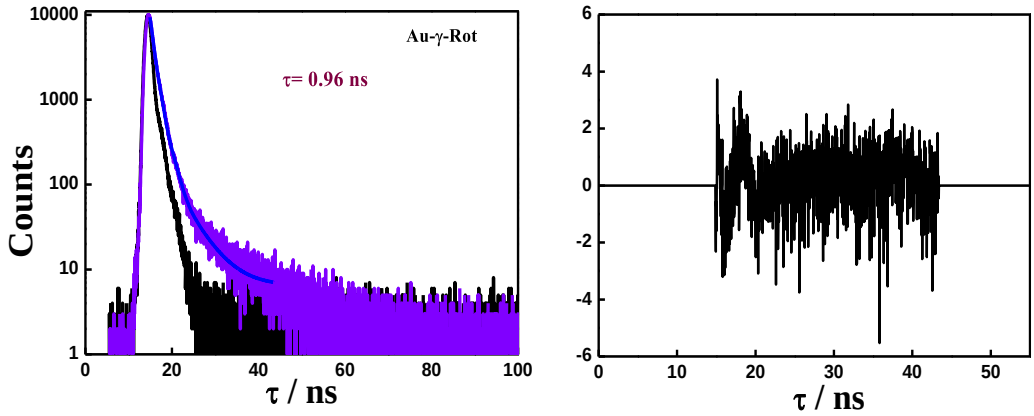


Figure S15. The fluorescence lifetime decay curves of **Au-γ-Rot** in H_2O at 25 ℃, λ_{ex} = 280 nm (Nano LED), λ_{em} =384 nm.

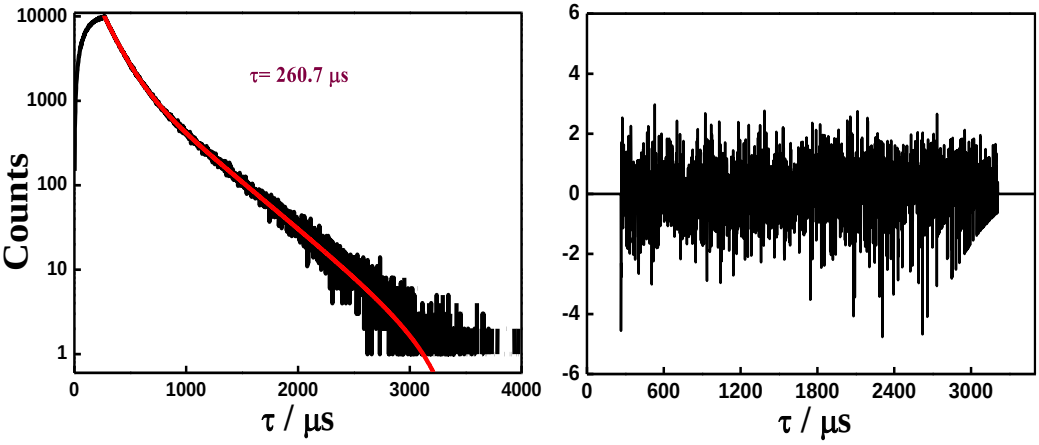


Figure S16. The phosphorescence lifetime decay curves of **Au-Axle** in deaerated H_2O at 25 ℃, λ_{ex} = 280 nm (Spectra LED), λ_{em} =541 nm.

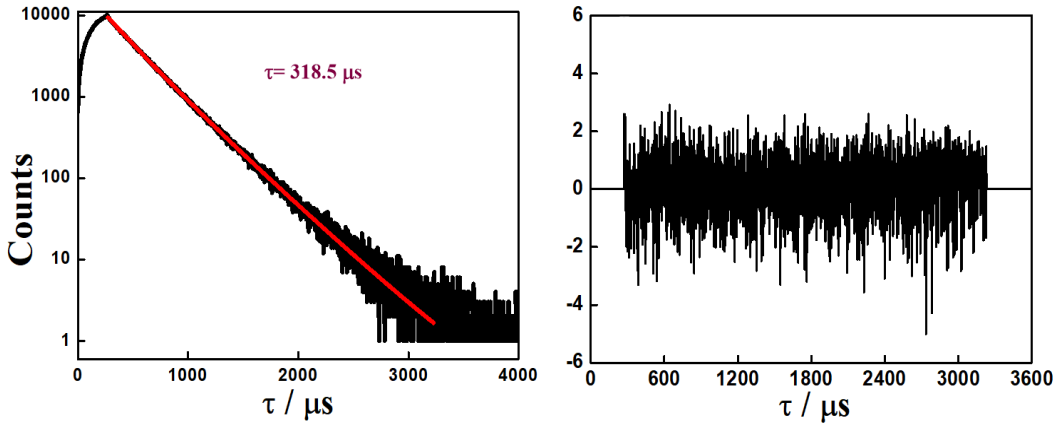


Figure S17. The phosphorescence lifetime decay curves of **Au-γ-Rot** in deaerated H_2O at 25 °C, λ_{ex} = 280 nm (Spectra LED), λ_{em} =537 nm.

4. The host-guest interactions between Au-γ-Rot and nitroaromatics

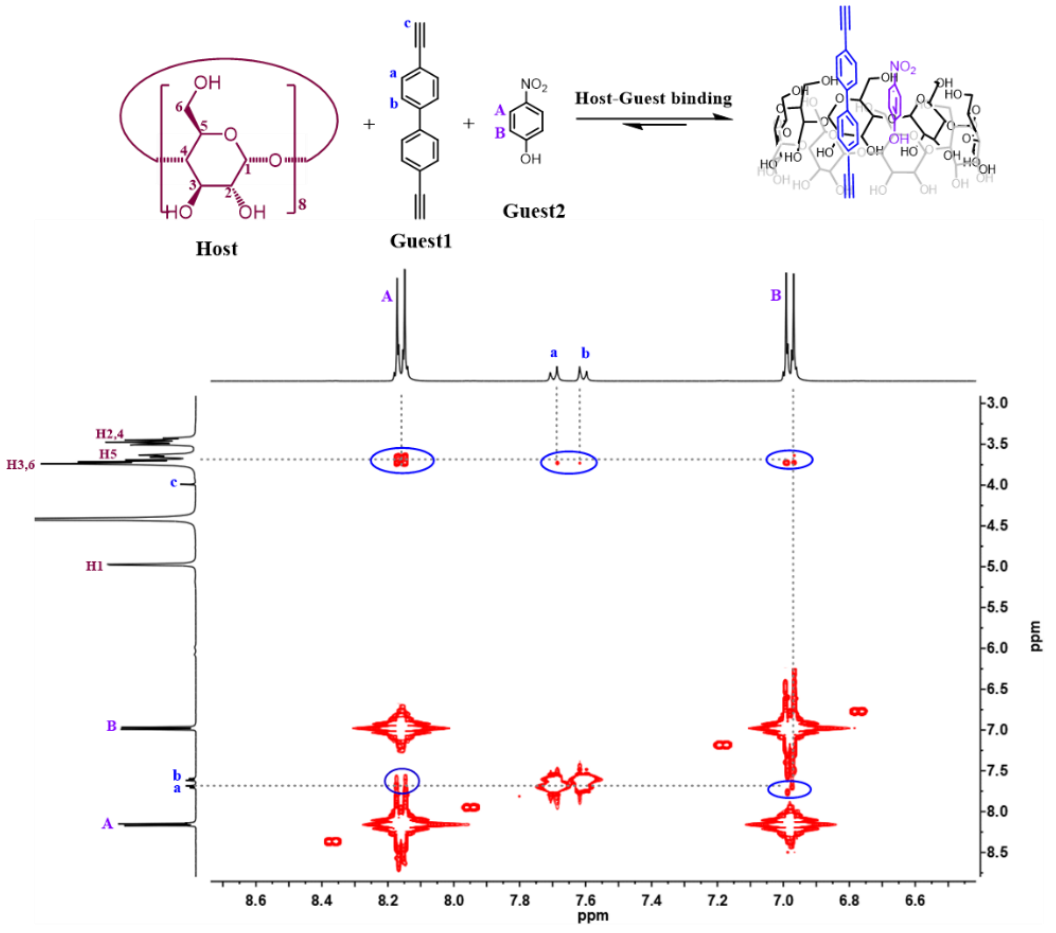


Figure S18. Partial NOESY spectra (400 MHz) of γ-CD, diethynylbiphenyl and *p*-NP in DMSO-d_6 / D_2O(50/50) at 25 °C.

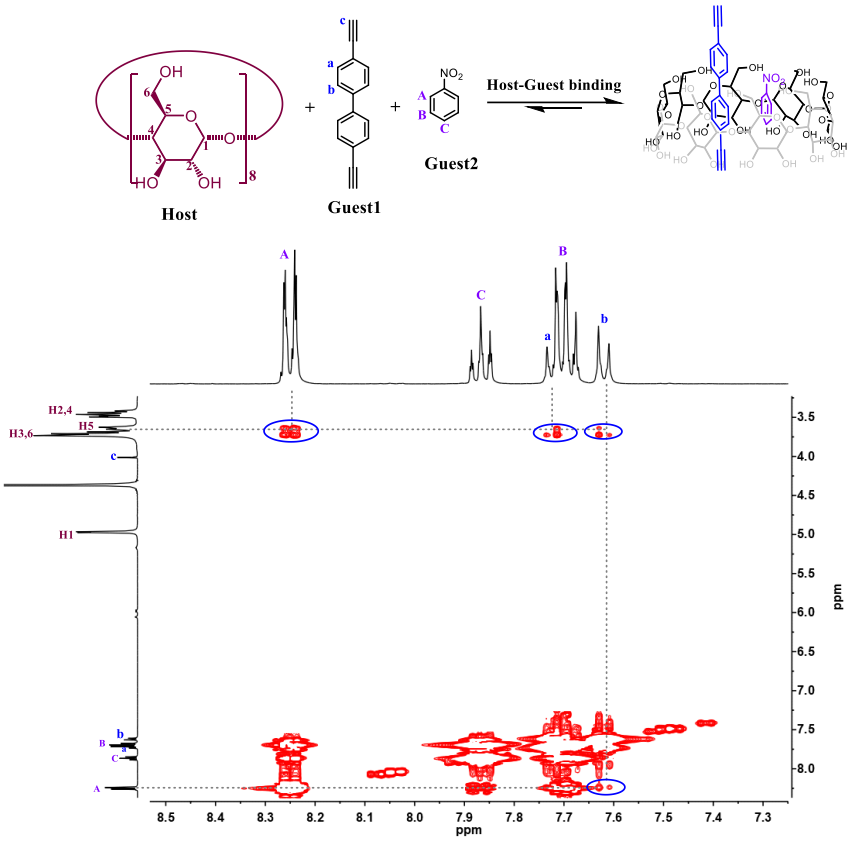


Figure S19. Partial NOESY spectra (400 MHz) of γ-CD, diethynylbiphenyl and NB in DMSO-d_6 / D_2O(50/50) at 25 °C.

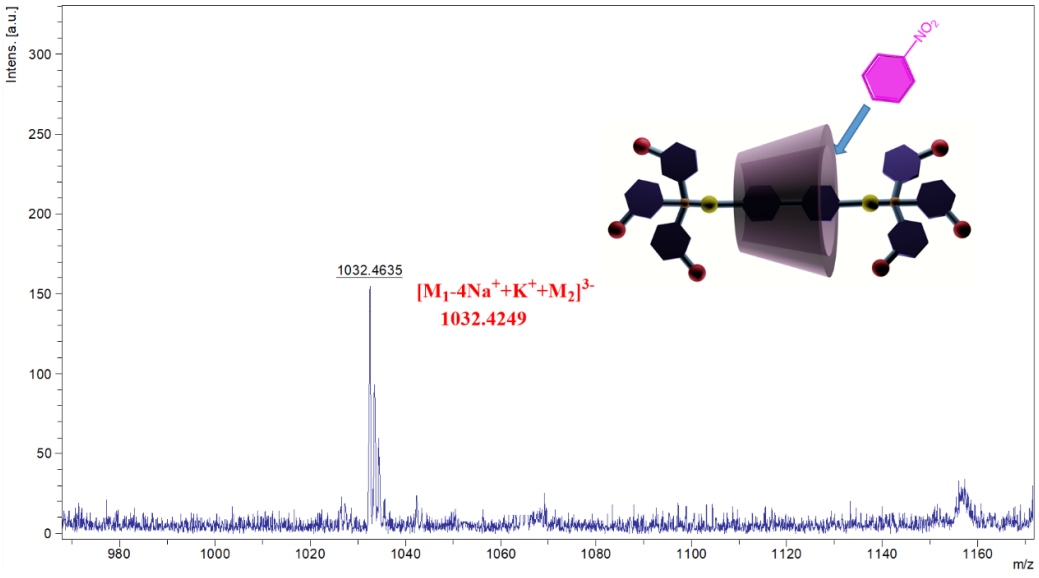


Figure S20. MALDI-TOF-HRMS spectrum of NB ⊂**Au-γ-Rot**, the M_1 represents **Au-γ-Rot**, the M_2 represents NB.

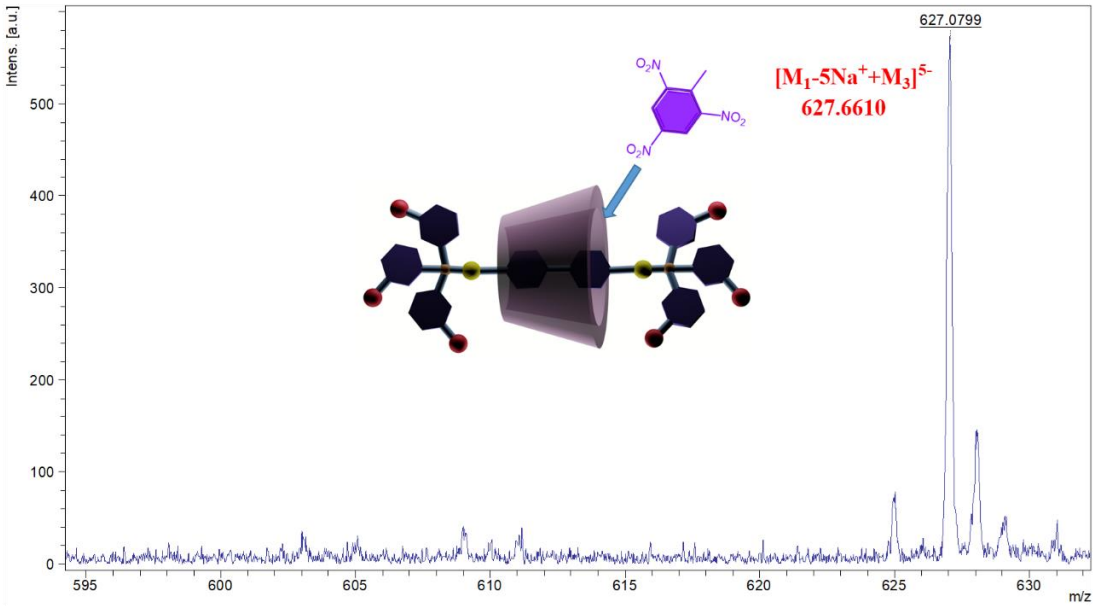


Figure S21. MALDI-TOF-HRMS spectrum of TNT ⊂**Au-γ-Rot**, the M_1 represents **Au-γ-Rot**, the M_3 represents TNT.

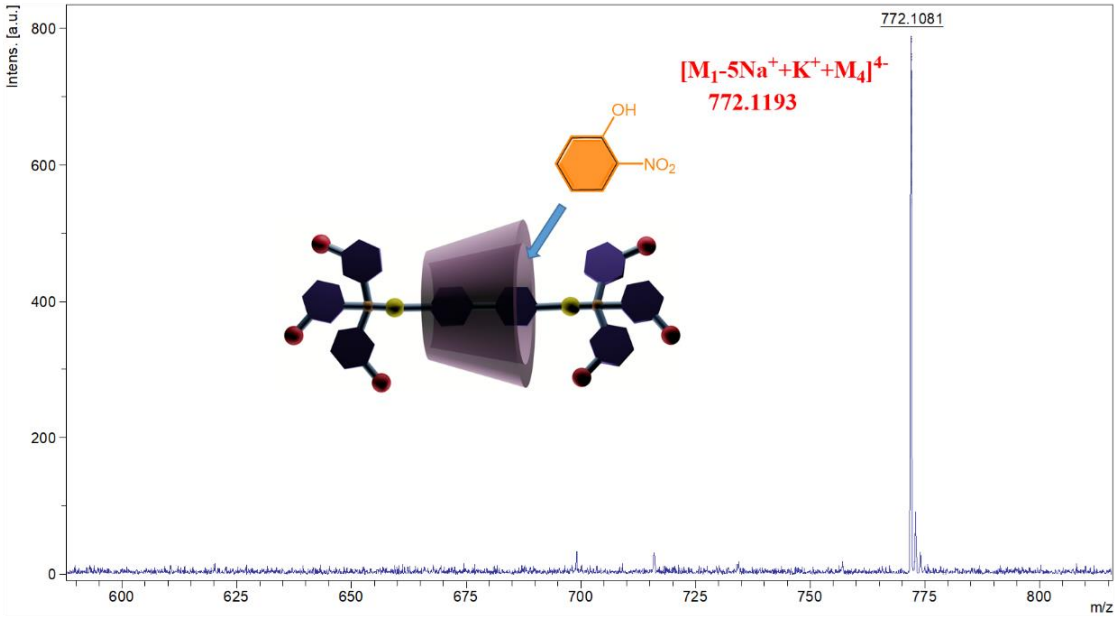


Figure S22. MALDI-TOF-HRMS spectrum of *o*-NP ⊂**Au-γ-Rot**, the M_1 represents **Au-γ-Rot**, the M_4 represents *o*-NP.

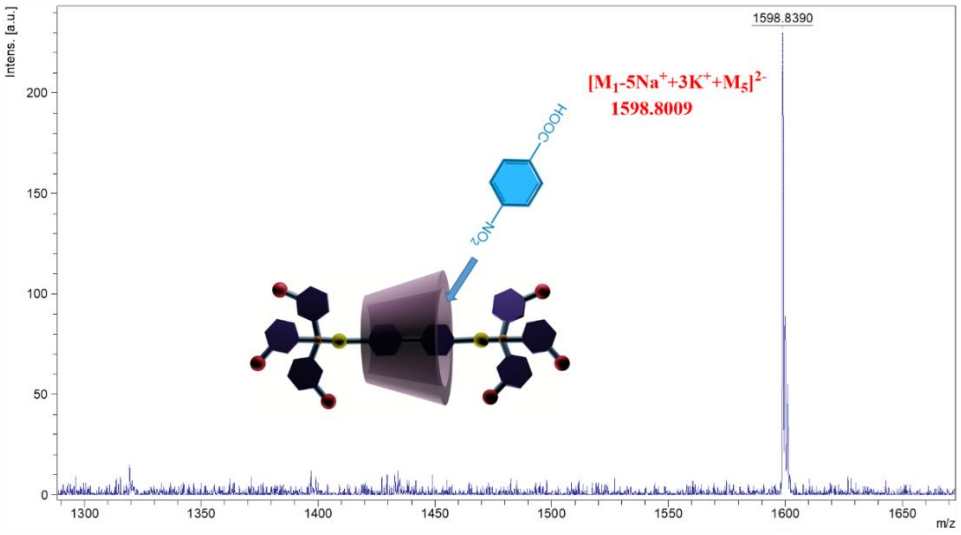


Figure S23. MALDI-TOF-HRMS spectrum of *p*-NBA ⊂**Au-γ-Rot**, the M_1 represents **Au-γ-Rot**, the M_5 represents *p*-NBA.

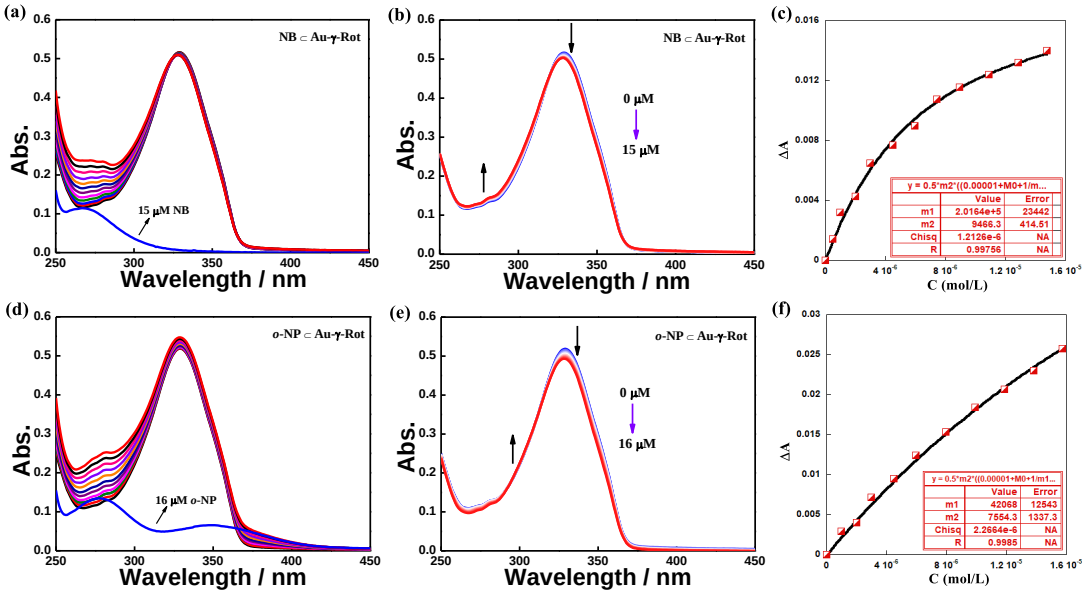


Figure S24. UV-Vis spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of NB (a) and *o*-NP (d), mixed solution of nitroaromatics and **Au-γ-Rot** after deducting the inherent absorption of NB (b) and *o*-NP (e) in aerated H_2O at 25 ℃. Nitroaromatic analytes were dissolved in DMF mother solution. Nonlinear curve fitting (UV titrations) for the complexation of NB with **Au-γ-Rot** (c, 329 nm) and *o*-NP with **Au-γ-Rot** (f, 328 nm), the association constant (K_a) for the complexes were 2.02 $\times 10^5$ M^{-1} and 4.21 $\times 10^4$ M^{-1}, respectively.

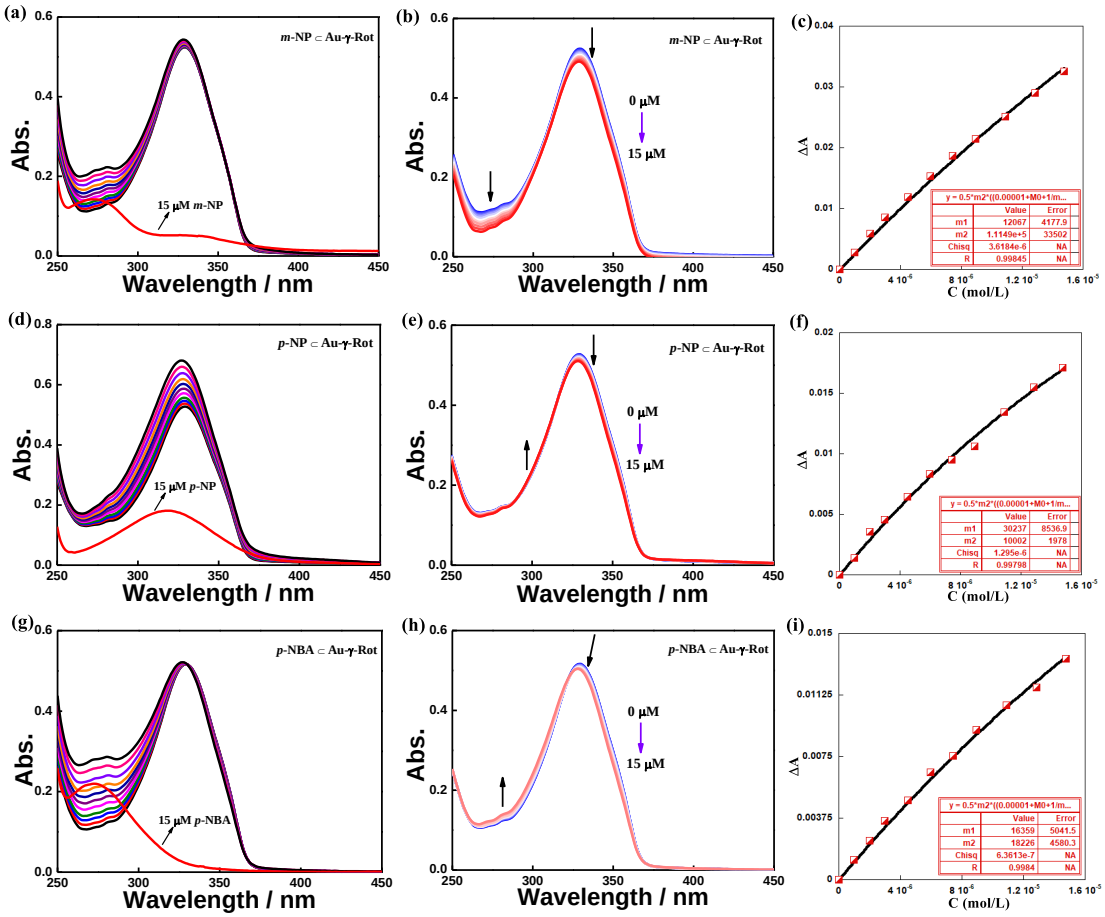


Figure S25. UV-Vis spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *m*-NP (a), *p*-NP (d) and *p*-NBA (g), mixed solution of nitroaromatics and **Au-γ-Rot** after deducting the inherent absorption of *m*-NP (b), *p*-NP (e) and *p*-NBA (h) in aerated H_2O at 25 ℃. Nitroaromatic analytes were dissolved in DMF mother solution. Nonlinear curve fitting (UV titrations) for the complexation of *m*-NP with **Au-γ-Rot** (c, 329 nm); *p*-NP with **Au-γ-Rot** (f, 328 nm) and *p*-NBA with **Au-γ-Rot** (i, 329 nm), the association constant (K_a) for the complexes were 1.11 $\times 10^4$ M^{-1}, 3.02 $\times 10^4$ M^{-1} and 1.64 $\times 10^4$ M^{-1}, respectively.

Table S2 The binding constants for **Au-γ-Rot** and various nitroaromatics through UV absorption titration [a]

	NB	TNT	*o*-NP	*m*-NP	*p*-NP	*p*-NBA
$K_a(M^{-1})$ [b]	2.02×10^5	2.21×10^5	4.21×10^4	1.11×10^4	3.02×10^4	1.64×10^4
R	0.998	0.988	0.998	0.998	0.998	0.998
λ_{Abs}(nm)	329	329	328	329	328	329

[a] All data were measured in H_2O, the concertration of **Au-γ-Rot** was 10 μM and nitroaromatic analytes were dissolved in DMF mother solution, 25°C. [b] UV titrations data of **Au-γ-Rot** complex with various nitroaromatics, association constant *K* / M^{-1}. [c] Selected wavelength values in the non-linear curve-fitting (UV titrations).

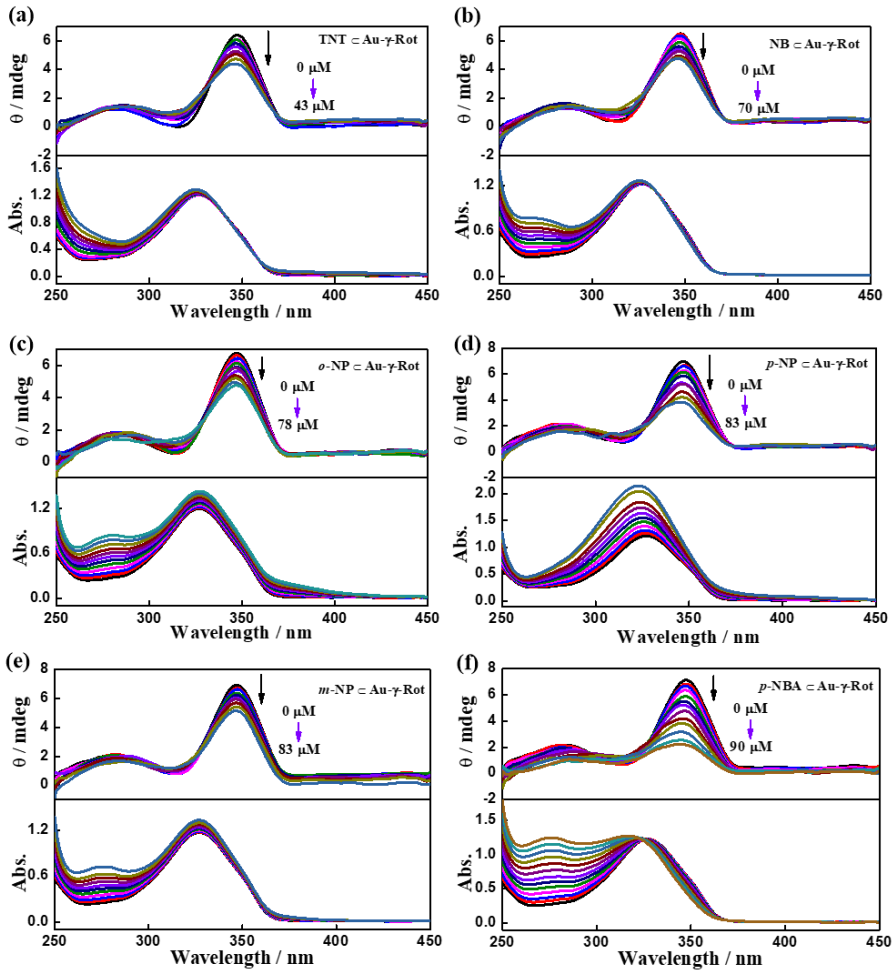


Figure S26. Circular dichroism spectra of 30 μM **Au-γ-Rot** in the presence of different concentration of TNT (a), NB (b), *o*-NP (c), *m*-NP (d), *p*-NP (e) and *p*-NBA (f) in aerated H_2O at 25 ℃. Nitroaromatic analytes were dissolved in DMF mother solution.

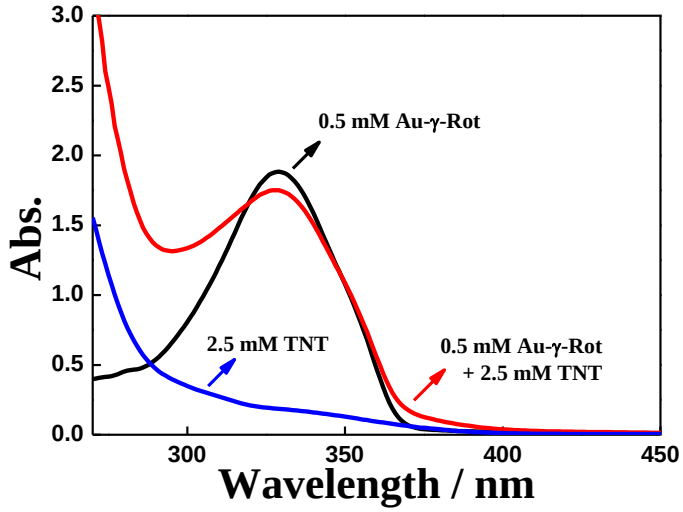


Figure S27. UV-Vis spectra of **Au-γ-Rot** (black line, 0.5 mM), TNT (blue line, 2.5 mM), 0.5 mM **Au-γ-Rot** + 2.5 mM TNT (red line) in H_2O at 25 ℃.

5. RTP of Au-γ-Rot for sensing of nitroaromatics

5.1 RTP of Au-γ-Rot for sensing of nitroaromatics in aerated H_2O

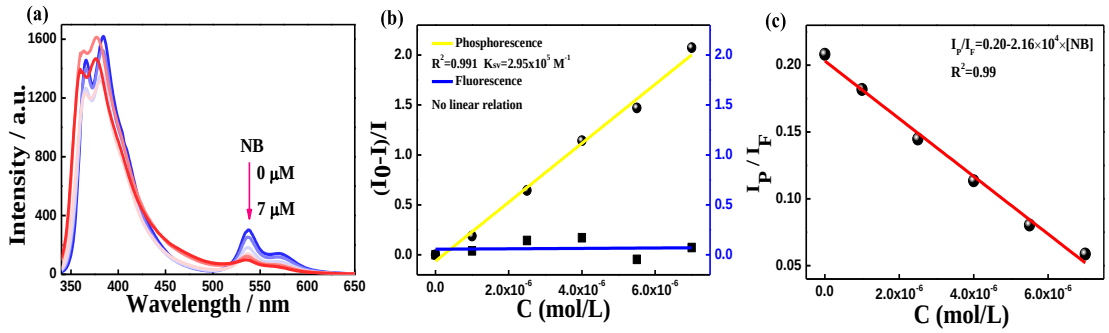


Figure S27. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of NB (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, NB dissolve in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of NB (b). Plot of phosphorescence and fluorescence intensities (I_P/I_F) versus the concentrations of NB (c).

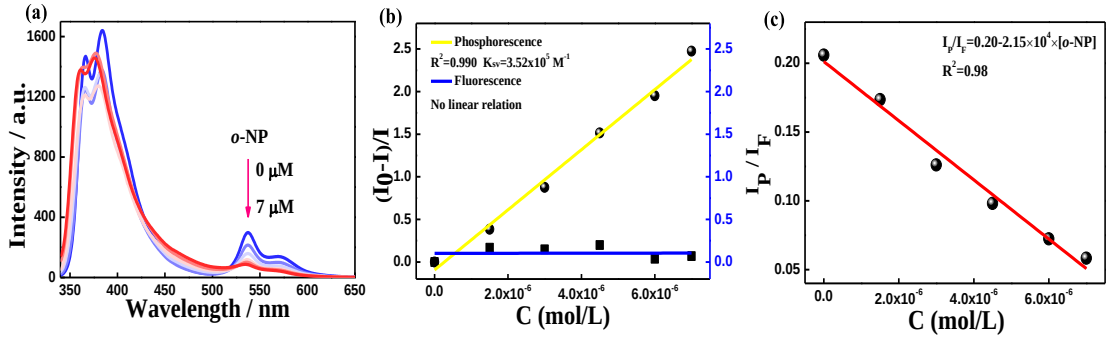


Figure S28. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *o*-NP (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, *o*-NP dissolve in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of *o*-NP (b). Plot of phosphorescence and fluorescence intensities (I_P/I_F) versus the concentrations of *o*-NP (c).

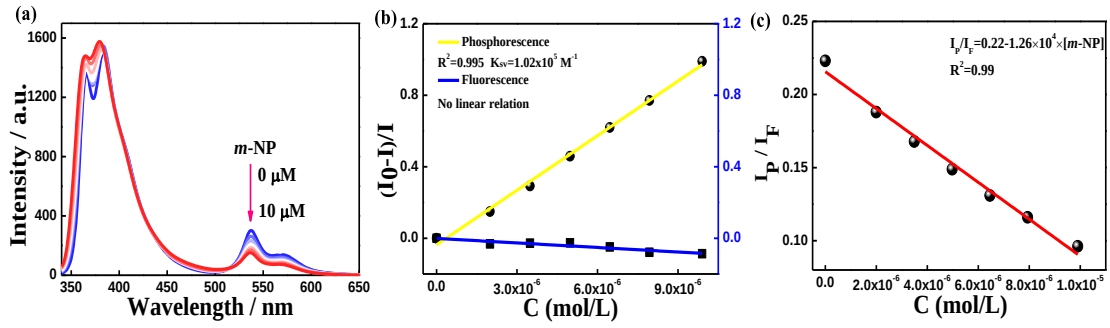


Figure S29. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *m*-NP (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, *m*-NP dissolve in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of *m*-NP (b). Plot of phosphorescence and fluorescence intensities (I_P/I_F) versus the concentrations of *m*-NP (c).

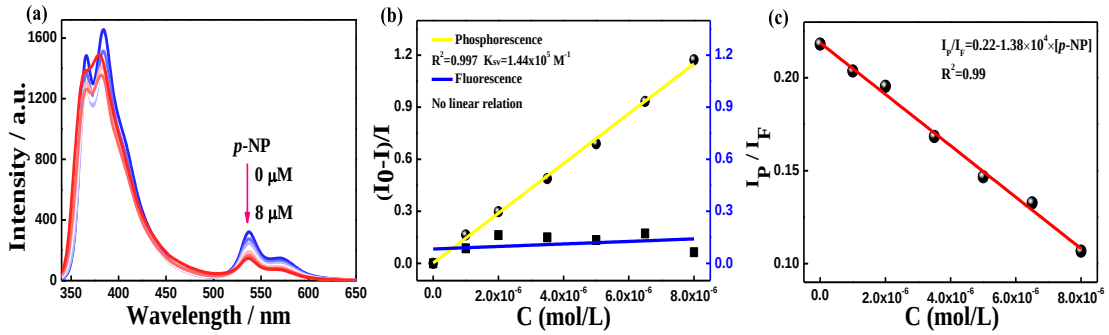


Figure S30. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *p*-NP (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, *p*-NP dissolve in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of the *p*-NP (b). Plot of phosphorescence and fluorescence intensities (I_P/I_F) versus the concentrations of *p*-NP (c).

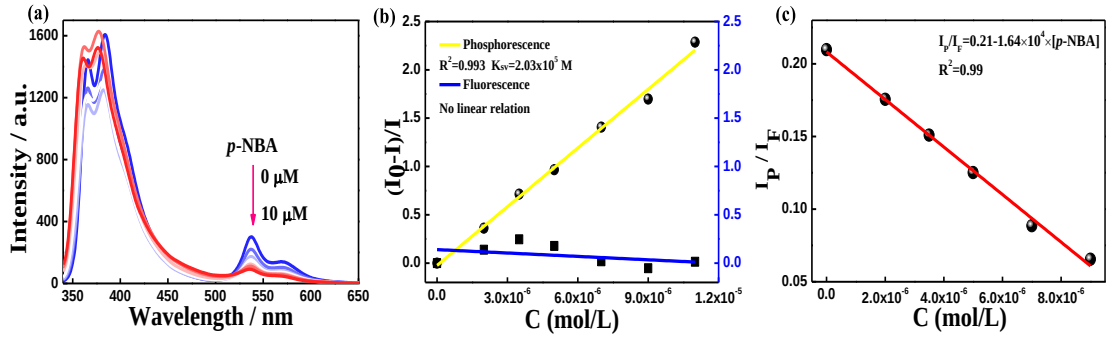


Figure S31. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *p*-NBA (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, *p*-NBA dissolve in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of *p*-NBA (b). Plot of phosphorescence and fluorescence intensities (I_P/I_F) versus the concentrations of *p*-NBA (c).

5.2 RTP of Au-γ-Rot for sensing of nitroaromatics in deaerated H_2O

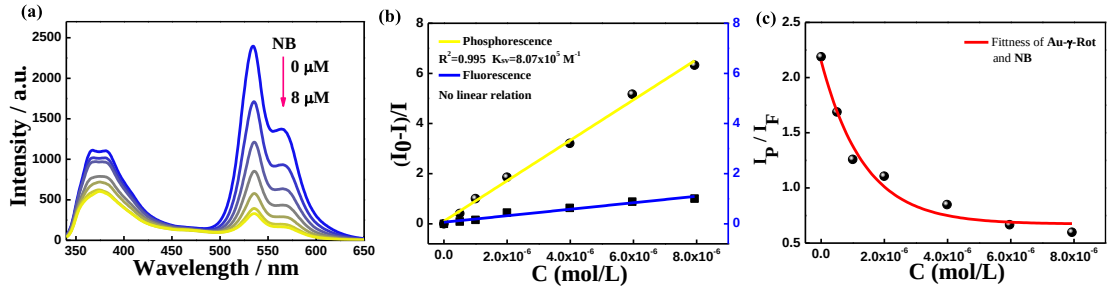


Figure S32. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of NB (a) in deaerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, NB were dissolved in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of NB (b). Plot of phosphorescence (λ_{em}=537 nm) and fluorescence (λ_{em}=365 nm) intensities (I_P/I_F) versus the concentrations of NB (c).

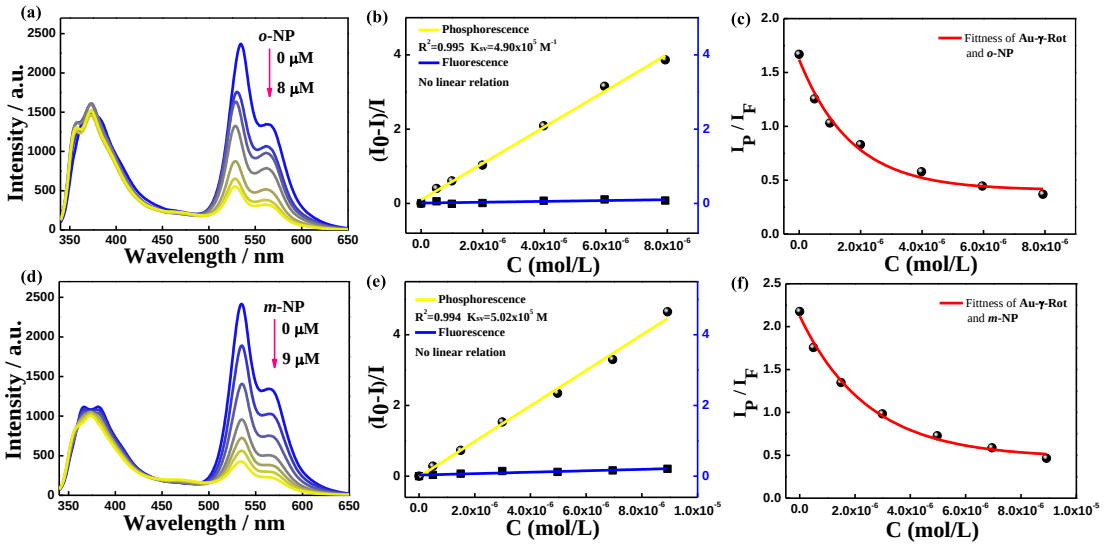


Figure S33. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *o*-NP (a) and *m*-NP (d) in deaerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, nitroaromatic analytes were dissolved in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of *o*-NP (b) and *m*-NP (e). Plot of phosphorescence (λ_{em}=537 nm) and fluorescence (λ_{em}=365 nm) intensities (I_P/I_F) versus the concentrations of *o*-NP (c) and *m*-NP (f).

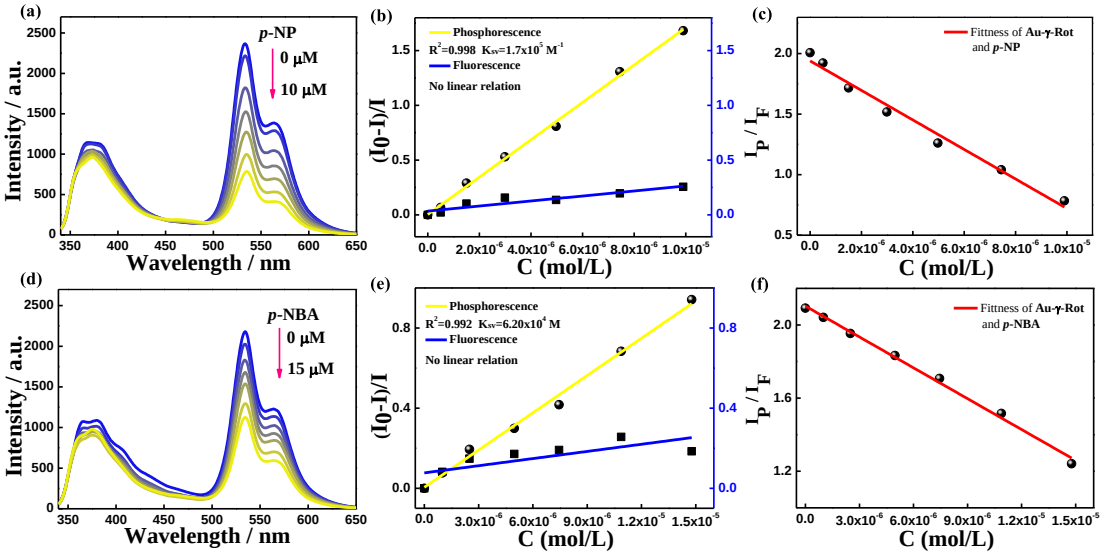


Figure S34. Emission spectra of 10 μM **Au-γ-Rot** in the presence of different concentration of *p*-NP (a) and *p*-NBA (d) in deaerated H_2O at 25 °C. λ_{ex}=330 nm in fluorescence mode, nitroaromatic analytes were dissolved in DMF mother solution. Plot of relative fluorescence (λ_{em}=365 nm) and phosphorescence (λ_{em}=537 nm) intensities (I_0/I-1) versus the concentrations of *p*-NP (b) and *p*-NBA (e). Plot of phosphorescence (λ_{em}=537 nm) and fluorescence (λ_{em}=365 nm) intensities (I_P/I_F) versus the concentrations of *p*-NP (c) and *p*-NBA (f).

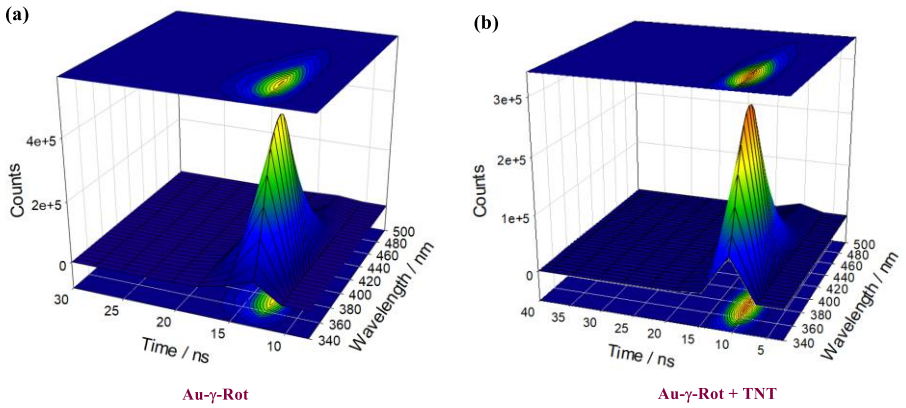


Figure S35. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and TNT⊂**Au-γ-Rot** (b) in H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of TNT was 20 μM, λ_{ex} = 280 nm (Nano LED).

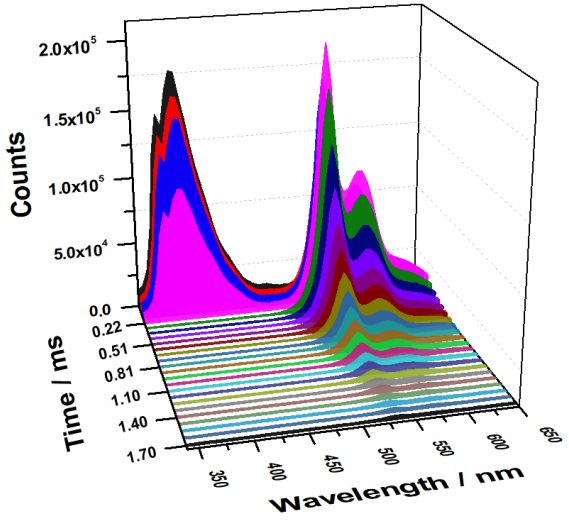


Figure S36. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM, λ_{ex} = 280 nm (Spectra LED).

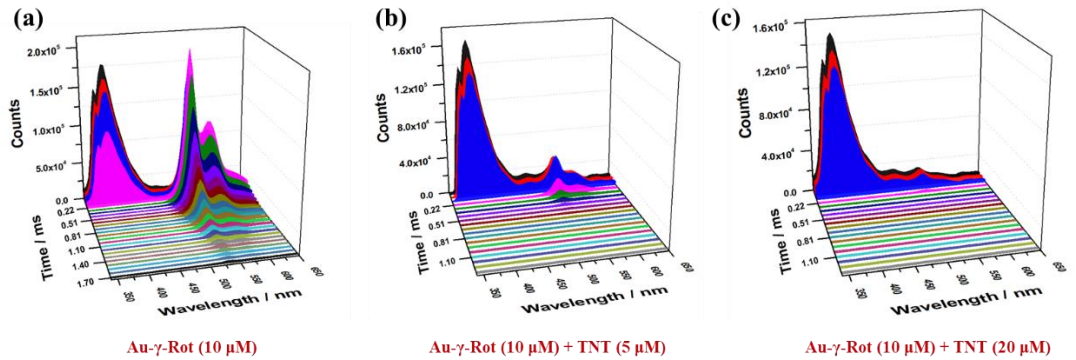


Figure S37. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and TNT⊂**Au-γ-Rot** (b,c) in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of TNT was 5 μM or 20 μM, λ_{ex} = 280 nm (Spectra LED).

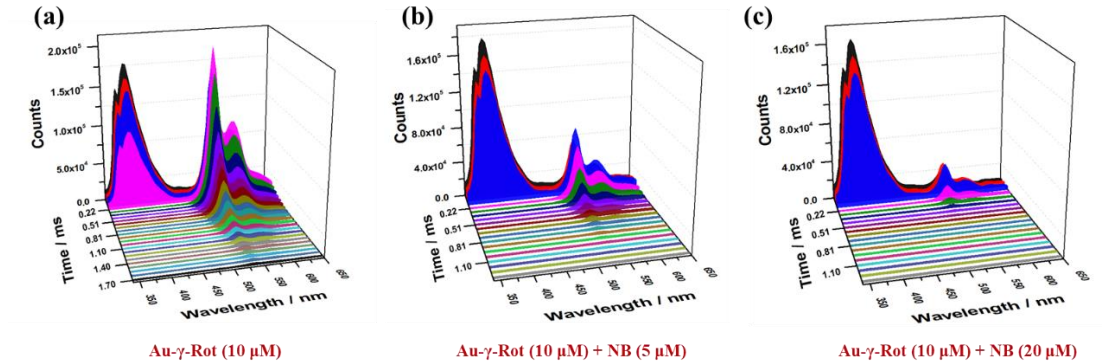


Figure S38. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and NB⊂**Au-γ-Rot** (b,c) in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of NB was 5 μM or 20 μM, λ_{ex} = 280 nm (Spectra LED).

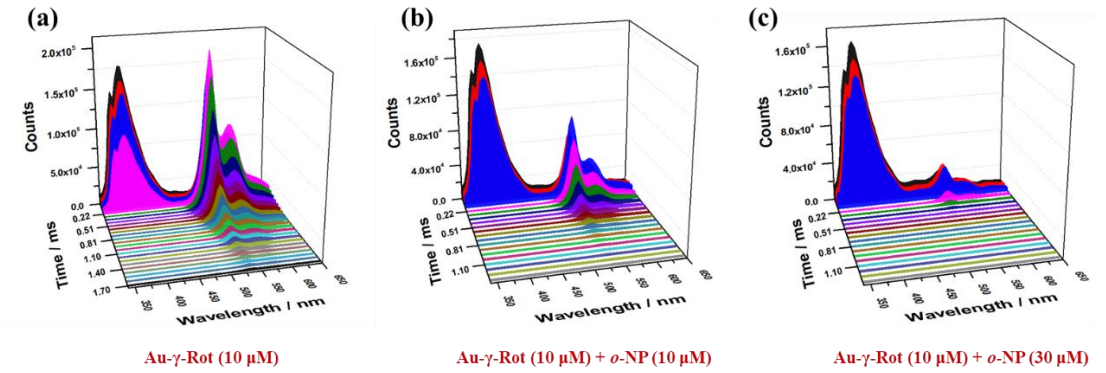


Figure S39. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and *o*-NP⊂**Au-γ-Rot** (b,c) in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of *o*-NP was 10 μM or 30 μM, λ_{ex} = 280 nm (Spectra LED).

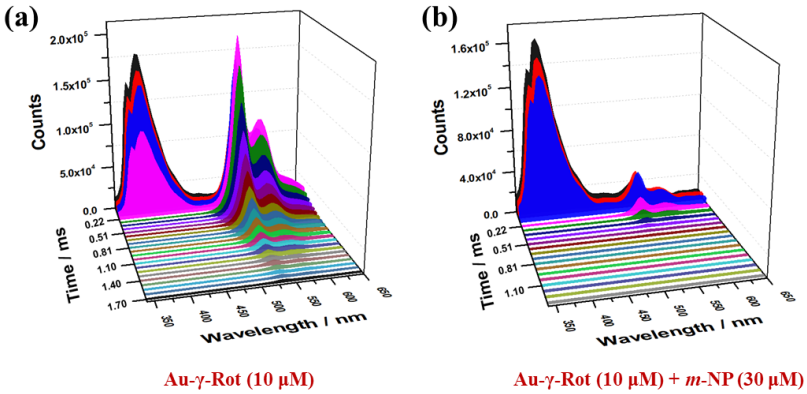


Figure S40. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and *m*-NP⊂**Au-γ-Rot** (b) in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of *m*-NP was 30 μM, λ_{ex} = 280 nm (Spectra LED).

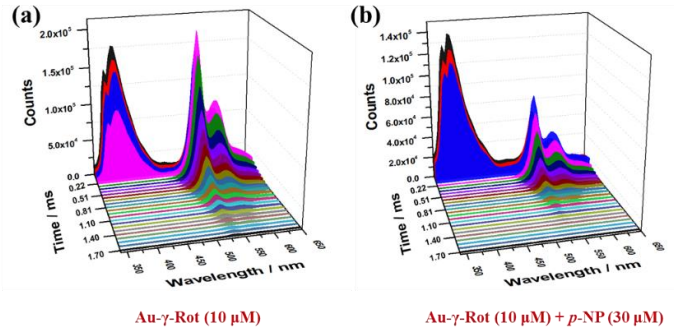
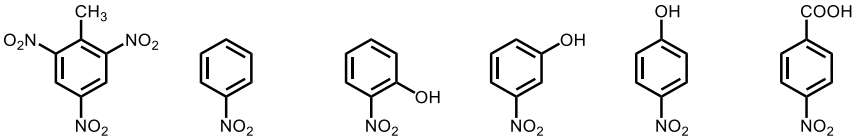


Figure S41. Time-resolved emission spectra (TRES) of the **Au-γ-Rot** (a) and *p*-NP⊂**Au-γ-Rot** (b) in deaerated H_2O at 25 ℃. The concertration of **Au-γ-Rot** was 10 μM and the concertration of *p*-NP was 30 μM, λ_{ex} = 280 nm (Spectra LED).

Table S3. Stern-Volmer quenching constants of a variety of nitroaromatics for **Au-γ-Rot**[a]

Quencher						
	TNT	NB	*o*-NP	*m*-NP	*p*-NP	*p*-NBA
K_{sv}[b] (M^{-1})	4.28(±0.10) ×10^5	2.95(±0.12) ×10^5	3.52(±0.15) ×10^5	1.02(±0.03) ×10^5	1.44(±0.03) ×10^5	2.03(±0.06) ×10^5
K_{sv}[c] (M^{-1})	1.78(±0.33) ×10^6	8.07(±0.23) ×10^5	4.90(±0.13) ×10^5	5.02(±0.16) ×10^5	1.71(±0.04) ×10^5	6.20(±0.22) ×10^4

[a] All data were measured in H_2O, λ_{ex}=330 nm in fluorescence mode and the concentration of **Au-γ-Rot** was 10 μM, 298 K. [b] The phosphorescence responses of **Au-γ-Rot** with nitroaromatics in aerated H_2O were analysed by fitting the data to a Stern-Volmer equation: $(I_0/I) = 1 + K_{SV}[Q]$, I_0 is the initial phosphorescence intensity before the addition of analyte, I is the phosphorescence intensity in the presence of analyte, [Q] is the molar concentration of analytes, and K_{SV} is the Stern-Volmer constant. [c] The phosphorescence responses of **Au-γ-Rot** with nitroaromatics in deaerated H_2O.

5.3 The limit of detection for nitroaromatics toward Au-γ-Rot

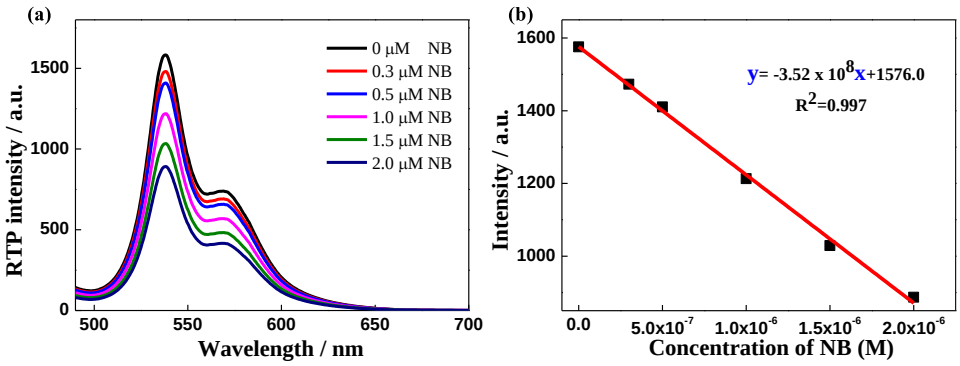


Figure 42. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **NB** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **NB** was dissolved in DMF mother solution.

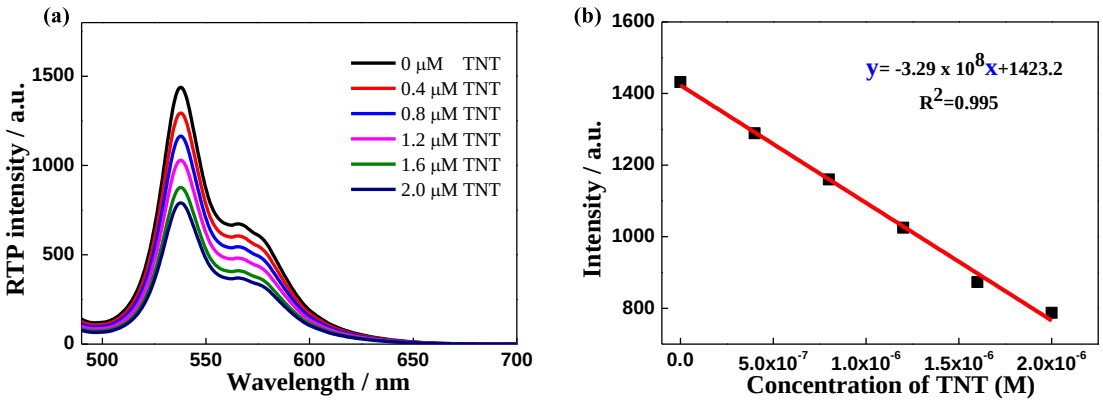


Figure S43. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **TNT** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **TNT** was dissolved in DMF mother solution.

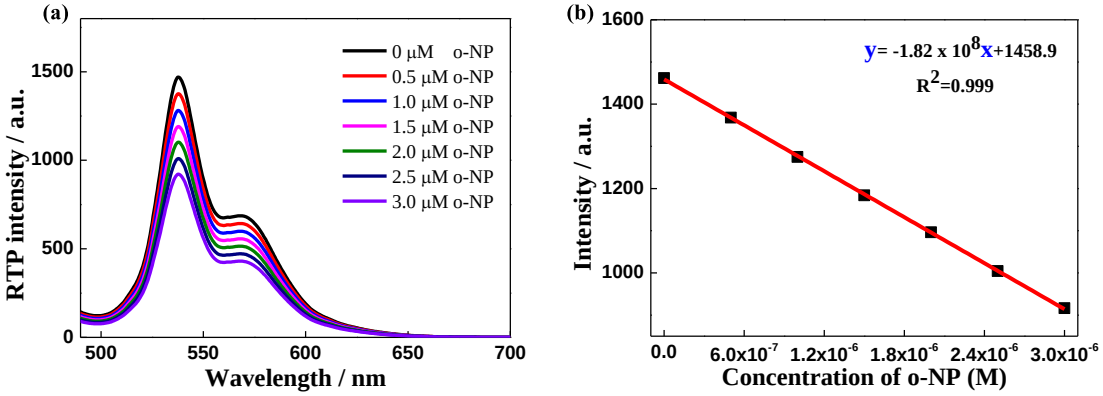


Figure S44. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **o-NP** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **o-NP** was dissolved in DMF mother solution.

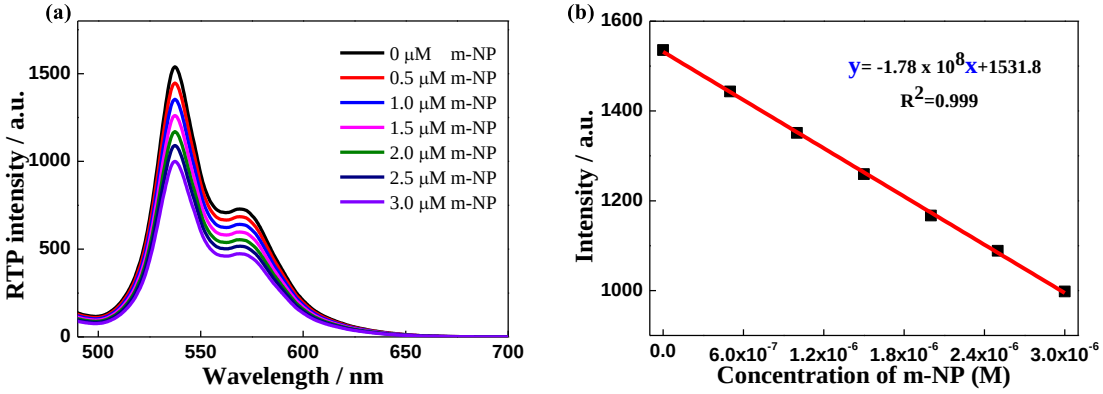


Figure S45. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **m-NP** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **m-NP** was dissolved in DMF mother solution.

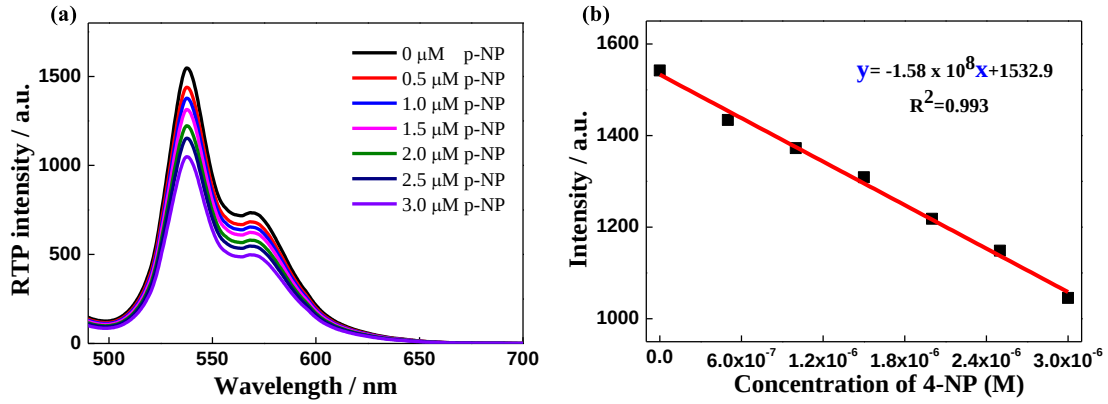


Figure S46. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **p-NP** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **p-NP** was dissolved in DMF mother solution.

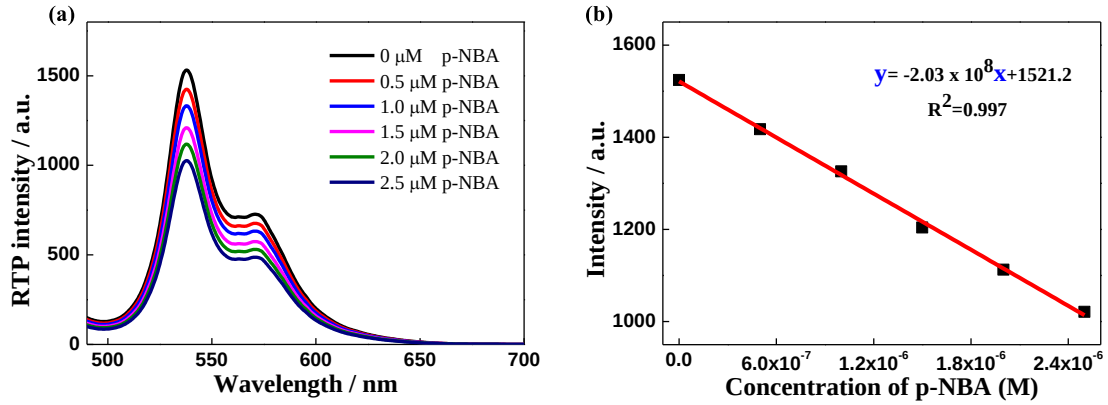


Figure S47. Emission spectra of 10 μM **Au-γ-Rot** in the presence of lower concentration of **p-NBA** (a) in aerated H_2O at 25 °C. λ_{ex}=330 nm in phosphorescence mode, and its corresponding detection limit plot (b). **p-NBA** was dissolved in DMF mother solution.

Table S4 The limit of detection for nitroaromatics toward **Au-γ-Rot**[a]

	NB	TNT	*o*-NP	*m*-NP	*p*-NP	*p*-NBA
LOD (μM)[b]	0.17	0.18	0.33	0.34	0.38	0.29
R^2	0.997	0.995	0.999	0.999	0.993	0.997

[a] Measured in aerated H_2O, λ_{ex}=330 nm in phosphorescence mode and the concentration of **Au-γ-Rot** was 10 μM. [b] The limit of detection (LOD) was calculated by using the equation: LOD = $3\sigma/K$, where σ is the standard deviation of initial intensity of **Au-γ-Rot** without analyte and K denotes the slope of the above-mentioned linear curve.

6. Effects of nitroaromatic on the emission lifetime of Au-γ-Rot

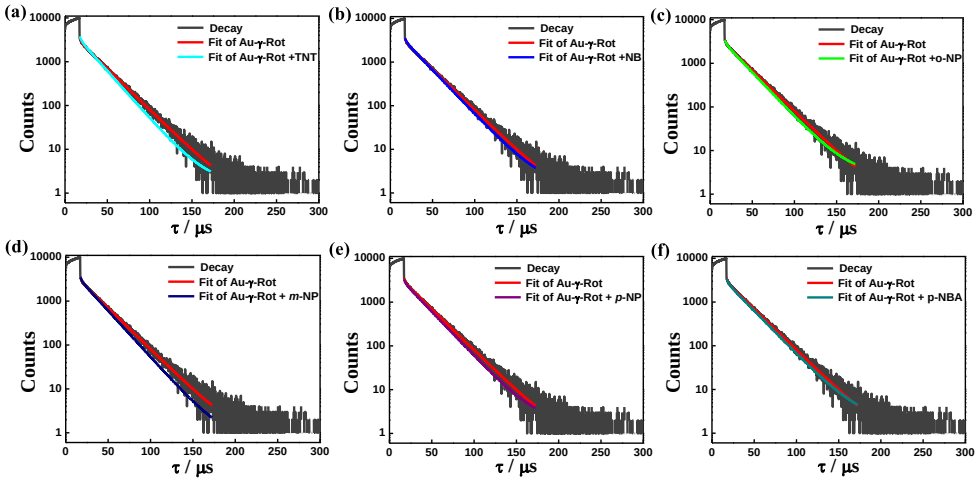


Figure S48. The phosphorescence lifetime decay curves of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** in aerated H_2O at 25 ℃, (a) **Au-γ-Rot** and TNT⊂**Au-γ-Rot**, (b) **Au-γ-Rot** and NB⊂**Au-γ-Rot**, (c) **Au-γ-Rot** and *o*-NP⊂**Au-γ-Rot**, (d) **Au-γ-Rot** and *m*-NP⊂**Au-γ-Rot**, (e) **Au-γ-Rot** and *p*-NP⊂**Au-γ-Rot**, (f) **Au-γ-Rot** and *p*-NBA⊂**Au-γ-Rot**, λ_{ex} = 280 nm (Spectra LED), λ_{em} =537 nm.

Table S5 The phosphorescence lifetime of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** [a]

	Au-γ-Rot	NB [b]	TNT	*o*-NP	*m*-NP	*p*-NP	*p*-NBA
τ (μs) [c]	22.7	21.2	19.7	20.9	20.2	21.1	21.5
CHISQ	1.10	1.14	1.13	1.17	1.12	1.04	1.12

[a] Measured in aerated H_2O at 25 ℃, the concentration of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** were 10 μM. [b] The phosphorescence lifetime of **Au-γ-Rot** after adding with nitroaromatics. [c] λ_{ex} = 280 nm (Spectra LED), λ_{em}=537 nm.

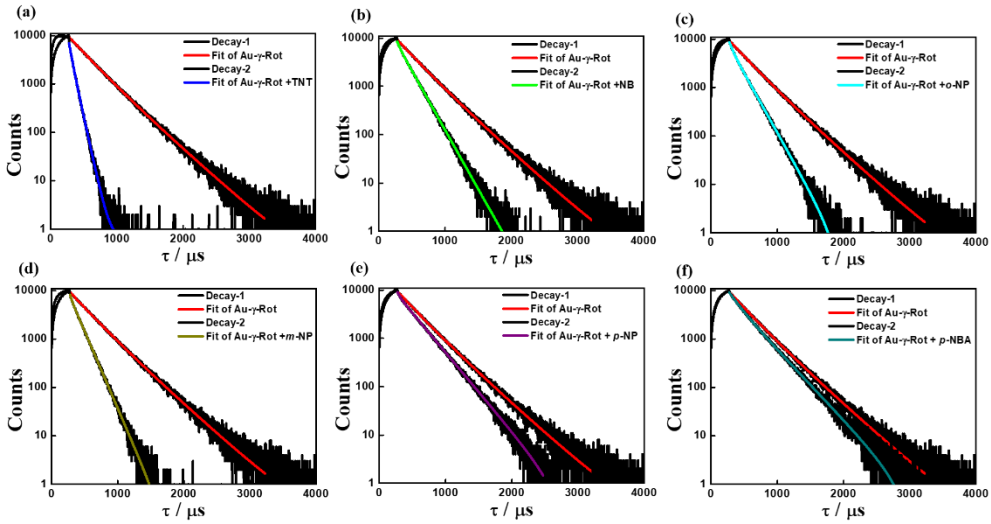


Figure S49. The phosphorescence lifetime decay curves of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** in deaerated H_2O at 25 ℃, (a) **Au-γ-Rot** and TNT⊂**Au-γ-Rot**, (b) **Au-γ-Rot** and NB⊂**Au-γ-Rot**, (c) **Au-γ-Rot** and *o*-NP⊂**Au-γ-Rot**, (d) **Au-γ-Rot** and *m*-NP⊂**Au-γ-Rot**, (e) **Au-γ-Rot** and *p*-NP⊂**Au-γ-Rot**, (f) **Au-γ-Rot** and *p*-NBA⊂**Au-γ-Rot**, λ_{ex} = 280 nm (Spectra LED), λ_{em} =537 nm.

Table S6 The phosphorescence lifetime of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** [a]

	Au-γ-Rot	NB [b]	TNT	*o*-NP	*m*-NP	*p*-NP	*p*-NBA
τ (μs) [c]	318.5	173.0	64.2	169.1	134.3	261.1	277.2
CHISQ	1.09	1.01	1.03	1.02	1.03	1.04	1.08

[a] Measured in deaerated H_2O at 25 ℃, the concentration of **Au-γ-Rot** and nitroaromatics ⊂**Au-γ-Rot** were 10 μM. [b] The phosphorescence lifetime of **Au-γ-Rot** after adding with nitroaromatics. [c] λ_{ex} = 280 nm (Spectra LED), λ_{em}=537 nm.

7. Calculations

7.1 Calculated Potential Profile of the compounds

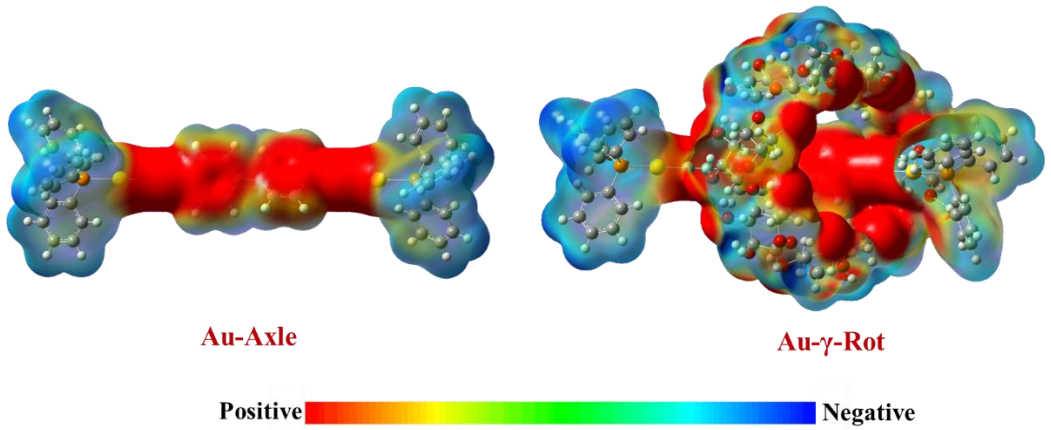


Figure S50. Calculated potential profile of **Au-Axle** and **Au-γ-Rot**.

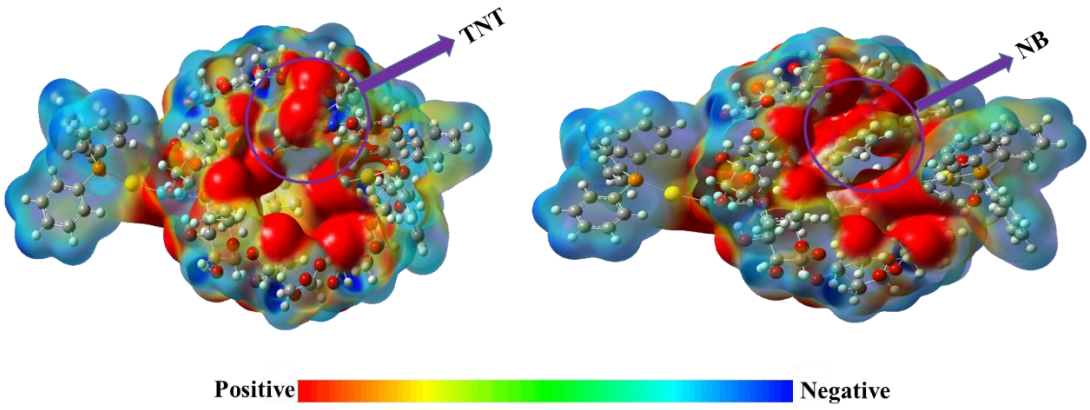


Figure S51. Calculated potential profile of TNT⊂**Au-γ-Rot** and NB⊂**Au-γ-Rot**.

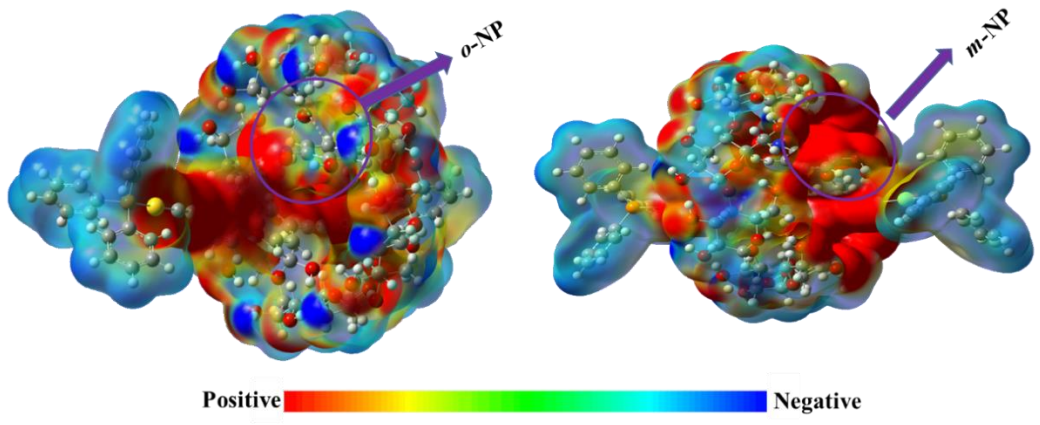


Figure S52. Calculated potential profile of *o*-NP⊂**Au-γ-Rot** and *m*-NP⊂**Au-γ-Rot**.

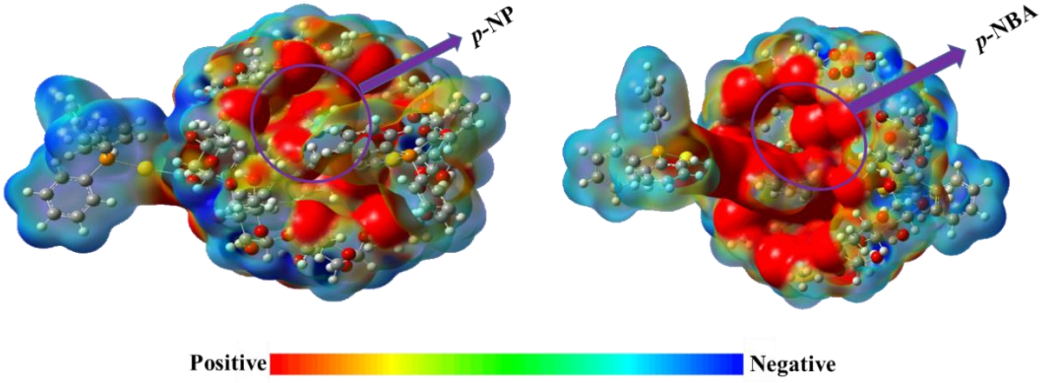


Figure S53. Calculated potential profile of *p*-NP⊂**Au-γ-Rot** and *p*-NBA⊂**Au-γ-Rot**.

7.2 Calculated HOMO-LUMO energy gaps of the nitroaromatics ⊂Au-γ-Rot.

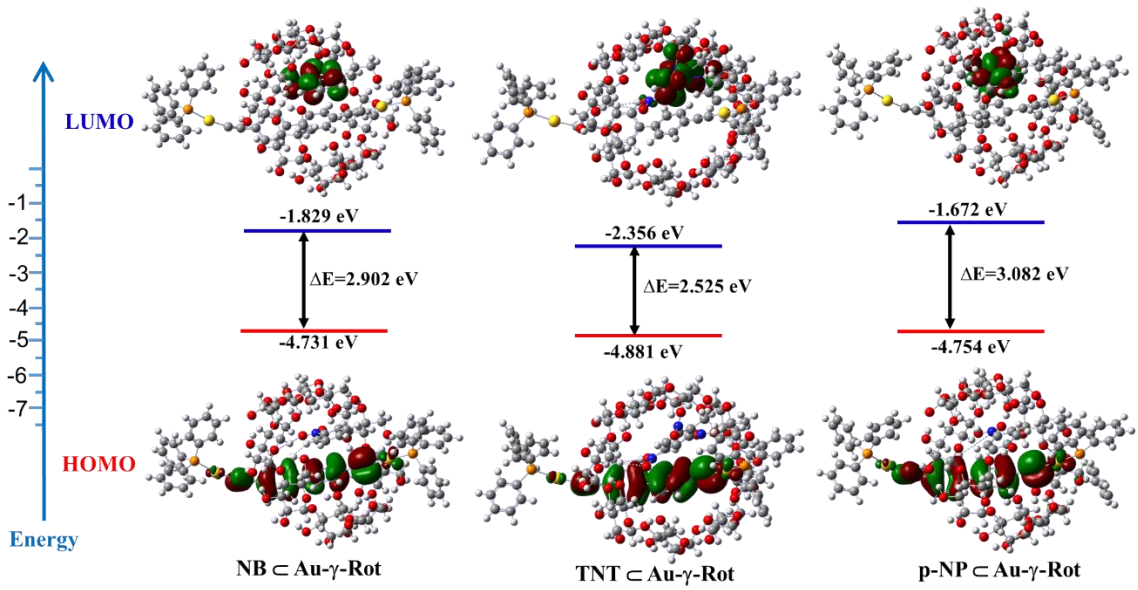


Figure S54. HOMO-LUMO energy gaps of NB⊂**Au-γ-Rot**, TNT⊂**Au-γ-Rot** and *p*-NP⊂**Au-γ-Rot**.

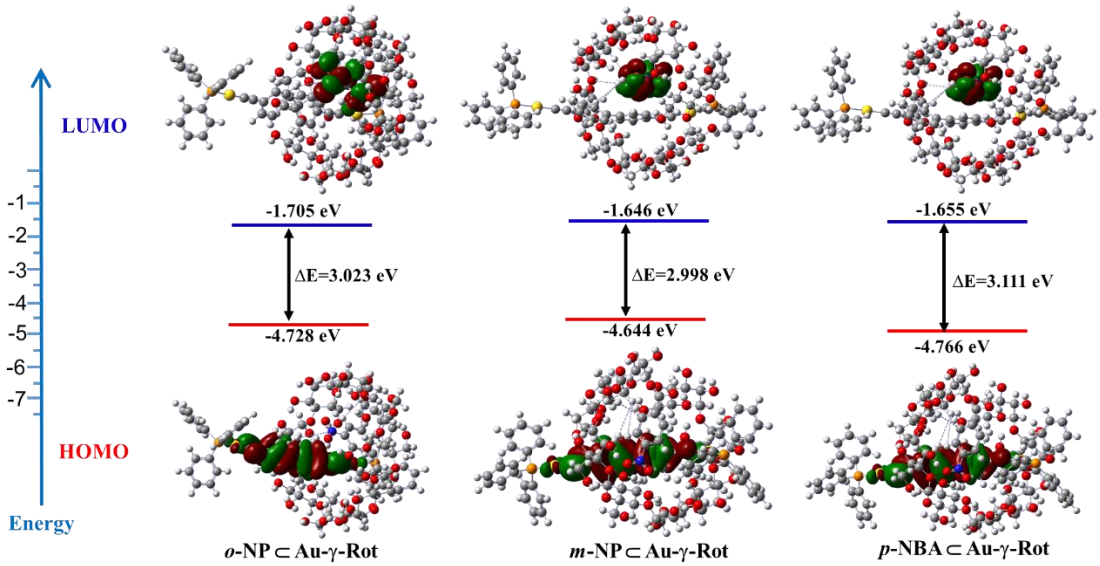


Figure S55. HOMO-LUMO energy gaps of *o*-NP ⊂**Au-γ-Rot**, *m*-NP⊂**Au-γ-Rot** and *p*-NBA⊂**Au-γ-Rot**.

7.3 Calculated for Au-Axle, Au-γ-Rot and nitroaromatics⊂Au-γ-Rot

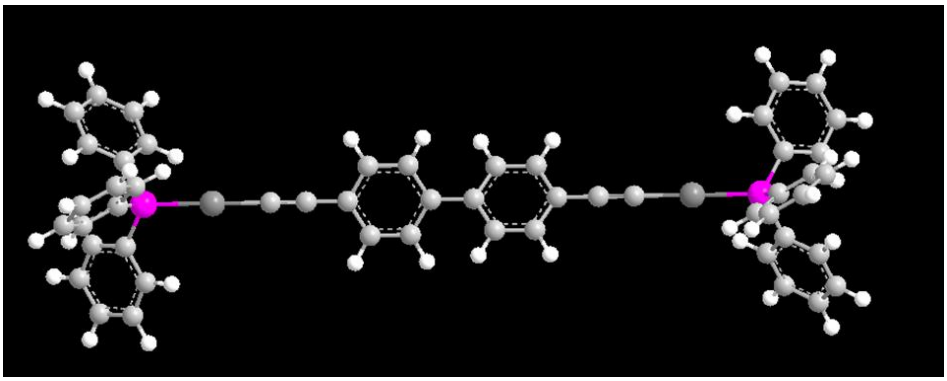


Figure S56. Calculated structure of **Au-Axle**.

The atomic coordinates of **Au-Axle**:

P	-10.599	0.001033	-0.00744
C	-11.3416	-0.26611	1.652762
C	-10.6607	0.239331	2.772145
C	-12.5542	-0.94745	1.837219
C	-11.1932	0.079725	4.051403
H	-9.70893	0.74739	2.64057
C	-13.0811	-1.10909	3.120013
H	-13.0818	-1.3614	0.983245
C	-12.4037	-0.5946	4.227154
H	-10.6564	0.472588	4.91024
H	-12.8134	-0.7261	5.224894
C	-11.3186	-1.30412	-1.08334
C	-10.6377	-2.5281	-1.1856

C	-12.5139	-1.12241	-1.79523
C	-11.1534	-3.55692	-1.97372
H	-9.6991	-2.66913	-0.65609
C	-13.0239	-2.15331	-2.58682
H	-13.0411	-0.1747	-1.74164
C	-12.3467	-3.37103	-2.67542
H	-13.9477	-2.00116	-3.13835
H	-12.7431	-4.16998	-3.29605
C	-11.3075	1.584994	-0.61427
C	-10.6036	2.289112	-1.60472
C	-12.5164	2.106858	-0.12954
C	-11.1098	3.485815	-2.11197
H	-9.65476	1.904014	-1.96903
C	-13.0168	3.307517	-0.63676
H	-13.0617	1.58397	0.650299
C	-12.3165	3.996664	-1.62878
H	-13.9514	3.706098	-0.25145
H	-12.7058	4.933369	-2.01833
Au	-8.23119	-0.00925	0.012528
C	-6.24063	-0.01294	0.024577
C	-5.01548	-0.01214	0.028623
C	-3.59029	-0.01013	0.03191
C	-2.85828	-1.15697	-0.33902
C	-2.86348	1.139351	0.404966
C	-1.46861	-1.15032	-0.33664
H	-3.39829	-2.04996	-0.63932
C	-1.47379	1.138151	0.405207
H	-3.40758	2.030299	0.703951
C	-0.74079	-0.00455	0.034635
H	-0.93423	-2.04096	-0.65572
H	-0.94348	2.03095	0.725084
C	0.74065	-0.00123	0.034277
C	1.473862	-1.14868	0.38938
C	1.468246	1.149377	-0.3222
C	2.863552	-1.14979	0.388541
H	0.943751	-2.04567	0.697654
C	2.857914	1.156151	-0.32508
H	0.933671	2.044114	-0.62928
C	3.59014	0.004579	0.030445
H	3.407826	-2.04458	0.675471
H	3.397754	2.053046	-0.61382
C	5.015328	0.006889	0.026932
C	6.240484	0.008177	0.022849
Au	8.231059	0.006431	0.011263

P	10.59882	0.000277	-0.00755
C	11.33732	-0.212	1.662365
C	11.32076	1.554957	-0.6712
C	11.30927	-1.34897	-1.03415
C	10.6547	-1.01415	2.591202
C	12.54848	0.390276	2.035233
C	10.63654	2.757929	-0.4328
C	12.52156	1.580708	-1.39657
C	10.61075	-1.74182	-2.1874
C	12.51471	-1.98997	-0.71048
C	11.18395	-1.22246	3.864784
H	9.704148	-1.46522	2.318622
C	13.07209	0.182951	3.31281
H	13.0776	1.029115	1.334619
C	11.15428	3.966542	-0.8984
H	9.693739	2.744243	0.10784
C	13.03365	2.792245	-1.8648
H	13.0513	0.656304	-1.60598
C	11.11886	-2.74708	-3.01008
H	9.664448	-1.26695	-2.43301
C	13.01708	-2.9991	-1.53428
H	13.0559	-1.71081	0.188488
C	12.39286	-0.62426	4.227386
H	14.00821	0.657762	3.593907
C	12.35305	3.985456	-1.61489
H	13.96177	2.801342	-2.42986
C	12.32219	-3.37711	-2.68476
H	10.56853	-3.04445	-3.89826
H	12.80008	-0.77996	5.222687
H	12.75125	4.926433	-1.98461
H	12.7129	-4.1661	-3.32159
H	10.64578	-1.84276	4.575945
H	10.61506	4.890662	-0.71025
H	13.94893	-3.49296	-1.27247
H	-10.5553	4.02314	-2.87619
H	-10.6167	-4.49858	-2.04737
H	-14.0184	-1.64255	3.253146

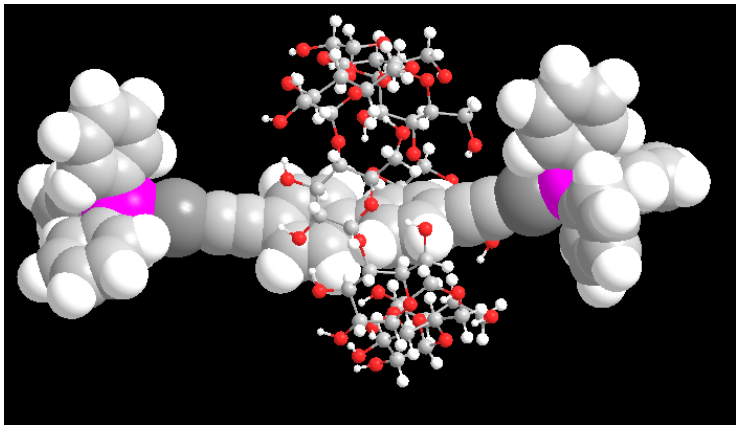


Figure S57. Calculated structure of **Au-γ-Rot**.

The atomic coordinates of **Au-γ-Rot**:

C	6.569645	-1.79227	4.557345
C	5.909194	-0.94308	5.643299
C	5.195317	0.254738	5.037878
C	6.194124	1.080342	4.232903
C	6.931717	0.223189	3.182917
C	8.190705	0.899279	2.603212
O	5.598195	-2.38158	3.728493
O	5.004792	-1.73064	6.411135
O	4.642722	0.960852	6.132616
O	7.463771	-0.9847	3.809931
O	7.961988	1.867211	1.60164
H	6.924353	1.518468	4.929431
H	7.200528	-2.56567	5.010337
H	6.710826	-0.57208	6.298555
H	4.406683	-0.09536	4.354919
H	6.2394	-0.04621	2.377307
H	8.782114	1.311741	3.43971
H	8.796433	0.120042	2.132686
H	4.444695	-1.08658	6.882516
H	4.475977	1.892905	5.872371
H	7.283742	2.517406	1.864921
C	5.902337	3.446023	3.674491
C	4.90885	4.324997	4.43351
C	3.614456	4.513509	3.655825
C	3.925481	5.036813	2.252682
C	4.912309	4.092327	1.536486
C	5.444767	4.606142	0.188645
O	5.440494	2.120953	3.604099
O	4.645229	3.76088	5.715404

O	2.846755	5.406184	4.438616
O	6.101083	3.969758	2.375544
O	4.479523	4.603068	-0.83813
H	4.382268	6.034206	2.335447
H	6.886126	3.483296	4.157074
H	5.373906	5.313747	4.55945
H	3.1095	3.540818	3.548743
H	4.462879	3.104354	1.3897
H	5.894268	5.603227	0.337804
H	6.242989	3.930002	-0.13064
H	3.868972	4.249429	6.046798
H	2.058065	5.697033	3.931158
H	3.840131	5.319374	-0.67878
C	2.281299	6.389281	1.052298
C	0.89535	6.773877	1.575944
C	-0.18322	5.865143	1.004745
C	-0.12917	5.913964	-0.52166
C	1.27908	5.542189	-1.02377
C	1.522557	5.777061	-2.52575
O	2.677099	5.138399	1.552601
O	0.873247	6.743669	2.998069
O	-1.40024	6.345284	1.540531
O	2.25725	6.396846	-0.36741
O	0.84708	4.868492	-3.36154
H	-0.37184	6.934486	-0.85254
H	3.014462	7.156758	1.324591
H	0.693536	7.799198	1.231992
H	0.011786	4.829298	1.324456
H	1.488238	4.493231	-0.78796
H	1.283075	6.828217	-2.76203
H	2.592071	5.635879	-2.70889
H	-0.07263	6.735878	3.235245
H	-2.15706	5.912338	1.087378
H	-0.1069	5.064373	-3.34894
C	-2.13771	5.496856	-1.8483
C	-3.51794	5.14138	-1.29623
C	-3.78383	3.645773	-1.37193
C	-3.59542	3.154313	-2.80798
C	-2.20916	3.557437	-3.34855
C	-2.01638	3.352913	-4.8624
O	-1.12016	5.001695	-1.01104
O	-3.64986	5.604158	0.044275
O	-5.10136	3.479843	-0.88954
O	-2.01879	4.990611	-3.16602

O	-1.93585	2.004376	-5.25498
H	-4.37684	3.597901	-3.44295
H	-2.04071	6.583216	-1.95329
H	-4.25821	5.651406	-1.93042
H	-3.062	3.113117	-0.73489
H	-1.42896	3.011829	-2.80622
H	-2.81466	3.900225	-5.39315
H	-1.06354	3.815035	-5.13789
H	-4.4231	5.124752	0.396167
H	-5.37334	2.538549	-0.99372
H	-2.80464	1.578442	-5.14136
C	-4.7523	1.12652	-3.54322
C	-5.61955	0.222543	-2.65849
C	-4.83469	-0.99272	-2.17664
C	-4.19317	-1.71018	-3.37021
C	-3.35181	-0.7456	-4.22411
C	-2.83532	-1.31383	-5.55878
O	-3.73564	1.730937	-2.78582
O	-6.13887	0.998405	-1.59019
O	-5.76194	-1.81649	-1.49866
O	-4.20198	0.370333	-4.61136
O	-1.75078	-2.20082	-5.42052
H	-4.99242	-2.13717	-3.9936
H	-5.37514	1.889298	-4.02413
H	-6.44664	-0.14303	-3.28587
H	-4.03115	-0.65964	-1.50296
H	-2.49957	-0.37478	-3.64457
H	-3.68088	-1.76297	-6.10857
H	-2.47146	-0.46981	-6.15174
H	-6.44617	0.409022	-0.87117
H	-5.35244	-2.68983	-1.3284
H	-2.06395	-3.03923	-5.03651
C	-3.58034	-4.07903	-3.29381
C	-3.8984	-5.03531	-2.1421
C	-2.69732	-5.23517	-1.22636
C	-1.48884	-5.68181	-2.05038
C	-1.21301	-4.67355	-3.18178
C	-0.12444	-5.08892	-4.18806
O	-3.39565	-2.7729	-2.82156
O	-5.01811	-4.55603	-1.40822
O	-3.11353	-6.18845	-0.26905
O	-2.42651	-4.55411	-3.97594
O	1.184478	-4.99201	-3.67755
H	-1.70347	-6.66515	-2.49368

H	-4.38193	-4.10707	-4.04038
H	-4.14287	-6.01025	-2.58964
H	-2.4462	-4.27524	-0.74724
H	-0.95057	-3.69712	-2.75988
H	-0.35583	-6.09795	-4.57086
H	-0.18129	-4.39709	-5.03364
H	-5.03045	-5.07937	-0.58646
H	-2.33106	-6.55023	0.200336
H	1.338074	-5.71259	-3.0412
C	0.329392	-7.00529	-1.09555
C	0.32539	-7.57728	0.322735
C	1.137642	-6.70805	1.270719
C	2.557767	-6.54135	0.728053
C	2.531431	-5.99061	-0.71047
C	3.885924	-6.03244	-1.44171
O	-0.38155	-5.79488	-1.14561
O	-1.00994	-7.71794	0.793119
O	1.087853	-7.37237	2.517953
O	1.671113	-6.83754	-1.52358
O	4.855371	-5.16057	-0.91005
H	3.053958	-7.52314	0.727659
H	-0.10195	-7.72865	-1.79647
H	0.801428	-8.56793	0.275517
H	0.675009	-5.71071	1.331133
H	2.145547	-4.96502	-0.70864
H	4.231783	-7.08004	-1.46838
H	3.714071	-5.71684	-2.47511
H	-0.92281	-7.84431	1.756335
H	1.629271	-6.88028	3.173298
H	5.134756	-5.48511	-0.03635
C	4.344648	-6.14319	2.340634
C	4.177794	-5.83052	3.827941
C	4.262337	-4.33336	4.084684
C	5.596961	-3.80389	3.560345
C	5.795077	-4.17044	2.076781
C	7.231104	-3.9695	1.560905
O	3.255453	-5.64792	1.605415
O	2.946501	-6.35052	4.314917
O	4.109715	-4.18858	5.482107
O	5.572744	-5.59696	1.885388
O	7.619229	-2.62486	1.396043
H	6.40763	-4.24879	4.156551
H	4.446232	-7.22343	2.188686
H	5.011311	-6.31631	4.356571

H	3.450896	-3.82624	3.539705
H	5.095937	-3.59908	1.455887
H	7.918365	-4.52255	2.224338
H	7.290134	-4.42866	0.570201
H	2.784907	-5.87622	5.151595
H	4.270644	-3.25327	5.737815
H	7.630831	-2.16268	2.254567
P	8.641929	0.614539	-2.23498
C	10.06625	-0.26008	-1.47374
C	9.805184	-1.32422	-0.59776
C	11.39605	0.111369	-1.73136
C	10.86188	-2.01482	-0.00077
H	8.784956	-1.60784	-0.35659
C	12.44771	-0.58595	-1.13571
H	11.60964	0.953132	-2.38401
C	12.18208	-1.65118	-0.2709
H	10.63898	-2.82724	0.684771
H	13.00339	-2.18722	0.197838
C	9.231324	2.346126	-2.44097
C	9.310866	3.148634	-1.2889
C	9.589065	2.884579	-3.68403
C	9.754719	4.466855	-1.38863
H	9.023621	2.74301	-0.32111
C	10.02535	4.209051	-3.77608
H	9.52321	2.276787	-4.58094
C	10.11043	5.000534	-2.63061
H	10.29544	4.619364	-4.74552
H	10.44777	6.031056	-2.7047
C	8.470185	-0.05919	-3.9372
C	7.212851	0.027269	-4.5575
C	9.537971	-0.64661	-4.63275
C	7.03263	-0.45154	-5.85548
H	6.373332	0.458029	-4.01826
C	9.351821	-1.12961	-5.92909
H	10.51095	-0.73949	-4.16032
C	8.101292	-1.03075	-6.54266
H	10.1838	-1.58888	-6.45635
H	7.95773	-1.4126	-7.54991
Au	6.626015	0.472393	-1.00329
C	4.866062	0.398104	-0.06055
C	3.726825	0.390765	0.392441
C	2.362355	0.425574	0.797738
C	1.545512	1.510325	0.413796
C	1.762109	-0.62557	1.520135

C	0.185	1.515408	0.69173
H	1.998607	2.323739	-0.14445
C	0.399014	-0.61435	1.79509
H	2.377417	-1.46141	1.840778
C	-0.42566	0.442362	1.368296
H	-0.4252	2.335798	0.322668
H	-0.03776	-1.43995	2.351138
C	-1.89546	0.399516	1.539949
C	-2.64789	1.566988	1.76819
C	-2.6002	-0.81086	1.399974
C	-4.03762	1.536942	1.805518
H	-2.13341	2.512438	1.917898
C	-3.98905	-0.85008	1.437013
H	-2.04877	-1.72622	1.203945
C	-4.73974	0.329523	1.615805
H	-4.60014	2.452833	1.955806
H	-4.51498	-1.78588	1.277016
C	-6.16403	0.30747	1.539242
C	-7.38392	0.289251	1.417213
Au	-9.36173	0.249894	1.166316
P	-11.703	0.194815	0.831604
C	-12.604	-0.70729	2.154675
C	-12.1775	-0.62466	-0.74274
C	-12.461	1.867315	0.766682
C	-12.1054	-0.63368	3.465457
C	-13.764	-1.45527	1.902485
C	-11.3737	-1.67539	-1.2139
C	-13.3082	-0.24088	-1.47986
C	-11.7148	2.91138	0.196001
C	-13.7485	2.131758	1.257435
C	-12.7658	-1.28449	4.507409
H	-11.1948	-0.07512	3.666119
C	-14.419	-2.10916	2.947854
H	-14.1503	-1.5372	0.891098
C	-11.706	-2.34056	-2.39413
H	-10.4826	-1.96372	-0.6625
C	-13.6344	-0.90683	-2.66267
H	-13.9272	0.58346	-1.13862
C	-12.2553	4.193826	0.104329
H	-10.7082	2.720592	-0.1671
C	-14.2834	3.418365	1.167881
H	-14.3295	1.338718	1.71834
C	-13.923	-2.02311	4.250122
H	-15.3138	-2.69014	2.741914

C	-12.8363	-1.95748	-3.11967
H	-14.5092	-0.59954	-3.22925
C	-13.5397	4.44914	0.590231
H	-11.6683	4.994335	-0.33699
H	-14.432	-2.53688	5.061004
H	-13.0896	-2.47069	-4.04329
H	-13.9566	5.450479	0.525962
H	-12.3697	-1.22273	5.517063
H	-11.075	-3.14966	-2.75072
H	-15.2795	3.614672	1.555022
H	9.81505	5.081005	-0.49401
H	13.47369	-0.2912	-1.3401
H	6.053942	-0.38261	-6.32177

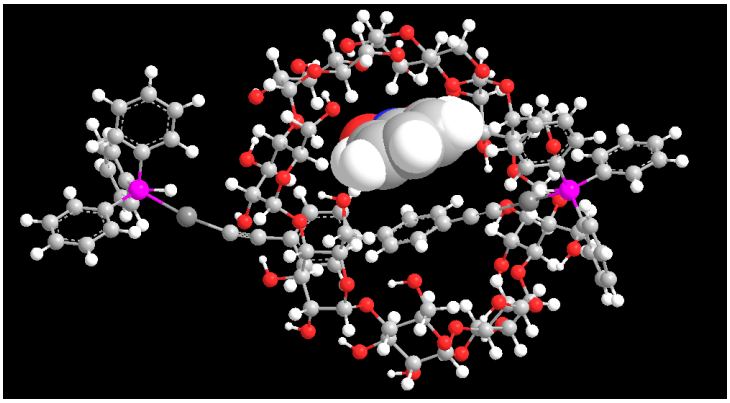


Figure S58. Calculated structure of NB⊂**Au-γ-Rot**.

The atomic coordinates of NB⊂**Au-γ-Rot**:

C	-4.49488	3.428011	2.935954
C	-4.92909	4.341669	1.789437
C	-3.75367	4.718763	0.897929
C	-2.63461	5.330468	1.744406
C	-2.24689	4.378481	2.891062
C	-1.27083	4.96152	3.927559
O	-4.0946	2.176816	2.444946
O	-5.95603	3.709436	1.028994
O	-4.28767	5.617204	-0.05627
O	-3.44704	4.062887	3.654283
O	0.043436	5.114425	3.442538
H	-2.98232	6.285479	2.165815
H	-5.3086	3.312302	3.661181
H	-5.32404	5.264571	2.239207
H	-3.35188	3.815403	0.415867
H	-1.82628	3.457666	2.475125
H	-1.6874	5.905399	4.319045

H	-1.21479	4.256896	4.762743
H	-6.01342	4.2289	0.205422
H	-3.55613	5.990821	-0.59464
H	0.068166	5.852369	2.807148
C	-1.01755	6.864048	0.731549
C	-1.00284	7.283216	-0.73936
C	0.007083	6.474196	-1.54254
C	1.387266	6.600714	-0.89635
C	1.318726	6.166775	0.579274
C	2.602536	6.392769	1.393538
O	-1.52379	5.562695	0.870091
O	-2.30448	7.159951	-1.30288
O	-0.05443	7.011763	-2.85074
O	0.30143	6.963547	1.25289
O	3.634465	5.481446	1.076172
H	1.718735	7.648328	-0.95458
H	-1.61063	7.570206	1.32377
H	-0.69314	8.338496	-0.77131
H	-0.27507	5.410964	-1.53083
H	1.047308	5.110009	0.629006
H	2.926712	7.441425	1.283925
H	2.359586	6.232376	2.44796
H	-2.16229	7.183483	-2.26729
H	0.679851	6.645905	-3.38938
H	3.982834	5.698744	0.192786
C	3.420618	6.348577	-2.22824
C	3.455655	6.071456	-3.73159
C	3.679454	4.59278	-4.01697
C	4.981119	4.144178	-3.35303
C	4.96447	4.460727	-1.8456
C	6.336482	4.339949	-1.15787
O	2.288393	5.769727	-1.64148
O	2.256193	6.521097	-4.34857
O	3.705786	4.494639	-5.42714
O	4.618051	5.859134	-1.63764
O	6.817605	3.022494	-1.01627
H	5.816833	4.681694	-3.82535
H	3.439952	7.428173	-2.04038
H	4.308321	6.630506	-4.14554
H	2.84955	4.00996	-3.58868
H	4.233289	3.81707	-1.34304
H	7.048472	4.987446	-1.69825
H	6.233635	4.740308	-0.14517
H	2.241667	6.075555	-5.21637

H	3.927916	3.574799	-5.69081
H	6.977607	2.626448	-1.89256
C	6.22263	2.287418	-4.34103
C	5.747657	1.416689	-5.50482
C	5.163318	0.104258	-5.00779
C	6.223014	-0.63425	-4.19685
C	6.782106	0.241126	-3.05533
C	8.107912	-0.28597	-2.46966
O	5.135708	2.734039	-3.56614
O	4.799412	2.115197	-6.30265
O	4.764059	-0.59294	-6.1719
O	7.155853	1.560707	-3.55835
O	7.999929	-1.37637	-1.57993
H	7.040096	-0.92167	-4.87521
H	6.788757	3.145613	-4.72037
H	6.633059	1.186559	-6.11597
H	4.302029	0.306963	-4.35317
H	6.027864	0.338516	-2.26595
H	8.79012	-0.51179	-3.30811
H	8.560527	0.52643	-1.89453
H	4.35304	1.425816	-6.82846
H	4.680885	-1.55142	-5.97334
H	7.43763	-2.09032	-1.93501
C	6.215071	-3.05917	-3.8422
C	5.330106	-3.99159	-4.66797
C	4.060911	-4.35703	-3.91493
C	4.414679	-4.94719	-2.54928
C	5.329271	-3.98953	-1.75726
C	5.948731	-4.59521	-0.48567
O	5.596239	-1.80837	-3.67171
O	5.011429	-3.38435	-5.917
O	3.379497	-5.26325	-4.76018
O	6.483474	-3.6558	-2.58802
O	5.028482	-4.80039	0.5611
H	4.933297	-5.90618	-2.69778
H	7.193523	-2.93921	-4.32229
H	5.90121	-4.91432	-4.84721
H	3.466953	-3.44617	-3.74412
H	4.786926	-3.07485	-1.49531
H	6.48417	-5.52122	-0.75951
H	6.691355	-3.88518	-0.11048
H	4.278644	-3.92115	-6.27278
H	2.593852	-5.62117	-4.29209
H	4.413322	-5.51621	0.323003

C	2.835658	-6.46734	-1.45258
C	1.460789	-6.86433	-1.99836
C	0.353642	-6.02368	-1.37392
C	0.425202	-6.15302	0.14697
C	1.824727	-5.73246	0.637711
C	2.087818	-5.92135	2.140968
O	3.175846	-5.16995	-1.86231
O	1.438029	-6.74927	-3.41664
O	-0.85317	-6.50228	-1.9362
O	2.810329	-6.56632	-0.03434
O	1.451653	-4.95022	2.941584
H	0.243626	-7.19995	0.430561
H	3.597269	-7.18592	-1.77589
H	1.291206	-7.9142	-1.71722
H	0.514247	-4.96672	-1.63482
H	2.006512	-4.68491	0.380847
H	1.8202	-6.95097	2.43394
H	3.163373	-5.80335	2.301639
H	0.494414	-6.76913	-3.6604
H	-1.61086	-6.26743	-1.35688
H	0.497207	-5.14084	2.976297
C	-1.51553	-5.88966	1.612148
C	-2.95487	-5.78674	1.106984
C	-3.45114	-4.34831	1.096819
C	-3.28425	-3.72871	2.485202
C	-1.82628	-3.86705	2.966653
C	-1.59704	-3.51798	4.447049
O	-0.61297	-5.32489	0.691257
O	-3.05802	-6.35864	-0.19246
O	-4.79694	-4.42691	0.675153
O	-1.41853	-5.2606	2.87791
O	-1.77092	-2.1506	4.747572
H	-3.94899	-4.2469	3.192402
H	-1.25428	-6.93747	1.797157
H	-3.58326	-6.35809	1.806608
H	-2.85139	-3.75837	0.388755
H	-1.17312	-3.24933	2.339401
H	-2.24569	-4.16207	5.063371
H	-0.55972	-3.7641	4.69286
H	-3.91781	-6.04484	-0.53122
H	-5.18444	-3.52124	0.652952
H	-2.71424	-1.92421	4.654417
C	-4.79593	-1.90474	3.081225
C	-5.74698	-1.15026	2.137256

C	-5.15673	0.187291	1.703467
C	-4.72957	0.989204	2.938183
C	-3.78633	0.179197	3.840516
C	-3.45159	0.820238	5.200664
O	-3.65205	-2.34758	2.394241
O	-6.06114	-1.99852	1.046279
O	-6.16318	0.861522	0.971198
O	-4.43061	-1.07865	4.177913
O	-2.47885	1.834554	5.127539
H	-5.63084	1.260366	3.507332
H	-5.32117	-2.75467	3.530456
H	-6.66006	-0.93537	2.713344
H	-4.26818	0.007705	1.079455
H	-2.85028	-0.02054	3.308214
H	-4.38569	1.163235	5.678445
H	-3.03377	0.033671	5.836188
H	-6.37261	-1.47507	0.278967
H	-5.88173	1.789538	0.832433
H	-2.86989	2.627054	4.715886
P	8.629534	-0.28883	2.344481
C	8.390882	0.1407	4.117157
C	7.26887	-0.39121	4.774798
C	9.273943	0.965381	4.829052
C	7.046013	-0.11554	6.12364
H	6.566424	-1.01292	4.225523
C	9.042085	1.246125	6.177352
H	10.13634	1.397739	4.331533
C	7.931512	0.704771	6.82684
H	6.174755	-0.5328	6.620858
H	7.751607	0.927572	7.875113
C	9.801963	0.949538	1.662819
C	9.29014	2.004102	0.891232
C	11.1873	0.860824	1.877488
C	10.15348	2.96243	0.35603
H	8.226269	2.076684	0.683493
C	12.04386	1.824328	1.34405
H	11.59771	0.032644	2.448331
C	11.52778	2.877508	0.583927
H	13.11445	1.747182	1.514539
H	12.19836	3.622259	0.163038
C	9.576201	-1.86699	2.348861
C	9.703726	-2.55619	1.130064
C	10.16598	-2.39373	3.506275
C	10.42357	-3.74984	1.078654

H	9.240657	-2.16146	0.228112
C	10.87908	-3.59374	3.446914
H	10.06517	-1.87496	4.454539
C	11.01001	-4.27201	2.234687
H	11.32851	-3.99712	4.350486
H	11.56261	-5.20687	2.191101
Au	6.585679	-0.418	1.161274
C	4.837242	-0.54414	0.206362
C	3.732068	-0.65467	-0.31187
C	2.412253	-0.83613	-0.8148
C	1.846208	0.015831	-1.78539
C	1.607793	-1.87359	-0.29844
C	0.523585	-0.14331	-2.18935
H	2.447153	0.822854	-2.19442
C	0.293669	-2.03593	-0.7172
H	2.018686	-2.51345	0.475937
C	-0.28544	-1.1625	-1.65648
H	0.106171	0.539163	-2.92471
H	-0.31092	-2.81888	-0.26824
C	-1.73129	-1.25897	-1.96364
C	-2.51972	-0.09428	-2.00783
C	-2.37962	-2.49992	-2.10804
C	-3.9024	-0.17027	-2.11816
H	-2.04868	0.874476	-1.87223
C	-3.76495	-2.581	-2.21962
H	-1.79268	-3.41518	-2.12149
C	-4.55777	-1.41712	-2.18982
H	-4.5021	0.734488	-2.09527
H	-4.25145	-3.5488	-2.29336
C	-5.98216	-1.4657	-2.12372
C	-7.19673	-1.41726	-1.95937
Au	-9.07581	-1.02317	-1.42351
P	-11.1583	-0.27769	-0.58929
C	-10.8947	0.864956	0.825338
C	-12.2779	-1.59379	0.035607
C	-12.1415	0.651433	-1.83384
C	-9.65245	1.508915	0.942683
C	-11.8901	1.113841	1.784908
C	-11.7001	-2.7264	0.631689
C	-13.675	-1.50169	-0.05352
C	-12.1391	0.178029	-3.15643
C	-12.8815	1.800416	-1.51879
C	-9.41713	2.407768	1.984582
H	-8.85557	1.294319	0.237315

C	-11.6508	2.010847	2.82643
H	-12.8449	0.598926	1.727475
C	-12.5082	-3.74068	1.144867
H	-10.618	-2.81547	0.684642
C	-14.4799	-2.52174	0.457563
H	-14.1347	-0.64142	-0.53077
C	-12.8788	0.832443	-4.14076
H	-11.5482	-0.69673	-3.41578
C	-13.616	2.45632	-2.50911
H	-12.8761	2.191818	-0.5064
C	-10.4178	2.662593	2.923654
H	-12.4257	2.196148	3.565505
C	-13.8988	-3.63979	1.058709
H	-15.5609	-2.44369	0.380266
C	-13.6185	1.972897	-3.8185
H	-12.8674	0.458171	-5.16056
H	-10.2368	3.359117	3.738144
H	-14.5273	-4.43424	1.451712
C	1.922733	2.253617	1.779543
C	0.638224	1.856061	1.404238
C	-0.09904	0.920325	2.133574
C	0.467298	0.362772	3.276246
C	1.752098	0.750705	3.670688
C	2.472542	1.691483	2.929296
H	2.465765	2.99339	1.203867
H	-1.08786	0.640756	1.793381
H	-0.09177	-0.36982	3.851154
H	3.468241	1.990117	3.241365
N	0.033082	2.437364	0.2084
O	0.750465	3.092414	-0.55351
O	-1.17291	2.2482	0.014744
H	-12.0507	-4.61348	1.60222
H	-8.4475	2.893191	2.05128
H	-14.1814	3.349047	-2.25588
H	-14.1873	2.487967	-4.58777
H	10.51875	-4.27724	0.133226
H	9.740335	3.764423	-0.24865
H	9.728947	1.8923	6.717401
H	2.193286	0.315833	4.56316

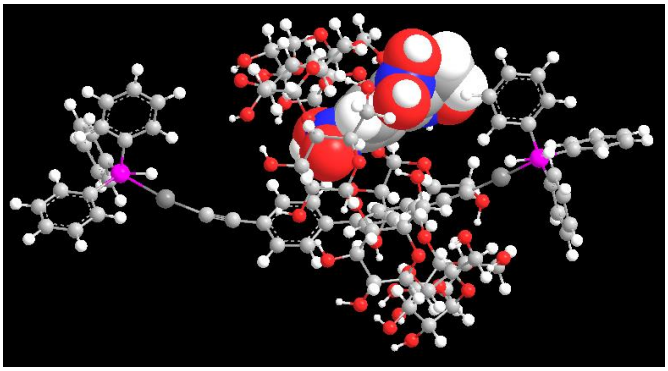


Figure S59. Calculated structure of TNT⊂**Au-γ-Rot**.

The atomic coordinates of TNT⊂**Au-γ-Rot**:

C	4.2001	3.4675	-2.4354
C	4.5847	4.3789	-1.2663
C	3.4126	4.5989	-0.3179
C	2.2184	5.1446	-1.1027
C	1.8639	4.1906	-2.2574
C	0.8053	4.723	-3.2387
O	3.9734	2.1615	-1.9931
O	5.7007	3.8377	-0.5713
O	3.893	5.495	0.6647
O	3.049	4.0061	-3.0805
O	-0.4921	4.7941	-2.6874
H	2.4873	6.1252	-1.5221
H	4.9826	3.4849	-3.2025
H	4.8583	5.3556	-1.6934
H	3.1218	3.6349	0.1278
H	1.5389	3.2238	-1.8556
H	1.1437	5.695	-3.6335
H	0.7521	4.0293	-4.0829
H	5.7302	4.3184	0.2762
H	3.1615	5.7373	1.2727
H	-0.5132	5.5373	-2.0586
C	0.625	6.5906	0.0401
C	0.5589	6.8884	1.5396
C	-0.5184	6.0654	2.2342
C	-1.8621	6.3281	1.5562
C	-1.7701	6.025	0.05
C	-2.9926	6.4752	-0.7722
O	1.1211	5.2968	-0.1919
O	1.828	6.6658	2.1416
O	-0.4784	6.4682	3.5884
O	-0.6626	6.7679	-0.534
O	-4.0908	5.5939	-0.7047

H	-2.1311	7.385	1.7006
H	1.256	7.3321	-0.4619
H	0.2883	7.9499	1.6439
H	-0.2838	4.9943	2.1309
H	-1.6131	4.9507	-0.0947
H	-3.2655	7.5041	-0.4837
H	-2.6869	6.5043	-1.8223
H	1.6554	6.629	3.1001
H	-1.31	6.202	4.0387
H	-4.4753	5.6109	0.1919
C	-4.0076	6.0708	2.7075
C	-4.1195	5.7905	4.2062
C	-4.3366	4.3085	4.4685
C	-5.5951	3.8404	3.7399
C	-5.5399	4.188	2.24
C	-6.9018	4.0995	1.5294
O	-2.8363	5.4906	2.1867
O	-2.9536	6.2495	4.882
O	-4.426	4.189	5.8748
O	-5.1632	5.587	2.0494
O	-7.4021	2.792	1.3566
H	-6.4681	4.3226	4.2049
H	-4.0079	7.1513	2.5223
H	-4.9957	6.341	4.5796
H	-3.4797	3.743	4.072
H	-4.8138	3.5415	1.7406
H	-7.6158	4.7472	2.0674
H	-6.7762	4.511	0.5246
H	-2.9849	5.8094	5.7525
H	-4.6351	3.2585	6.1119
H	-7.5378	2.3532	2.2161
C	-6.7762	1.8714	4.5978
C	-6.293	0.9858	5.7454
C	-5.5563	-0.2364	5.2178
C	-6.4795	-1.0137	4.283
C	-7.0419	-0.1124	3.1625
C	-8.2334	-0.7354	2.4083
O	-5.6866	2.4178	3.8997
O	-5.4612	1.7261	6.6328
O	-5.1708	-0.9664	6.3661
O	-7.6057	1.1047	3.738
O	-7.8988	-1.7004	1.4329
H	-7.3117	-1.4215	4.8757
H	-7.425	2.6693	4.9773

H	-7.185	0.6419	6.2891
H	-4.6762	0.0877	4.642
H	-6.2421	0.1423	2.4581
H	-8.9469	-1.1361	3.1494
H	-8.7422	0.069	1.8706
H	-4.9907	1.0538	7.1595
H	-5.0151	-1.9063	6.126
H	-7.3095	-2.3913	1.7901
C	-6.221	-3.3957	3.7711
C	-5.3509	-4.2974	4.6459
C	-3.9837	-4.5268	4.021
C	-4.1514	-5.0912	2.6101
C	-5.046	-4.1688	1.757
C	-5.4889	-4.7777	0.4152
O	-5.7075	-2.0856	3.7313
O	-5.2146	-3.737	5.9485
O	-3.322	-5.4084	4.9072
O	-6.3014	-3.9387	2.4686
O	-4.4438	-4.9342	-0.5168
H	-4.6183	-6.0852	2.6787
H	-7.2519	-3.3873	4.1449
H	-5.8596	-5.2698	4.7215
H	-3.4531	-3.5656	3.9425
H	-4.5434	-3.2126	1.577
H	-6.0135	-5.7278	0.6173
H	-6.2113	-4.0938	-0.0394
H	-4.4782	-4.2347	6.3518
H	-2.4394	-5.6381	4.5421
H	-3.8397	-5.633	-0.2104
C	-2.3569	-6.4935	1.7235
C	-0.9884	-6.7314	2.3702
C	0.0843	-5.8507	1.7408
C	0.1291	-6.1415	0.2419
C	-1.2556	-5.8696	-0.3785
C	-1.4013	-6.2571	-1.8611
O	-2.8431	-5.2134	2.034
O	-1.0527	-6.5152	3.7746
O	1.2839	-6.1547	2.4279
O	-2.2453	-6.6781	0.3183
O	-0.7775	-5.3538	-2.7423
H	0.3872	-7.1997	0.0889
H	-3.0681	-7.2602	2.0506
H	-0.7207	-7.7813	2.1791
H	-0.1854	-4.794	1.8839

H	-1.5084	-4.8099	-0.2696
H	-1.0533	-7.2953	-1.9999
H	-2.4696	-6.2371	-2.0971
H	-0.1265	-6.418	4.0627
H	2.0604	-5.9769	1.8527
H	0.1886	-5.4689	-2.6941
C	2.1418	-5.9295	-1.1277
C	3.5337	-5.6925	-0.5441
C	3.9301	-4.2296	-0.6409
C	3.8359	-3.751	-2.0889
C	2.4558	-4.0625	-2.7072
C	2.4045	-3.9658	-4.2455
O	1.1501	-5.3157	-0.3329
O	3.5765	-6.1367	0.8089
O	5.2427	-4.1578	-0.1214
O	2.1039	-5.4563	-2.4583
O	2.4287	-2.6608	-4.7653
H	4.6215	-4.2483	-2.6773
H	1.9431	-7.0044	-1.2039
H	4.2421	-6.2837	-1.1429
H	3.2368	-3.6234	-0.0398
H	1.6988	-3.4026	-2.2693
H	3.2136	-4.5971	-4.6545
H	1.4561	-4.4072	-4.567
H	4.392	-5.7453	1.1739
H	5.5966	-3.249	-0.2589
H	3.2567	-2.2088	-4.5213
C	5.1	-1.7851	-2.828
C	6.0533	-0.9527	-1.9549
C	5.4034	0.3396	-1.4684
C	4.6859	1.0746	-2.6088
C	3.7465	0.1352	-3.3793
C	3.0887	0.7195	-4.6403
O	4.073	-2.3408	-2.0534
O	6.5101	-1.769	-0.8854
O	6.4494	1.1295	-0.9259
O	4.56	-0.9724	-3.8591
O	2.0629	1.6548	-4.3611
H	5.4407	1.4755	-3.3013
H	5.6619	-2.5728	-3.3432
H	6.9032	-0.671	-2.5945
H	4.652	0.0954	-0.7031
H	2.9644	-0.2435	-2.7164
H	3.8646	1.1473	-5.2967

H	2.6166	-0.1077	-5.1754
H	6.8165	-1.2079	-0.1435
H	6.0775	1.9883	-0.6347
H	2.4709	2.4815	-4.045
P	-7.9854	-0.6604	-2.4602
C	-7.5363	-0.0605	-4.1398
C	-6.257	-0.3743	-4.6309
C	-8.406	0.7002	-4.9353
C	-5.8597	0.0569	-5.897
H	-5.5694	-0.9485	-4.0149
C	-8.0031	1.135	-6.1999
H	-9.3913	0.9655	-4.5652
C	-6.7325	0.8153	-6.6817
H	-4.8636	-0.1781	-6.2597
H	-6.4169	1.1631	-7.6615
C	-9.389	0.3763	-1.8928
C	-9.1344	1.4134	-0.9831
C	-10.7045	0.149	-2.3306
C	-10.1809	2.2191	-0.5288
H	-8.1314	1.5915	-0.6063
C	-11.7446	0.9613	-1.8783
H	-10.918	-0.6698	-3.012
C	-11.4837	1.9979	-0.9777
H	-12.7594	0.7783	-2.2217
H	-12.2979	2.6232	-0.6203
C	-8.7175	-2.3306	-2.7007
C	-9.0116	-3.0842	-1.5504
C	-8.9812	-2.8691	-3.9669
C	-9.5716	-4.355	-1.6764
H	-8.8019	-2.6762	-0.5638
C	-9.5354	-4.1467	-4.0841
H	-8.7504	-2.2988	-4.8612
C	-9.8321	-4.8897	-2.9414
H	-9.7314	-4.5587	-5.0704
H	-10.2606	-5.8841	-3.0348
Au	-6.1155	-0.6693	-1.0106
C	-4.4629	-0.7036	0.1129
C	-3.3842	-0.7496	0.694
C	-2.0689	-0.86	1.2302
C	-1.5355	0.0717	2.1447
C	-1.2241	-1.8927	0.7709
C	-0.2018	-0.0027	2.5372
H	-2.1722	0.8691	2.5158
C	0.1041	-1.9603	1.1674

H	-1.6221	-2.6059	0.0562
C	0.6523	-1.0036	2.0417
H	0.1885	0.7334	3.2354
H	0.743	-2.7283	0.7414
C	2.1071	-1.0034	2.3132
C	2.8258	0.2057	2.3164
C	2.8348	-2.1995	2.4581
C	4.2132	0.2191	2.3824
H	2.2893	1.1424	2.1944
C	4.2246	-2.1935	2.5229
H	2.3056	-3.1481	2.5074
C	4.9449	-0.9849	2.4462
H	4.7544	1.1592	2.332
H	4.772	-3.128	2.5879
C	6.3658	-0.9608	2.326
C	7.5711	-0.8785	2.1155
Au	9.4274	-0.5352	1.4749
P	11.4817	0.0441	0.4622
C	11.1965	0.5876	-1.2696
C	12.7147	-1.314	0.3606
C	12.3424	1.431	1.306
C	9.9333	1.0979	-1.6115
C	12.1935	0.5022	-2.255
C	12.2417	-2.6244	0.1839
C	14.0967	-1.0878	0.4447
C	12.2941	1.4798	2.7088
C	13.0374	2.43	0.6086
C	9.681	1.5324	-2.9135
H	9.1332	1.1405	-0.878
C	11.9349	0.938	-3.5553
H	13.1656	0.0826	-2.0125
C	13.1382	-3.6872	0.0764
H	11.1716	-2.8106	0.1387
C	14.9903	-2.1557	0.3415
H	14.4756	-0.0822	0.6009
C	12.9449	2.5006	3.4011
H	11.7371	0.7238	3.2565
C	13.6829	3.4535	1.3055
H	13.0656	2.4179	-0.4766
C	10.6799	1.4561	-3.8856
H	12.7116	0.8649	-4.3118
C	14.5134	-3.4545	0.1552
H	16.0589	-1.9716	0.4121
C	13.6401	3.489	2.7004

H	12.8989	2.5293	4.4861
H	10.4804	1.7887	-4.9008
H	15.2108	-4.2843	0.0794
C	-1.6786	1.4945	-1.5724
C	-0.9574	0.97	-2.6316
C	-1.3475	1.1695	-3.9468
C	-2.4613	1.9711	-4.1813
C	-3.2782	2.5081	-3.163
C	-2.8426	2.1995	-1.8572
H	-1.3719	1.3254	-0.5492
H	-0.7779	0.7455	-4.763
N	0.2354	0.168	-2.3491
O	0.8558	0.4267	-1.3177
O	0.5305	-0.707	-3.1569
H	12.7615	-4.6972	-0.0588
H	8.6948	1.9171	-3.1562
H	14.2141	4.2259	0.756
H	14.1396	4.2891	3.2398
H	-9.7977	-4.9322	-0.7837
H	-9.9611	3.0042	0.188
H	-8.6821	1.7307	-6.8042
N	-2.7449	2.2103	-5.6139
O	-2.6422	1.2395	-6.3635
O	-3.0204	3.3501	-5.9768
N	-3.6201	2.6083	-0.6742
O	-4.8369	2.6948	-0.7751
O	-2.9857	2.8135	0.363
C	-4.5286	3.3065	-3.4362
H	-5.4081	2.6744	-3.2757
H	-4.6068	4.1455	-2.7402
H	-4.5354	3.6823	-4.4555

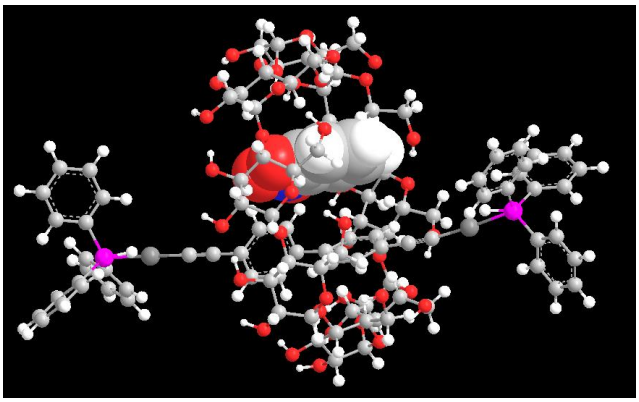


Figure S60. Calculated structure of *o*-NP⊂**Au-γ-Rot**.

The atomic coordinates of *o*-NP ⊂**Au-γ-Rot**:

C	1.5634	4.2967	5.8349
C	0.2175	4.9691	5.5505
C	0.0559	5.2869	4.0717
C	1.2202	6.1618	3.6096
C	2.5668	5.4869	3.9219
C	3.8099	6.379	3.7461
O	1.6032	3.0023	5.2911
O	-0.8502	4.1493	6.009
O	-1.1975	5.9353	3.9597
O	2.6144	5.1065	5.3261
O	4.1473	6.6368	2.4044
H	1.163	7.134	4.1211
H	1.7427	4.2582	6.9151
H	0.2103	5.9194	6.1055
H	0.0759	4.3512	3.4928
H	2.6718	4.5984	3.2902
H	3.6684	7.3037	4.3314
H	4.6584	5.8439	4.1832
H	-1.6457	4.4898	5.56
H	-1.3028	6.285	3.0487
H	3.4862	7.2348	2.0113
C	0.9842	7.6457	1.6755
C	-0.268	7.7929	0.8097
C	-0.1757	6.9225	-0.4352
C	1.1184	7.2177	-1.1959
C	2.3447	7.1015	-0.2714
C	3.6733	7.5955	-0.8727
O	1.06	6.3468	2.198
O	-1.4243	7.4626	1.5716
O	-1.338	7.2073	-1.187
O	2.1282	7.9517	0.8902
O	4.226	6.7165	-1.8254
H	1.0663	8.2359	-1.6084
H	0.9828	8.3875	2.4819
H	-0.3252	8.844	0.4911
H	-0.1498	5.8655	-0.1274
H	2.469	6.0628	0.0529
H	3.5312	8.6141	-1.2724
H	4.3978	7.6618	-0.0561
H	-2.137	7.3408	0.9181
H	-1.2638	6.7912	-2.0733
H	3.6931	6.7398	-2.6404
C	1.3392	6.7055	-3.583

C	0.2147	6.1643	-4.4657
C	0.2944	4.6496	-4.6165
C	1.6943	4.247	-5.087
C	2.7673	4.8338	-4.1514
C	4.2229	4.61	-4.5913
O	1.1776	6.2634	-2.2626
O	-1.0474	6.5492	-3.9307
O	-0.7234	4.3225	-5.5406
O	2.5877	6.2763	-4.1133
O	4.6666	3.2833	-4.3721
H	1.8536	4.6384	-6.1021
H	1.3685	7.8	-3.6245
H	0.3406	6.6095	-5.4635
H	0.1101	4.1757	-3.6405
H	2.6461	4.4327	-3.1409
H	4.3471	4.9165	-5.6424
H	4.8585	5.2555	-3.9793
H	-1.7002	5.9933	-4.3946
H	-0.6399	3.379	-5.7981
H	4.2607	2.6992	-5.0404
C	2.0863	2.1761	-6.3206
C	0.9819	1.2178	-6.7734
C	0.8971	-0.0107	-5.8796
C	2.2575	-0.7059	-5.8645
C	3.3576	0.2645	-5.3958
C	4.7956	-0.2506	-5.5949
O	1.7483	2.8125	-5.1114
O	-0.2692	1.89	-6.8234
O	-0.1277	-0.8041	-6.4415
O	3.3147	1.476	-6.2056
O	5.1553	-1.2999	-4.7314
H	2.4903	-1.0402	-6.8864
H	2.2674	2.9282	-7.0963
H	1.2506	0.877	-7.7849
H	0.6458	0.2991	-4.8528
H	3.2	0.5158	-4.3401
H	4.9238	-0.5165	-6.6583
H	5.4794	0.5769	-5.3828
H	-0.9341	1.1769	-6.8592
H	-0.1752	-1.6658	-5.9713
H	4.6596	-2.101	-4.9799
C	2.354	-3.1193	-5.5532
C	1.1893	-4.0497	-5.2048
C	1.1818	-4.4157	-3.729

C	2.5314	-5.0179	-3.3429
C	3.6858	-4.0692	-3.7116
C	5.0897	-4.6973	-3.6281
O	2.1639	-1.8402	-4.9973
O	-0.0469	-3.4549	-5.5837
O	0.1102	-5.3269	-3.5745
O	3.5728	-3.6976	-5.1182
O	5.6055	-4.8255	-2.3225
H	2.6572	-5.9753	-3.8707
H	2.4558	-3.0418	-6.6413
H	1.3384	-4.9753	-5.7809
H	1.0229	-3.51	-3.1251
H	3.6406	-3.1748	-3.0798
H	5.0795	-5.6618	-4.1646
H	5.7758	-4.0347	-4.163
H	-0.7311	-3.948	-5.0948
H	0.1663	-5.7459	-2.6888
H	5.0642	-5.4467	-1.7984
C	2.7981	-6.5056	-1.4127
C	1.6415	-7.0251	-0.5576
C	1.4496	-6.154	0.6738
C	2.7585	-6.0354	1.4556
C	3.9144	-5.5707	0.5492
C	5.3164	-5.691	1.1724
O	2.4819	-5.2441	-1.9326
O	0.4476	-7.0645	-1.3334
O	0.4167	-6.772	1.4208
O	3.973	-6.4464	-0.6184
O	5.5947	-4.7224	2.1584
H	3.0023	-7.0153	1.8924
H	3.0283	-7.2119	-2.219
H	1.9016	-8.0426	-0.2304
H	1.1553	-5.1461	0.3492
H	3.7383	-4.5377	0.2309
H	5.4533	-6.7193	1.5502
H	6.0488	-5.536	0.3757
H	-0.2728	-7.152	-0.6823
H	0.296	-6.2859	2.2639
H	5.0378	-4.8874	2.9402
C	2.712	-5.4717	3.8382
C	1.4631	-5.1803	4.6733
C	1.2278	-3.6838	4.8353
C	2.4866	-3.0182	5.3907
C	3.7087	-3.3462	4.5125

C	5.0641	-2.8954	5.0862
O	2.5166	-5.0867	2.5072
O	0.3287	-5.8084	4.087
O	0.1098	-3.5725	5.6935
O	3.8218	-4.7938	4.4152
O	5.3135	-1.5136	4.9391
H	2.6658	-3.3931	6.409
H	2.9685	-6.5353	3.8981
H	1.638	-5.6014	5.6744
H	1.0164	-3.2375	3.8514
H	3.5826	-2.9167	3.5122
H	5.141	-3.222	6.1371
H	5.8467	-3.4122	4.5245
H	-0.4432	-5.4126	4.5306
H	0.0363	-2.6493	6.0183
H	4.7281	-1.0111	5.536
C	2.4336	-0.9224	6.6419
C	1.1516	-0.229	7.1117
C	0.7828	0.9592	6.2324
C	1.9736	1.9153	6.1468
C	3.2048	1.159	5.614
C	4.5159	1.9601	5.6029
O	2.2251	-1.6084	5.4364
O	0.0843	-1.1677	7.1652
O	-0.3541	1.5303	6.8478
O	3.4687	0.0415	6.5075
O	4.5177	3.0171	4.6683
H	2.2012	2.2976	7.1528
H	2.7902	-1.6122	7.415
H	1.3479	0.1571	8.1233
H	0.5528	0.6093	5.2139
H	3.0007	0.7821	4.605
H	4.7287	2.3098	6.6266
H	5.3232	1.2819	5.3115
H	-0.7226	-0.6273	7.2519
H	-0.5958	2.3613	6.3838
H	3.9442	3.7263	5.01
P	7.7601	-1.1014	-0.243
C	8.2789	-0.2289	1.289
C	7.6463	-0.5798	2.4927
C	9.2859	0.7487	1.3017
C	8.032	0.019	3.6925
H	6.8432	-1.3115	2.4977
C	9.6626	1.3521	2.5032

H	9.768	1.047	0.3756
C	9.0409	0.9846	3.6986
H	7.5263	-0.2753	4.6069
H	9.3357	1.459	4.6311
C	8.2575	-0.0126	-1.6392
C	7.3026	0.867	-2.1735
C	9.5522	-0.0272	-2.1807
C	7.638	1.7335	-3.2156
H	6.2892	0.8619	-1.7816
C	9.8863	0.8369	-3.2249
H	10.2953	-0.7202	-1.7974
C	8.9328	1.718	-3.7398
H	10.8908	0.8157	-3.6395
H	9.1963	2.3865	-4.5554
C	8.8504	-2.5762	-0.3541
C	8.3891	-3.6834	-1.083
C	10.1147	-2.6268	0.2528
C	9.1931	-4.8166	-1.2162
H	7.3996	-3.6801	-1.5315
C	10.9125	-3.7646	0.1175
H	10.4718	-1.7863	0.8405
C	10.4546	-4.8593	-0.6192
H	11.8888	-3.7966	0.594
H	11.0762	-5.7455	-0.7185
Au	5.4426	-1.5815	-0.2598
C	3.464	-1.8645	-0.2769
C	2.2396	-1.9288	-0.2824
C	0.8151	-1.9323	-0.2968
C	0.1067	-1.2798	-1.3286
C	0.0618	-2.5372	0.7316
C	-1.2806	-1.2007	-1.3071
H	0.6665	-0.8269	-2.1414
C	-1.3275	-2.4642	0.7399
H	0.5876	-3.0475	1.5331
C	-2.0307	-1.778	-0.2665
H	-1.795	-0.6824	-2.1108
H	-1.8786	-2.9077	1.5652
C	-3.5048	-1.6419	-0.2282
C	-4.123	-0.4342	-0.6032
C	-4.3304	-2.7023	0.1855
C	-5.5058	-0.2964	-0.5734
H	-3.5038	0.4149	-0.8807
C	-5.7138	-2.57	0.2164
H	-3.8801	-3.6527	0.4608

C	-6.3345	-1.3627	-0.1657
H	-5.965	0.6461	-0.8562
H	-6.3354	-3.4043	0.5277
C	-7.7531	-1.2251	-0.1389
C	-8.9725	-1.1086	-0.1172
Au	-10.9543	-0.9236	-0.0869
P	-13.3121	-0.7078	-0.0528
C	-13.8797	0.9675	0.447
C	-14.1269	-1.8711	1.1143
C	-14.0921	-1.0237	-1.6871
C	-13.0961	2.0714	0.0734
C	-15.0587	1.1788	1.1777
C	-13.451	-2.2008	2.3004
C	-15.3887	-2.4316	0.8652
C	-13.4971	-1.974	-2.5326
C	-15.2515	-0.3573	-2.1122
C	-13.495	3.3645	0.4114
H	-12.1693	1.9151	-0.4723
C	-15.4516	2.4746	1.5181
H	-15.6643	0.3337	1.4906
C	-14.0358	-3.0636	3.2274
H	-12.4632	-1.7894	2.4906
C	-15.9681	-3.2987	1.7937
H	-15.9148	-2.2014	-0.0563
C	-14.0624	-2.2634	-3.7745
H	-12.5857	-2.4776	-2.221
C	-15.8111	-0.6466	-3.3582
H	-15.7114	0.3942	-1.4777
C	-14.6728	3.568	1.1341
H	-16.3638	2.6277	2.0884
C	-15.2946	-3.6138	2.9753
H	-16.9436	-3.7316	1.5893
C	-15.2196	-1.6002	-4.189
H	-13.5919	-2.9985	-4.4213
H	-14.9783	4.5751	1.4044
H	-15.7456	-4.2926	3.694
C	2.0529	2.3033	-1.3843
C	1.0699	2.2048	-0.3829
C	1.4217	2.2425	0.9918
C	2.7797	2.403	1.3196
C	3.7361	2.521	0.3225
C	3.3806	2.4692	-1.0387
H	1.7424	2.2494	-2.4205
H	3.059	2.4294	2.3684

H	4.1288	2.5653	-1.8188
N	-0.3034	2.0726	-0.7949
O	-0.5773	2.0489	-1.9945
O	-1.1911	1.9917	0.0873
H	-13.5026	-3.3134	4.1403
H	-12.8797	4.2108	0.1192
H	-16.7062	-0.1217	-3.6807
H	-15.6544	-1.8199	-5.1603
H	8.8188	-5.6664	-1.7803
H	6.8836	2.4038	-3.6197
H	10.4385	2.1132	2.5022
H	4.7762	2.6528	0.6052
O	0.536	2.1431	1.9956
H	-0.3503	2.02	1.5743

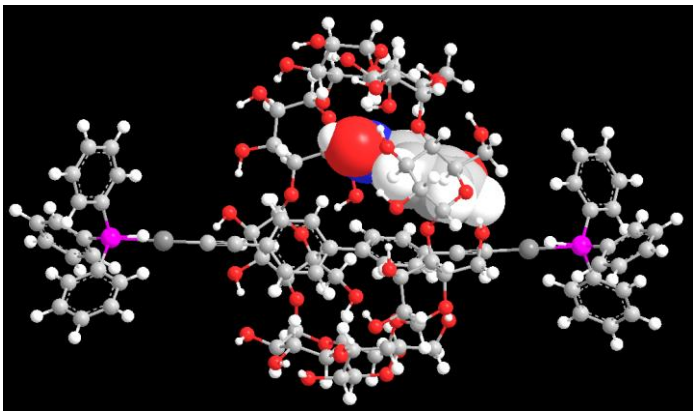


Figure S61. Calculated structure of *m*-NP⊂**Au-γ-Rot**.

The atomic coordinates of *m*-NP ⊂**Au-γ-Rot**:

C	0.585	-4.3828	-5.9604
C	-0.6472	-5.2489	-5.6898
C	-0.8043	-5.5423	-4.2054
C	0.471	-6.1944	-3.6733
C	1.7043	-5.3294	-3.9931
C	3.0608	-6.0068	-3.7217
O	0.4149	-3.0905	-5.4299
O	-1.8174	-4.6216	-6.2024
O	-1.941	-6.376	-4.1045
O	1.7322	-5.017	-5.4157
O	3.4008	-6.0773	-2.3589
H	0.5854	-7.1844	-4.1392
H	0.7788	-4.3266	-7.0372
H	-0.489	-6.2043	-6.2118
H	-0.9562	-4.5962	-3.6629

H	1.6515	-4.3996	-3.4186
H	3.0703	-6.9949	-4.2138
H	3.8322	-5.3977	-4.203
H	-2.561	-5.0712	-5.7599
H	-1.9999	-6.7398	-3.1932
H	2.8174	-6.7123	-1.9042
C	0.4432	-7.6032	-1.6695
C	-0.8189	-7.9765	-0.8908
C	-1.0063	-7.0906	0.3322
C	0.2522	-7.127	1.2008
C	1.4934	-6.7563	0.3664
C	2.8431	-6.9558	1.0772
O	0.3032	-6.3358	-2.2604
O	-1.9605	-7.9038	-1.7409
O	-2.1522	-7.605	0.9857
O	1.5575	-7.6378	-0.7936
O	3.0963	-6.0091	2.0887
H	0.3784	-8.1392	1.6134
H	0.6561	-8.3584	-2.435
H	-0.6906	-9.0128	-0.5444
H	-1.1622	-6.0498	0.0142
H	1.4122	-5.7182	0.0297
H	2.9014	-7.9943	1.4467
H	3.6316	-6.8298	0.3289
H	-2.7223	-7.8952	-1.132
H	-2.2622	-7.1522	1.8504
H	2.5088	-6.1771	2.8473
C	0.1158	-6.629	3.5975
C	-1.1714	-6.2785	4.3469
C	-1.3278	-4.7734	4.5141
C	-0.0856	-4.2009	5.1963
C	1.1794	-4.5892	4.4073
C	2.5157	-4.2123	5.0664
O	0.0502	-6.1906	2.2657
O	-2.302	-6.8273	3.6759
O	-2.5111	-4.6072	5.2757
O	1.2164	-6.0414	4.2771
O	2.8132	-2.836	4.9765
H	-0.0173	-4.6018	6.2188
H	0.2986	-7.7091	3.6363
H	-1.0934	-6.7261	5.3488
H	-1.4174	-4.2988	3.5261
H	1.1361	-4.136	3.4151
H	2.5283	-4.5749	6.1087

H	3.3095	-4.7369	4.5268
H	-3.0678	-6.3513	4.0468
H	-2.5646	-3.6803	5.5925
H	2.2234	-2.3397	5.5725
C	-0.1389	-2.1168	6.4759
C	-1.4126	-1.3354	6.8082
C	-1.6052	-0.1414	5.8815
C	-0.3556	0.7401	5.9158
C	0.8856	-0.0941	5.5468
C	2.2343	0.6259	5.7174
O	-0.2653	-2.7786	5.2493
O	-2.5436	-2.197	6.7557
O	-2.7664	0.5078	6.3596
O	0.9648	-1.22	6.4661
O	2.4401	1.674	4.7964
H	-0.2263	1.1353	6.934
H	0.086	-2.8307	7.2767
H	-1.2969	-0.948	7.8317
H	-1.7443	-0.5009	4.8499
H	0.795	-0.4645	4.5191
H	2.3216	0.9677	6.7623
H	3.0281	-0.1059	5.542
H	-3.3127	-1.5977	6.7411
H	-2.903	1.3453	5.8651
H	1.8564	2.4182	5.0285
C	-0.5788	3.137	5.5216
C	-1.851	3.8792	5.1025
C	-1.8529	4.1982	3.6158
C	-0.5992	4.9965	3.2635
C	0.6721	4.2517	3.7086
C	1.97	5.08	3.6503
O	-0.5574	1.8288	5.0024
O	-3.0062	3.128	5.455
O	-3.048	4.9211	3.3907
O	0.5587	3.8809	5.1137
O	2.4764	5.2711	2.3521
H	-0.65	5.9756	3.7627
H	-0.51	3.1043	6.6145
H	-1.8572	4.8329	5.6517
H	-1.8411	3.2608	3.0386
H	0.7969	3.3552	3.0938
H	1.8084	6.0317	4.1867
H	2.7342	4.523	4.2009
H	-3.7276	3.4992	4.914

H	-3.0353	5.2975	2.4842
H	1.8844	5.8561	1.8459
C	-0.521	6.4664	1.3044
C	-1.7035	6.7463	0.3752
C	-1.6505	5.853	-0.8546
C	-0.2966	5.9834	-1.5553
C	0.8639	5.741	-0.57
C	2.265	6.0946	-1.1009
O	-0.6174	5.1758	1.8429
O	-2.9292	6.5602	1.0756
O	-2.7347	6.2633	-1.6678
O	0.685	6.6261	0.5733
O	2.7463	5.2109	-2.0862
H	-0.2094	6.9944	-1.9795
H	-0.4751	7.2157	2.103
H	-1.6228	7.7934	0.0478
H	-1.7691	4.8079	-0.5344
H	0.8571	4.6984	-0.2353
H	2.2582	7.1438	-1.444
H	2.96	6.0276	-0.2591
H	-3.6105	6.4931	0.3816
H	-2.7062	5.7727	-2.5164
H	2.2365	5.3255	-2.9072
C	-0.0925	5.4395	-3.9375
C	-1.2172	4.9399	-4.847
C	-1.1779	3.4264	-5.0237
C	0.2147	2.9892	-5.4812
C	1.2893	3.524	-4.5157
C	2.7456	3.276	-4.9441
O	-0.2963	5.0151	-2.6171
O	-2.4792	5.3531	-4.3357
O	-2.1965	3.1384	-5.9605
O	1.1491	4.9704	-4.4475
O	3.1585	1.9387	-4.7594
H	0.4031	3.395	-6.4856
H	-0.0252	6.5321	-3.9825
H	-1.0561	5.3945	-5.8357
H	-1.3842	2.9423	-4.0563
H	1.1449	3.1014	-3.517
H	2.8858	3.6159	-5.9841
H	3.3862	3.8896	-4.3053
H	-3.1394	4.8287	-4.8241
H	-2.1065	2.2108	-6.2683
H	2.7315	1.3787	-5.4323

C	0.5786	0.9273	-6.7389
C	-0.5408	0.0221	-7.2595
C	-0.7219	-1.2152	-6.3913
C	0.6079	-1.963	-6.2925
C	1.7061	-1.0279	-5.7518
C	3.1353	-1.5944	-5.8287
O	0.2112	1.5533	-5.536
O	-1.7588	0.7495	-7.3555
O	-1.7396	-1.9623	-7.0261
O	1.7659	0.1642	-6.5836
O	3.379	-2.6699	-4.9498
H	0.8952	-2.3099	-7.2961
H	0.8302	1.6811	-7.4931
H	-0.2394	-0.3152	-8.2627
H	-1.0234	-0.9094	-5.3771
H	1.4768	-0.7475	-4.7169
H	3.3505	-1.8595	-6.877
H	3.8255	-0.7946	-5.5442
H	-2.4503	0.0683	-7.4517
H	-1.8472	-2.8275	-6.5731
H	2.8883	-3.455	-5.2548
P	10.2158	1.2888	0.3617
C	10.9788	0.5735	-1.1492
C	10.3585	0.8178	-2.3852
C	12.1496	-0.1986	-1.1092
C	10.9102	0.3111	-3.5618
H	9.4382	1.3948	-2.423
C	12.6957	-0.7077	-2.2891
H	12.6285	-0.4129	-0.1586
C	12.079	-0.4522	-3.5154
H	10.4198	0.5034	-4.5118
H	12.5029	-0.8544	-4.4315
C	10.8201	0.2605	1.7592
C	10.0532	-0.8504	2.1465
C	12.0121	0.5444	2.4431
C	10.48	-1.6712	3.1904
H	9.117	-1.0654	1.6383
C	12.4335	-0.2777	3.4898
H	12.605	1.4115	2.1682
C	11.6703	-1.3859	3.8631
H	13.3553	-0.0472	4.017
H	11.9975	-2.0205	4.6822
C	11.0027	2.9348	0.5827
C	10.3238	3.8956	1.3497

C	12.2471	3.2586	0.0213
C	10.8889	5.1526	1.5637
H	9.349	3.6615	1.7696
C	12.8067	4.5199	0.2343
H	12.7744	2.5325	-0.5899
C	12.1306	5.4665	1.0064
H	13.7687	4.7631	-0.2086
H	12.5661	6.4491	1.1664
Au	7.8555	1.3947	0.2499
C	5.8639	1.4667	0.1746
C	4.6392	1.5282	0.1341
C	3.2114	1.5287	0.1057
C	2.4739	1.4383	1.3038
C	2.5091	1.5354	-1.1164
C	1.0876	1.3347	1.274
H	2.9892	1.4338	2.2586
C	1.1214	1.4416	-1.1309
H	3.0563	1.5846	-2.0528
C	0.378	1.3377	0.0591
H	0.5463	1.26	2.2131
H	0.6052	1.3991	-2.0863
C	-1.0999	1.2391	0.0349
C	-1.7959	0.4156	0.9396
C	-1.859	1.9773	-0.8926
C	-3.1849	0.344	0.9263
H	-1.2387	-0.2079	1.6334
C	-3.2479	1.9126	-0.9077
H	-1.3489	2.6383	-1.5879
C	-3.9451	1.0961	0.0066
H	-3.7009	-0.3092	1.6235
H	-3.8135	2.504	-1.622
C	-5.3692	1.0345	0.0018
C	-6.5933	0.9833	0.0017
Au	-8.5814	0.8845	0.0117
P	-10.9455	0.7511	0.0291
C	-11.5676	-0.978	-0.0153
C	-11.731	1.5932	-1.4037
C	-11.7047	1.5092	1.5216
C	-10.8125	-1.9705	0.6304
C	-12.7602	-1.3353	-0.6623
C	-11.0528	1.5798	-2.6333
C	-12.9736	2.2384	-1.3126
C	-11.0788	2.633	2.0851
C	-12.8777	1.0108	2.1084

C	-11.2525	-3.294	0.6417
H	-9.8753	-1.7066	1.1135
C	-13.1944	-2.6622	-0.6526
H	-13.3444	-0.5823	-1.1827
C	-11.6167	2.1873	-3.7551
H	-10.0791	1.1024	-2.7069
C	-13.5321	2.8495	-2.437
H	-13.5007	2.2741	-0.364
C	-11.6271	3.256	3.2062
H	-10.157	3.0112	1.651
C	-13.4202	1.6346	3.2335
H	-13.3619	0.1309	1.6957
C	-12.4435	-3.6417	0.0004
H	-14.1168	-2.93	-1.1607
C	-12.8567	2.8229	-3.6586
H	-14.4927	3.3508	-2.3552
C	-12.798	2.7577	3.782
H	-11.1329	4.1231	3.6352
H	-12.7812	-4.6745	0.0023
H	-13.2914	3.3032	-4.531
C	2.5782	-2.1505	1.2976
C	1.6249	-2.6419	0.4077
C	1.8605	-2.7707	-0.9629
C	3.1043	-2.3839	-1.4544
C	4.0754	-1.8768	-0.5904
C	3.8144	-1.749	0.7828
H	2.3808	-2.0577	2.3581
H	1.0754	-3.1424	-1.6074
H	3.3146	-2.4621	-2.5171
N	0.2956	-2.9802	0.9119
O	-0.0034	-2.6244	2.0592
O	-0.476	-3.5925	0.169
H	-11.0821	2.1725	-4.7007
H	-10.6588	-4.0538	1.1421
H	-14.3262	1.2381	3.6838
H	-13.2196	3.2383	4.6606
H	10.3532	5.8888	2.1562
H	9.8755	-2.5246	3.4838
H	13.5996	-1.3093	-2.2475
H	5.0366	-1.5522	-0.9778
O	4.7226	-1.2252	1.6485
H	5.2238	-0.5186	1.1903

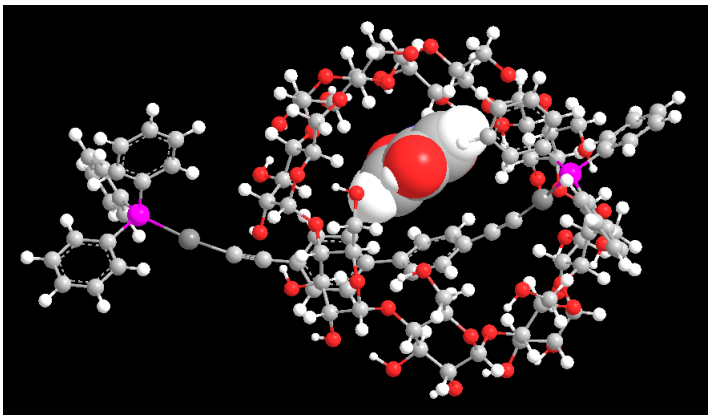


Figure S62. Calculated structure of *p*-NP⊂**Au-γ-Rot**.

The atomic coordinates of *p*-NP⊂**Au-γ-Rot**:

C	-4.23632	-3.5219	-2.47421
C	-4.52359	-4.39254	-1.25001
C	-3.24883	-4.73432	-0.48895
C	-2.24064	-5.37783	-1.44339
C	-1.98275	-4.45556	-2.65009
C	-1.12124	-5.06473	-3.77054
O	-3.81048	-2.24468	-2.07925
O	-5.46299	-3.74365	-0.39891
O	-3.6647	-5.59685	0.551442
O	-3.26207	-4.16106	-3.28554
O	0.243377	-5.168	-3.43867
H	-2.64798	-6.33442	-1.80302
H	-5.1286	-3.44705	-3.10667
H	-4.95672	-5.33456	-1.61814
H	-2.79614	-3.8156	-0.08642
H	-1.51843	-3.52259	-2.3128
H	-1.5573	-6.03282	-4.07168
H	-1.18271	-4.39549	-4.6341
H	-5.40195	-4.21515	0.452175
H	-2.87623	-5.99719	0.979326
H	0.363201	-5.88116	-2.78537
C	-0.51958	-6.91753	-0.63766
C	-0.37894	-7.38643	0.811789
C	0.704701	-6.61867	1.555238
C	2.020947	-6.70954	0.781302
C	1.821702	-6.21944	-0.66539
C	3.026533	-6.41602	-1.59947
O	-1.04156	-5.6135	-0.69753
O	-1.62612	-7.27528	1.490165
O	0.766159	-7.22563	2.834393
O	0.746711	-6.99335	-1.27479

O	4.080871	-5.51179	-1.34966
H	2.361063	-7.7562	0.767958
H	-1.16113	-7.60754	-1.19756
H	-0.07913	-8.44467	0.777279
H	0.428727	-5.55746	1.629476
H	1.549808	-5.16126	-0.65231
H	3.357373	-7.46768	-1.55189
H	2.688447	-6.22532	-2.6225
H	-1.39965	-7.33807	2.436628
H	1.533552	-6.86325	3.327008
H	4.50335	-5.7515	-0.5055
C	4.163586	-6.47967	1.941861
C	4.326574	-6.24298	3.444666
C	4.54744	-4.76749	3.75193
C	5.770998	-4.27025	2.982489
C	5.607086	-4.54113	1.475003
C	6.888334	-4.33925	0.648371
O	2.97858	-5.90119	1.476496
O	3.194144	-6.73444	4.151148
O	4.704203	-4.70538	5.156156
O	5.296583	-5.94798	1.265195
O	7.280889	-2.9942	0.488784
H	6.659139	-4.80525	3.350745
H	4.183363	-7.55297	1.719761
H	5.222528	-6.79508	3.766176
H	3.669532	-4.19247	3.419453
H	4.799969	-3.91813	1.072805
H	7.689515	-4.95502	1.091677
H	6.696071	-4.72559	-0.35676
H	3.247543	-6.31377	5.029526
H	4.963751	-3.79547	5.419197
H	7.541261	-2.61717	1.349552
C	7.085729	-2.41239	3.873315
C	6.747575	-1.60254	5.126144
C	6.074012	-0.28685	4.769391
C	6.988054	0.51312	3.845136
C	7.379134	-0.30975	2.600535
C	8.558754	0.277774	1.79927
O	5.91789	-2.86585	3.235152
O	5.927167	-2.36176	6.006521
O	5.832025	0.356108	6.006315
O	7.881915	-1.62084	3.004629
O	8.249939	1.382628	0.976604
H	7.893432	0.795562	4.403461

H	7.724673	-3.26315	4.136373
H	7.699686	-1.37304	5.627536
H	5.13342	-0.48672	4.234125
H	6.501725	-0.42663	1.955786
H	9.378476	0.508455	2.502144
H	8.91962	-0.505	1.126401
H	5.538833	-1.70801	6.616983
H	5.635213	1.305407	5.850608
H	7.838052	2.104233	1.488918
C	6.853646	2.952283	3.632225
C	6.012649	3.829776	4.561063
C	4.678831	4.199144	3.927456
C	4.917903	4.851456	2.566112
C	5.768711	3.933314	1.666669
C	6.257283	4.579688	0.359029
O	6.262928	1.690386	3.473556
O	5.809823	3.167839	5.805641
O	4.053517	5.059997	4.86062
O	6.999563	3.603616	2.381459
O	5.249346	4.74556	-0.61211
H	5.44381	5.806218	2.714614
H	7.872446	2.85261	4.025438
H	6.576023	4.759203	4.730939
H	4.085658	3.28586	3.767737
H	5.217798	3.014914	1.436147
H	6.767618	5.529444	0.597125
H	7.00129	3.911019	-0.08123
H	5.096934	3.668916	6.243142
H	3.260868	5.4676	4.45081
H	4.636978	5.446668	-0.32799
C	3.286764	6.409135	1.611575
C	1.991872	6.86009	2.292303
C	0.797418	6.063657	1.787192
C	0.714072	6.157793	0.263069
C	2.045501	5.730669	-0.38682
C	2.163237	6.009569	-1.89573
O	3.624414	5.10315	1.992302
O	2.112166	6.740509	3.704506
O	-0.32978	6.617523	2.438777
O	3.121044	6.510221	0.203106
O	1.352548	5.175122	-2.69236
H	0.49467	7.198691	-0.01582
H	4.101583	7.101692	1.850297
H	1.836612	7.916252	2.026352

H	0.934372	5.00707	2.061854
H	2.220878	4.66426	-0.20958
H	1.967599	7.080189	-2.07633
H	3.198649	5.810339	-2.18622
H	1.200887	6.804272	4.044685
H	-1.14917	6.225148	2.068254
H	0.419827	5.427013	-2.57316
C	-1.42883	5.875558	-0.87898
C	-2.78176	5.58831	-0.22528
C	-3.20072	4.12524	-0.33828
C	-3.1139	3.667064	-1.79645
C	-1.70719	3.96046	-2.35279
C	-1.51859	3.679539	-3.85116
O	-0.37491	5.312732	-0.14505
O	-2.75886	5.996527	1.137123
O	-4.50906	4.090592	0.187349
O	-1.45096	5.381988	-2.21479
O	-1.47928	2.293449	-4.16334
H	-3.8534	4.222685	-2.39085
H	-1.28444	6.956363	-0.98319
H	-3.52813	6.183218	-0.77259
H	-2.51693	3.49898	0.255628
H	-0.95383	3.400969	-1.78618
H	-2.30315	4.189509	-4.42856
H	-0.55352	4.091146	-4.15634
H	-3.56119	5.608377	1.531849
H	-4.90245	3.199829	0.04206
H	-2.37646	1.913257	-4.07424
C	-4.51621	1.834386	-2.6122
C	-5.5264	1.049379	-1.75989
C	-4.98413	-0.31249	-1.34947
C	-4.48644	-1.08347	-2.57593
C	-3.52823	-0.26109	-3.44985
C	-3.26407	-0.851	-4.84891
O	-3.41272	2.264507	-1.84336
O	-5.89167	1.846591	-0.64724
O	-6.04941	-0.99583	-0.7166
O	-4.08148	1.059198	-3.71833
O	-2.37419	-1.93928	-4.85135
H	-5.36229	-1.38502	-3.16988
H	-5.01441	2.702175	-3.05785
H	-6.4072	0.878124	-2.39828
H	-4.13802	-0.16972	-0.6608
H	-2.57425	-0.16695	-2.92435

H	-4.23123	-1.0915	-5.32406
H	-2.79696	-0.06665	-5.45383
H	-6.29296	1.285427	0.049866
H	-5.74231	-1.89173	-0.45799
H	-2.78909	-2.70784	-4.41697
P	7.228904	0.587683	-3.01628
C	6.213761	0.270441	-4.51685
C	4.867071	0.672317	-4.49508
C	6.717823	-0.3669	-5.66052
C	4.041132	0.446356	-5.59705
H	4.458604	1.148733	-3.60797
C	5.889715	-0.59061	-6.7624
H	7.749188	-0.70447	-5.6878
C	4.553423	-0.18638	-6.73224
H	2.997274	0.742499	-5.54776
H	3.909172	-0.37492	-7.5869
C	8.613538	-0.61713	-3.04255
C	8.555568	-1.72667	-2.18689
C	9.733166	-0.44373	-3.87374
C	9.597265	-2.65686	-2.17598
H	7.717752	-1.86438	-1.50993
C	10.76647	-1.38055	-3.86405
H	9.805472	0.430351	-4.5149
C	10.6989	-2.48961	-3.01587
H	11.62866	-1.23881	-4.51044
H	11.51005	-3.21313	-3.00357
C	8.053382	2.209453	-3.28882
C	8.777248	2.759051	-2.21604
C	7.992398	2.898532	-4.50677
C	9.440421	3.975458	-2.37451
H	8.814095	2.240032	-1.26037
C	8.652651	4.121383	-4.65464
H	7.4279	2.487091	-5.33776
C	9.37872	4.659383	-3.59209
H	8.59581	4.651396	-5.60175
H	9.890859	5.610859	-3.70903
Au	5.863272	0.546341	-1.0857
C	4.522687	0.580681	0.397249
C	3.545436	0.659736	1.134296
C	2.298046	0.812739	1.803257
C	1.714642	-0.20686	2.582522
C	1.535723	1.977065	1.570016
C	0.392187	-0.11045	3.005894
H	2.287134	-1.10522	2.792893

C	0.217091	2.065582	1.991678
H	1.980353	2.776895	0.987939
C	-0.40278	1.002922	2.675962
H	-0.04373	-0.93338	3.564464
H	-0.36699	2.935848	1.705331
C	-1.87164	1.007478	2.864685
C	-2.60627	-0.18045	2.681369
C	-2.59447	2.197239	3.074856
C	-3.99446	-0.16519	2.627813
H	-2.07921	-1.11286	2.503094
C	-3.98445	2.218334	3.022119
H	-2.05702	3.123327	3.261938
C	-4.71264	1.041527	2.756589
H	-4.54183	-1.08199	2.430411
H	-4.52268	3.152407	3.148334
C	-6.11839	1.058524	2.517168
C	-7.30375	1.013875	2.205888
Au	-9.1286	0.741477	1.452115
P	-11.1649	0.260182	0.356278
C	-10.8608	-0.2271	-1.38971
C	-12.3538	1.658808	0.281186
C	-12.0855	-1.13299	1.122232
C	-9.62476	-0.80833	-1.71895
C	-11.8218	-0.03834	-2.39585
C	-11.8379	2.960507	0.17265
C	-13.7436	1.471874	0.322183
C	-12.054	-1.25438	2.521115
C	-12.8112	-2.06755	0.368633
C	-9.36801	-1.2109	-3.03031
H	-8.85215	-0.93308	-0.96495
C	-11.557	-0.4403	-3.70593
H	-12.7714	0.433534	-2.16077
C	-12.6996	4.05398	0.089508
H	-10.762	3.11552	0.162629
C	-14.6023	2.570157	0.243669
H	-14.156	0.472767	0.426006
C	-12.7508	-2.28302	3.154641
H	-11.4742	-0.54943	3.111408
C	-13.5031	-3.09889	1.006824
H	-12.8275	-1.99975	-0.71476
C	-10.3316	-1.03016	-4.02435
H	-12.3062	-0.28684	-4.47789
C	-14.0825	3.860435	0.125007
H	-15.6772	2.41605	0.280889

C	-13.4762	-3.20666	2.398447
H	-12.7171	-2.36875	4.237051
H	-10.1267	-1.33929	-5.04581
H	-14.7529	4.713685	0.068627
C	1.62547	-1.90516	-1.44477
C	0.556104	-1.77159	-0.54716
C	-0.40605	-0.77107	-0.70713
C	-0.30348	0.100889	-1.77866
C	0.72985	-0.05395	-2.72359
C	1.699321	-1.05732	-2.53763
H	2.370024	-2.6773	-1.29064
H	-1.2037	-0.67147	0.017978
H	-1.02005	0.906797	-1.8885
H	2.497457	-1.15788	-3.2647
N	0.445769	-2.67228	0.576421
O	1.432943	-3.35472	0.879614
O	-0.62891	-2.73108	1.191026
O	0.832588	0.733801	-3.81105
H	0.035718	1.3072	-3.90015
H	-12.2899	5.056813	0.007763
H	-8.40736	-1.6589	-3.26793
H	-14.0578	-3.8212	0.414149
H	-14.0113	-4.01323	2.892008
H	10.00026	4.393581	-1.54209
H	9.542006	-3.50062	-1.49462
H	6.288464	-1.09228	-7.64019

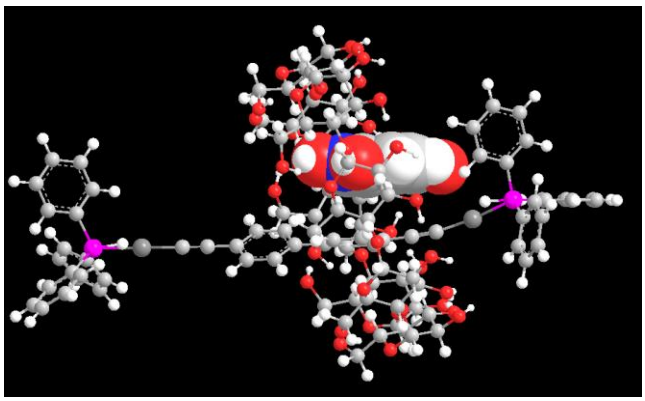


Figure S63. Calculated structure of *p*-NBA⊂**Au-γ-Rot**.

The atomic coordinates of *p*-NBA⊂**Au-γ-Rot**:

C	1.0947	-4.979	-4.8952
C	-0.2304	-5.7363	-5.0018
C	-1.0097	-5.6638	-3.6961
C	-0.1461	-6.1867	-2.5476

C	1.1951	-5.4298	-2.4831
C	2.2456	-6.0378	-1.5337
O	0.8637	-3.5996	-4.7648
O	-0.9996	-5.2214	-6.0808
O	-2.1801	-6.4289	-3.9082
O	1.8283	-5.4942	-3.7953
O	1.9722	-5.84	-0.1696
H	0.0506	-7.2566	-2.7116
H	1.7194	-5.179	-5.773
H	0.0132	-6.7915	-5.1953
H	-1.2576	-4.6115	-3.4848
H	1.0206	-4.385	-2.2043
H	2.376	-7.1039	-1.791
H	3.196	-5.5348	-1.7351
H	-1.901	-5.564	-5.9406
H	-2.6332	-6.5779	-3.05
H	1.2002	-6.372	0.0933
C	-1.1496	-7.13	-0.5246
C	-2.6499	-7.2985	-0.2734
C	-3.1942	-6.1636	0.5794
C	-2.394	-6.0547	1.8794
C	-0.8888	-5.9078	1.5816
C	0.0371	-6.0317	2.8056
O	-0.9119	-6.016	-1.3482
O	-3.3454	-7.3789	-1.5152
O	-4.5658	-6.464	0.7937
O	-0.4824	-7.0129	0.7186
O	0.0058	-4.9178	3.6658
H	-2.5622	-6.9587	2.4848
H	-0.7394	-8.0361	-0.9849
H	-2.7835	-8.2398	0.2795
H	-3.0813	-5.214	0.0388
H	-0.7005	-4.9529	1.0813
H	-0.1911	-6.9762	3.3302
H	1.0626	-6.1041	2.4318
H	-4.2838	-7.2468	-1.2903
H	-4.9121	-5.8905	1.5121
H	-0.8539	-4.8739	4.1203
C	-3.38	-5.0203	3.8767
C	-4.8039	-4.4665	3.9589
C	-4.825	-2.9618	3.7053
C	-3.9003	-2.2899	4.7235
C	-2.4782	-2.8635	4.5527
C	-1.426	-2.3437	5.5447

O	-2.9077	-4.9097	2.5653
O	-5.6481	-5.1483	3.0339
O	-6.1861	-2.5817	3.7977
O	-2.5556	-4.3005	4.7836
O	-1.0223	-1.0188	5.2728
H	-4.2521	-2.5189	5.7404
H	-3.3466	-6.0614	4.2192
H	-5.1722	-4.6455	4.9794
H	-4.4329	-2.7539	2.699
H	-2.1191	-2.6804	3.5341
H	-1.799	-2.4647	6.5755
H	-0.5365	-2.9713	5.4393
H	-6.4612	-4.6127	2.9897
H	-6.2532	-1.6327	4.0487
H	-1.7246	-0.4124	5.5684
C	-4.2716	-0.0456	5.607
C	-5.5259	0.7807	5.3083
C	-5.2494	1.8087	4.225
C	-4.0975	2.7118	4.6662
C	-2.8479	1.8866	5.0238
C	-1.7622	2.6669	5.7879
O	-3.9497	-0.8748	4.5123
O	-6.5896	-0.093	4.9461
O	-6.4584	2.5319	4.0436
O	-3.1989	0.8119	5.9433
O	-1.104	3.6461	5.0217
H	-4.4171	3.2992	5.5408
H	-4.4317	-0.6578	6.5017
H	-5.7948	1.3118	6.2341
H	-4.951	1.303	3.2975
H	-2.4222	1.4691	4.1057
H	-2.2151	3.0826	6.7049
H	-0.9973	1.9489	6.0997
H	-7.2659	0.4601	4.5144
H	-6.3035	3.237	3.3756
H	-1.726	4.3602	4.7953
C	-3.9918	4.9672	3.7233
C	-4.8431	5.5191	2.5769
C	-4.1044	5.4048	1.2515
C	-2.7562	6.1185	1.3549
C	-1.9345	5.5666	2.5376
C	-0.667	6.3632	2.8979
O	-3.8083	3.5877	3.5727
O	-6.0967	4.8446	2.5164

O	-4.9639	5.9898	0.2871
O	-2.7481	5.6522	3.7446
O	0.3961	6.1985	1.9914
H	-2.9329	7.1937	1.5061
H	-4.4571	5.1928	4.69
H	-5.017	6.5854	2.784
H	-3.9235	4.3431	1.0273
H	-1.6631	4.5226	2.3479
H	-0.942	7.4234	3.0378
H	-0.3125	5.9875	3.8619
H	-6.4209	4.986	1.6084
H	-4.4725	6.1058	-0.5528
H	0.1841	6.6425	1.1513
C	-1.6056	7.0238	-0.6062
C	-2.1515	7.0508	-2.038
C	-1.5753	5.9276	-2.8933
C	-0.0489	5.932	-2.8041
C	0.3902	5.8543	-1.3301
C	1.9036	5.924	-1.068
O	-2.1	5.9158	0.0939
O	-3.5735	6.9897	-2.0081
O	-2.0619	6.1491	-4.2038
O	-0.1848	7.0096	-0.6585
O	2.5668	4.7171	-1.3753
H	0.3353	6.8651	-3.2407
H	-1.8645	7.9538	-0.0879
H	-1.8336	8.0042	-2.4849
H	-1.933	4.9618	-2.5015
H	0.007	4.9392	-0.8666
H	2.3353	6.7867	-1.6024
H	2.0442	6.0936	0.0028
H	-3.847	6.8369	-2.9298
H	-1.4803	5.6937	-4.8496
H	2.6757	4.6464	-2.3406
C	1.436	5.0128	-4.5132
C	0.9782	4.6311	-5.9198
C	0.7236	3.1358	-6.0452
C	1.923	2.3287	-5.5392
C	2.392	2.8032	-4.1526
C	3.763	2.2534	-3.7238
O	0.4006	4.8163	-3.5835
O	-0.1969	5.3643	-6.2538
O	0.4555	2.9216	-7.4198
O	2.5778	4.2431	-4.1773

O	3.768	0.8585	-3.5113
H	2.7504	2.444	-6.2541
H	1.7751	6.0543	-4.4935
H	1.7903	4.9002	-6.6108
H	-0.1465	2.8722	-5.4271
H	1.6389	2.5443	-3.3999
H	4.5137	2.5633	-4.4691
H	4.0324	2.714	-2.769
H	-0.5393	4.9294	-7.0566
H	0.201	1.9793	-7.5518
H	3.6536	0.4088	-4.3668
C	2.0458	0.0664	-6.4465
C	0.8962	-0.7025	-7.1339
C	0.3532	-1.8492	-6.2818
C	1.4923	-2.6838	-5.6765
C	2.5281	-1.8077	-4.9565
C	3.8036	-2.5342	-4.4887
O	1.5349	0.9471	-5.4674
O	-0.1286	0.1949	-7.5475
O	-0.4849	-2.6241	-7.1047
O	3.0103	-0.8041	-5.8872
O	3.6166	-3.3387	-3.3515
H	1.9873	-3.2424	-6.4839
H	2.5932	0.6395	-7.2019
H	1.3048	-1.1429	-8.0504
H	-0.2065	-1.4255	-5.4315
H	2.0675	-1.3195	-4.0893
H	4.2266	-3.0935	-5.3411
H	4.5312	-1.7654	-4.2113
H	-0.7885	0.2815	-6.8307
H	-0.7386	-3.4369	-6.619
H	3.1174	-4.1379	-3.5986
P	12.3514	-0.0402	1.692
C	12.9334	-1.6891	1.1233
C	12.2155	-2.3277	0.0991
C	14.0586	-2.3239	1.6709
C	12.6272	-3.5717	-0.3792
H	11.3278	-1.855	-0.3128
C	14.4645	-3.5709	1.1922
H	14.6107	-1.8521	2.4782
C	13.7518	-4.1948	0.1663
H	12.0616	-4.0578	-1.1691
H	14.0664	-5.168	-0.2006
C	13.0046	0.1449	3.4008

C	12.2025	-0.2955	4.4661
C	14.2632	0.7014	3.6743
C	12.6598	-0.1954	5.78
H	11.2162	-0.7056	4.2649
C	14.7149	0.8042	4.9915
H	14.8861	1.0647	2.8625
C	13.9162	0.3545	6.0446
H	15.6891	1.2414	5.1934
H	14.2679	0.4401	7.0692
C	13.2779	1.1838	0.6794
C	12.7343	2.4709	0.5381
C	14.4959	0.8813	0.0522
C	13.407	3.442	-0.2035
H	11.779	2.7062	1
C	15.1635	1.8549	-0.6935
H	14.9185	-0.1155	0.1353
C	14.6221	3.1356	-0.8203
H	16.1038	1.6091	-1.1796
H	15.1413	3.8901	-1.405
Au	10.0026	0.2189	1.5579
C	8.0281	0.4271	1.4469
C	6.8104	0.5439	1.3802
C	5.3928	0.6786	1.3055
C	4.6105	0.7664	2.4759
C	4.7291	0.7226	0.0624
C	3.2283	0.8935	2.4038
H	5.1051	0.7377	3.4421
C	3.3478	0.8599	-0.0029
H	5.3028	0.631	-0.8546
C	2.5678	0.9499	1.1639
H	2.6511	0.9775	3.3206
H	2.8702	0.8567	-0.9783
C	1.0942	1.0786	1.0836
C	0.2521	0.3583	1.9501
C	0.4911	1.9163	0.1247
C	-1.1316	0.4387	1.8407
H	0.6799	-0.2974	2.7025
C	-0.8935	2.006	0.0159
H	1.1237	2.531	-0.5109
C	-1.7372	1.2547	0.8605
H	-1.7568	-0.1486	2.5059
H	-1.341	2.6572	-0.73
C	-3.157	1.2632	0.713
C	-4.3759	1.1823	0.6003

Au	-6.3075	0.7178	0.4569
P	-8.5242	-0.1012	0.3087
C	-8.4957	-1.8563	-0.2429
C	-9.6024	0.7911	-0.8813
C	-9.4335	-0.0944	1.9038
C	-7.5182	-2.7025	0.3123
C	-9.3679	-2.3599	-1.2177
C	-8.9977	1.4453	-1.9667
C	-10.9984	0.8375	-0.744
C	-9.1735	0.9455	2.8117
C	-10.3724	-1.0811	2.2387
C	-7.4135	-4.0278	-0.1105
H	-6.8442	-2.3261	1.0778
C	-9.2639	-3.6904	-1.6322
H	-10.1202	-1.716	-1.6626
C	-9.7779	2.1199	-2.9062
H	-7.9155	1.4337	-2.0671
C	-11.7749	1.517	-1.684
H	-11.4791	0.3543	0.1011
C	-9.8547	1.0031	4.0292
H	-8.4211	1.6952	2.5852
C	-11.0502	-1.02	3.4585
H	-10.5648	-1.9037	1.5561
C	-8.2862	-4.5216	-1.0849
H	-9.9427	-4.0711	-2.3906
C	-11.1669	2.1565	-2.7664
H	-12.8545	1.5511	-1.5663
C	-10.795	0.021	4.3529
H	-9.6395	1.8116	4.7224
H	-8.1987	-5.5518	-1.4192
H	-11.7734	2.6889	-3.4939
C	-3.1799	-1.3609	-1.7206
C	-1.8248	-1.5528	-1.4619
C	-0.8203	-0.9673	-2.2312
C	-1.1938	-0.1839	-3.317
C	-2.5533	-0.0078	-3.6234
C	-3.5432	-0.583	-2.8145
H	-3.9222	-1.8094	-1.0743
H	0.2189	-1.1225	-1.9692
H	-0.4384	0.297	-3.9289
H	-4.5906	-0.4243	-3.0409
N	-1.4394	-2.4207	-0.3377
O	-2.3366	-2.8132	0.4115
O	-0.2544	-2.7208	-0.2259

H	-9.2993	2.6252	-3.7404
H	-6.6367	-4.6688	0.2976
H	-11.7721	-1.7917	3.7115
H	-11.3196	0.062	5.3034
H	12.9755	4.4336	-0.3077
H	12.0293	-0.537	6.5961
H	15.3342	-4.0568	1.6264
C	-2.9056	0.7714	-4.8347
O	-2.1184	1.0968	-5.7126
O	-4.21	1.1009	-4.9093
H	-4.321	1.582	-5.7512

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