

Supporting information

Self-assembled metallasupramolecular cages towards light harvesting systems for oxidative cyclization

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Experimental section

Materials and methods

The chemicals and solvents used in the present study were purchased from commercial sources and used without further purification. NMR spectra were recorded in a Bruker 400 MHz spectrometer and the chemical shifts (δ) in the ^1H NMR spectra are reported in ppm relative to tetramethylsilane (Me_4Si) as an internal standard (0.0 ppm) or proton resonance resulting from incomplete deuteration of the solvents CDCl_3 (7.26 ppm), CD_3OD (3.30 ppm) and CD_3CN (1.94 ppm). ^{13}C NMR spectra were recorded at 100 MHz, and the chemical shifts (δ) are reported in ppm relative to external CDCl_3 at 77.8–77.2 ppm. $^{31}\text{P}\{\text{H}\}$ NMR spectra were recorded at 162 MHz spectrometer using an external unlocked sample of 85% H_3PO_4 ($\delta = 0$) as reference. Electrospray ionization mass spectrometry (ESI-MS) experiments were carried out in Agilent 6538 Ultra-High Definition (UHD) Accurate Mass Q-TOF spectrometer using standard spectroscopic-grade solvents. IR spectra were recorded with a Bruker ALPHA FTIR spectrometer. Analab μ -ThermoCal10 instrument was used for melting point determination. UV/Vis and fluorescence spectra were recorded with PerkinElmer Lambda-750 and Horiba Jobin Yvon Fluoromax4 spectrophotometers, respectively. The 1931 Commission Internationale de l'eclairage (CIE) chromaticity coordinates for the corresponding photoluminescence spectra were calculated by "GOCIE" software.^{s1} Time resolved fluorescence measurements were carried out on Fluorolog 04 using 325 and 340 nm nano-LED source. The absolute fluorescence quantum yields were measured by Quanta- ϕ Horiba Instrument coupled with Fluorolog spectrophotometer. Transmission Electron Microscopy (TEM) was performed with a JEOL JEM-2100F instrument operating at 200 kV. Dynamic Light Scattering (DLS) measurements were performed with a Zetaseizer instrument ZEN3600 (Malvern, UK) with a 1738 back scattering angle and He-Ne laser ($\lambda=633$ nm). Scanning Electron Microscopy (SEM) image was obtained using Zeiss Ultra-55 SEM instrument with the sample deposited on a silicon wafer. The MeCN/water mixtures with various water fractions were prepared by slowly adding ultrapure water into the MeCN solution of samples. Starting materials for the synthesis of ligand **C1** and *trans*-Pt acceptors **A1**, **A2** and **A3** were prepared according to the reported procedures.^{s2} Philips 40W LED bulb (4000 Lm, 6500K) has been used as a white light source for catalysis.

Computational methodology

Full geometry optimizations were performed using the Gaussian 09 package.^{s3} The hybrid B3LYP functional was used in all calculations as implemented in the Gaussian 09 package, mixing the exact Hartree–Fock-type exchange with Becke's expression for the exchange functional^{s4} that was proposed by Lee, Yang, and Parr for the correlation contribution.^{s5} The LanL2DZ basis set was used in the case of the platinum atom and the 6-31g(d) basis set for all other atoms in all calculations. The calculations were carried out methodically with the cationic units in gas phase. Solvent molecules or solvent model or any counter ions were not considered in the calculations.

Synthesis of C1

Compound **C1** was prepared according to the slightly modified reported procedure.^{s2a} 1,1,2,2-tetra-p-tolylethene (1 g, 2.57 mmol), N-bromosuccinimide (2.01 g, 11.30 mmol), benzoyl peroxide (31 mg, 0.12 mmol) and CCl₄ (30 mL) were taken in 100 mL round-bottom flask and heated to reflux for 24 h. The reaction mixture was then cooled to ambient temperature and filtered to remove by-product. Crude product was purified by column chromatography using silica 60 – 120 (hexane/ethyl acetate: 70/30) as pale yellow solid. Yield: 1.61 g (89%). m.p. 140 °C. ¹H NMR (400 MHz; CDCl₃) δ (ppm): 7.13 (d, 8H, J= 8 Hz), 6.96 (d, 8H, J= 8 Hz), 4.42 (s, 8H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 143.6, 136.7, 132.0, 129.0, 126.5, 33.8. FT-IR (KBr), v (cm⁻¹): 3925, 3024, 2968, 1915, 1705, 1605, 1509, 1410, 1227, 1097, 1018, 789, 611, 489. ESI MS (m/z): Calcd. For [M+Na]⁺ 726.83, found 726.84 for [M+Na]⁺.

Synthesis of L

Imidazole (0.77 g, 11.36 mmol), KOH (0.64 g, 11.36 mmol) and 25 mL of acetonitrile were taken in a 50 mL round bottom flask and the reaction mixture was stirred for 2 h at room temperature. Then compound **C1** (1 g, 1.42 mmol) was added and stirring continued for further 36 h. Subsequently, solvent was evaporated, and water was added to it and extracted with ethyl acetate. Crude product was purified by column chromatography using neutral alumina (CHCl₃/methanol: 95/5) as yellow solid. Yield: 0.62 g (67%). m.p. 190 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.44 (4H, s, 7.03)4H, s(, 6.84 – 6.93)20H, m(, 5.00)8H, s(. ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 143.4, 140.9, 137.7, 135.1, 132.1, 129.9, 127.3, 119.8, 50.9. FT-IR (KBr), v (cm⁻¹): 3388, 3112, 3023, 2926, 1923, 1669, 1509, 1282, 1231, 1108, 1076, 1020, 914, 821, 744, 662. ESI MS (m/z): Calcd. For [M+Na]⁺ 675.30, found, 675.28 for [M+Na]⁺.

Self-assembly of 1a

Ligand **L** (50.0 mg, 0.07 mmol) and acceptor **A1** (85.1 mg, 0.15 mmol) were mixed in 5 mL methanol followed by stirring at 50 °C for 24 h. Then the reaction mixture was centrifuged and obtained clear solution was concentrated and precipitated with excess diethyl ether to obtain the product as white powder by filtration. Isolated yield: 116.1 mg (86%). m.p. >200 °C. ¹H NMR (400 MHz, CD₃OD) δ (ppm): 8.51 (8H), 7.30 (12H), 6.86 – 6.96 (36H), 5.15 (16H), 1.89 (48H), 1.26- 1.29 (72H). ³¹P{¹H} NMR (CD₃OD, 162 MHz) δ (ppm): 1.12 ¹⁹⁵Pt satellites, δ (ppm): 10.93 ppm (d, ¹J_{Pt-P} = 3924 Hz), -8.51 ppm (d, ¹J_{Pt-P} = 3912 Hz).

Self-assembly of 1b

1a (100 mg, 0.03 mmol) was dissolved in 2 mL methanol and excess KF₆ (66.26 mg, 0.36 mmol) was added to it. Then the reaction mixture was stirred at room temperature for 24 h. The obtained precipitate was filtered off and washed several times with methanol and dried in vacuum to get pure metal complex as white powder. Isolated yield: 109 mg (92%). m.p. >200 °C. ¹H NMR (400 MHz, CD₃OD) δ (ppm): 8.01 (8H), 6.86 – 7.09 (48H), 5.01-5.03 (16H), 1.80 (48H), 1.19- 1.24 (72H). ³¹P{¹H} NMR (CD₃OD, 162 MHz) δ (ppm): 1.35 ¹⁹⁵Pt satellites, δ (ppm): 11.30 ppm (d, ¹J_{Pt-P} = 3980 Hz), -8.34 ppm (d, ¹J_{Pt-P} = 3976 Hz). DOSY (400 MHz, CD₃CN) : logD = -9.38 ESI-MS (m/z): 1950.01 [(**1b**) – 2PF₆]²⁺, 1252.10 [(**1b**) –

$3\text{PF}_6]^{3+}$. FT-IR (KBr), ν (cm^{-1}): 3663, 3594, 3439, 3150, 2977, 2939, 2882, 1671, 1533, 1459, 1417, 1243, 1110, 1037, 848, 557.

Self-assembly of **2a**

Ligand **L** (30 mg, 0.045 mmol) and acceptor **A2** (102 mg, 0.09 mmol) were mixed in 5 mL methanol followed by stirring at 50°C for 24 h. Then reaction mixture was centrifuged and obtained clear solution was concentrated and precipitated with excess diethyl ether to obtain the product as white powder by filtration. Isolated yield: 115 mg (87%). m.p. >200 °C. ^1H NMR)400 MHz, CD_3OD (δ (ppm): 8.34 (8H), 7.45 - 7.56 (64H), 5.56 (16H), 2.15 (94H), 1.48 – 1.51 (144H). $^{31}\text{P}\{\text{H}\}$ NMR (CD_3OD , 162 MHz) δ (ppm): 15.78 ^{195}Pt satellites, δ (ppm): 22.96 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2872$ Hz), 8.55 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2892$ Hz).

Self-assembly of **2b**

2a (100 mg, 0.017 mmol) was dissolved in 2 mL methanol and excess KF_6 (38 mg, 0.21 mmol) was added to it. Then the reaction mixture was stirred at room temperature for 24h. The obtained precipitate was filtered off and washed several times with methanol which was dried in vacuum to get pure metal complex as white powder. m.p. >200 °C. Isolated yield: 104 mg (94%); ^1H NMR)400 MHz, CD_3CN (δ (ppm): 7.94 (8H), 7.05 - 7.25 (64H), 5.16 (16H), 1.74 (94H), 1.07 (144H). $^{31}\text{P}\{\text{H}\}$ NMR (CD_3CN , 162 MHz) δ (ppm): 16.34 ^{195}Pt satellites, δ (ppm): 23.56 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2888$ Hz), 9.14 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2880$ Hz); δ (ppm) for PF_6^- (septate): -131.34, -135.71, -140.08, -144.44, -148.81, -153.18, -157.50. DOSY (400 MHz, CD_3CN) : logD = -9.78. ESI MS (m/z): 3061.67 [**2b**] – $2\text{PF}_6]^{2+}$, 1992.54 [**2b**] – $3\text{PF}_6]^{3+}$, 1458.31 [**2b**] – $4\text{PF}_6]^{4+}$, 1137.49 [**2b**] – $5\text{PF}_6]^{5+}$. FT-IR (KBr), ν (cm^{-1}): 3646, 3444, 3147, 2973, 2938, 2879, 2123, 1531, 1456, 1414, 1379, 1240, 1109, 1036, 847, 764, 558.

Self-assembly of **3a**

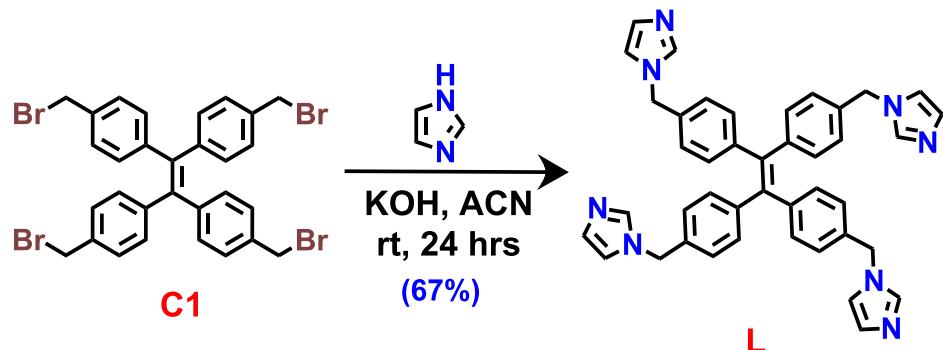
Ligand **L** (40 mg, 0.06 mmol) and acceptor **A3** (136 mg, 0.12 mmol) were mixed in 5 mL methanol followed by stirring at 50°C for 24 h. Then reaction mixture was centrifuged and obtained clear solution was concentrated and precipitated with excess diethyl ether to obtain the product as white powder by filtration. Isolated yield: 145 mg (82%). m.p.> 200°C. ^1H NMR)400 MHz, CD_3OD (δ (ppm): 8.00 (8H), 7.11- 7.21 (64H), 5.22 (16H), 1.81 (94H), 1.13- 1.16 (144H). $^{31}\text{P}\{\text{H}\}$ NMR (CD_3OD , 162 MHz) δ (ppm): 15.65. ^{195}Pt satellites, δ (ppm): 22.81 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2904$ Hz), 8.31 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2936$ Hz).

Self-assembly of **3b**

3a (100 mg, 0.017 mmol) was dissolved in 2 mL methanol and excess KF_6 (38 mg, 0.21 mmol) was added to it. Then the reaction mixture was stirred at room temperature for 24 h. The obtained precipitate was filtered off and washed several times with methanol which was dried in vacuum to get pure metal complex as white powder. m.p.> 200°C. Isolated yield: 100 mg (90%); ^1H NMR)400 MHz, CD_3CN (δ (ppm): 8.23 (8H), 7.34 - 7.73 (64H), 5.45 (16H), 1.74 (94H), 1.07 (144H). $^{31}\text{P}\{\text{H}\}$ NMR (CD_3CN , 162 MHz) δ (ppm): 16.42 ^{195}Pt satellites, δ (ppm): 23.58 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2864$ Hz), 9.09 ppm (d, $^1\text{J}_{\text{Pt-P}} = 2932$ Hz); δ (ppm) for PF_6^- (septate): -131.34, -135.71, -140.08, -144.44, -148.81, -153.18, -157.50. DOSY (400

MHz, CD₃CN) : logD = -9.81. ESI MS (m/z): 1992.54 [(3b) – 3PF₆]³⁺, 1137.49 [(3b) – 5PF₆]⁵⁺, 923.80 [(3b) – 6PF₆]⁶⁺. FT-IR (KBr), ν (cm⁻¹): 3508, 3133, 2969, 2939, 2881, 2126, 1586, 1530, 1457, 1417, 1272, 1158, 1032, 767, 638, 537, 517.

Reaction scheme



Scheme S1 Reaction scheme for synthesis of **L**.

Spectroscopic characterization

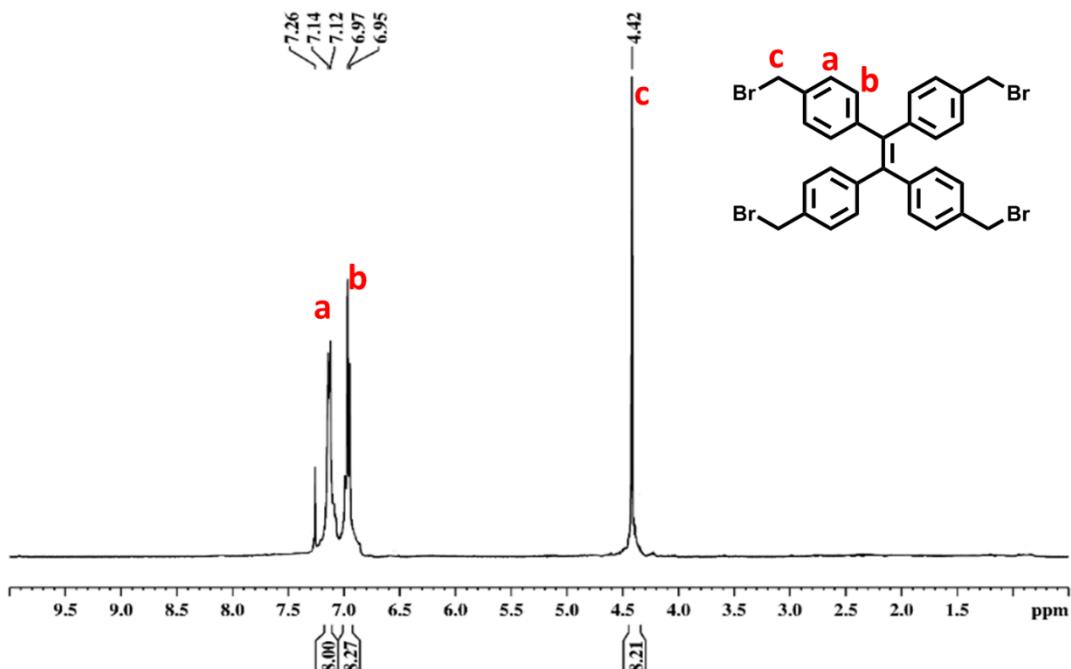


Fig. S1 ¹H NMR (CDCl₃, 400 MHz) of **C1**.

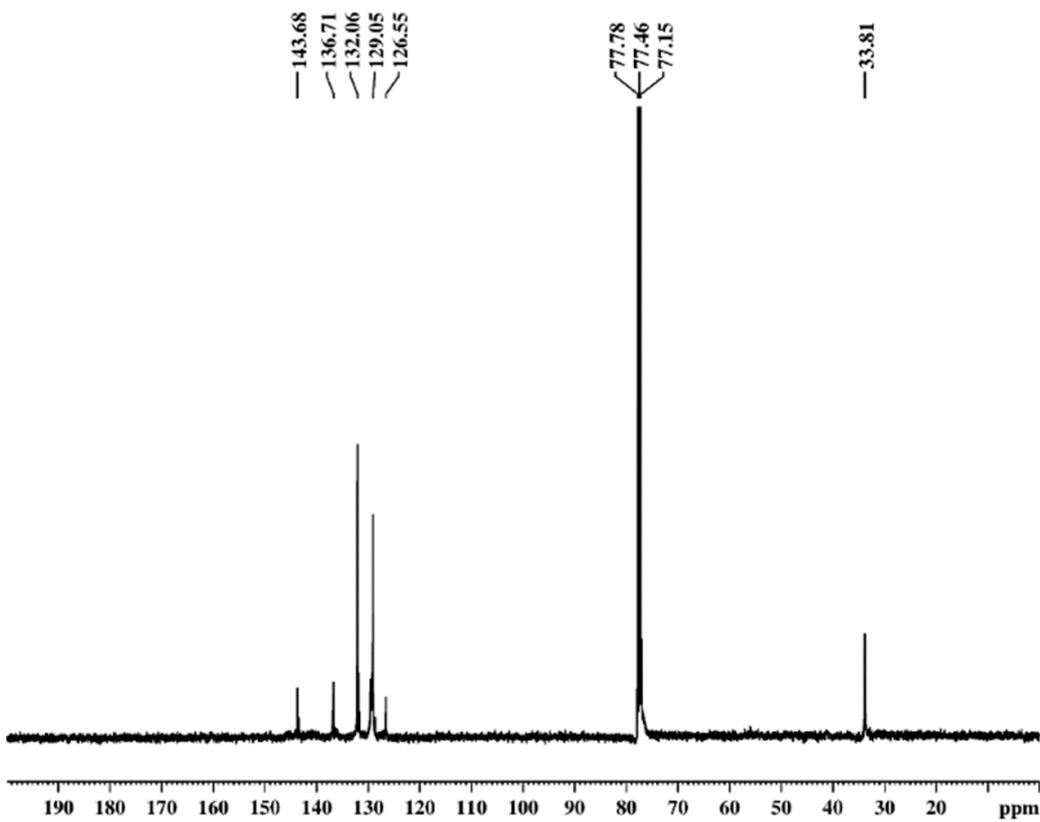


Fig. S2 ^{13}C NMR (CDCl_3 , 100 MHz) of **C1**.

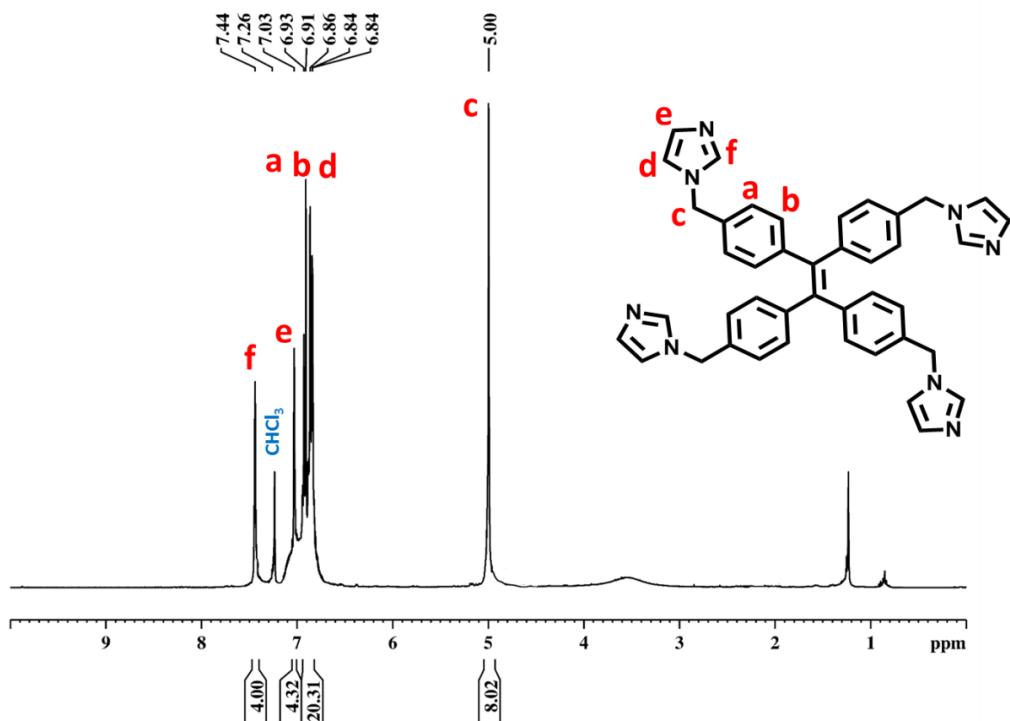


Fig. S3 ^1H NMR (CDCl_3 , 400 MHz) of **L**.

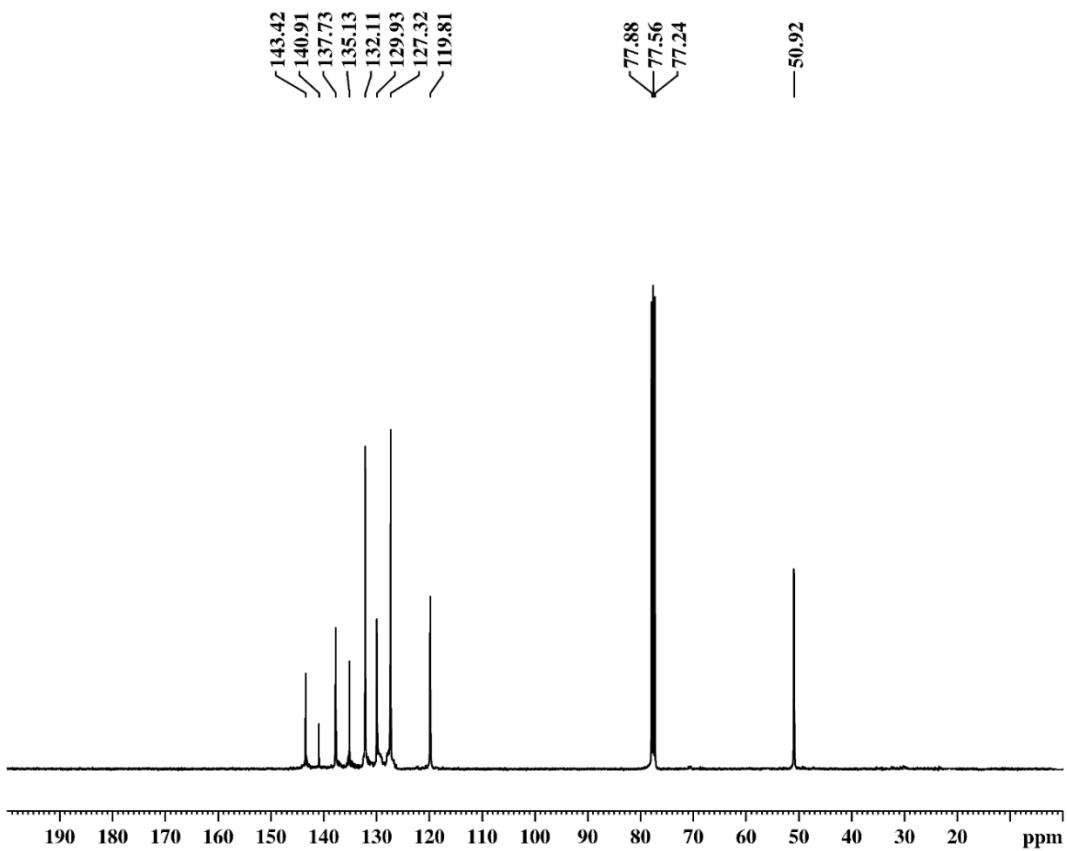


Fig. S4 ^{13}C NMR (CDCl_3 , 100 MHz) of ligand **L**.

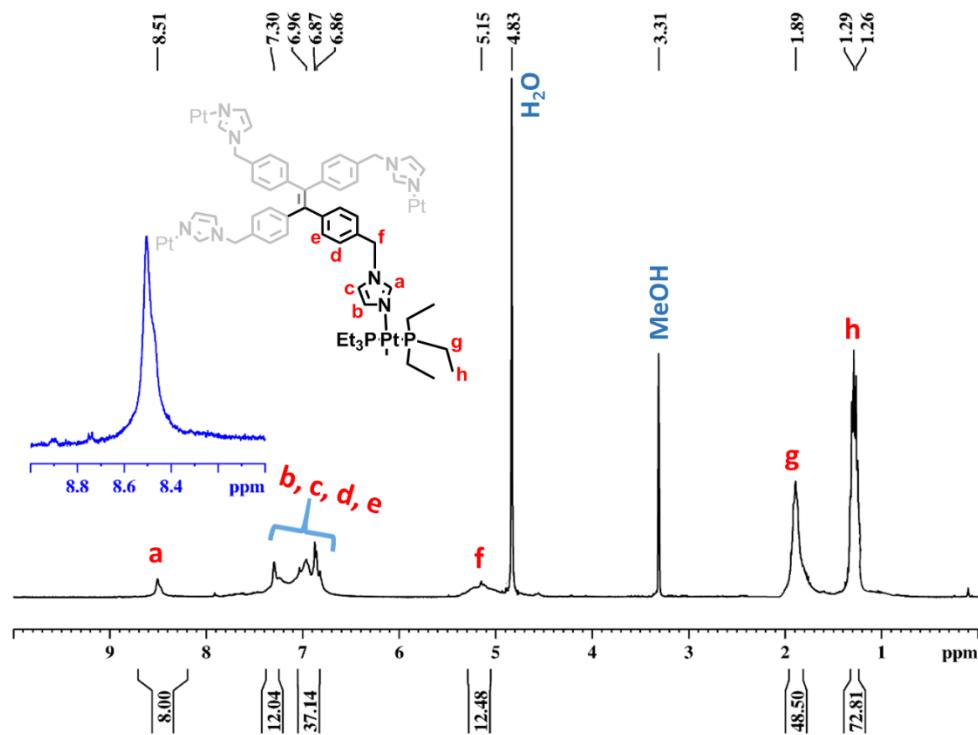


Fig. S5 ^1H NMR (CD_3OD , 400 MHz) of cage **1a**.

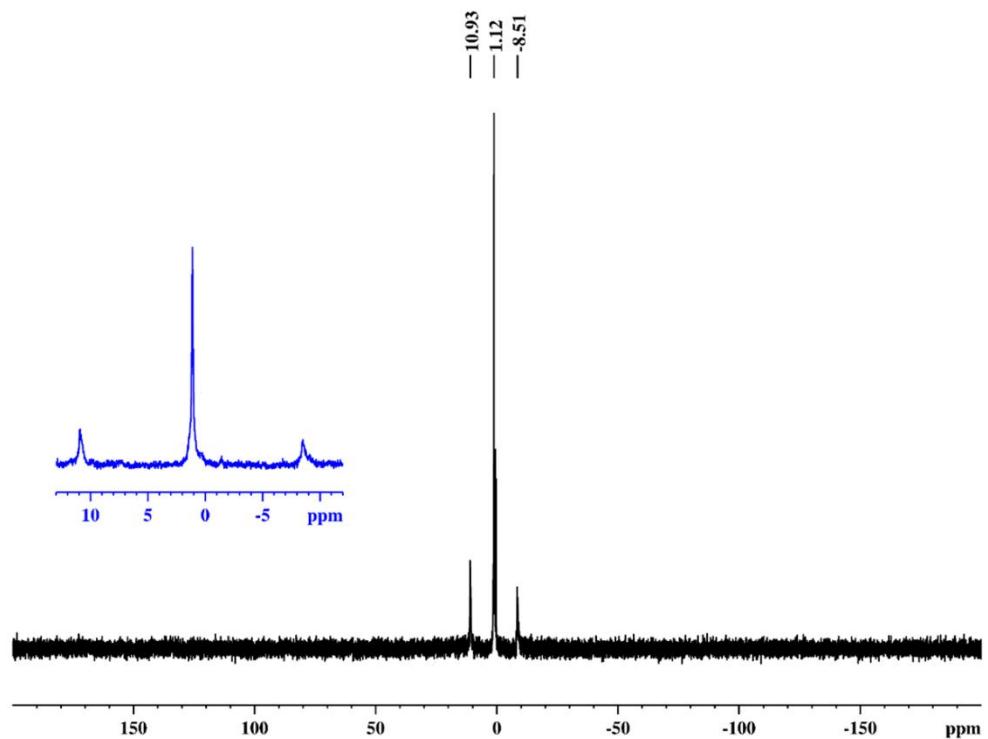


Fig. S6 $^{31}\text{P}\{\text{H}\}$ NMR (CD_3OD , 162 MHz) of cage **1a**.

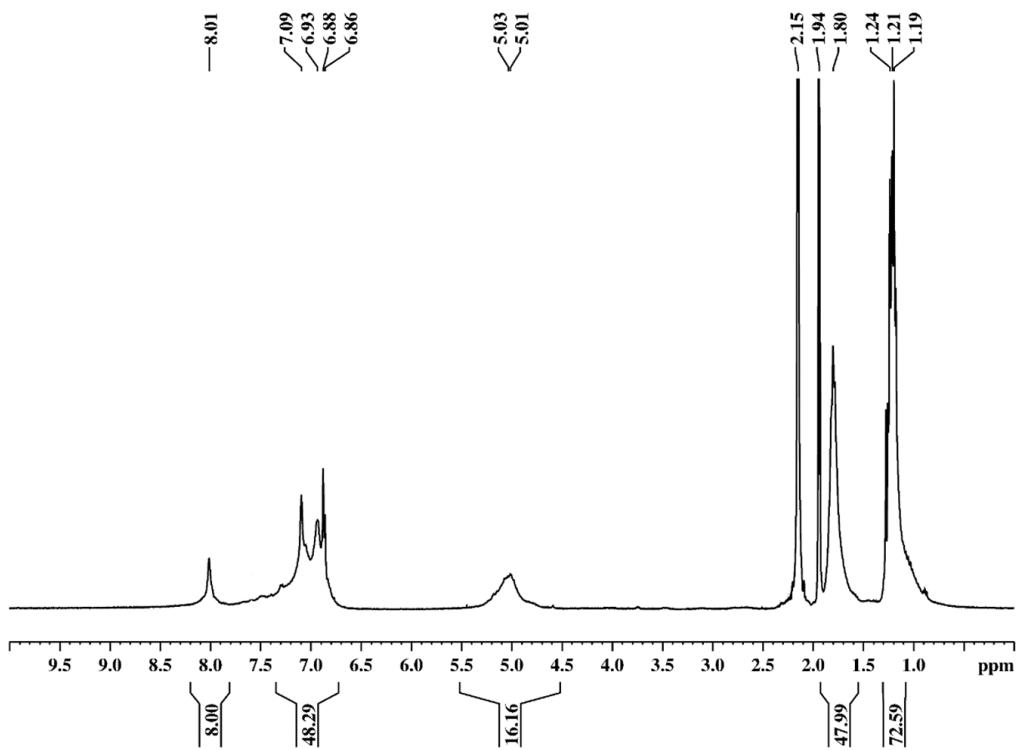


Fig. S7 ^1H NMR (CD_3CN , 400 MHz) of cage **1b**.

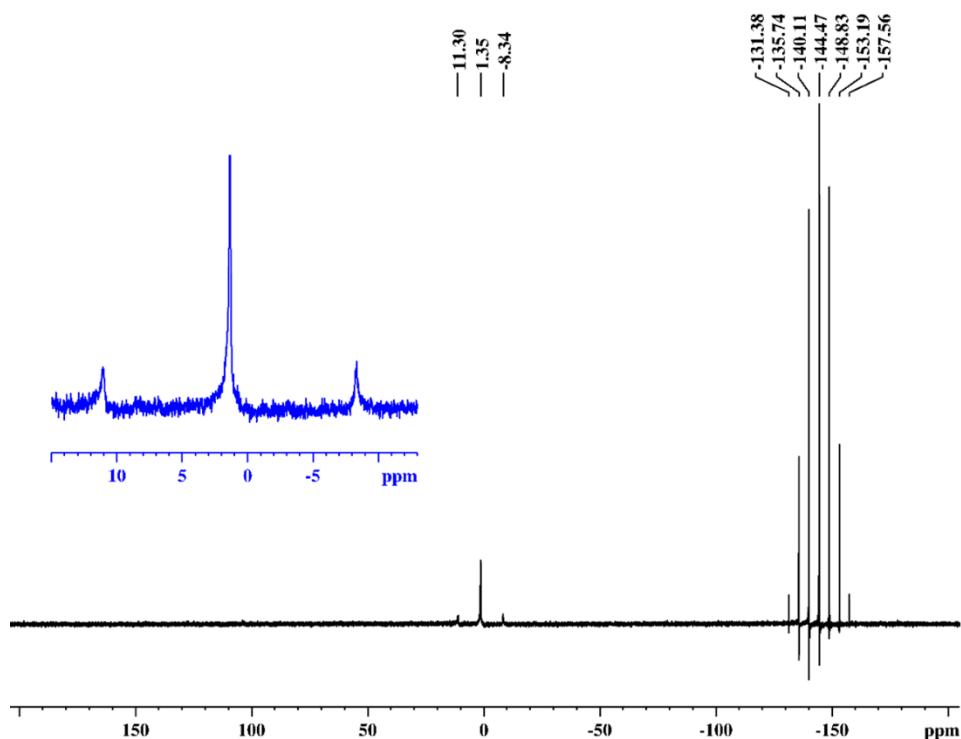


Fig. S8 $^{31}\text{P}\{\text{H}\}$ NMR (CD_3CN , 162 MHz) of cage **1b**.

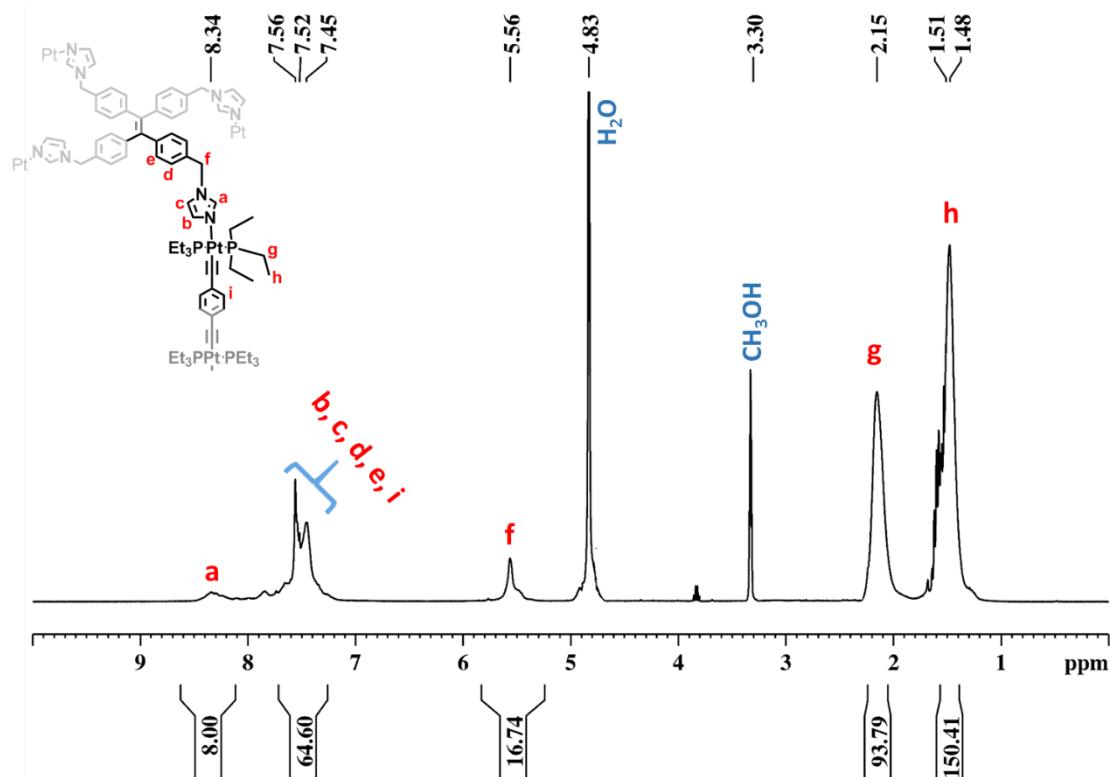


Fig. S9 ^1H NMR (CD_3OD , 400 MHz) of cage **2a**.

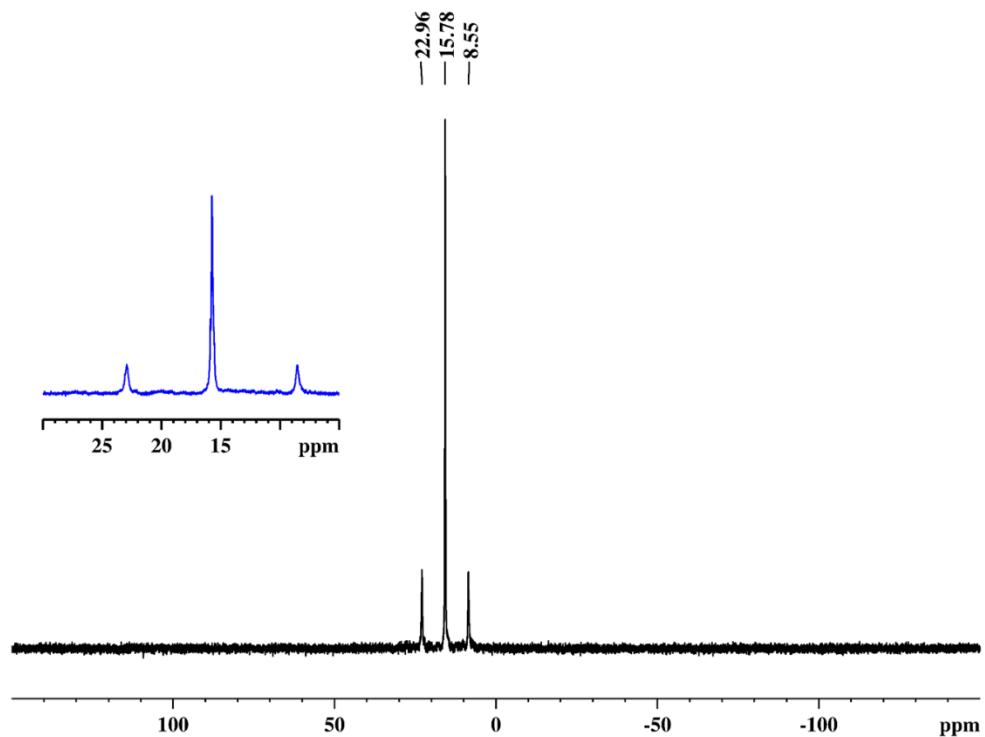


Fig. S10 $^{31}\text{P}\{\text{H}\}$ NMR (CD_3OD , 162 MHz) of cage **2a**.

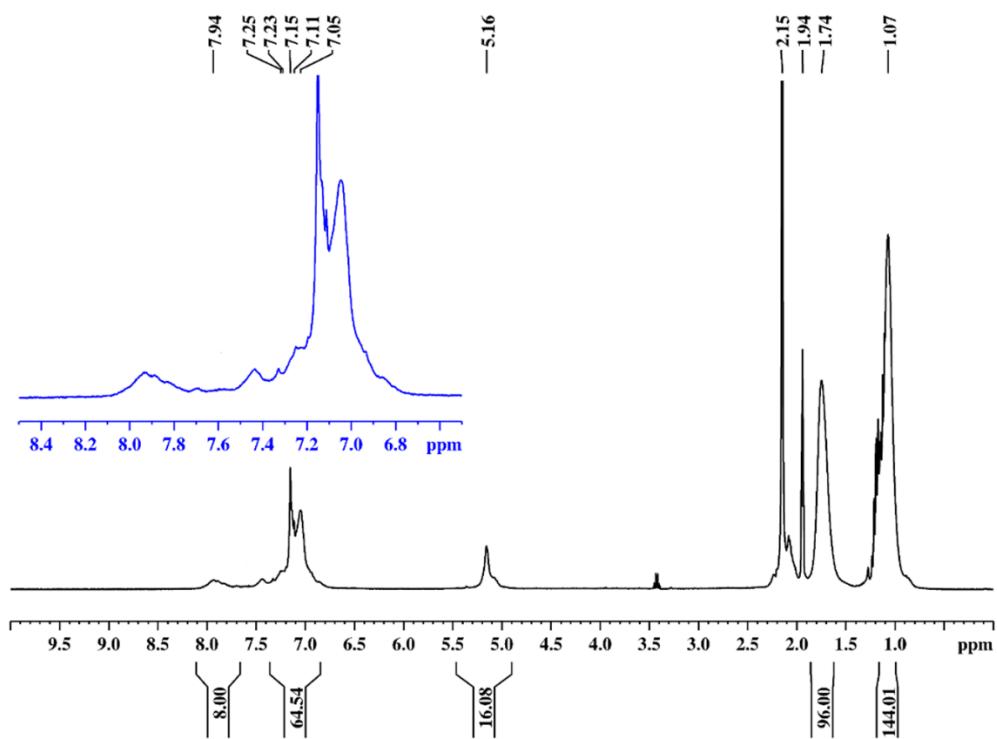


Fig. S11 ^1H NMR (CD_3CN , 400 MHz) of cage **2b**.

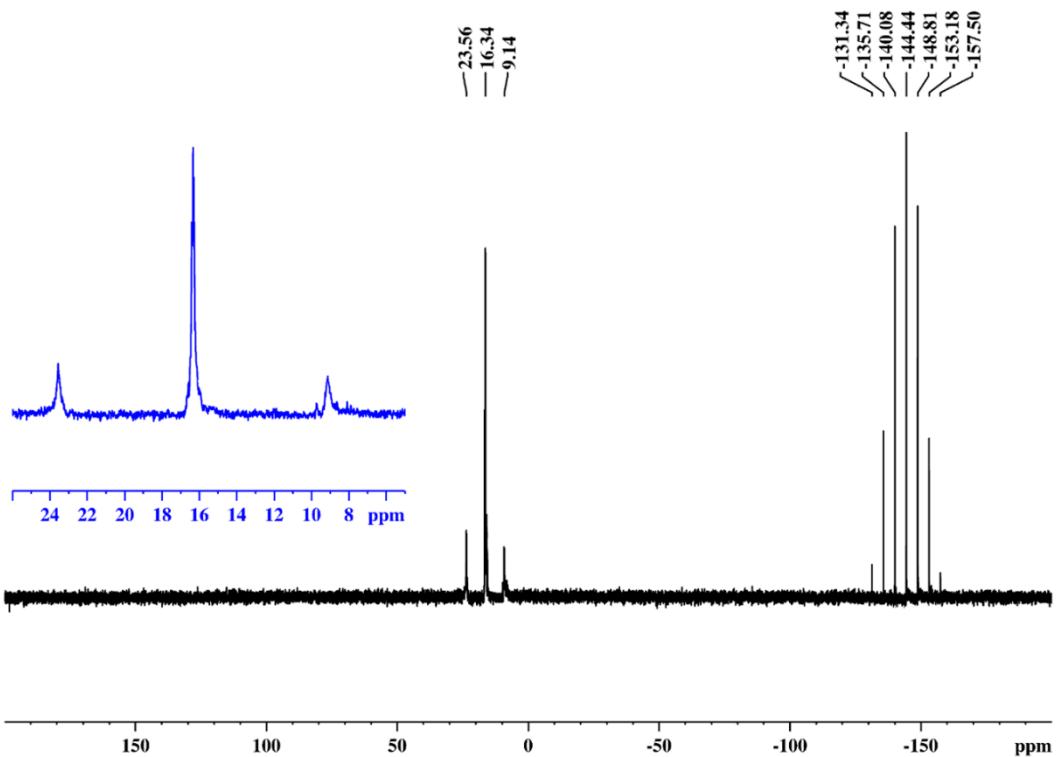


Fig. S12 $^{31}\text{P}\{\text{H}\}$ NMR (CD_3CN , 162 MHz) of cage **2b**.

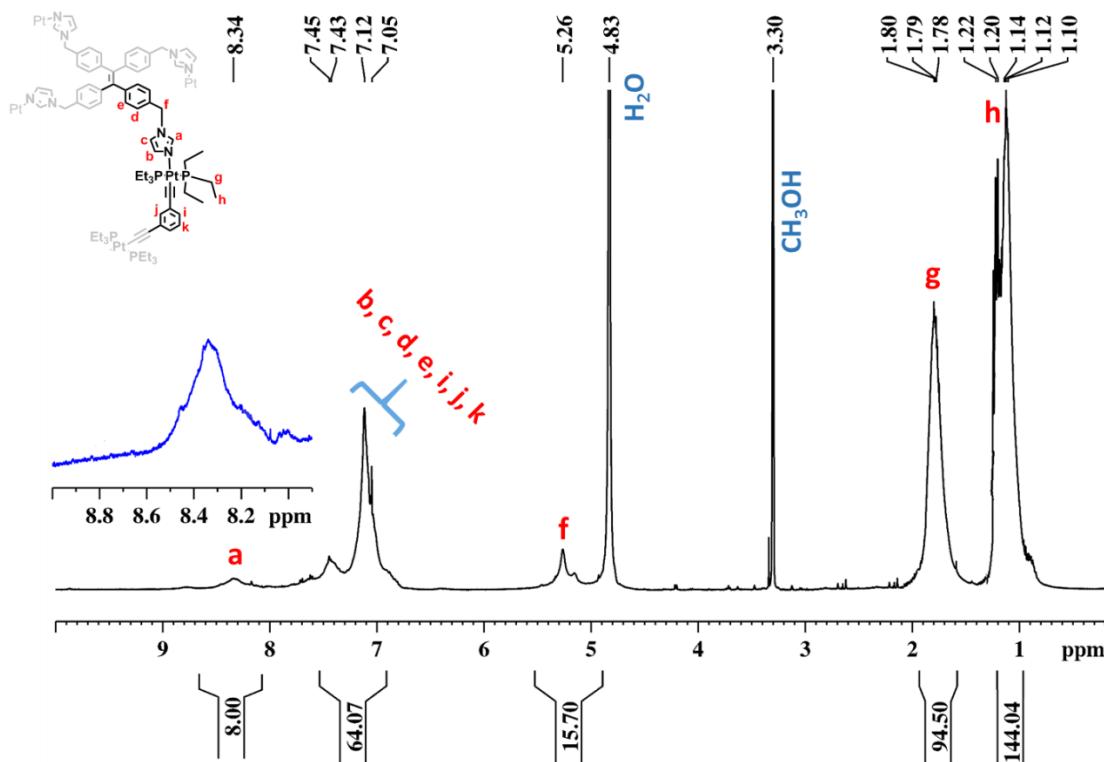


Fig. S13 ^1H NMR (CD_3OD , 400 MHz) of cage **3a**.

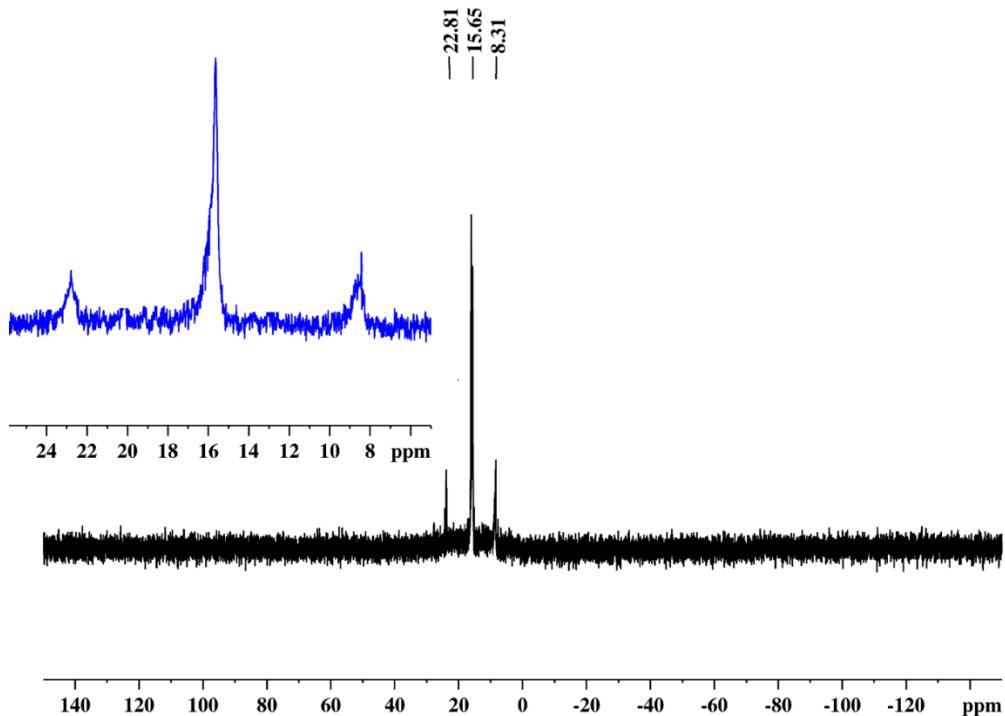


Fig. S14 $^{31}\text{P}\{\text{H}\}$ NMR (CD_3OD , 162 MHz) of cage **3a**.

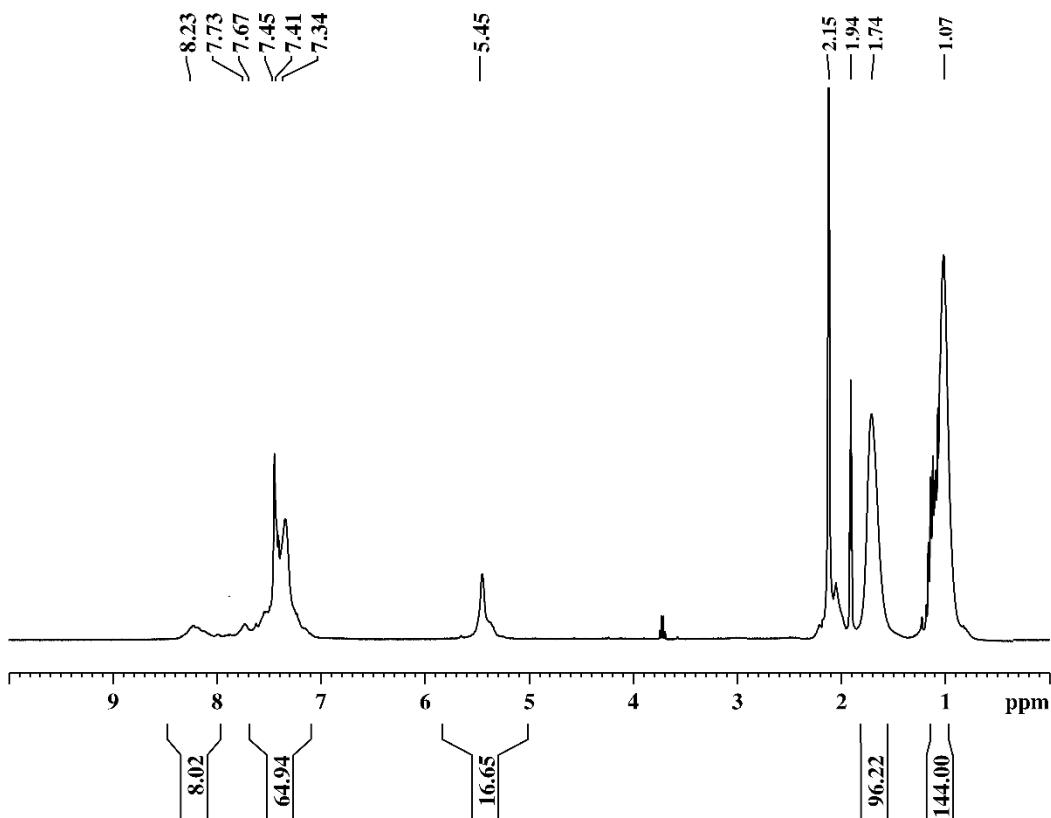


Fig. S15 ^1H NMR (CD_3CN , 400 MHz) of cage **3b**.

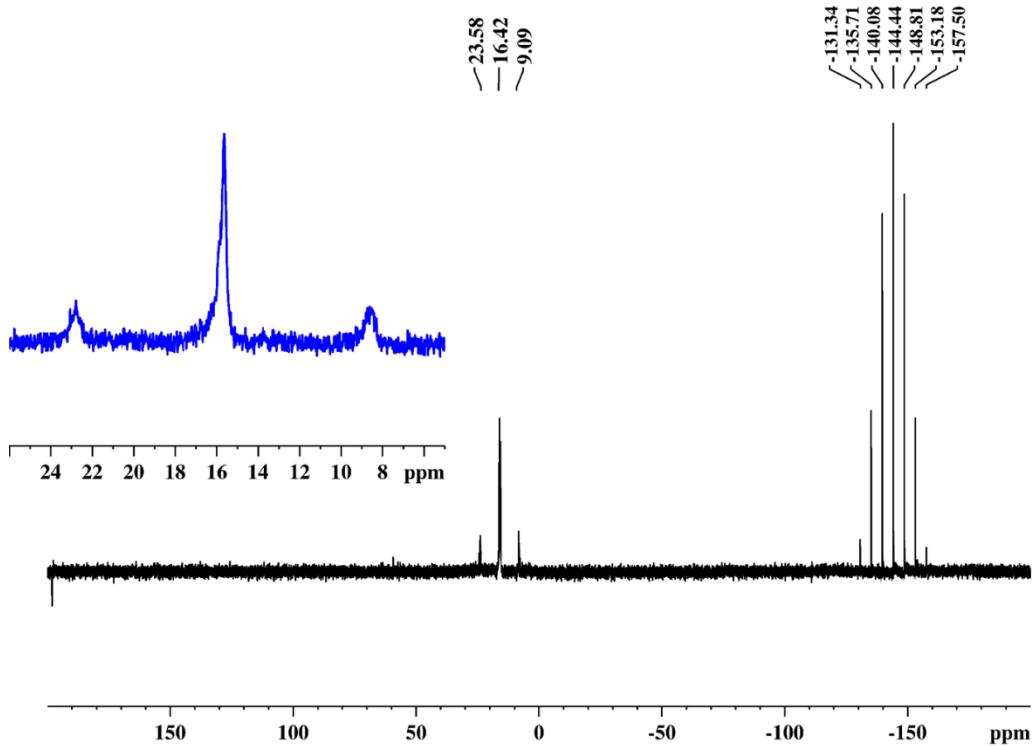


Fig. S16 $^{31}\text{P}\{\text{H}\}$ NMR (CD₃CN, 162 MHz) of cage **3b**.

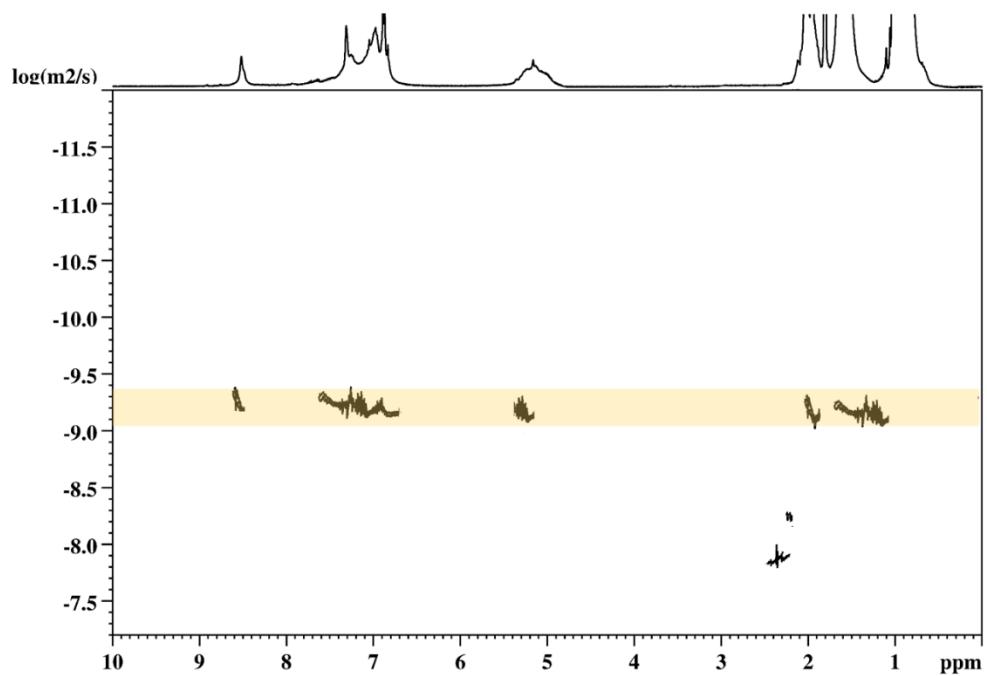


Fig. S17 DOSY NMR (CD₃CN, 400 MHz) of compound **1b**.

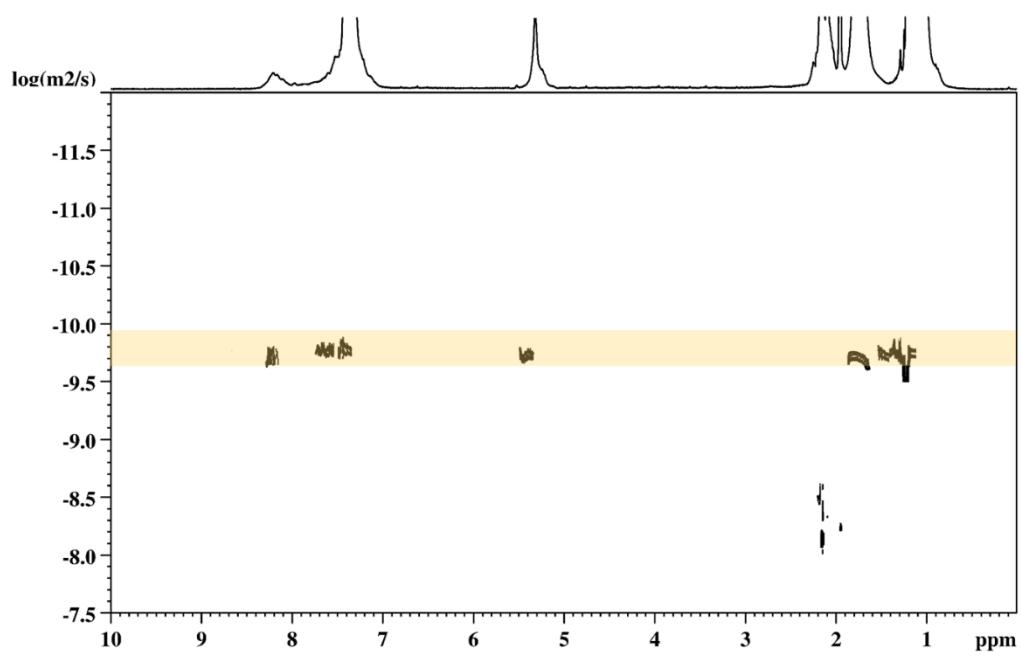


Fig. S18 DOSY NMR (CD_3CN , 400 MHz) of compound **2b**.

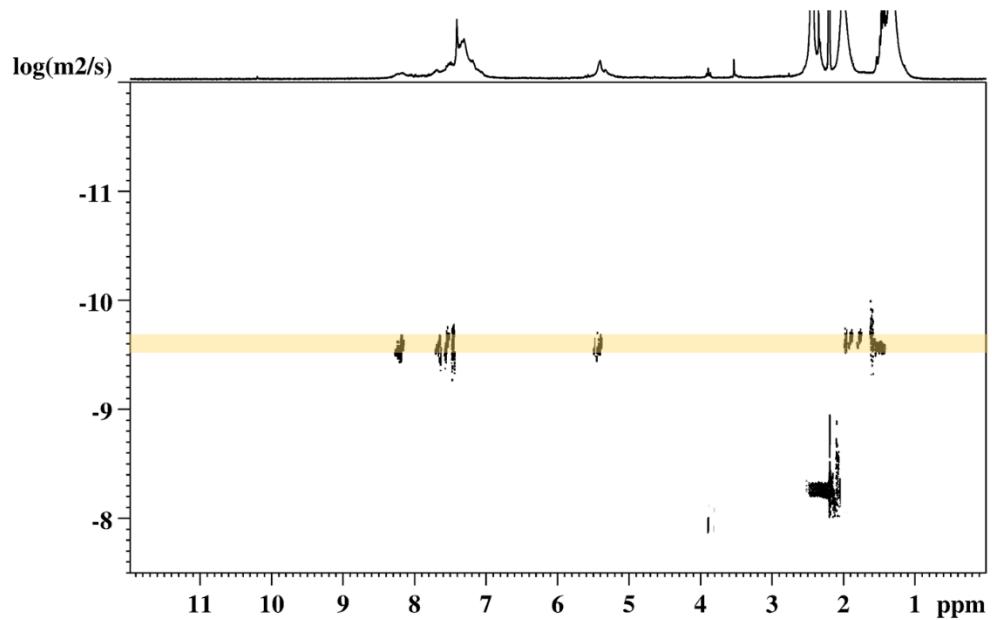


Fig. S19 DOSY NMR (CD_3CN , 400 MHz) of compound **3b**.

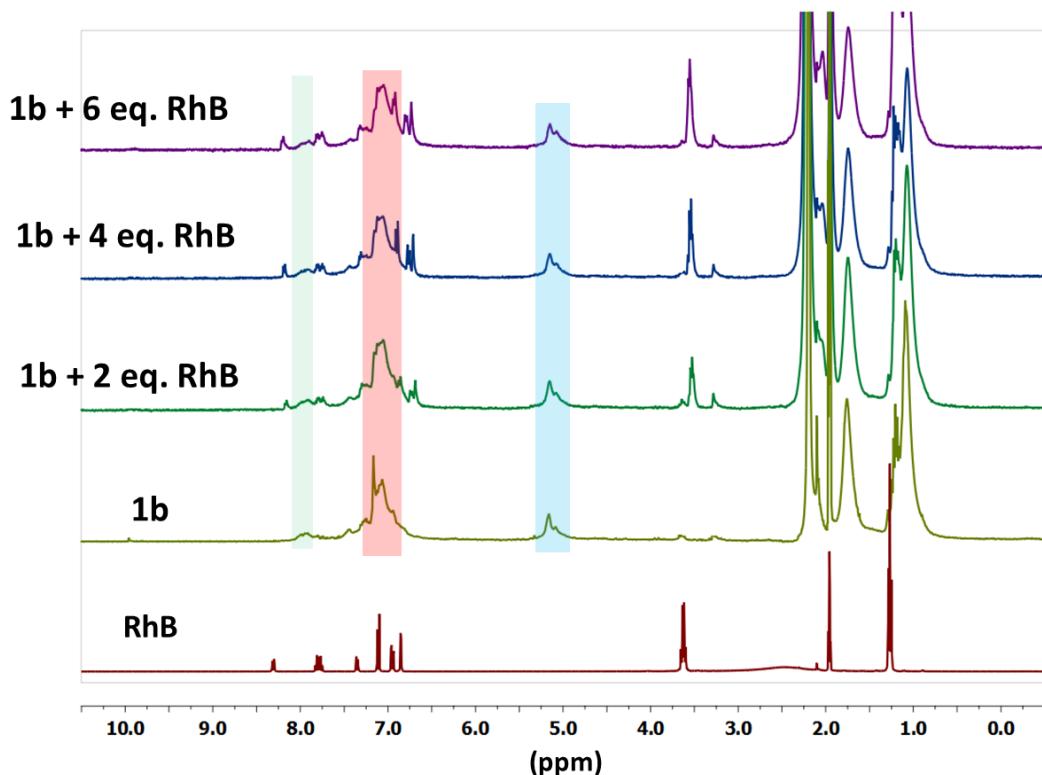


Fig. S20 ^1H NMR (CD₃CN, 400 MHz) titration of 10⁻³ M solution of **2b** with **RhB**.

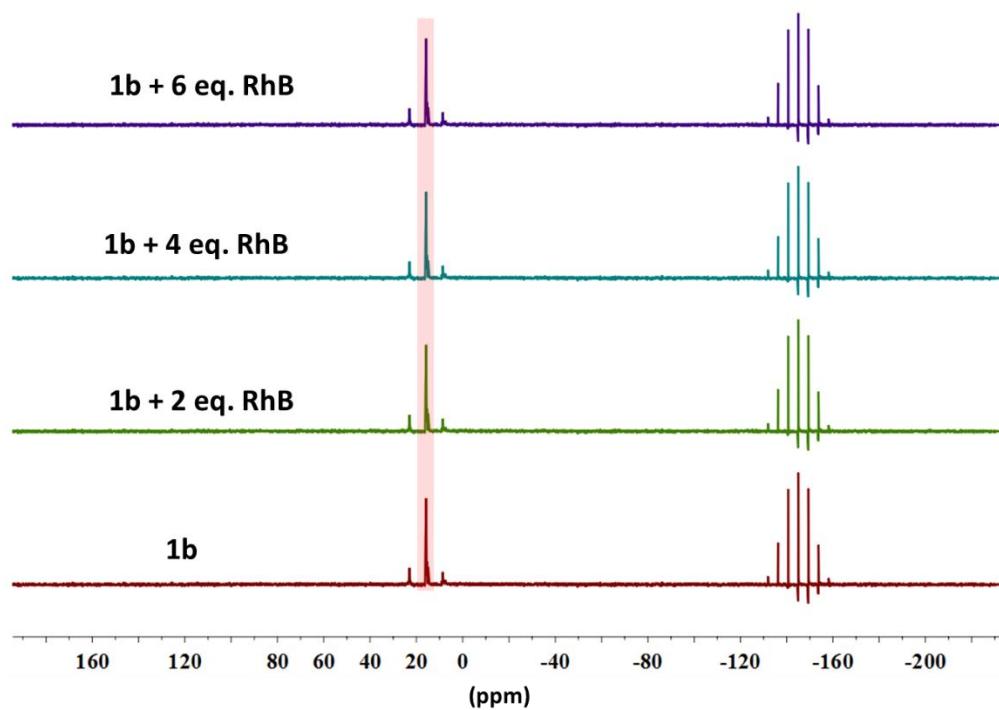


Fig. S21 ^{31}P NMR (CD₃CN, 162 MHz) titration of 10⁻³ M solution of **2b** with **RhB**.

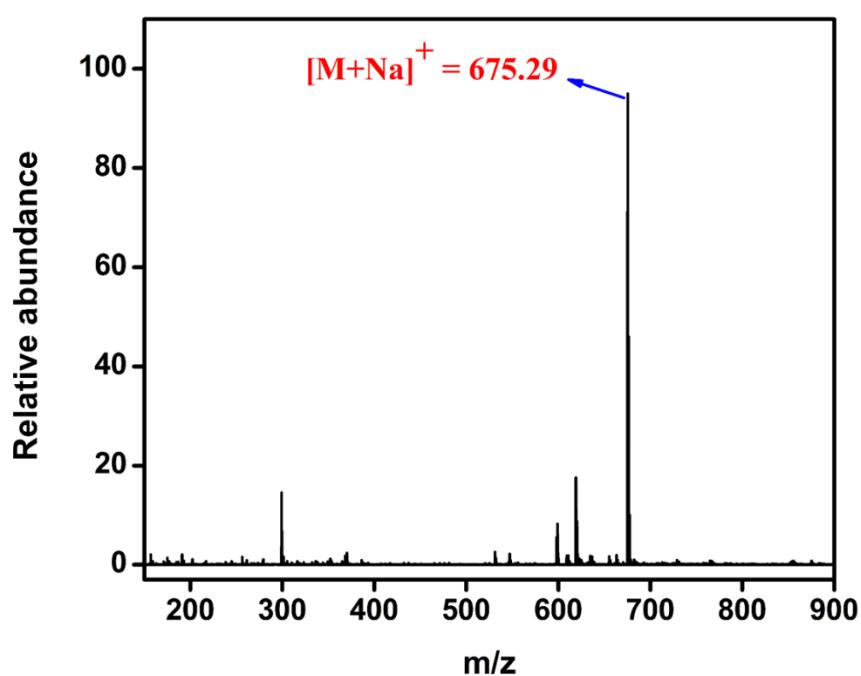


Fig. S22 ESI-MS spectrum of **L** in acetonitrile.

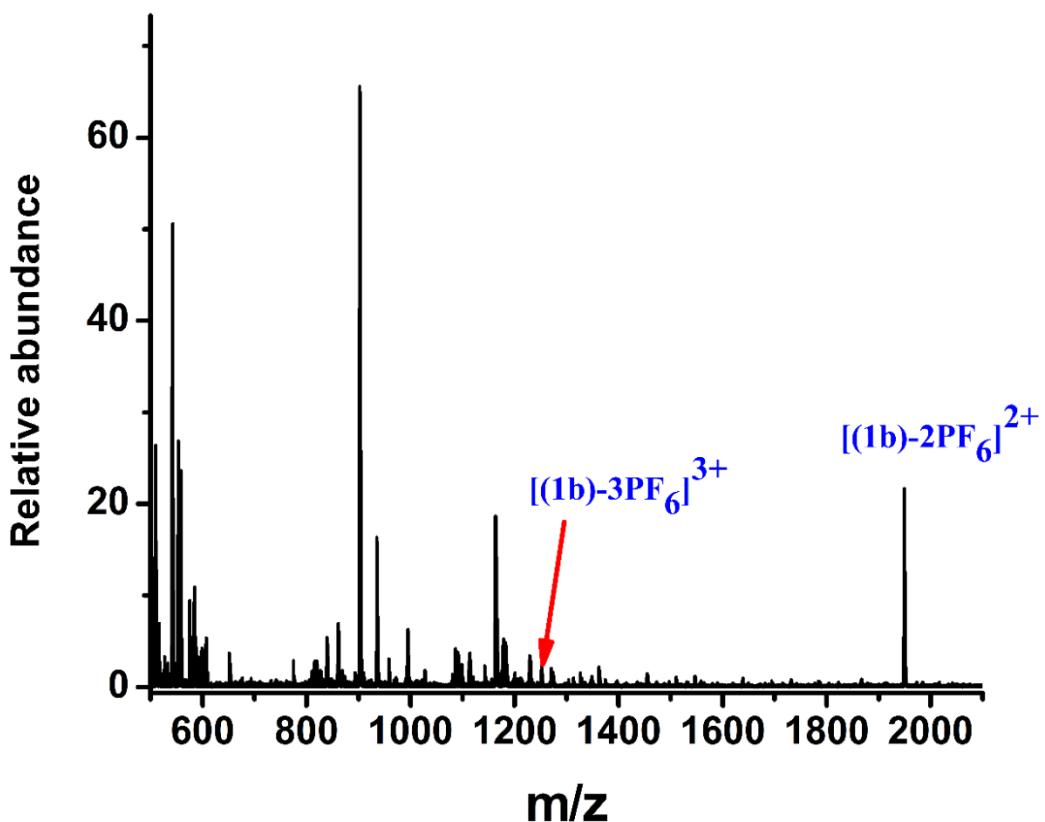


Fig. S23 ESI-MS spectrum of **1b** in acetonitrile.

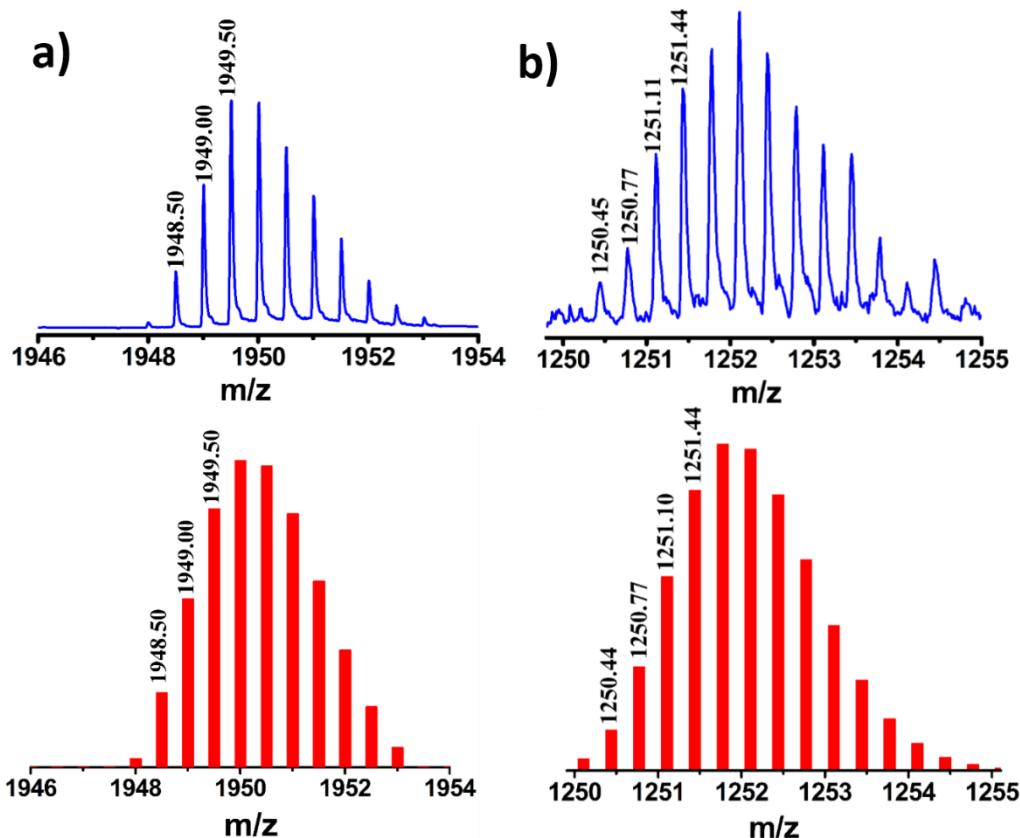


Fig. S24 Experimental (top) and theoretical (bottom) isotopic distribution patterns of the peaks corresponding to a) $[(1b)\text{-}2\text{PF}_6^-]^{2+}$ and b) $[(1b)\text{-}3\text{PF}_6^-]^{3+}$ fragments.

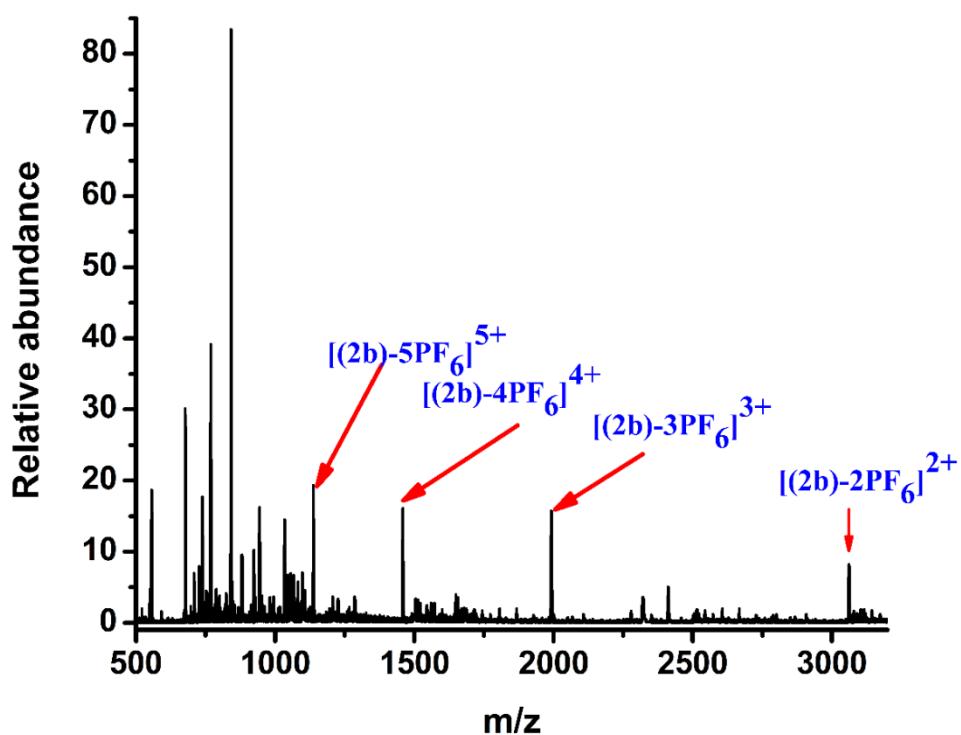


Fig. S25 ESI-MS spectrum of **2b** recorded in acetonitrile.

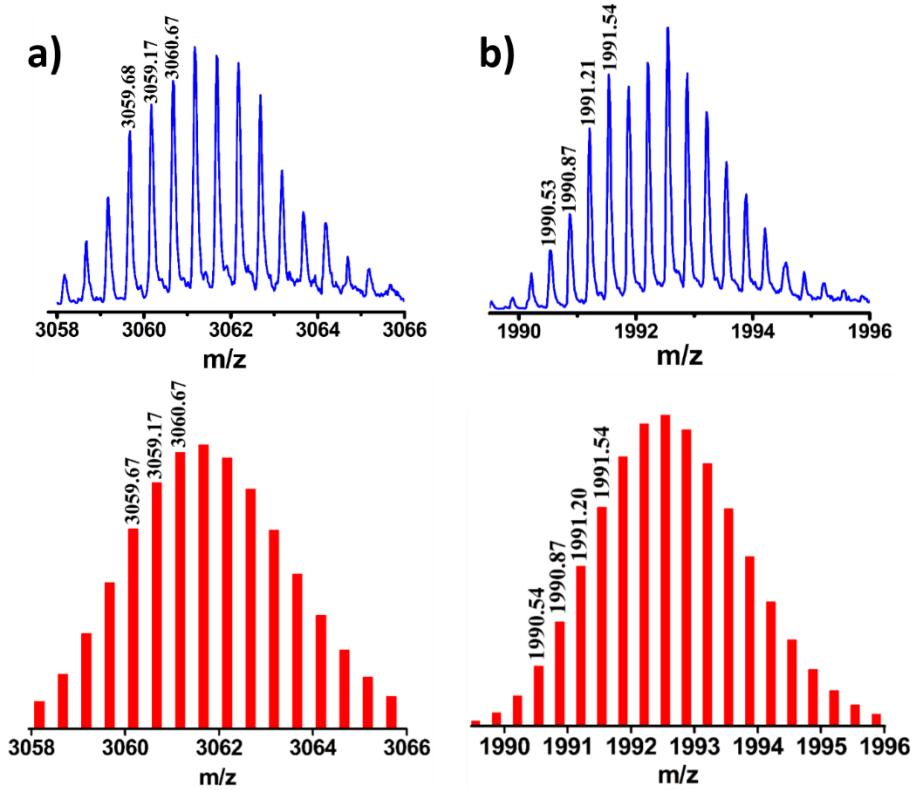


Fig. S26 Experimental (top) and theoretical (bottom) isotopic distribution patterns of the peaks corresponding to a) $[(2b)-2\text{PF}_6]^{2+}$ and b) $[(2b)-3\text{PF}_6]^{3+}$ fragments.

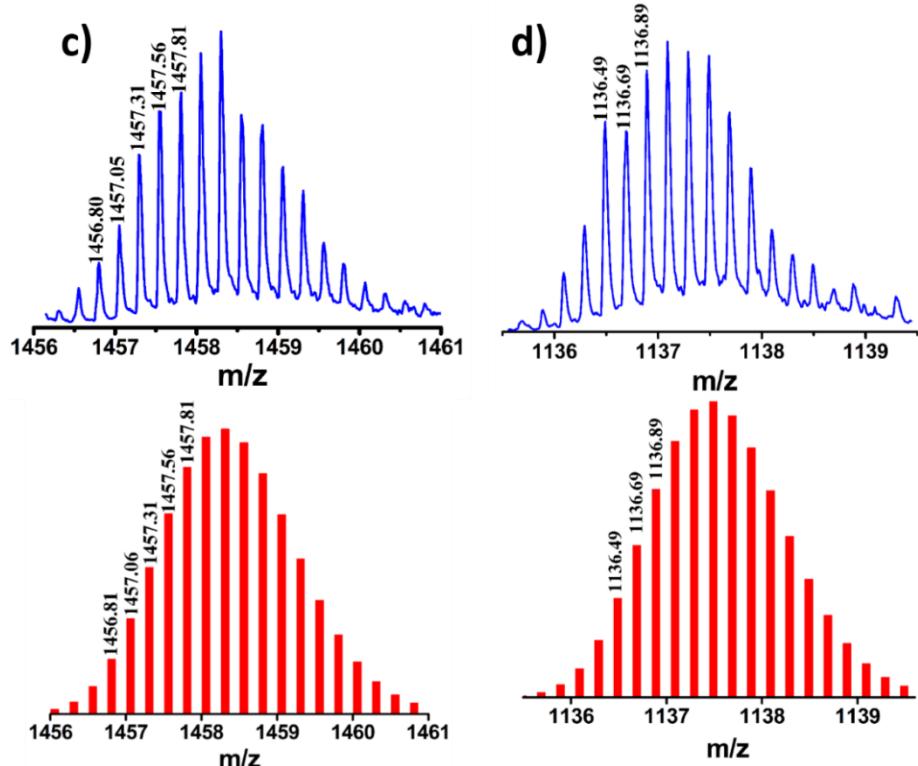


Fig. S27 Experimental (top) and theoretical (bottom) isotopic distribution patterns of the peaks corresponding to fragments a) $[(2b)-4\text{PF}_6]^{4+}$ and b) $[(2b)-5\text{PF}_6]^{5+}$.

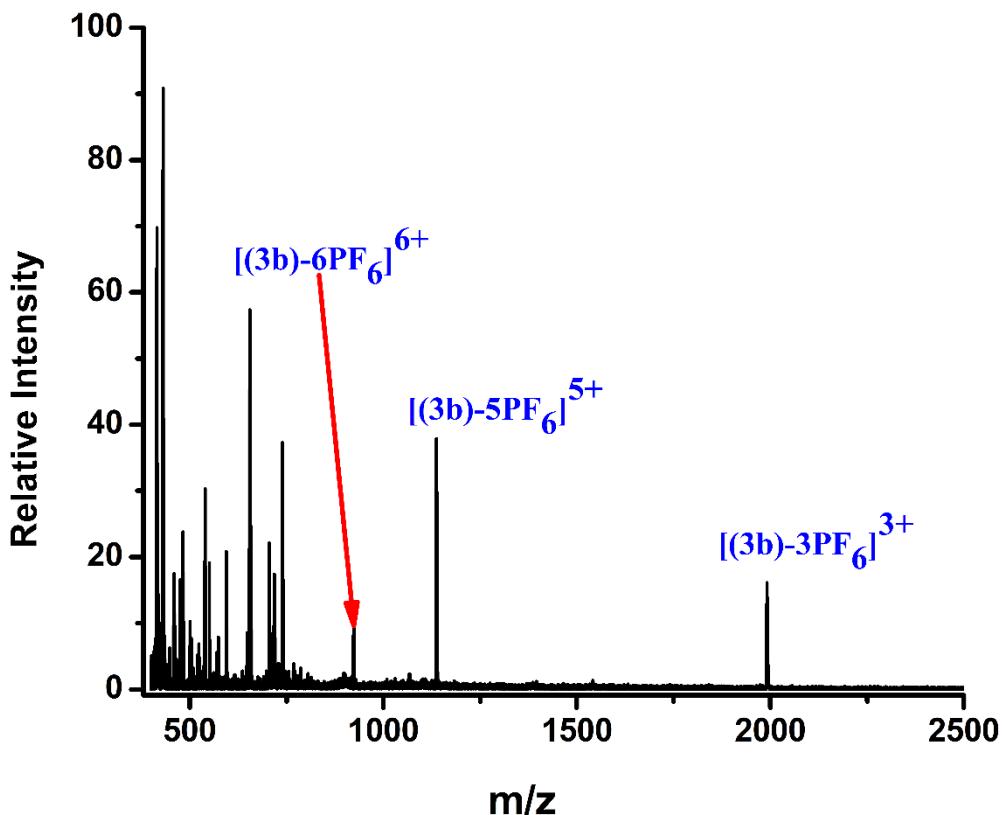


Fig. S28 ESI-MS spectrum of **3b** recorded in acetonitrile.

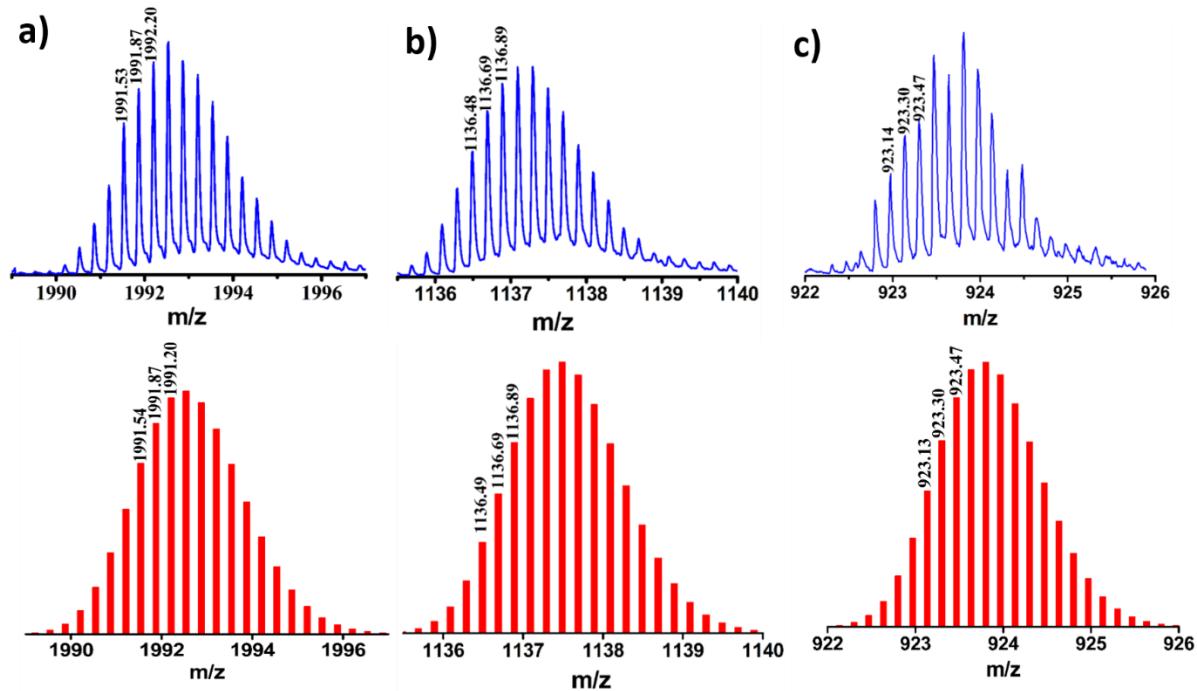


Fig. S29 Experimental (top) and theoretical (bottom) isotopic distribution patterns of the peaks corresponding to a) $[(3b)-3PF_6]^{3+}$; b) $[(3b)-5PF_6]^{5+}$ and c) $[(3b)-6PF_6]^{6+}$.

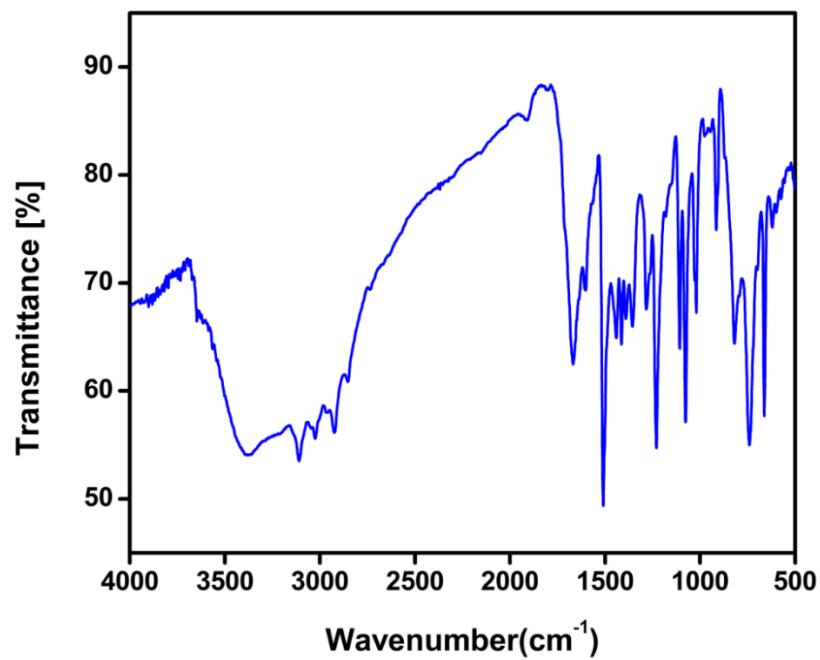


Fig. S30 FT-IR spectrum of **L**.

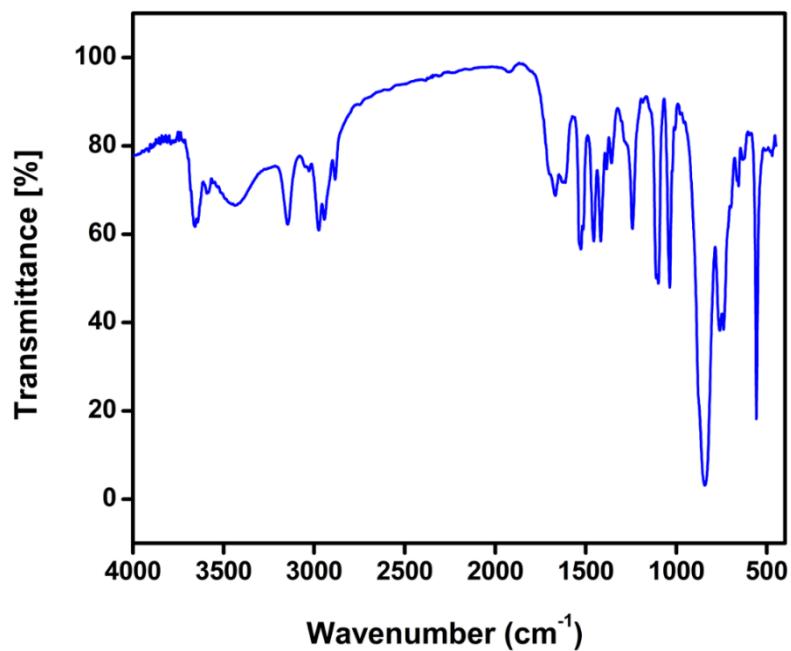


Fig. S31 FT-IR spectrum of **1b**.

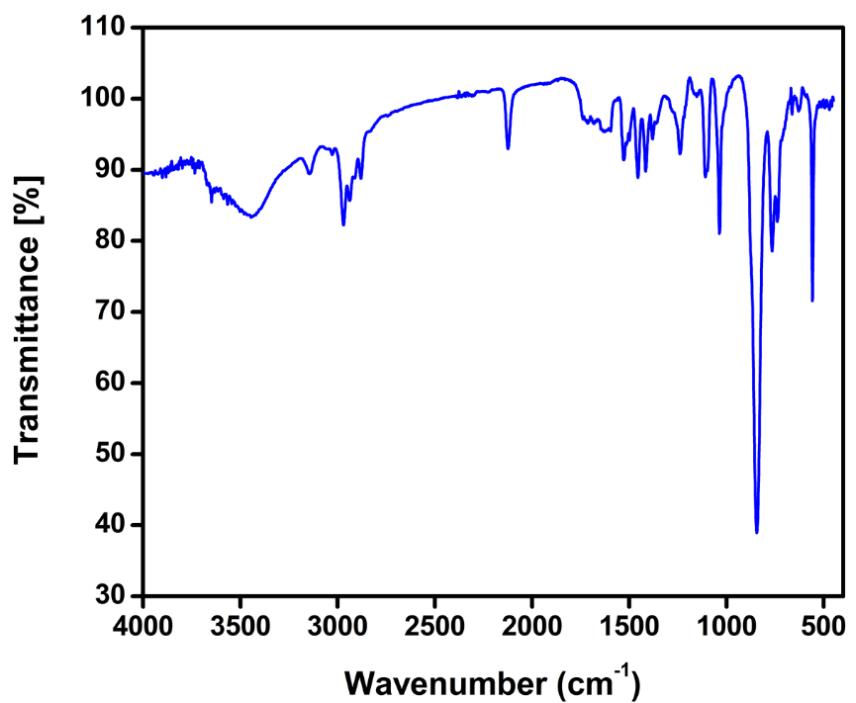


Fig. S32 FT-IR spectrum of **2b**.

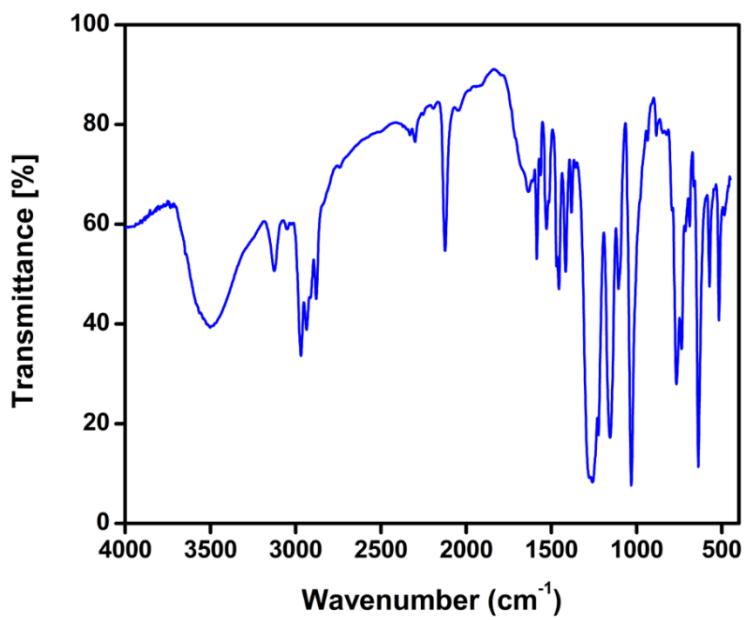


Fig. S33 FT-IR spectrum of **3b**.

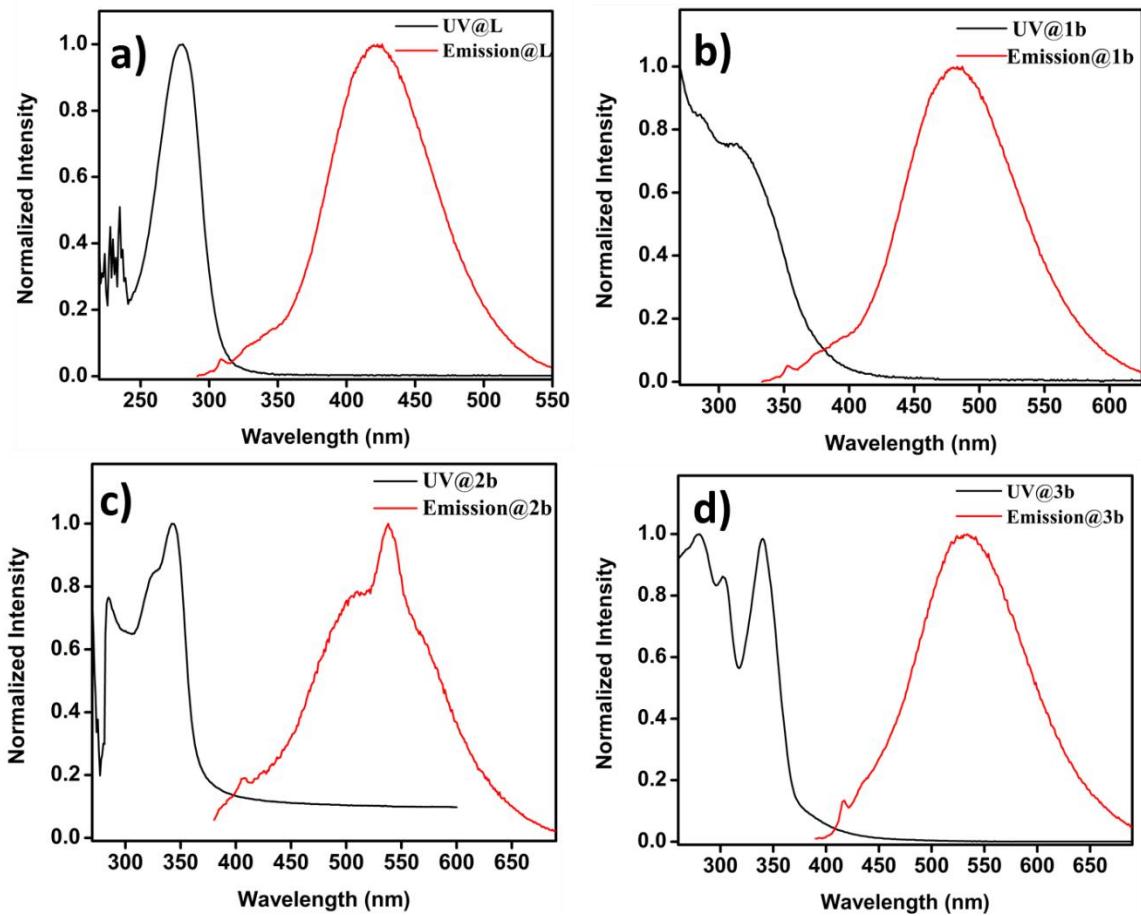


Fig. S34 Normalized UV-Vis and emission spectra in MeCN for a) **L**; b) **1b**; c) **2b** and d) **3b**.

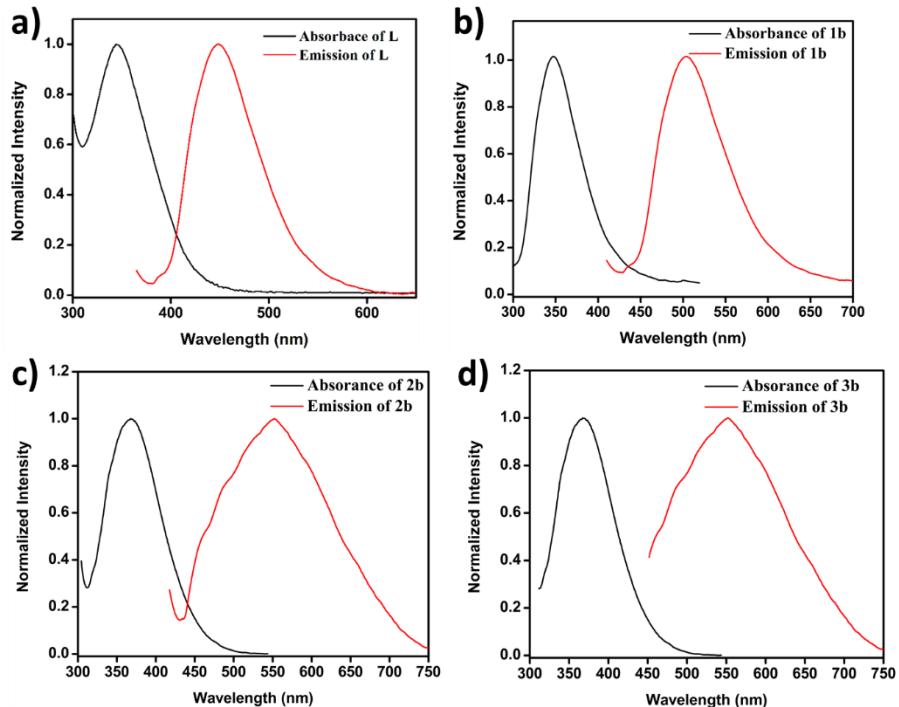


Fig. S35 Normalized UV-Vis and emission spectra in solid state for a) **L**; b) **1b**; c) **2b** and d) **3b**.

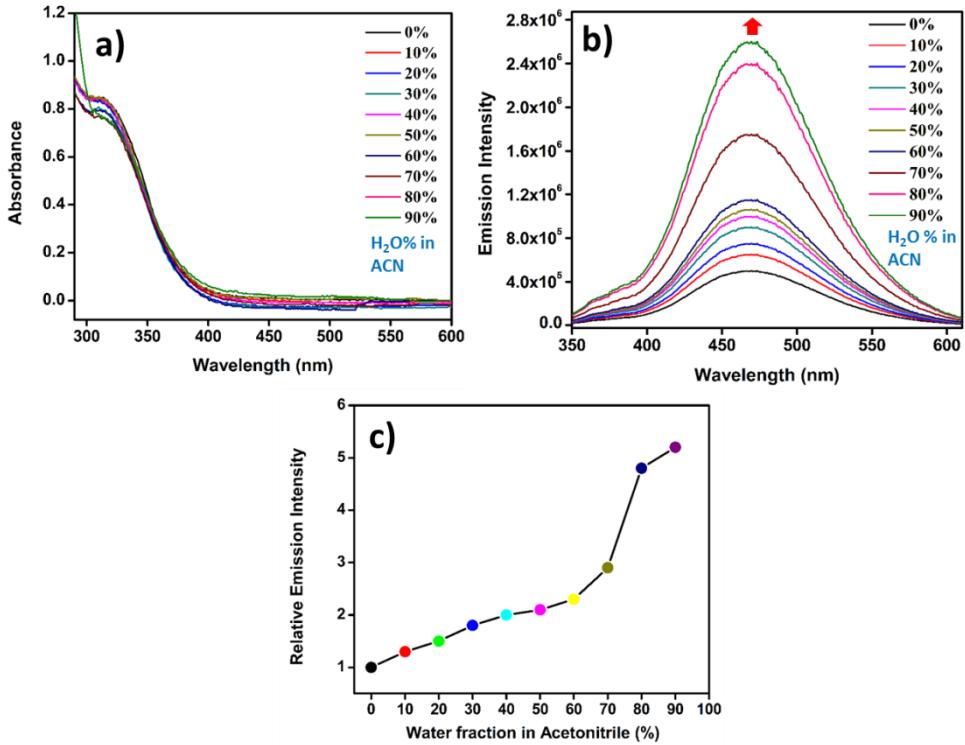


Fig. S36 a) UV-Vis spectra of **1b** in the water/MeCN mixture; b) Fluorescence emission spectra in the water/MeCN mixture ($\lambda_{ex} = 325\text{ nm}$, $c = 10^{-5}\text{ M}$); c) Plot of variation of relative emission intensity vs water fraction (%) in MeCN.

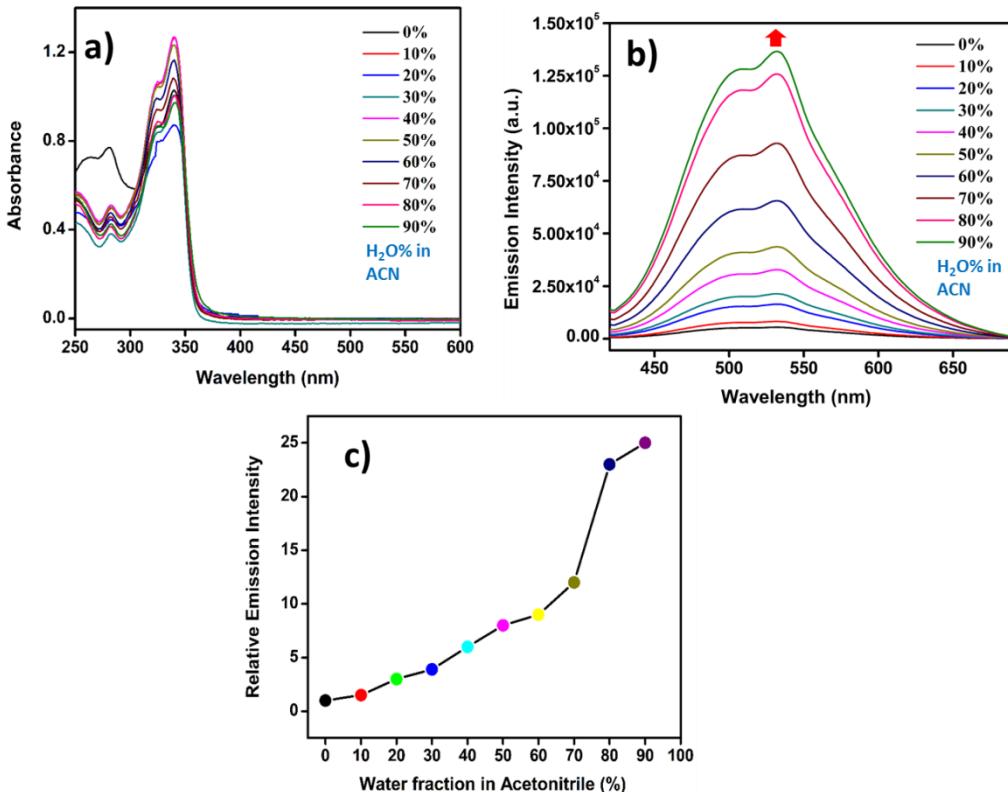


Fig. S37 a) UV-Vis spectra of **2b** in the water /MeCN mixture; b) Fluorescence Emission spectra in the water/MeCN mixture ($\lambda_{ex} = 345\text{ nm}$, $c = 10^{-5}\text{M}$); c) Plot of variation of relative emission intensity vs water fraction (%) in MeCN.

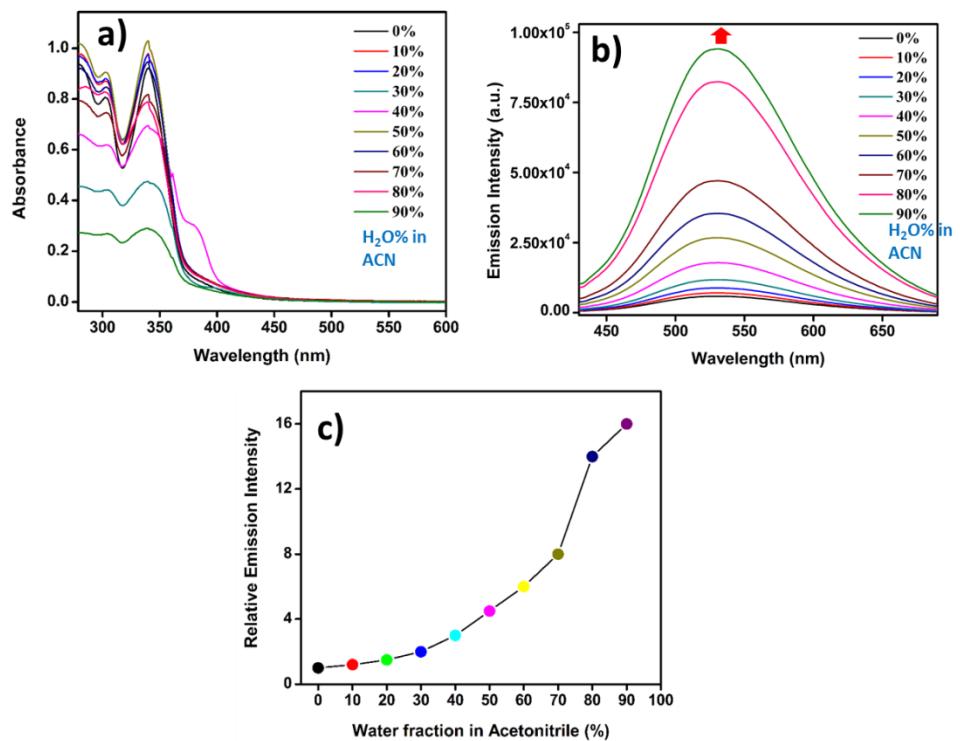


Fig. S38 a) UV-Vis spectra of **3b** in the water /MeCN mixture; b) Fluorescence Emission spectra in water/MeCN mixture ($\lambda_{ex} = 340\text{ nm}$, $c = 10^{-5}\text{M}$); c) Plot of variation of relative emission intensity vs water fraction (%) in MeCN.

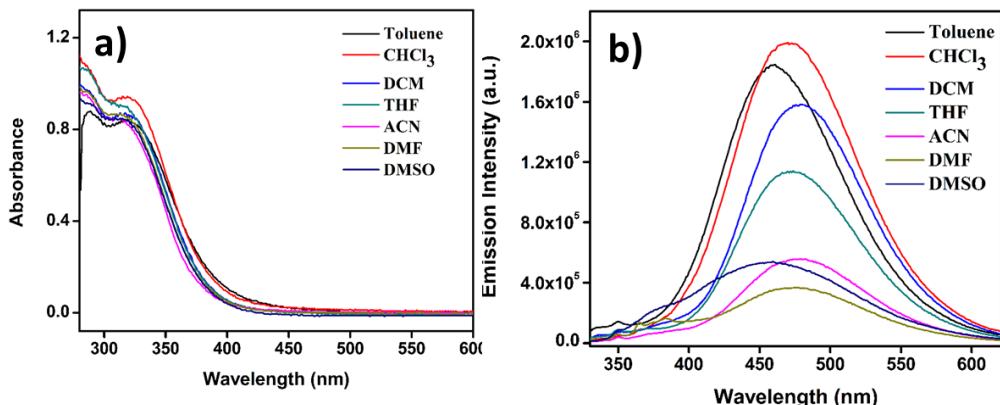


Fig. S39 a) UV-Vis spectra of **1b** in different solvents ($c = 10^{-5}\text{M}$); b) Fluorescence emission spectra of **1b** in different solvents ($\lambda_{ex} = 325\text{ nm}$, $c = 10^{-5}\text{M}$).

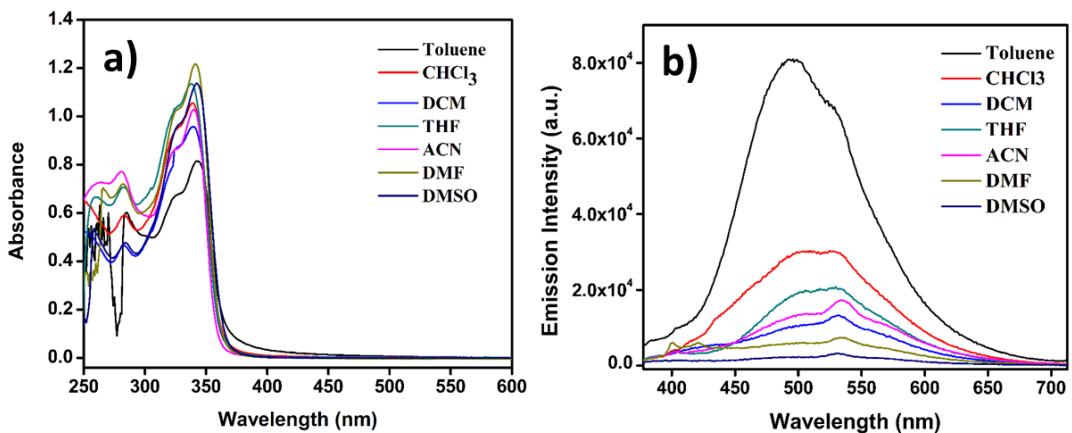


Fig. S40 a) UV-Vis spectra of **2b** in different solvents ($c = 10^{-5}$ M); b) Fluorescence emission spectra of **2b** in different solvents ($\lambda_{ex} = 345$ nm, $c = 10^{-5}$ M).

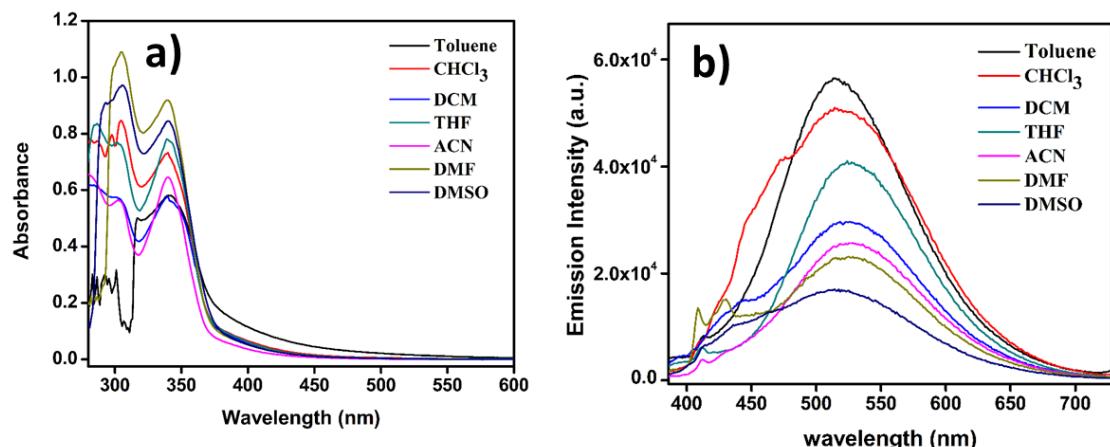


Fig. S41 a) UV-Vis spectra of **3b** in different solvents ($c = 10^{-5}$ M); b) Fluorescence emission spectra of **3b** in different solvents ($\lambda_{ex} = 340$ nm, $c = 10^{-5}$ M).

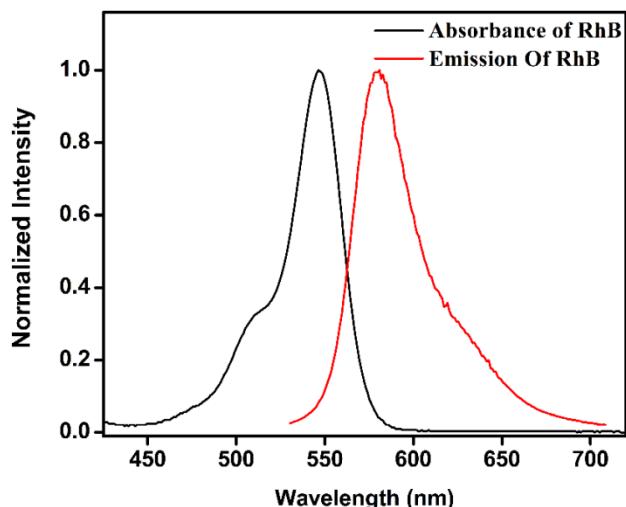


Fig. S42 a) UV-Vis spectra of **RhB** in 90% water in MeCN ($c = 10^{-5}$ M); b) Fluorescence emission spectra of **RhB** in 90% water in MeCN ($\lambda_{ex} = 547$ nm, $c = 10^{-5}$ M).

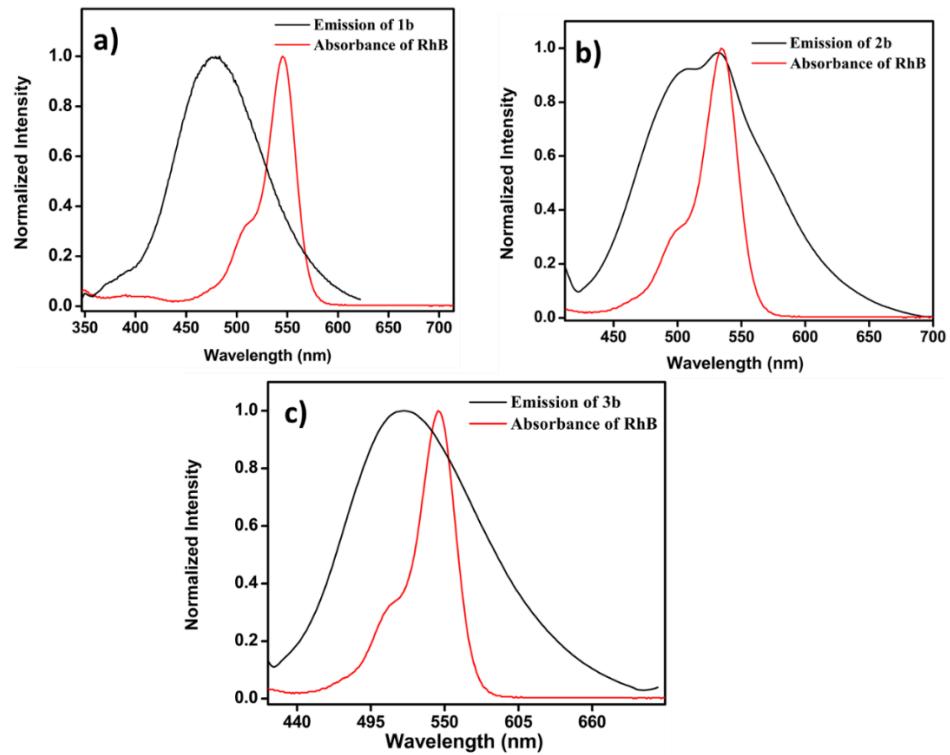


Fig. S43 Normalized plots of a) Emission of **1b** and absorbance of **RhB**; b) Emission of **2b** and absorbance of **RhB**; c) Emission of **3b** and absorbance of **RhB**.

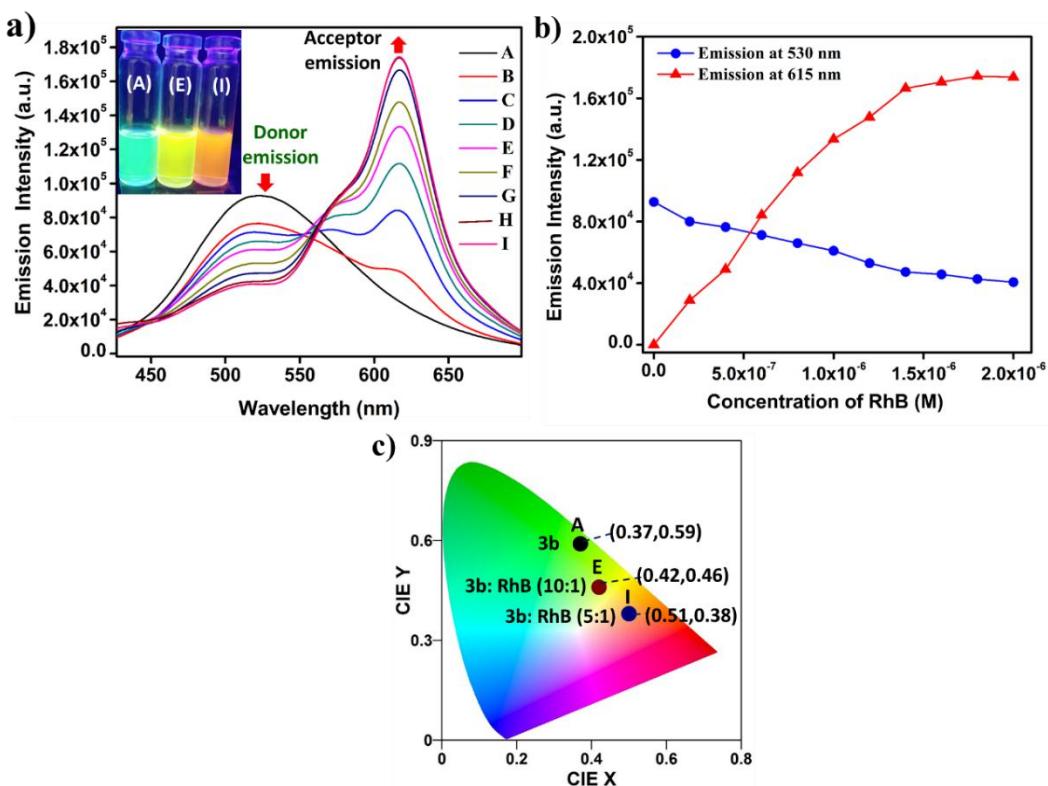


Fig. S44 a) Fluorescence spectra of metallacage **3b** with gradual addition of **RhB** ($\lambda_{ex} = 345\text{ nm}$) in 90% $\text{H}_2\text{O}/\text{MeCN}$ mixture. (Inset) photograph of **3b** (left), (**3b+RhB**) (10:1 equiv.) (middle), (**3b+RhB**) (5:1 equiv.) (right) under UV irradiation at 365 nm, b)

Fluorescence intensity change in **3b** at 530 and 615nm, c) the 1931 CIE chromaticity coordinate changes of **3b** (10^{-5} M in 90% water-MeCN mixture) titrated by **RhB** (0 to 0.2 equiv.).

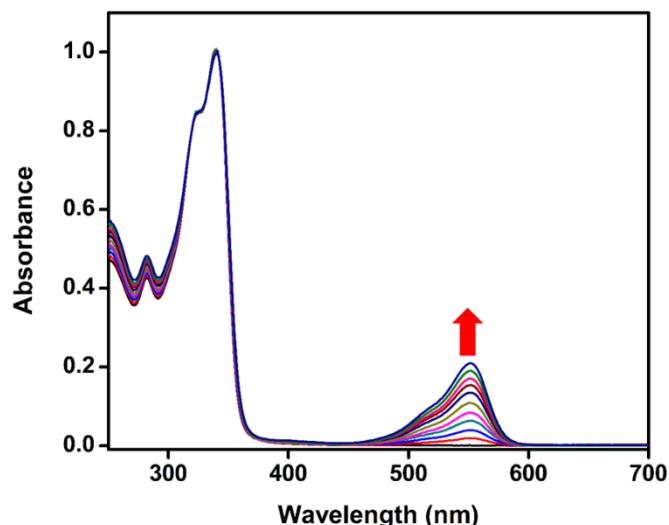


Fig. S45 UV-visible of **2b** ($\lambda_{\text{max}} = 345$ nm) with gradual addition of **RhB** in 90% water in MeCN {2 ml of 10^{-5} M cage solution (90% water/MeCN mixture) was titrated with 2×10^{-5} M solution of **RhB** ($\lambda_{\text{max}} = 547$ nm) in 90% water/MeCN mixture.

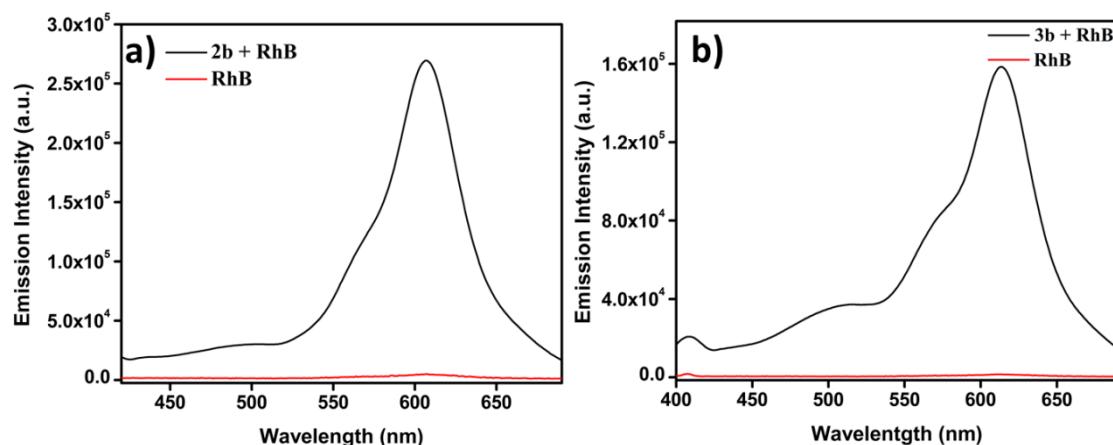


Fig. S46 a) Fluorescence emission spectra ($\lambda_{\text{ex}} = 345$ nm) of **RhB** in presence of **2b** (**2b** : **RhB** :: 5:1) (black line) and in absence of **2b** (red line). b) Fluorescence emission spectra ($\lambda_{\text{ex}} = 340$ nm) of **RhB** in presence of **2b** (**2b** : **RhB** :: 5:1). 90% water/MeCN medium was used for this study.

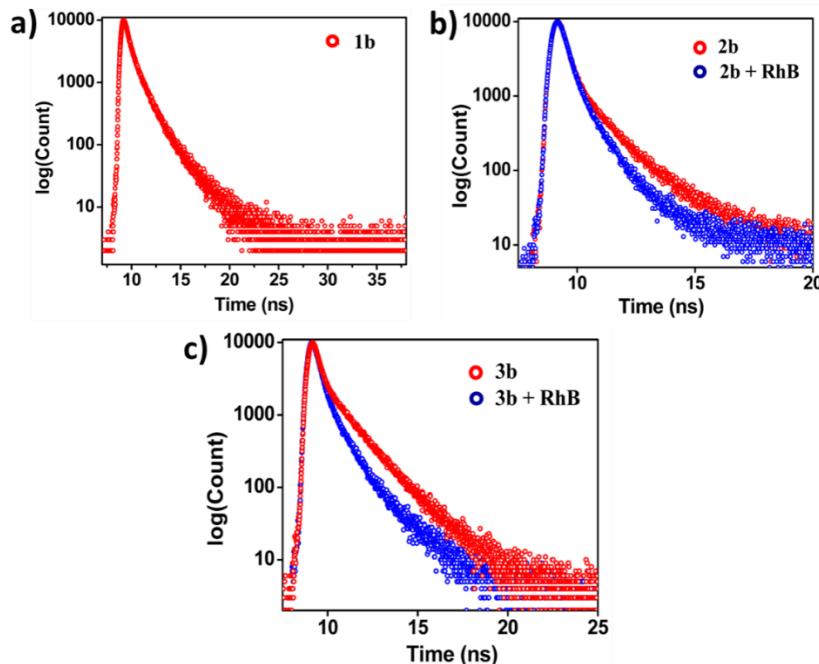


Fig. S47 Fluorescence decay profile for a) **1b** (red, $\lambda_{ex} = 320$ nm) {[**1b**] = 10^{-5} M} in 90% water/MeCN; b) **2b** (red, $\lambda_{ex} = 340$ nm) and (**2b+RhB**) (blue, $\lambda_{ex} = 340$ nm) {[**2b**] = 10^{-5} M, [RhB] = 2×10^{-6} M} in 90% water/MeCN; c) **3b** (red, $\lambda_{ex} = 340$ nm) and (**3b+RhB**) (blue, $\lambda_{ex} = 340$ nm) {[**3b**] = 10^{-5} M, [RhB] = 2×10^{-6} M} in 90% water/MeCN.

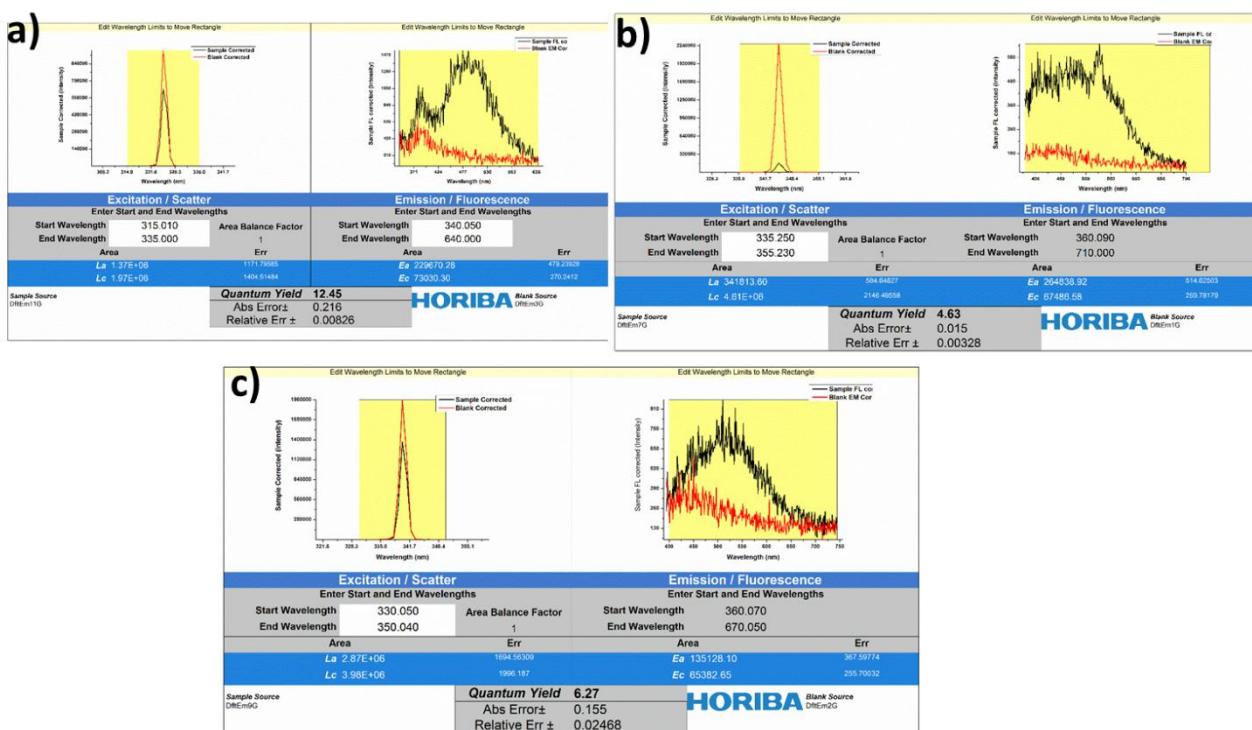


Fig. S48 Absolute fluorescence quantum yields of the cages in MeCN (a) **1b**; b) **2b**; and c) **3b**. [$c = 10^{-5}$ M; excitation/emission slit width: 2/2].

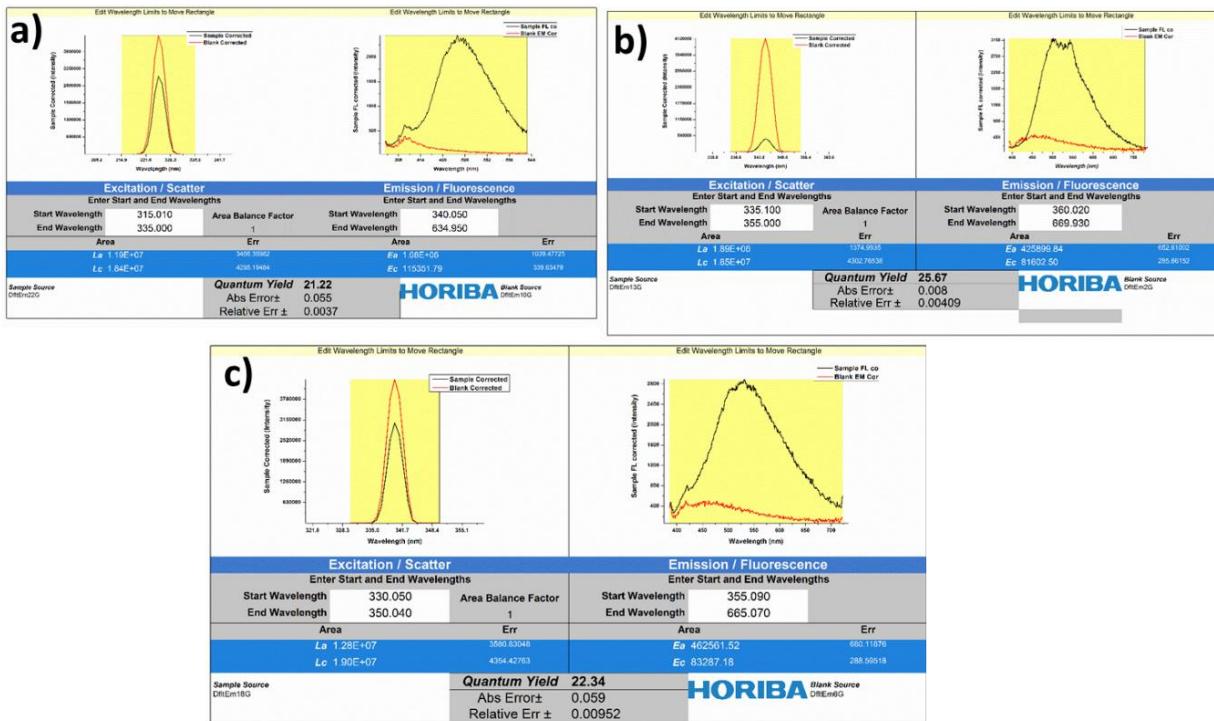


Fig. S49 Absolute fluorescence quantum yields in 90% water/MeCN for (a) **1b**; b) **2b**; and c) **3b**. [c = 10⁻⁵M; excitation/emission slit width: 2/2].

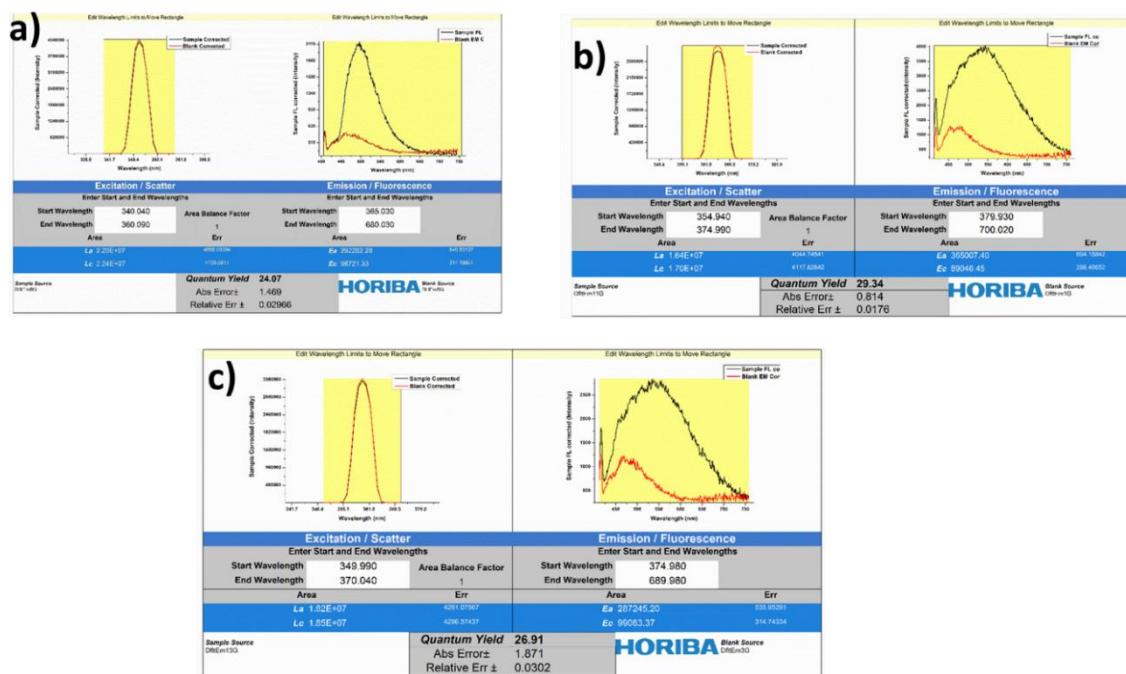


Fig. S50 Absolute fluorescence quantum yields in solid state for (a) **1b**; b) **2b**; and c) **3b**.

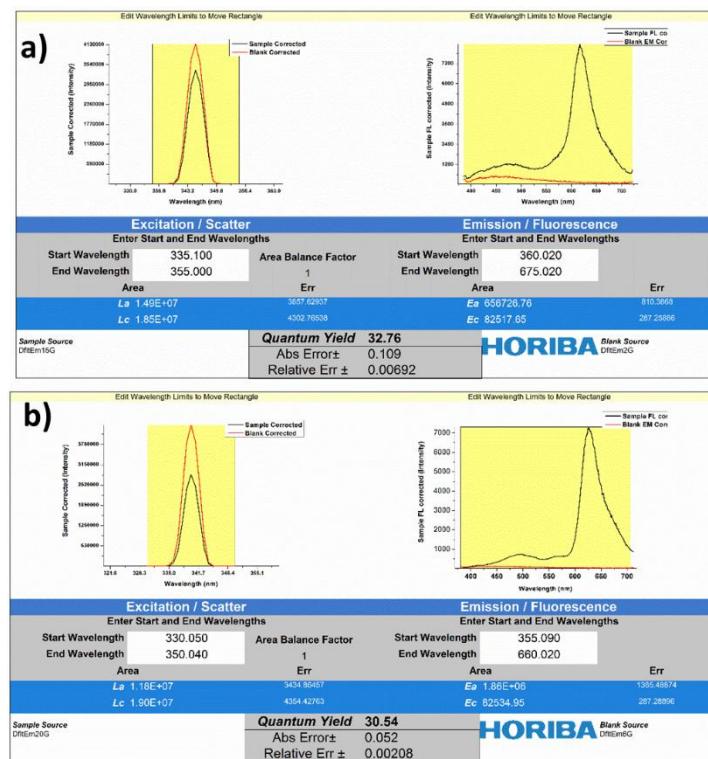


Fig. S51 Absolute fluorescence quantum yields for a) **2b + RhB** ($[2b] = 10^{-5}$ M, $[RhB] = 2 \times 10^{-6}$ M) and b) **3b + RhB** ($[3b] = 10^{-5}$ M, $[RhB] = 2 \times 10^{-6}$ M).

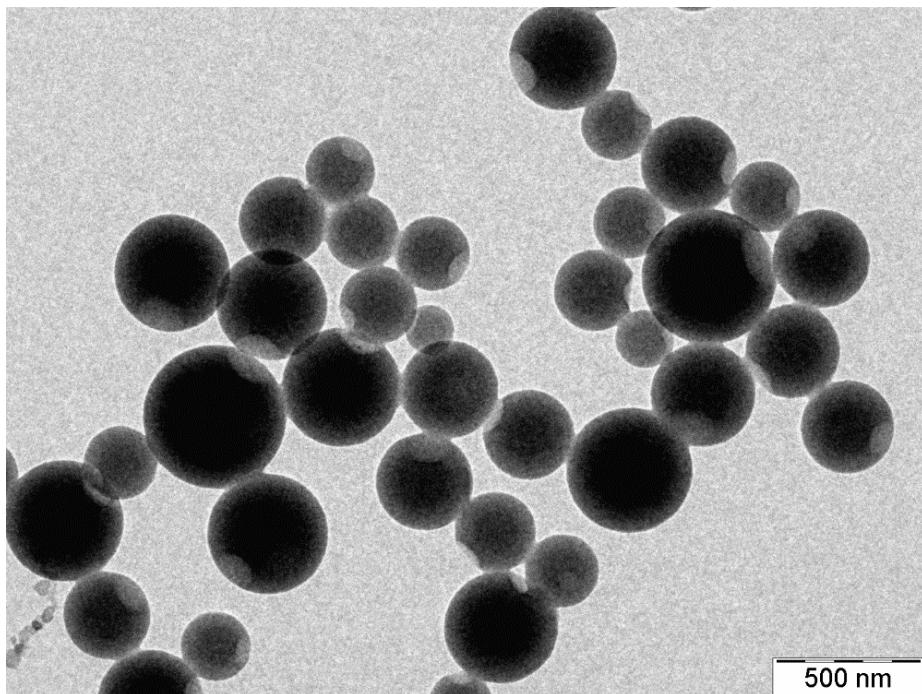


Fig. S52 TEM image showing the formation of aggregated spherical nano-aggregates of **1b** in 90% water-MeCN mixture.

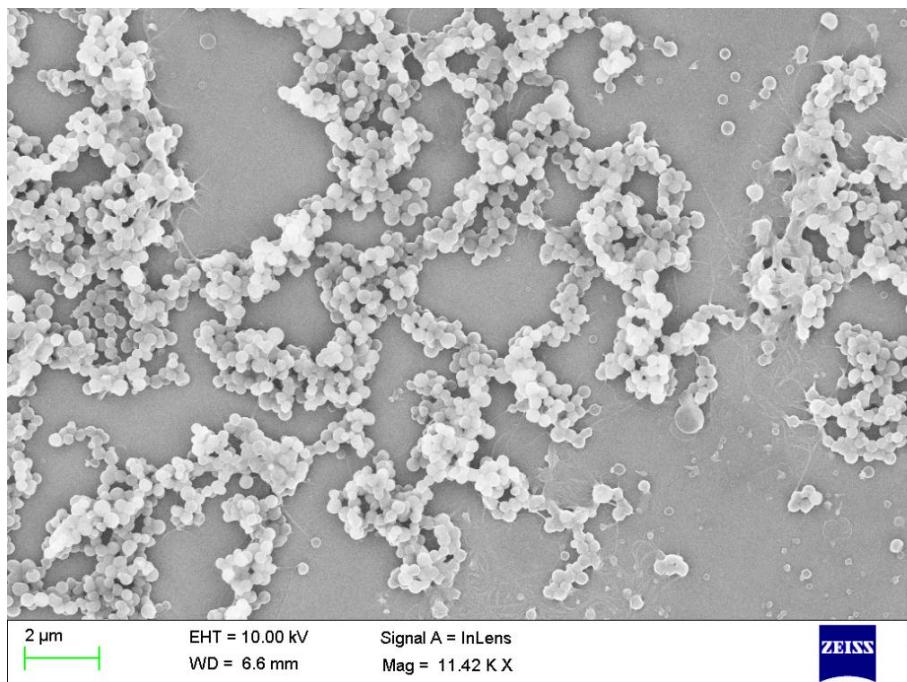


Fig. S53 SEM image showing the formation of spherical nano-aggregate of **1b** in 90% water-MeCN mixture.

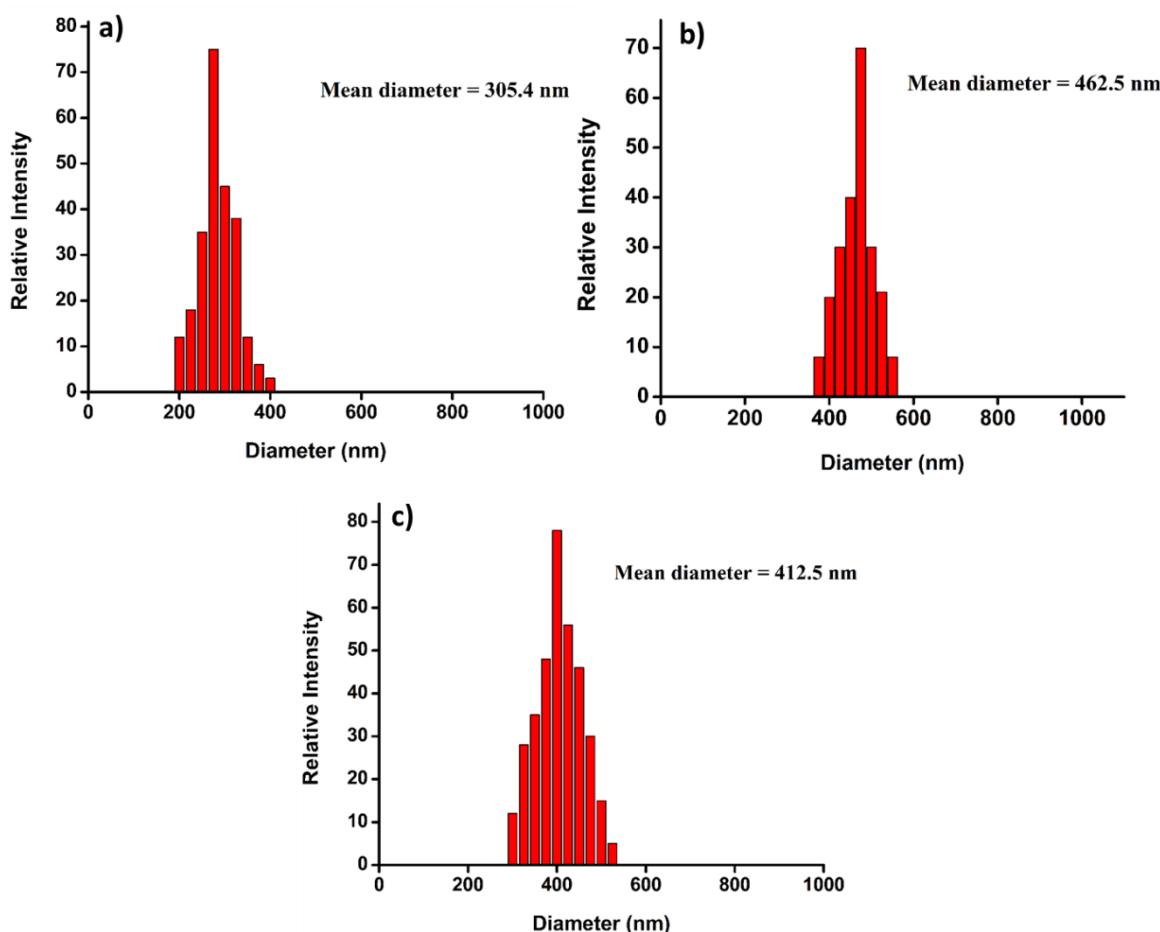


Fig. S54 DLS data profile in 90% H₂O/MeCN fraction: Size distributions patterns for a) **1b**; b) **2b** and c) **3b**.

Table S1 Photophysical data of the ligand and cages.

| Systems | Solution | | Solid | |
|-----------|--|---------------------------|----------------------|---------------------------|
| | λ_{max} (nm) | $\lambda_{emission}$ (nm) | λ_{max} (nm) | $\lambda_{emission}$ (nm) |
| L | $280 (\varepsilon_{max} = 3.02 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$ | 420 | 345 | 448 |
| 1b | $290 (\varepsilon_{max} = 1.85 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$, $325 (\varepsilon_{max} = 3.90 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$. | 480 | 345 | 510 |
| 2b | $284 (\varepsilon_{max} = 7.05 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$, $345 (\varepsilon_{max} = 5.28 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$. | 540 | 365 | 555 |
| 3b | $282 (\varepsilon_{max} = 4.92 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$, $340 (\varepsilon_{max} = 5.01 \times 10^4 \text{ molL}^{-1} \text{ cm}^{-1})$. | 530 | 360 | 550 |

Table S2 Fluorescence emission maxima in different solvents.

| | Metal complex ($\lambda_{emission}$ in nm) | | |
|-------------------|---|-----|-----|
| Solvents | 1b | 2b | 3b |
| Toluene | 460 | 495 | 515 |
| CHCl ₃ | 472 | 527 | 516 |
| DCM | 477 | 532 | 527 |
| THF | 474 | 531 | 526 |
| ACN | 480 | 538 | 530 |
| DMF | 479 | 538 | 531 |
| DMSO | 457 | 534 | 520 |

Table S3 Absolute fluorescence quantum yields of compounds under different conditions.

| Quantum Yield (Φ){ % } | | | |
|--|-----------------|------------------|-------------|
| Systems | 0% water in ACN | 90% water in ACN | Solid State |
| L | 3.46 | 15.05 | 23.22 |
| 1b | 12.45 | 21.22 | 24.07 |
| 2b | 4.63 | 25.67 | 29.34 |
| 2b + RhB* {[2b] = 10 ⁻⁵ M, [RhB] = 2 × 10 ⁻⁶ M} | ----- | 32.76 | ---- |
| 3b | 6.27 | 22.34 | 26.91 |
| 3b + RhB* {[2b] = 10 ⁻⁵ M, [RhB] = 2 × 10 ⁻⁶ M} | ----- | 30.54 | ----- |

*Solution of **2b+RhB** and **3b+RhB** were excited corresponding to λ_{max} for **2b** and **3b** respectively.

Table S4 Fluorescence lifetime parameters.

| Systems | τ_1 | B1 | τ_2 | B2 | χ^2 | τ_{av} |
|---------|----------|-------|----------|-------|----------|-------------|
| 1b | 1.09 | 58.37 | 4.23 | 41.63 | 1.09 | 2.36 |
| 2b | 0.97 | 70.60 | 3.90 | 29.40 | 1.02 | 1.83 |

| | | | | | | |
|--|------|-------|------|-------|------|------|
| 2b+RhB {[2b] = 10 ⁻⁵ M, [RhB] = 2 × 10 ⁻⁶ M} | 0.74 | 78.96 | 2.98 | 21.04 | 0.98 | 1.20 |
| 3b | 0.80 | 58.06 | 3.98 | 41.94 | 0.97 | 2.09 |
| 3b+RhB {[3b] = 10 ⁻⁵ M, [RhB] = 2 × 10 ⁻⁶ M} | 0.70 | 68.71 | 3.21 | 31.29 | 1.05 | 1.47 |

- Bi-exponential fitting
- τ_1 and τ_2 represents life time
- B1 and B2 are real amplitude corresponding to τ_1 and τ_2 respectively.
- τ_{av} calculated via following Equation (S1):

$$\tau_{av} = \frac{(\tau_1 \times B1 + \tau_2 \times B2)}{(B1 + B2)} \quad \text{Equation S1}$$

Energy transfer efficiency

Energy transfer efficiency is calculated by following Equation (S2):

$$\Phi_{ET} = 1 - \frac{I_{DA}}{I_D} \quad \text{Equation S2}$$

Where

I_{DA} = Intensity of donor emission in presence of acceptor

I_D = Intensity of donor emission in absence of acceptor

Φ_{ET} = fractional energy transfer efficiency

Table S5 Energy transfer efficiency for **2b+RhB** and **3b+RhB**.

| LHSs | λ_{ex} | I_{DA} | I_D | $\Phi_{ET}(\%)$ |
|---------------|----------------|----------|--------|-----------------|
| 2b+RhB | 340 | 30183 | 133588 | 77 |
| 3b+RhB | 345 | 40704 | 92807 | 58 |

Antenna effect

The antenna effect calculated for certain concentration of donor and acceptor equal to the ratio of emission intensity at 610 (for 2b) {Equation S3} and 615 (for 3b) {Equation S4} upon excitation of the donor.

(a) Antenna effect for **2b+RhB**:

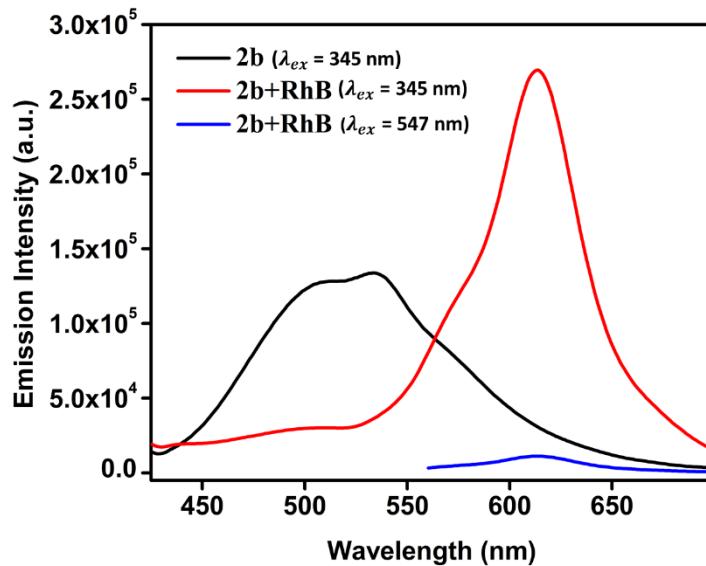


Fig. S55 Fluorescence emission intensity of **2b** ($\lambda_{ex} = 345 \text{ nm}$), **2b+RhB** {[**2b**] = 10^{-5}M } and {[**RhB**] = $2 \times 10^{-6}\text{M}$ } ($\lambda_{ex} = 345 \text{ nm}$) and **2b+RhB** {[**2b**] = 10^{-5}M } and {[**RhB**] = $2 \times 10^{-6}\text{M}$ } ($\lambda_{ex} = 547 \text{ nm}$).

$$\text{Antenna effect} = \frac{I_{A+D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}} - I_{D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}}}{I_{A+D(\lambda_{ex}=547 \text{ nm})}^{610 \text{ nm}}} \quad \text{Equation S3 (for } \mathbf{2b}\text{)}$$

$I_{D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}}$ = Emission intensity of donor at 610 nm upon excitation at 345 nm.

$I_{A+D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}}$ = Emission intensity of (donor+ acceptor) {[**2b**] = 10^{-5}M } and {[**RhB**] = $2 \times 10^{-6}\text{M}$ } at 610 nm upon excitation at 345 nm.

$I_{A+D(\lambda_{ex}=547 \text{ nm})}^{610 \text{ nm}}$ = Emission intensity of (donor+ acceptor) {[**2b**] = 10^{-5}M } and {[**RhB**] = $2 \times 10^{-6}\text{M}$ } at 610 nm upon excitation at 547 nm.

Table S6 Energy transfer efficiency for **2b+RhB**.

| LHSs | $I_{A+D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}}$ | $I_{D(\lambda_{ex}=345 \text{ nm})}^{610 \text{ nm}}$ | $I_{A+D(\lambda_{ex}=547 \text{ nm})}^{610 \text{ nm}}$ | Antenna effect |
|---------------|---|---|---|----------------|
| 2b+RhB | 266740 | 33222 | 11120 | 21 |

(b) Antenna effect for **3b+RhB**:

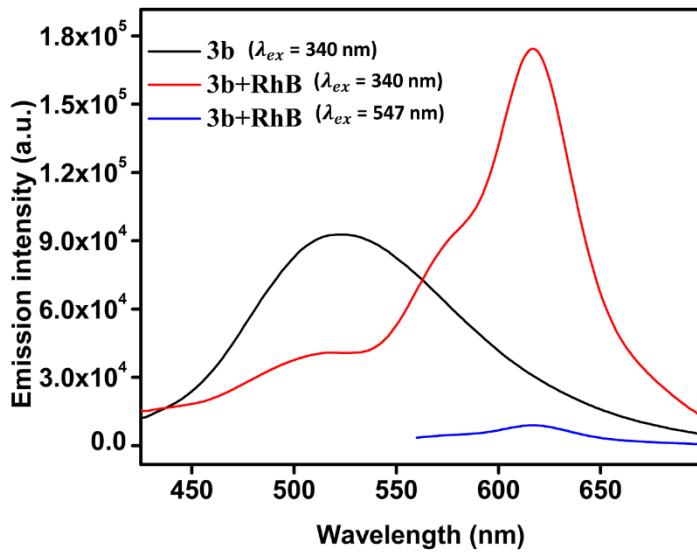


Fig. S56 Fluorescence emission intensity of **3b** ($\lambda_{ex} = 340\text{ nm}$), **3b+RhB** {[**3b**] = 10^{-5}M and [**RhB**] = $2 \times 10^{-6}\text{M}$ } ($\lambda_{ex} = 340\text{ nm}$) and **3b+RhB** {[**3b**] = 10^{-5}M and [**RhB**] = $2 \times 10^{-6}\text{M}$ } ($\lambda_{ex} = 547\text{ nm}$).

$$\text{Antenna effect} = \frac{I_{A+D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}} - I_{D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}}}{I_{A+D(\lambda_{ex}=547\text{ nm})}^{615\text{ nm}}} \quad \text{Equation S4 (for } \mathbf{3b}\text{)}$$

$I_{D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}}$ = Emission intensity of donor (**3b**) at 615 nm upon excitation at 340 nm.

$I_{A+D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}}$ = Emission intensity of (donor+ acceptor) {[**3b**] = 10^{-5}M and [**RhB**] = $2 \times 10^{-6}\text{M}$ } at 615 nm upon excitation at 340 nm.

$I_{A+D(\lambda_{ex}=547\text{ nm})}^{615\text{ nm}}$ = Emission intensity of (donor+ acceptor) {[**3b**] = 10^{-5}M and [**RhB**] = $2 \times 10^{-6}\text{M}$ } at 615 nm upon excitation at 547 nm.

Table S7 Energy transfer efficiency for **3b+RhB**.

| LHSs | $I_{A+D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}}$ | $I_{D(\lambda_{ex}=340\text{ nm})}^{615\text{ nm}}$ | $I_{A+D(\lambda_{ex}=547\text{ nm})}^{615\text{ nm}}$ | Antenna effect |
|---------------|---|---|---|----------------|
| 3b+RhB | 174372 | 31709 | 8916 | 16 |

General procedure for the synthesis of 6a-6f.

In air, *N,N*-dimethylaniline (5 mg, 0.0412 mmol), *N*-aryl/alkyl maleimide derivatives (0.0412 mmol), catalyst cage **2b** (13.2 mg, 0.002 mmol, 5 mol%) and rhodamine B (0.2 mg, 0.0004 mmol, 1 mol%) were successively added to a 0.5 mL acetonitrile (MeCN). To this solution 4.5 mL water was added to make the final solution as 90% water/ MeCN mixture.^a Then this reaction mixture was transferred to a quartz glass vial containing a magnetic stir bar

and then placed in white light LED photoreactor and stirred for 12 h. The vial was irradiated with visible light (white light) and maintained at 25 °C (room temperature). After the completion of reaction, solvent was evaporated under reduced pressure. Then crude product was extracted with CDCl₃ (0.5 mL) and 1,3,5-trimethoxybenzene (6.9 mg, 0.0412 mmol) was added as the reference to calculate the conversions of the reaction based on the ¹H integrals.

^aFor substrate **5f** reaction was performed in 70% water/MeCN mixture; ^bCrude products were purified by flash chromatography using 5-10% ethyl acetate/hexane mixture.

Synthesis of **6a**:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.47 (1H, d, J = 8 Hz), 7.35 (3H, m, 7.27) 1H, d, J = 8 Hz, 7.20 (3H, m, 6.84) 1H, m, 6.69 (1H, d, J = 8 Hz, 4.09) 1H, d, J = 12 Hz, 3.55 (1H, dd, J = 12, 2 Hz, 3.48) 1H, ddd, J = 12, 8, 4 Hz, 3.07 (1H, dd, J = 8, 4 Hz), 2.78 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 178.1, 176.2, 148.8, 132.5, 130.8, 129.4, 129.1, 128.9, 126.8, 120.2, 119.1, 113.1, 51.1, 43.9, 42.5 and 39.9. ESI MS (m/z): Calcd. For [M+H]⁺ 293.12, found, 293.13 for [M+H]⁺; Calcd. For [M+Na]⁺ 315.10, found, 315.11 for [M+Na]⁺.

Synthesis of **6b**:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.47 (1H, d, J = 4 Hz), 7.20 (1H, dd, J = 4, 4 Hz, 6.89) 1H, dd, J = 4, 4 Hz, 6.70 (1H, d, J = 4 Hz), 3.97 (1H, d, J = 12 Hz, 3.47 - 3.56) 3H, m, 3.34 (1H, ddd, J = 12, 8, 4 Hz, 3.03) 1H, dd, J = 8, 4 Hz, 2.79 (s, 3H), 1.13 (3H, t, J = 8 Hz). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 178.9, 177.0, 148.9, 130.7, 129.0, 120.0, 119.3, 112.9, 51.5, 43.9, 42.4, 39.8, 34.7 and 13.4. ESI MS (m/z): ESI MS (m/z): Calcd. For [M+H]⁺ 245.12, found, 245.13 for [M+H]⁺; Calcd. For [M+Na]⁺ 267.12, found, 267.12 for [M+Na]⁺.

Synthesis of **6c**:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.46 (1H, d, J = 4 Hz), 7.20 (1H, dd, J = 8, 8 Hz, 6.88) 1H, dd, J = 8, 8 Hz, 6.70 (1H, d, J = 8 Hz), 3.91 (1H, d, J = 12 Hz, 3.91) 1H, d, J = 12 Hz, 3.45 (1H, d, J = 12 Hz, 3.28) 1H, ddd, J = 12, 8, 4 Hz, 3.17 (1H, s) 3.03 (1H, dd, J = 12, 4 Hz), 2.79 (s, 3H), 2.04 - 2.10 (2H, m), 1.77 (2H, d, J = 12 Hz), 1.53 – 1.61 (4H, m), 1.21 – 1.26 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 179.2, 177.3, 148.9, 130.7, 128.9, 119.9, 119.6, 112.8, 52.6, 51.3, 43.5, 42.2, 39.8, 29.3, 26.2 and 25.2. ESI MS (m/z): Calcd. For [M+H]⁺ 299.17, found, 299.18 for [M+H]⁺; Calcd. For [M+Na]⁺ 321.17, found, 321.16 for [M+Na]⁺.

Synthesis of **6d**:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.45 (1H, d, J = 8 Hz), 7.15 (3H, m, 7.03 (2H, m), 6.82) 1H, m, 6.86 (1H, d, J = 8 Hz), 4.06 (1H, d, J = 8 Hz, 3.52) 1H, dd, J = 12, 4 Hz, 3.44 (1H, ddd, J = 12, 8, 4 Hz, 3.03) 1H, dd, J = 8, 4 Hz, 2.76 (s, 3H), 2.27 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 178.3, 176.4, 149.0, 139.0, 130.8, 130.1, 129.9, 129.1, 126.7, 120.1, 119.2, 113.0, 51.2, 44.0, 42.6, 39.9 and 21.7. ESI MS (m/z): Calcd. For [M+H]⁺ 307.14, found, 307.15 for [M+H]⁺; Calcd. For [M+Na]⁺ 329.12, found, 329.13 for [M+Na]⁺.

Synthesis of 6e:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.43 – 7.48 (3H, m, J = 8 Hz), 7.18 (1H, d, J = 8 Hz), 7.10 – 7.15 (2H, m), 6.84 (1H, t, J = 8 Hz), 6.67 (1H, d, J = 8 Hz), 4.08 (1H, d, J = 12 Hz), 3.53 (1H, dd, J = 12, 4 Hz), 3.46 (1H, ddd, J = 12, 8, 4 Hz), 3.04 (1H, dd, J = 8, 4 Hz), 2.76 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 177.8, 175.9, 149.0, 132.6, 131.5, 130.8, 129.3, 128.3, 122.7, 120.2, 118.8, 113.1, 51.1, 44.1, 42.6 and 39.9. ESI MS (m/z): Calcd. For [M+H]⁺ 371.04, found, 371.04 for [M+H]⁺.

Synthesis of 6f:

¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.82 – 7.97 (5H, m, 7.27 - 7.46 (4H, m, 7.14 -7.18 (2H, m), 6.88 (1H, t, J = 8Hz), 6.66 (1H, m), 4.07 (1H, d, J = 8 Hz), 3.52 (1H, dd, J = 12, 4 Hz), 3.45 (1H, ddd, J = 12, 8, 4 Hz), 3.04 (1H, dd, J = 8, 4 Hz), 2.76 (s, 3H). ¹³C NMR (100 MHz, CD₃CN) δ (ppm): 178.7, 176.8, 133.2, 132.8, 130.8, 129.5, 129.0, 128.9, 128.2, 127.3, 126.9, 126.6, 125.7, 124.1, 123.6, 123.3, 121.5, 119.7, 117.8, 114.1, 113.0, 51.4, 44.1, 42.7 and 39.4. ESI MS (m/z): Calcd. For [M+Na]⁺ 439.09, found, 439.08 for [M+Na]⁺.

Recyclability studies of catalyst 2a

In air, *N,N*-dimethylaniline (5.0 mg, 0.0412 mmol), *N*-phenyl maleimide **5a** (7.7 mg, 0.0412 mmol), catalyst cage **2b** (13.2 mg, 0.002 mmol, 5 mol%) and rhodamine B (0.2 mg, 0.0004 mmol,1 mol%) were successively added to 0.5 mL acetonitrile (MeCN). To this solution 4.5 mL water was added to make the final solution 90% water/ MeCN mixture*. Then this reaction mixture was transferred to a quartz glass vial containing a magnetic stir bar and then placed in white light LED photoreactor and magnetically stirred for 12 h. The vial was irradiated with visible light (white light) and maintained at 25 °C (room temperature). After the completion of reaction, solvent was evaporated under reduced pressure. Then crude product was extracted with CDCl₃ and ¹H NMR checked with internal standard 1,3,5-trimethoxy benzene. Then solid cage **2b** was washed three times with CHCl₃ to remove Rhodamine-B dye and added fresh 1 mol% RhB and used for next run.

Detection of H₂O₂: Formation of H₂O₂ as by-product during catalytic reaction was confirmed by adding the reaction mixture **B** to the KI/starch solution which turns the colorless solution of (KI/starch) to dark blue due to oxidation of potassium iodide by hydrogen peroxide (Table S8)^{S6}.

Table S8 Detection of H₂O₂ by KI/starch indicator

| Solution under visible light | A | B | C | D | E |
|------------------------------|---|--|---|--|---|
| Solution | Starch +KI solution as an indicator in water ^a | Reaction mixture ^b at t = 0 h | Reaction mixture ^b at t = 12 h | Addition of 0.5 ml reaction mixture ^b at t = 12 h to solution A | Addition of 0.5 ml 30% H ₂ O ₂ solution to solution A |
| Color | Colorless | Light orange | Light orange | Dark blue | Blue-violet |

^aSolution of Starch (0.04 mmol) +KI (0.04 mmol) Solution in 5 ml water; ^bReaction mixture: N,N-Dimethylaniline **4** (0.04 mmol), N-alkyl/aryl maleimides **5** (0.04 mmol), catalyst **A** (5 mol%), **RhB** (1 mol%) in water (4.5 mL) + MeCN (0.5 ml) mixture.

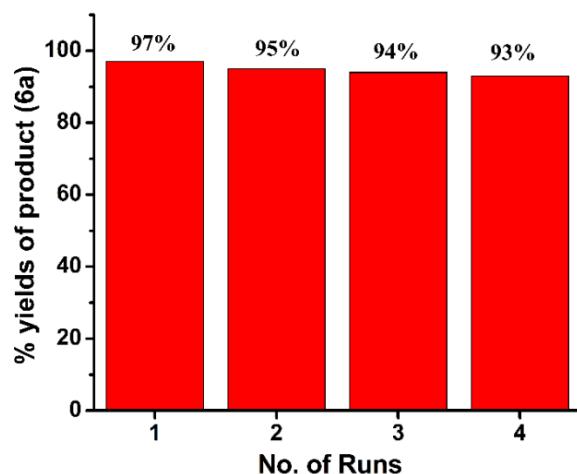


Fig. S57 Reusability studies of **2b** catalyst for the synthesis of **6a**.

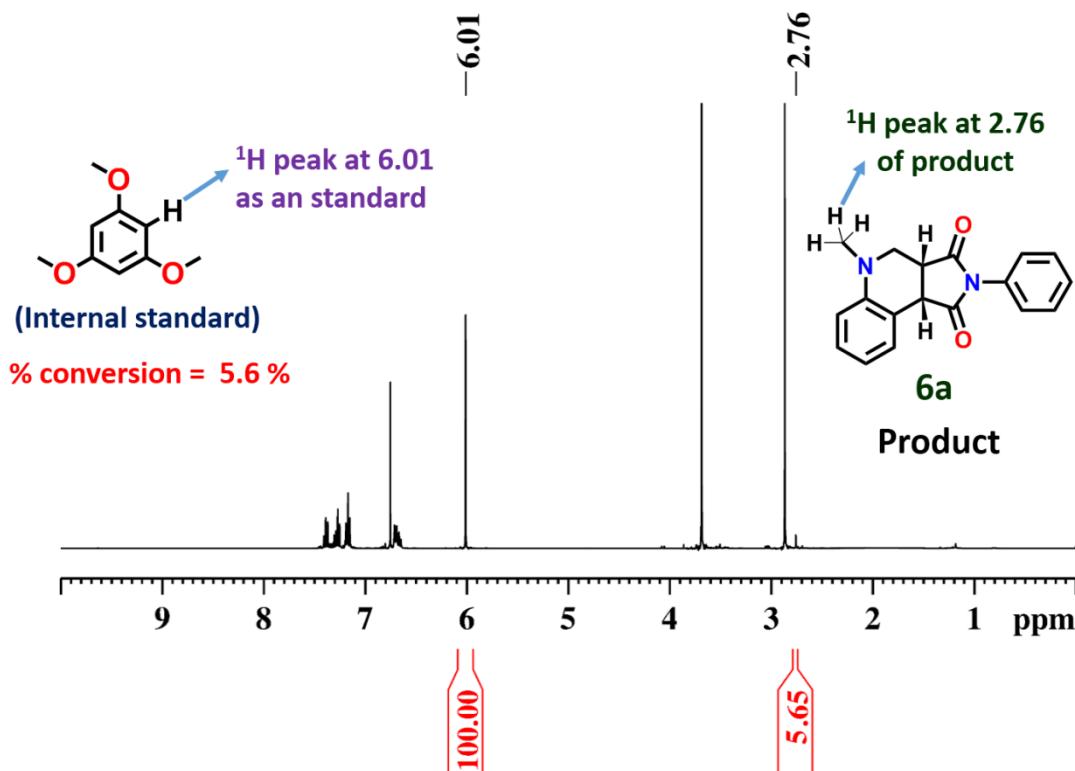


Fig. S58 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4 + 5a**) using {1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

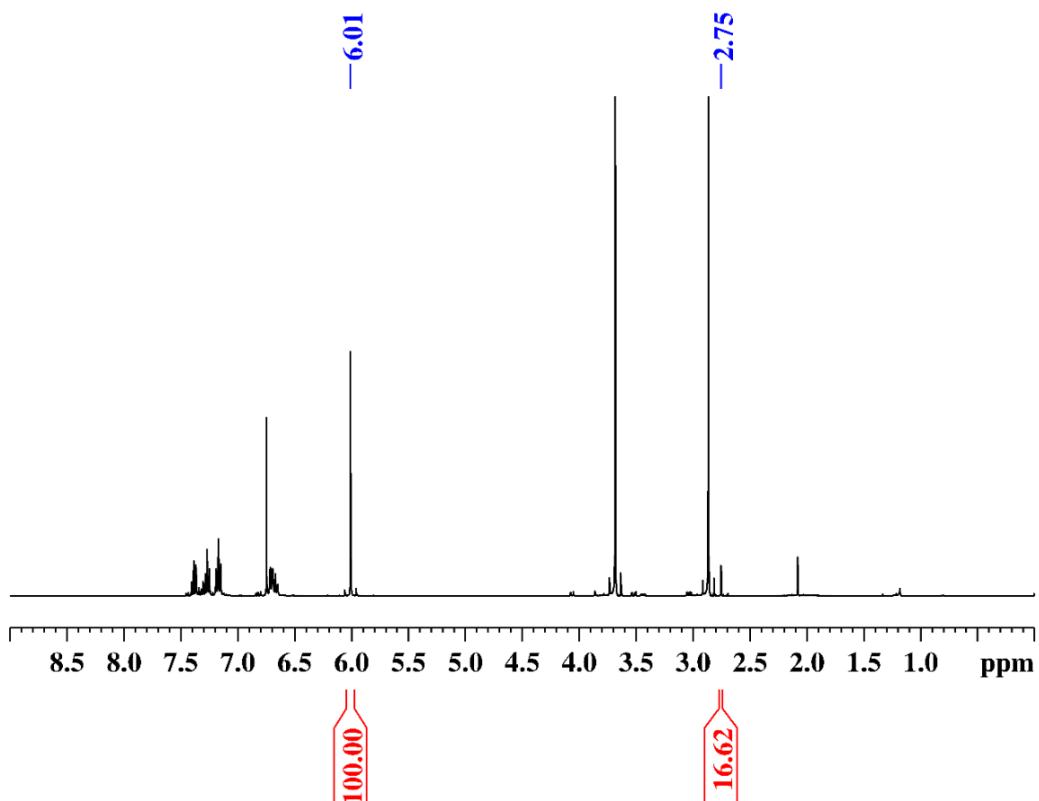


Fig. S59 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4 + 5a**) using {5 mol% **RhB**} as the photocatalyst at 12 h under visible light.

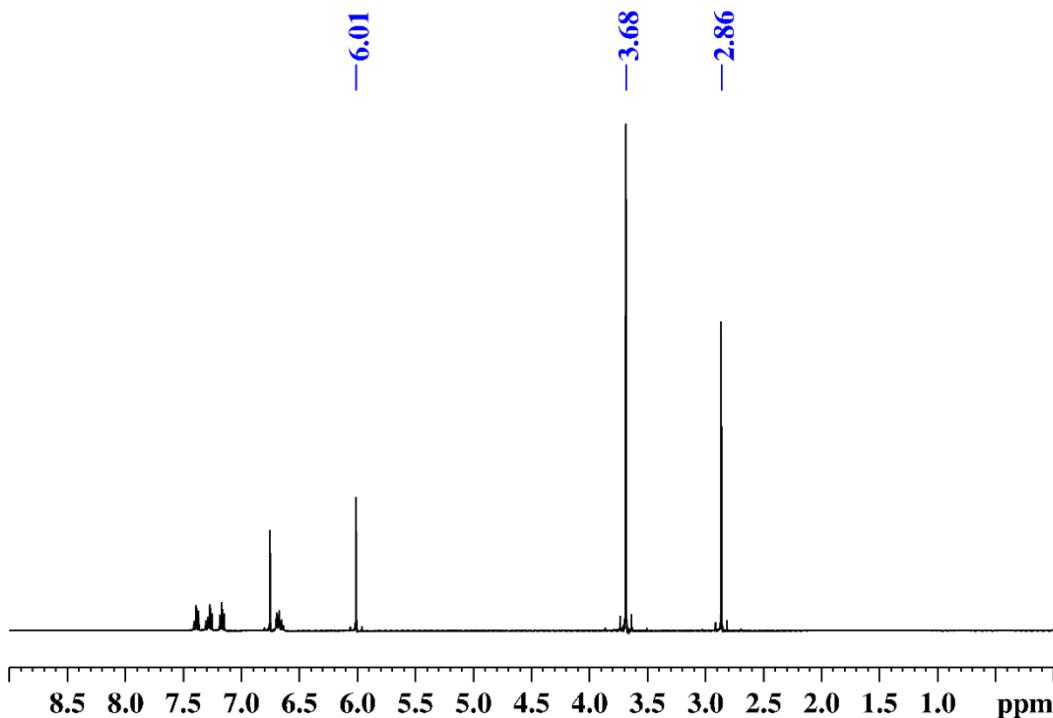


Fig. S60 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% cage **2b**} as the photocatalyst at 12 h under visible light.

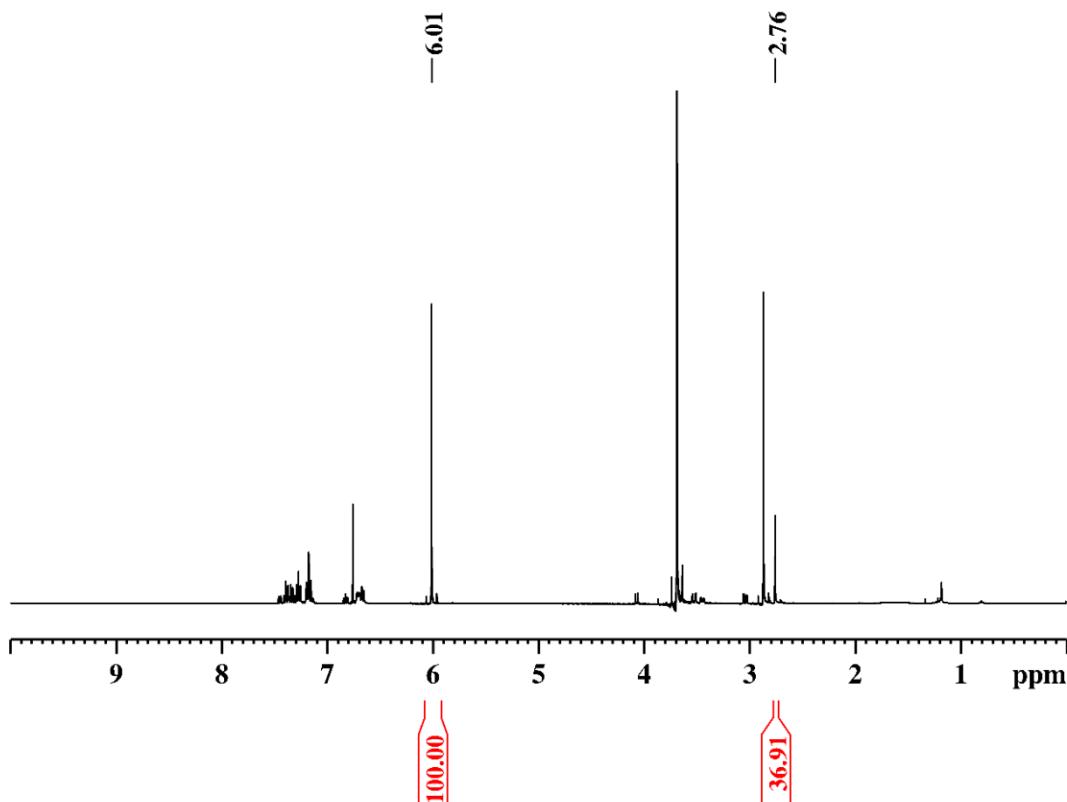


Fig. S61 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% cage **2b + 1** mol% **RhB**} as the photocatalyst for 4 h under visible light.

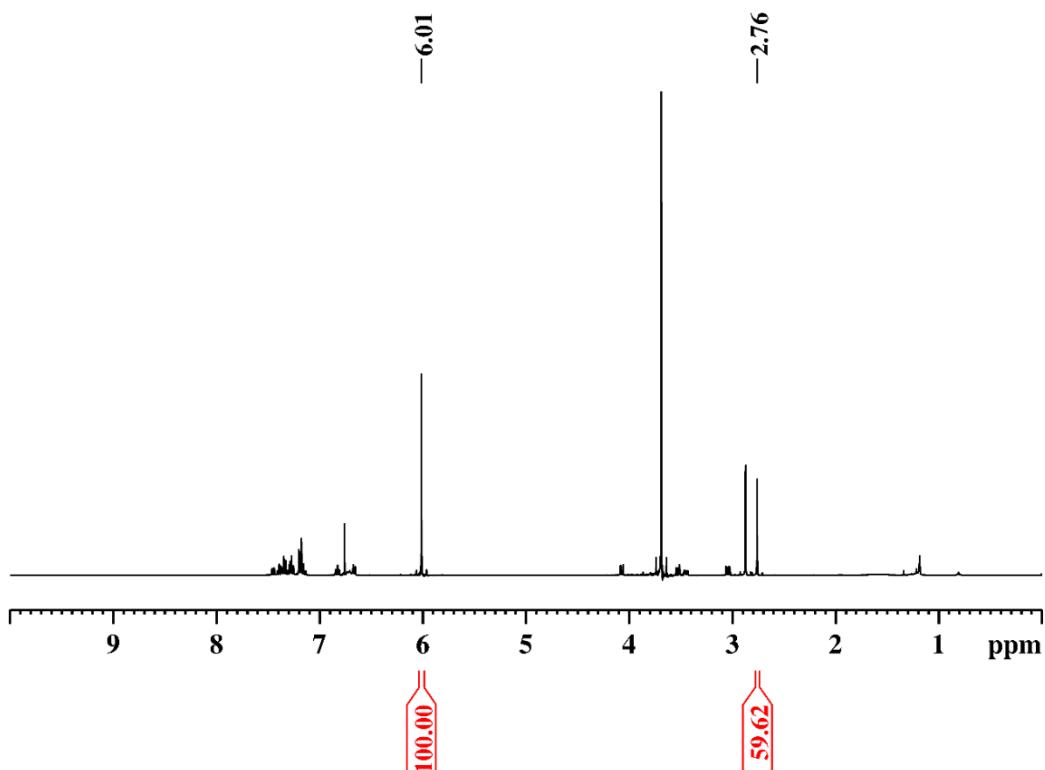


Fig. S62 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 8 h under visible light.

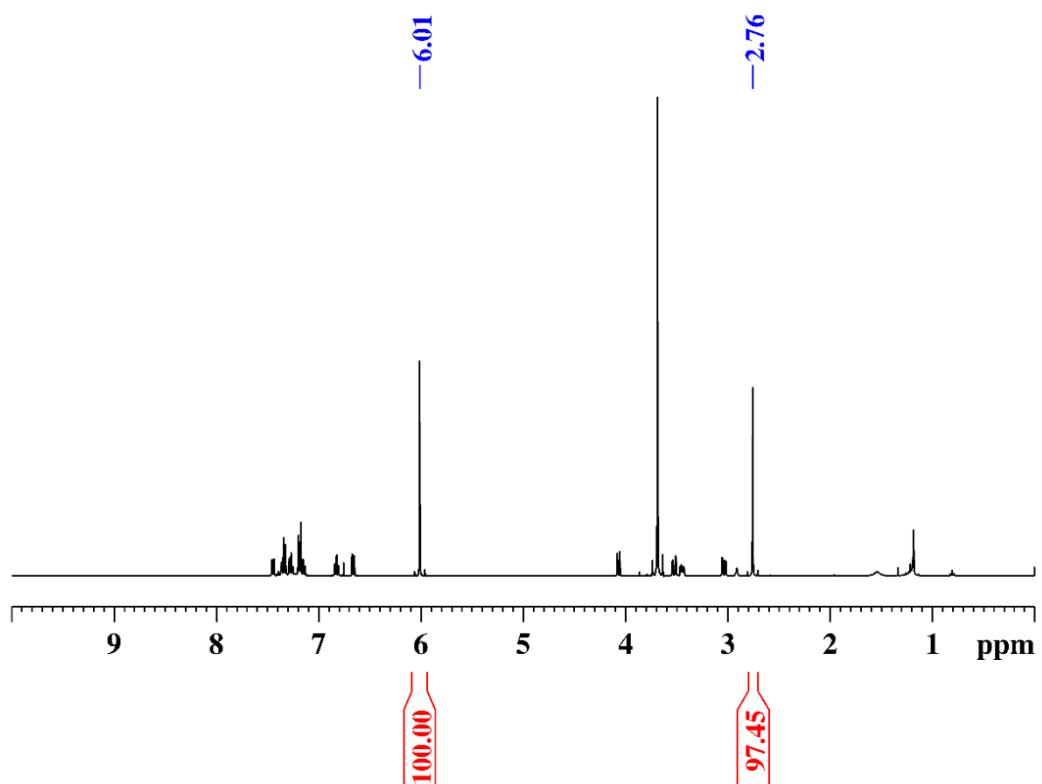


Fig. S63 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

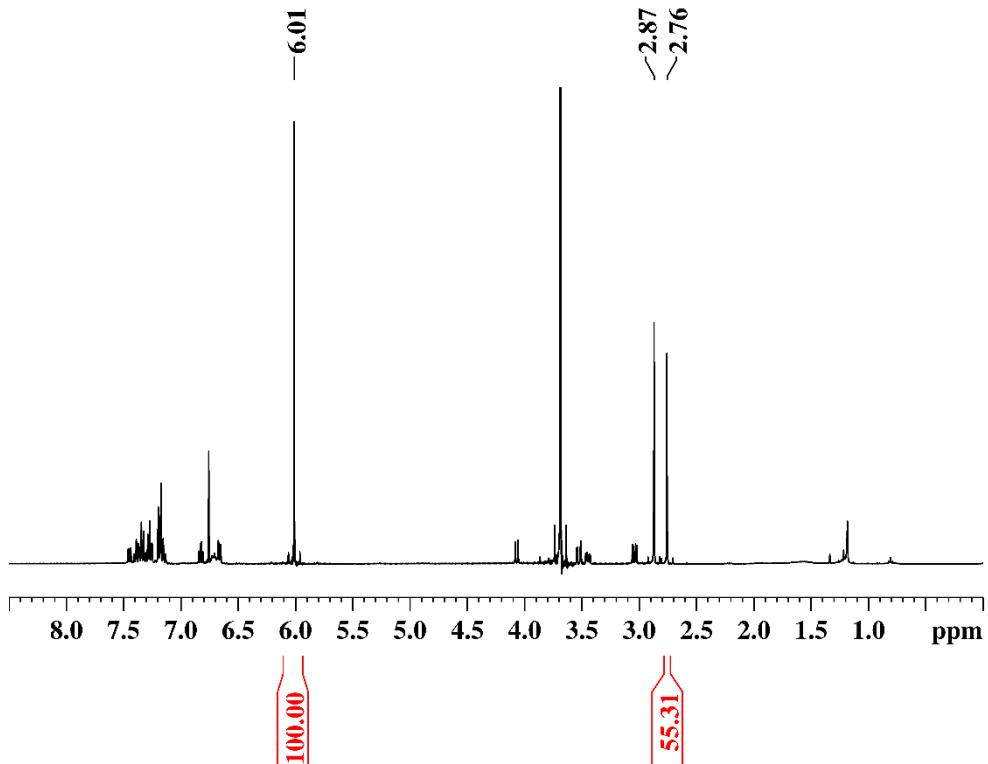


Fig. S64 ¹H NMR (400 MHz, CDCl_3) of the reaction of (**4 + 5a**) using {2.5 mol% cage **2b** + 0.5 mol% **RhB**} as the photocatalyst for 12 h under visible light.

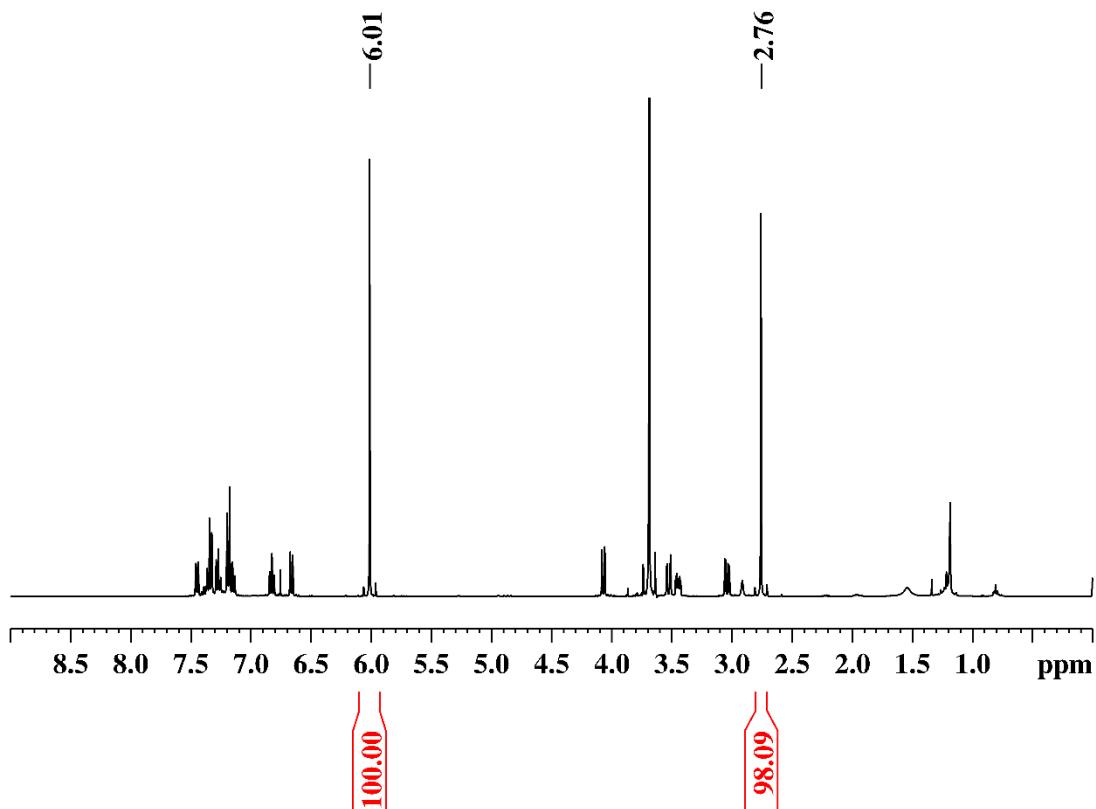


Fig. S65 ¹H NMR (400 MHz, CDCl_3) of the reaction of (**4 + 5a**) using {7.5 mol% cage **2b** + 1.5 mol% **RhB**} as the photocatalyst for 12 h under visible light.

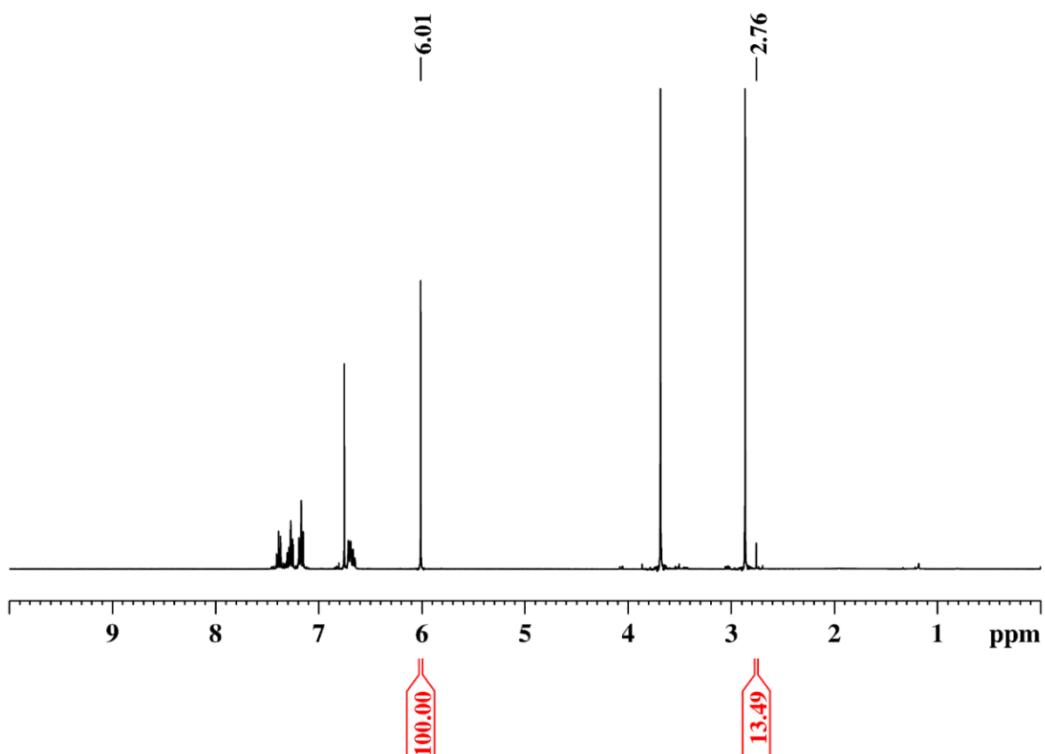


Fig. S66 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under dark condition.

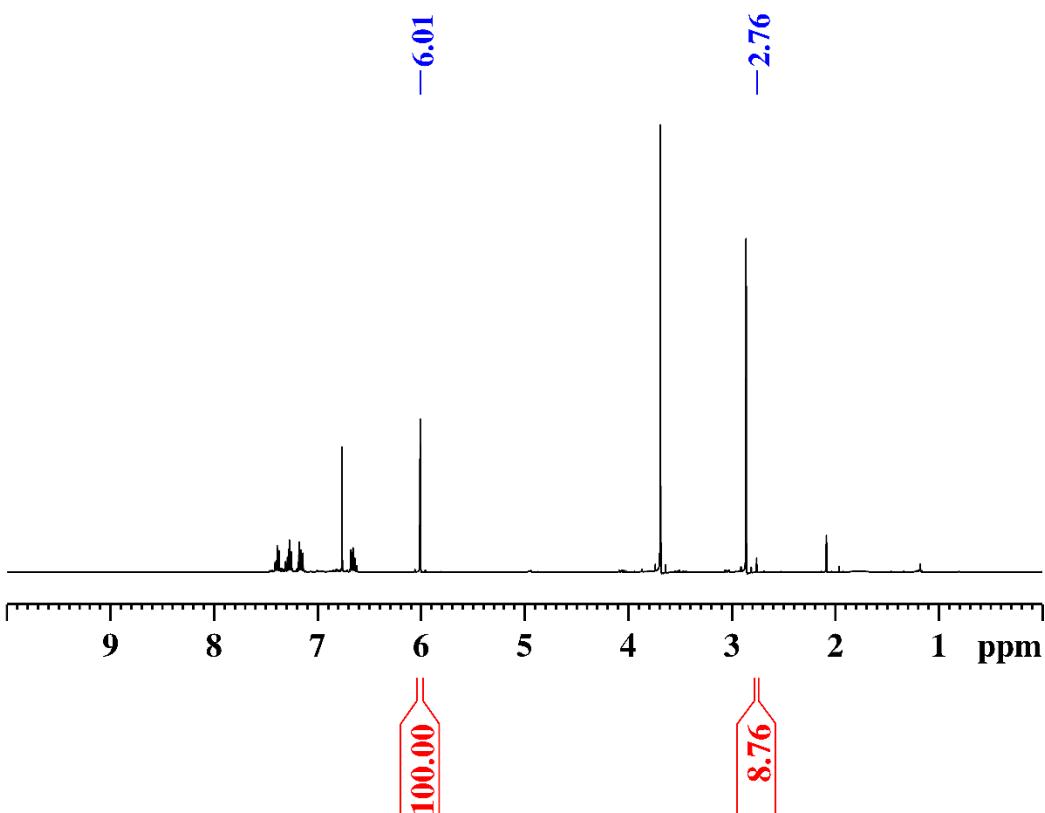


Fig. S67 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4 + 5a**) using {5 mol% ligand **L** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

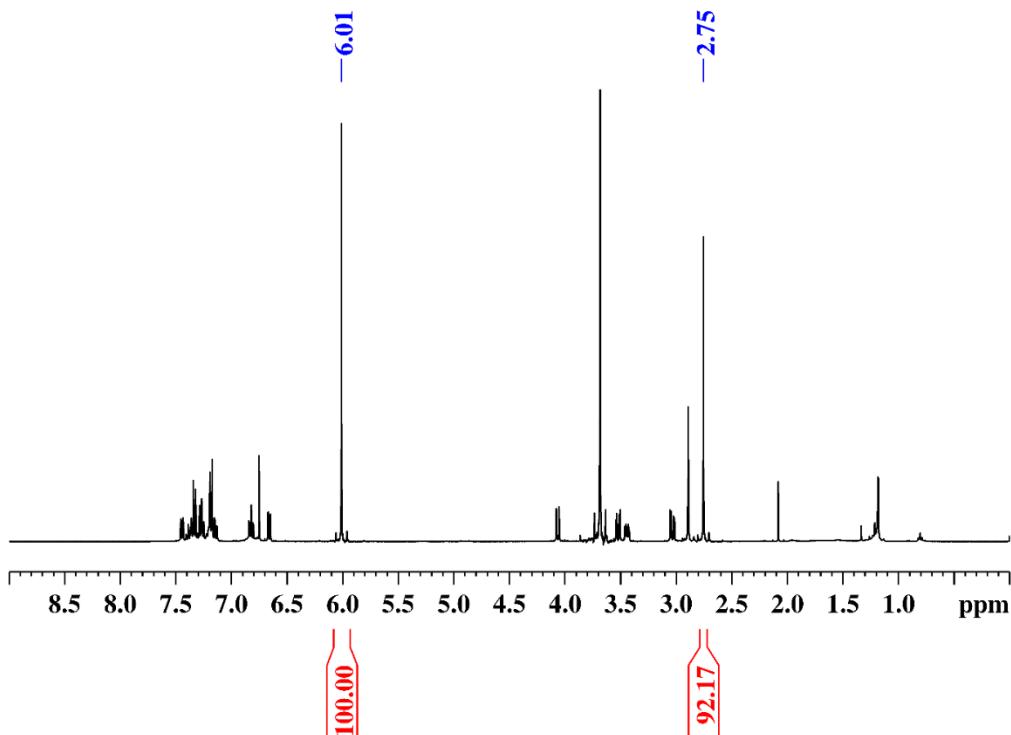


Fig. S68 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4** + **5a**) using {5 mol% cage **3b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

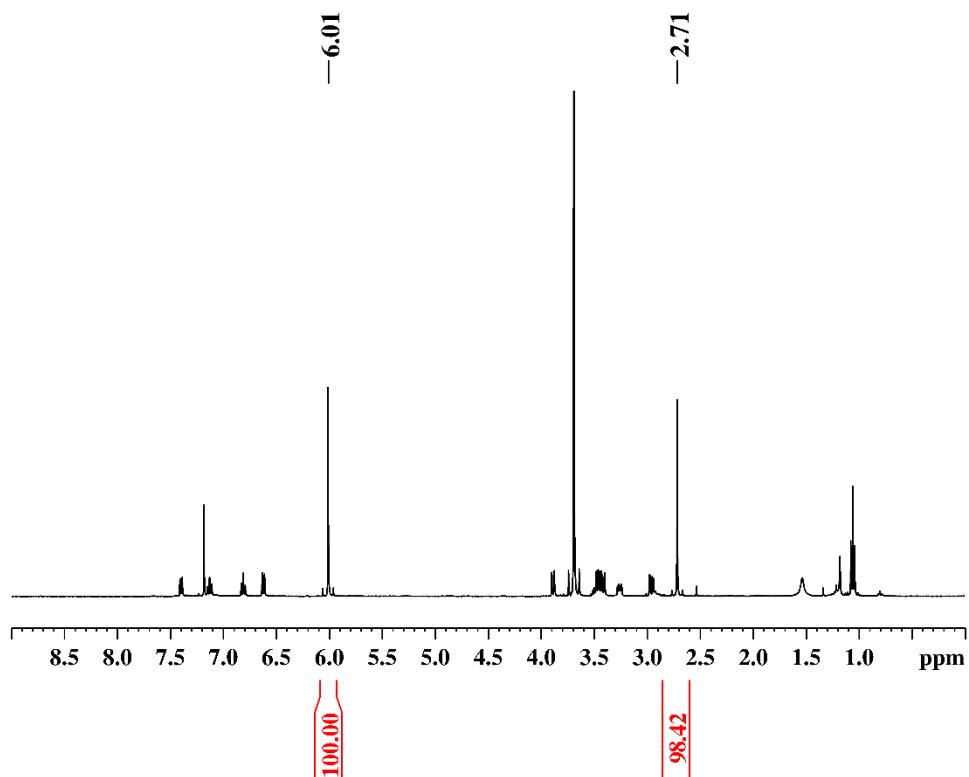


Fig. S69 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4** + **5b**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

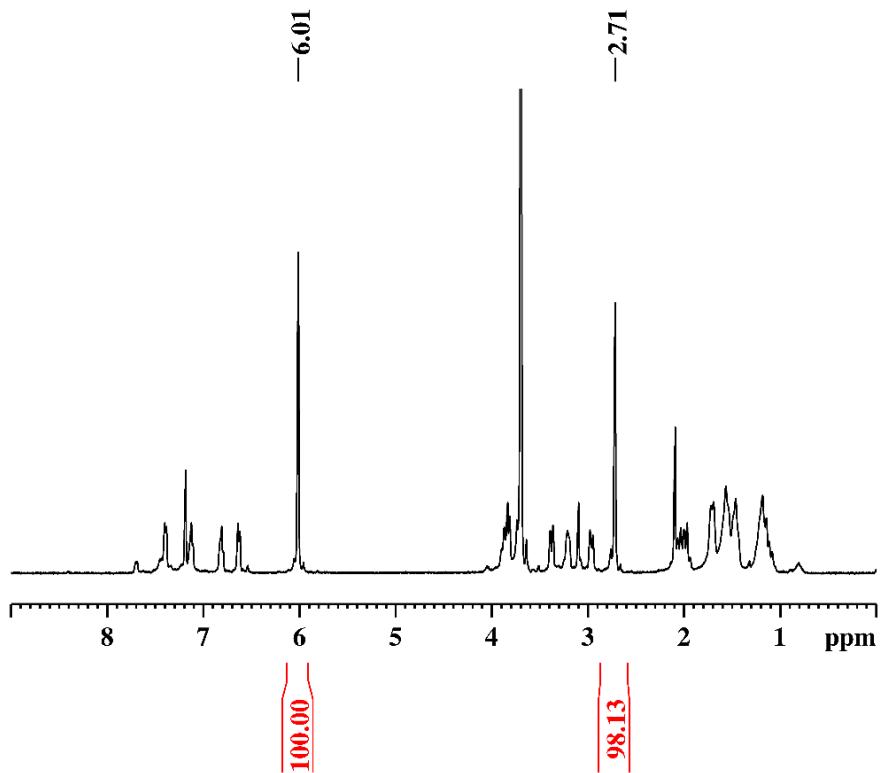


Fig. S70 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4** + **5c**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

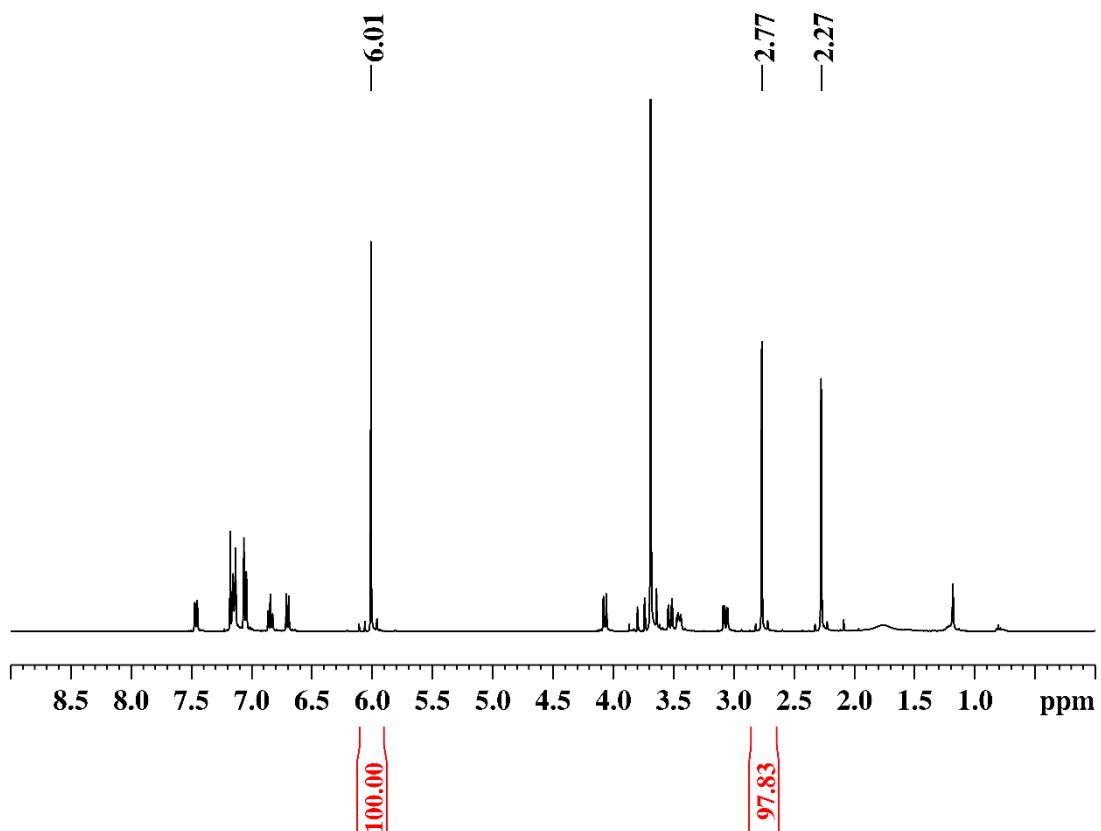


Fig. S71 ^1H NMR (400 MHz, CDCl_3) of the reaction of (**4** + **5d**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

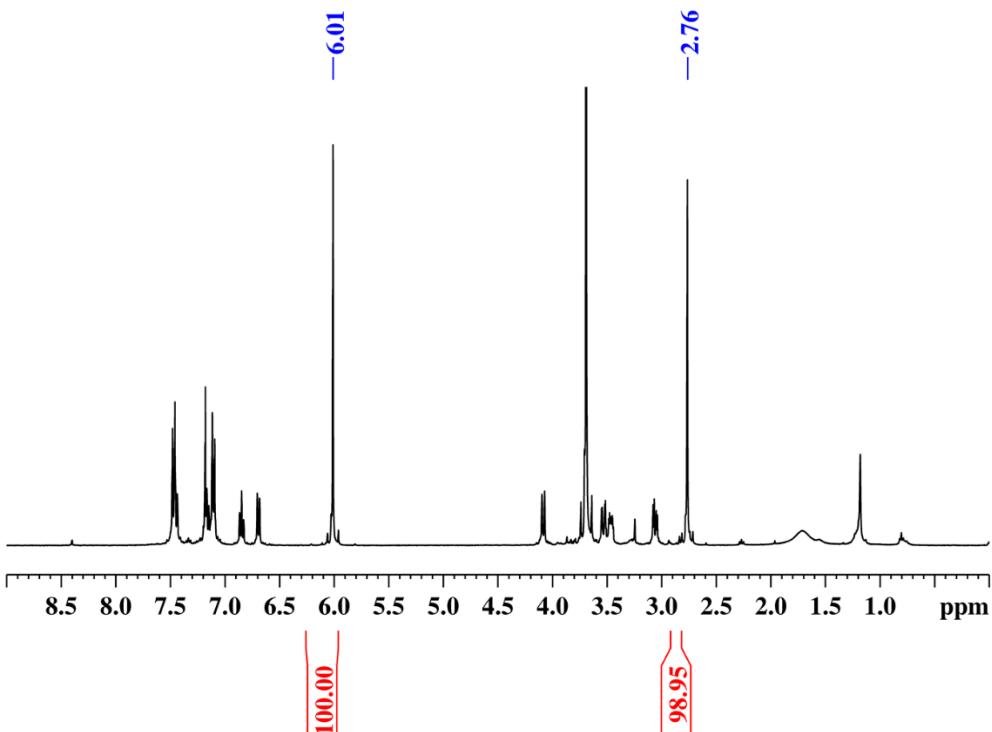


Fig. S72 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4** + **5e**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light.

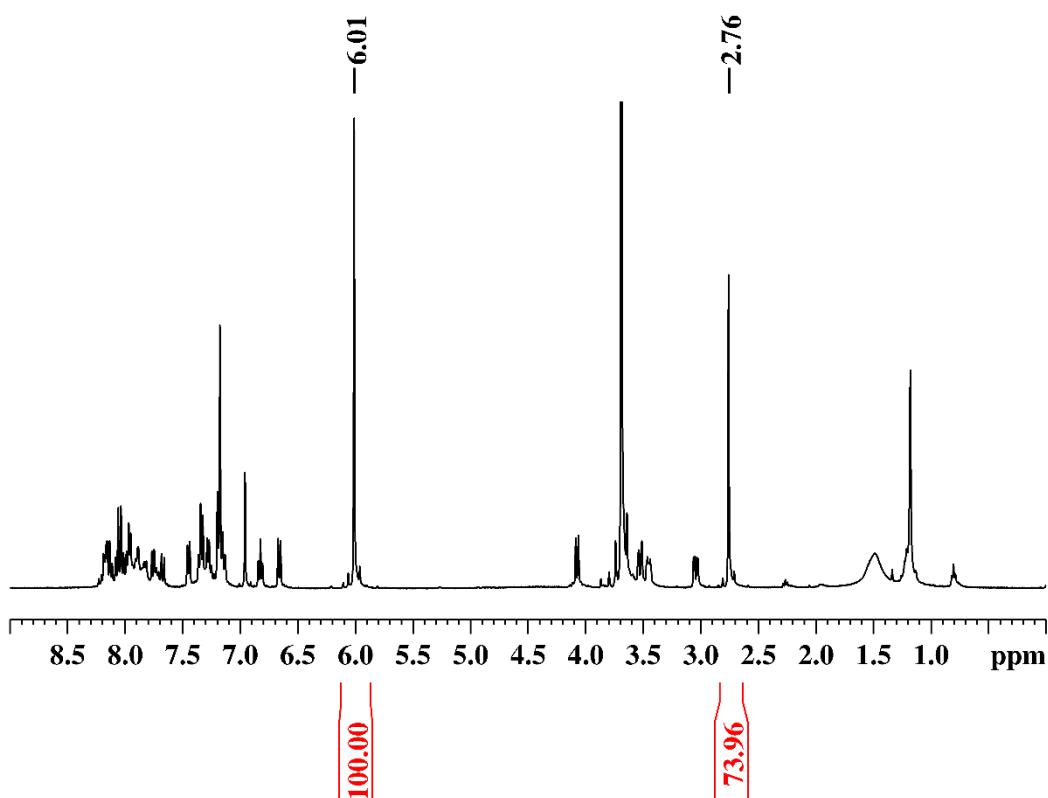


Fig. S73 ¹H NMR (400 MHz, CDCl₃) of the reaction of (**4** + **5f**) using {5 mol% cage **2b** + 1 mol% **RhB**} as the photocatalyst for 12 h under visible light in 70% water/MeCN mixture.

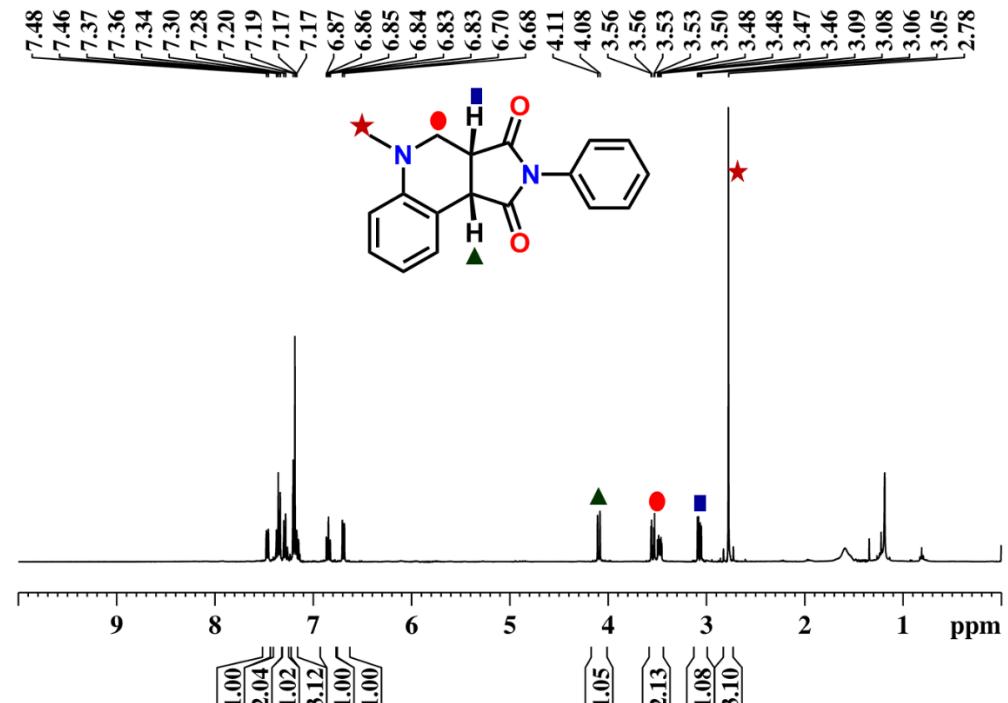


Fig. S74 ^1H NMR (CDCl_3 , 400 MHz) of **6a**.

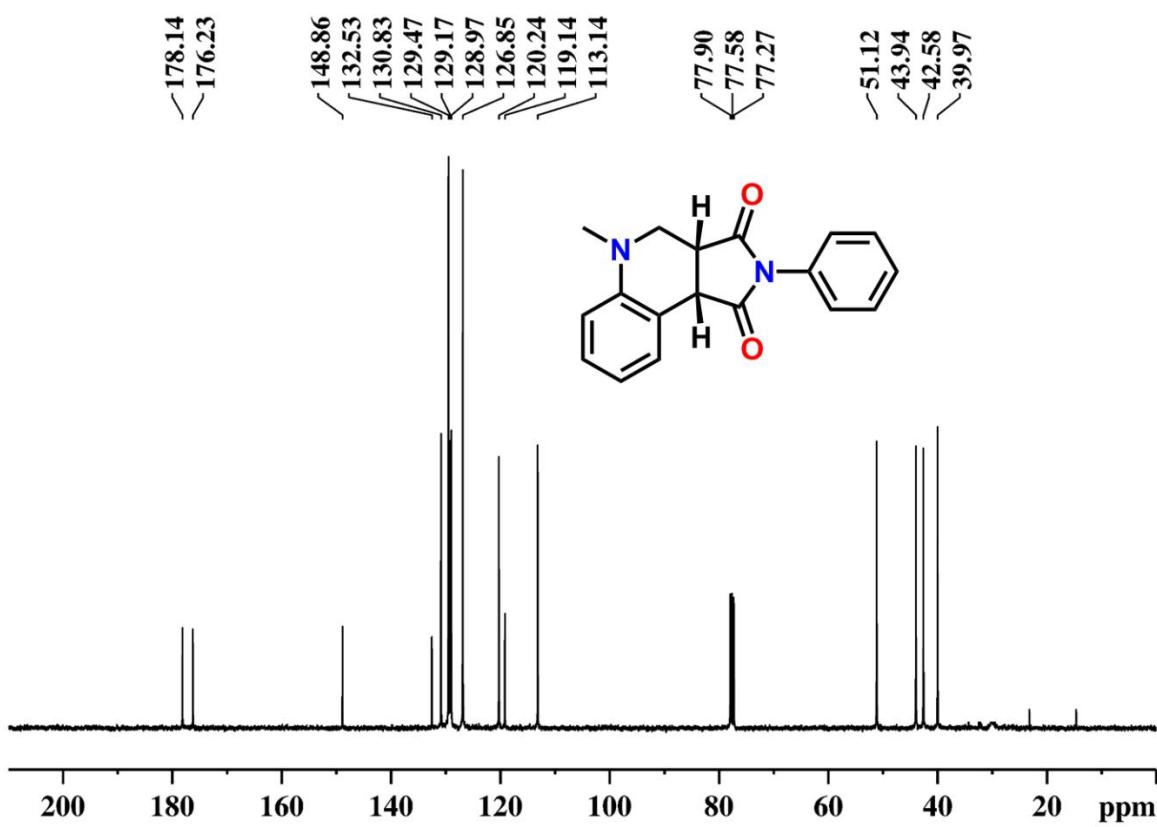


Fig. S75 ^{13}C NMR (CDCl_3 , 100 MHz) of **6a**.

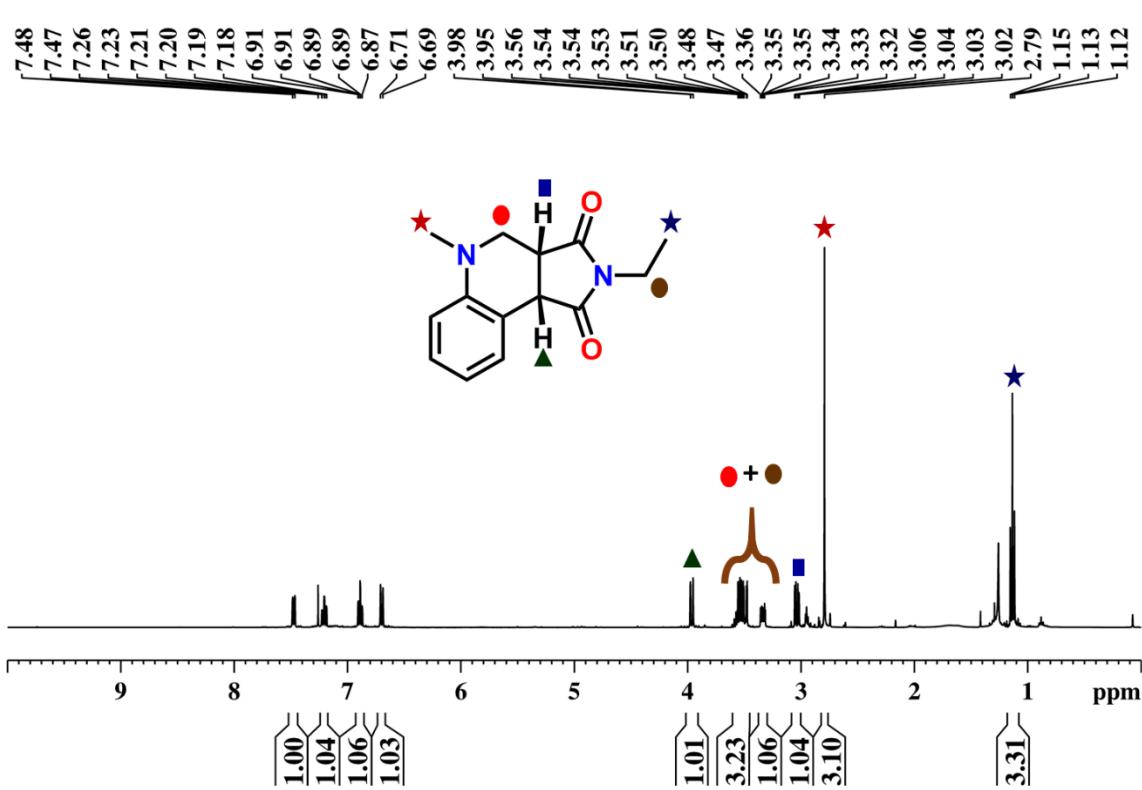


Fig. S76 ^1H NMR (CDCl_3 , 400 MHz) of **6b**.

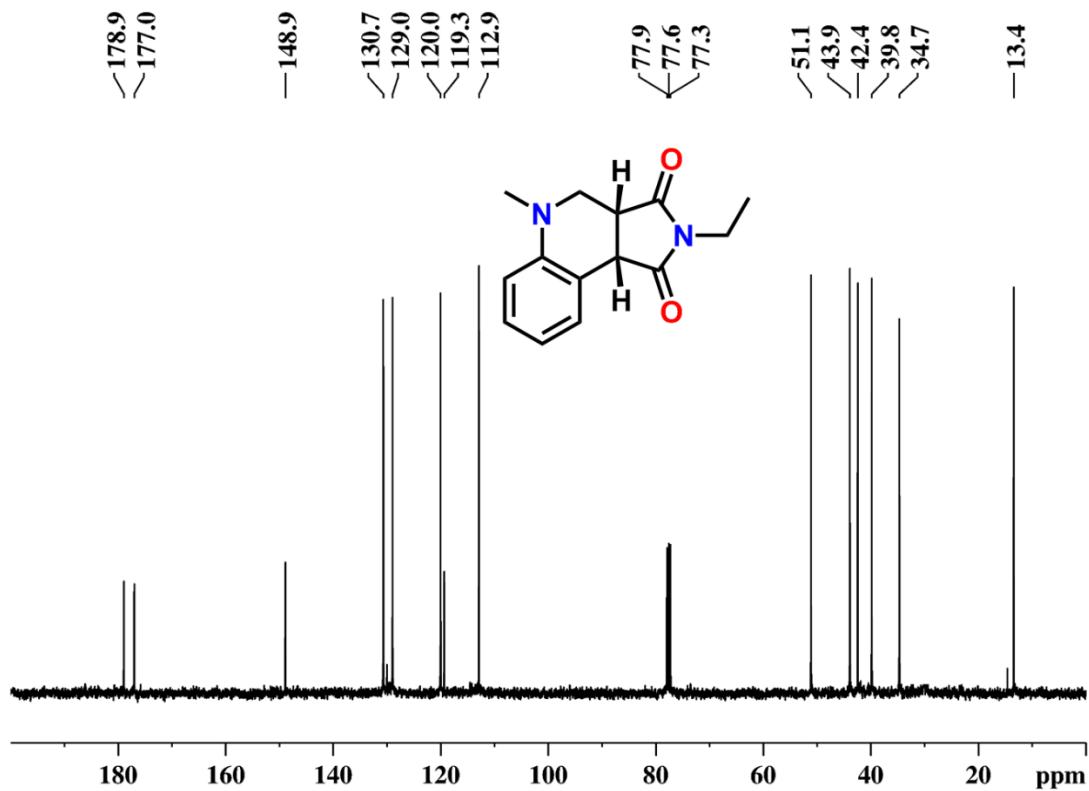


Fig. S77 ^{13}C NMR (CDCl_3 , 100 MHz) of **6b**.

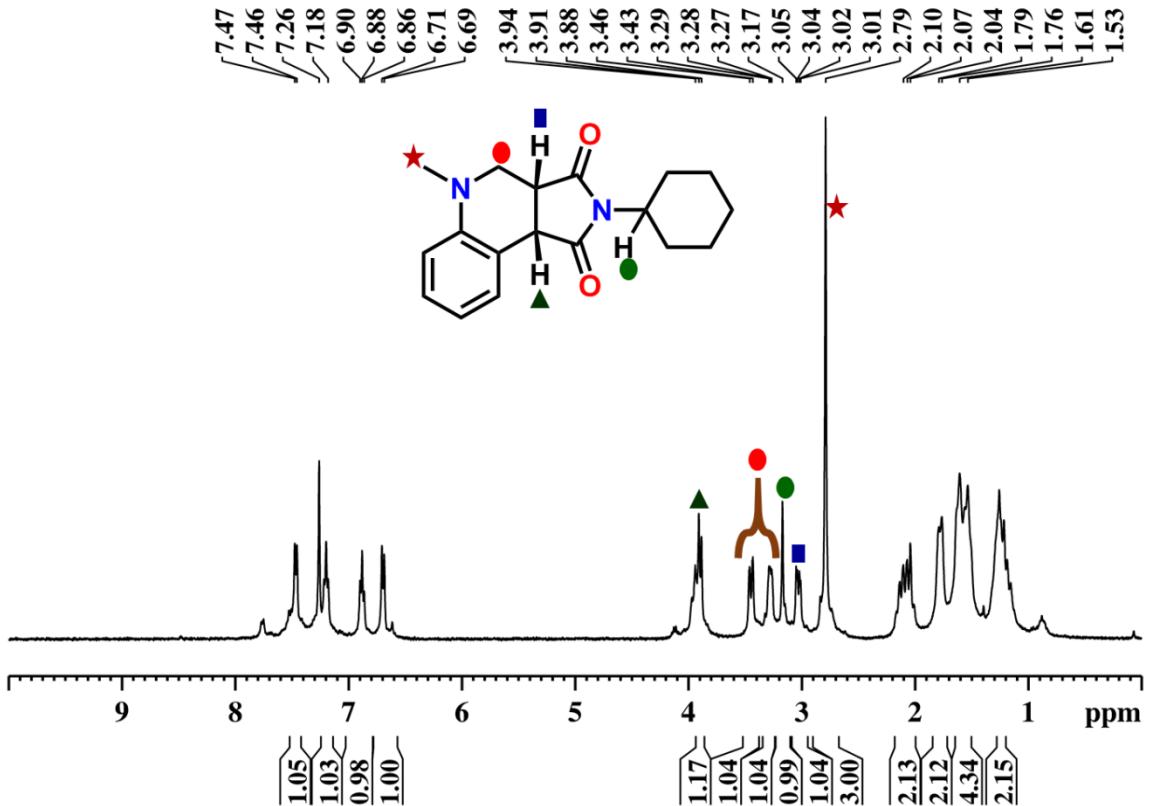


Fig. S78 ^1H NMR (CDCl_3 , 400 MHz) of **6c**.

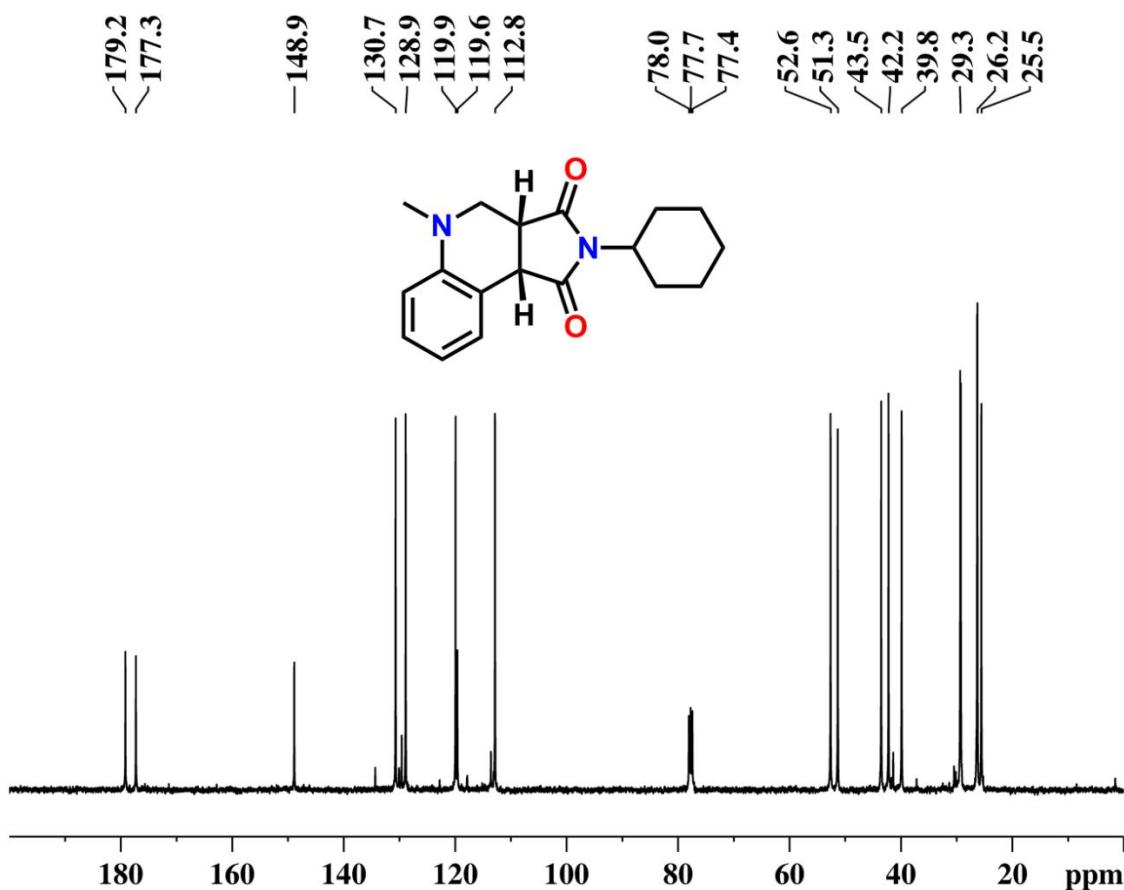


Fig. S79 ^{13}C NMR (CDCl_3 , 100 MHz) of **6c**.

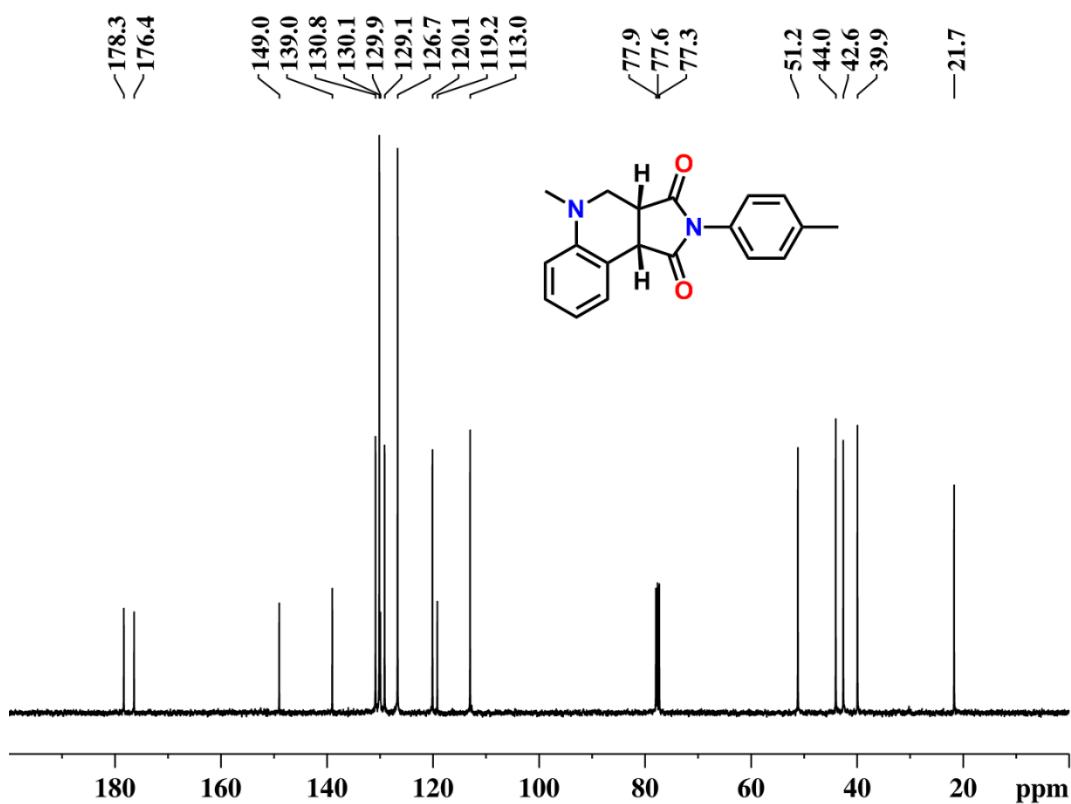
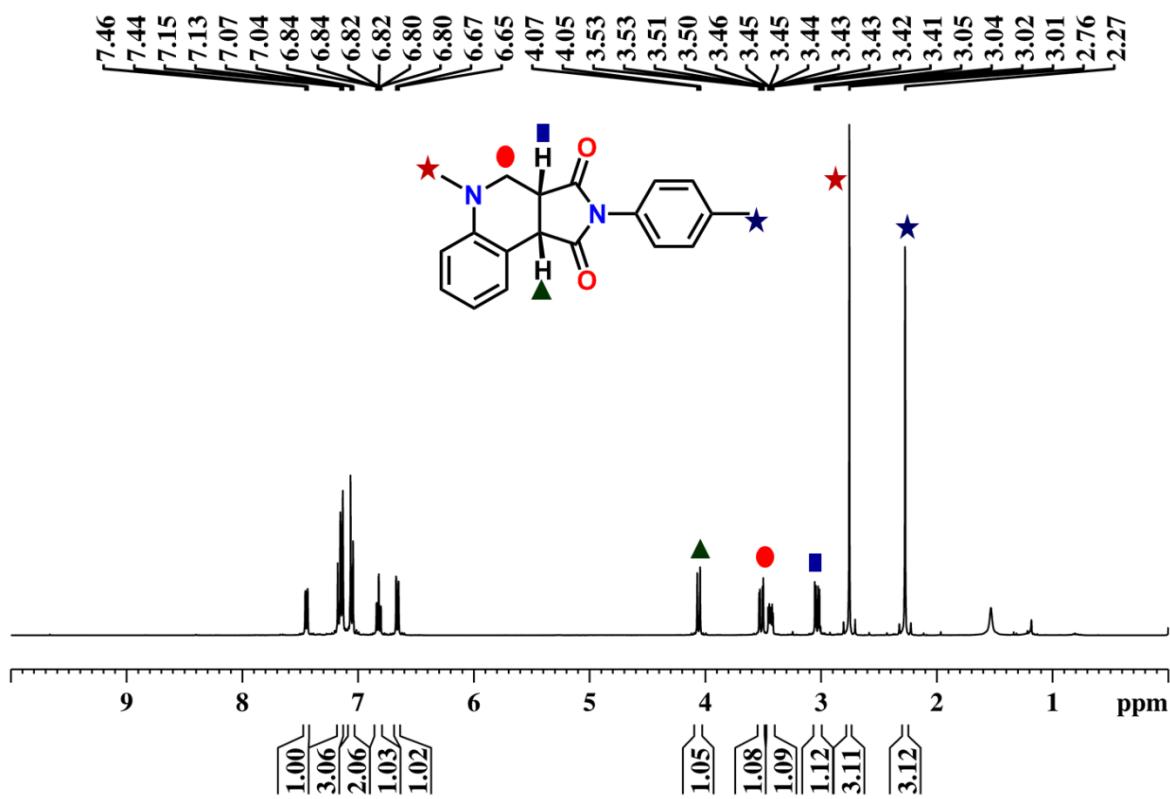


Fig. S81 ^{13}C NMR (CDCl_3 , 100 MHz) of **6d**.

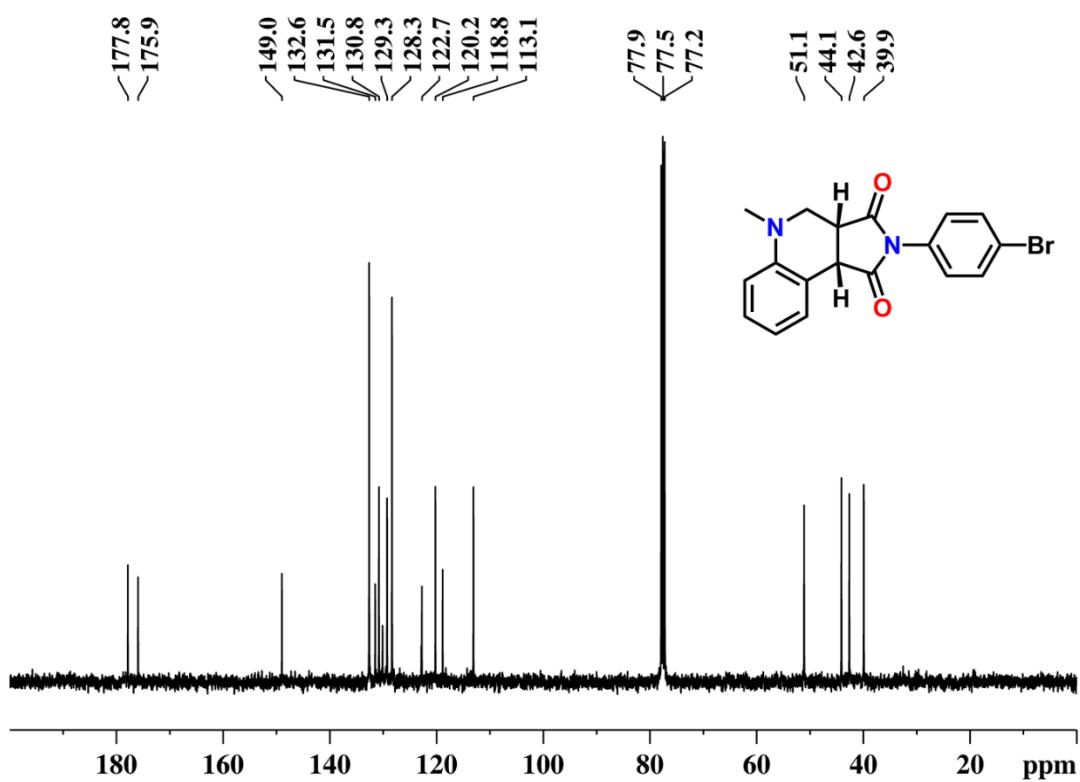
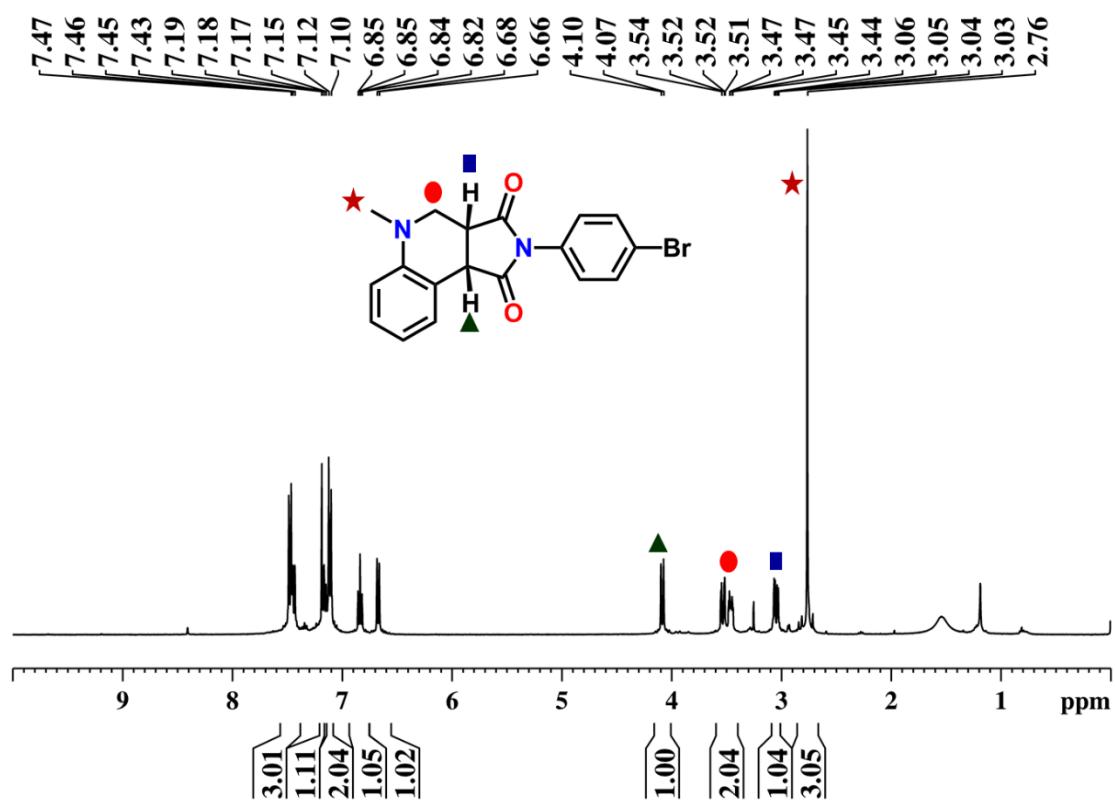


Fig. S83 ^{13}C NMR (CDCl_3 , 100 MHz) of **6e**.

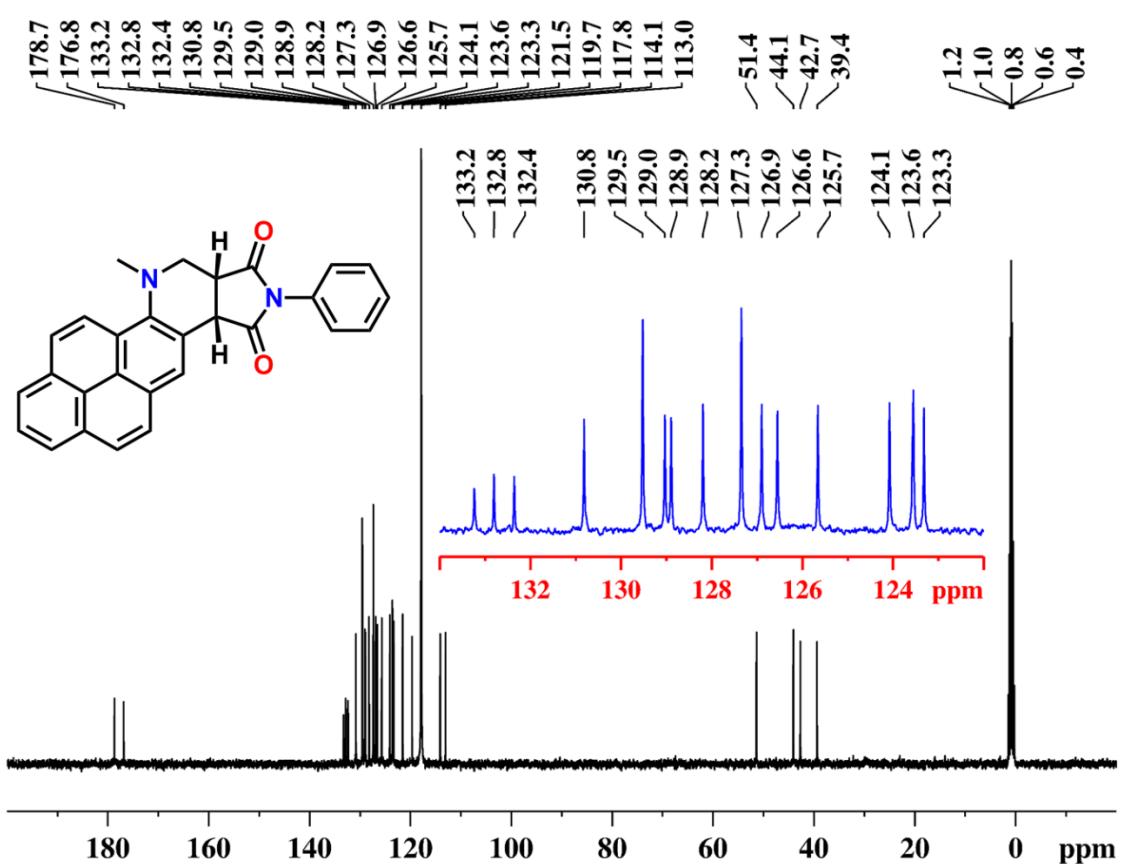
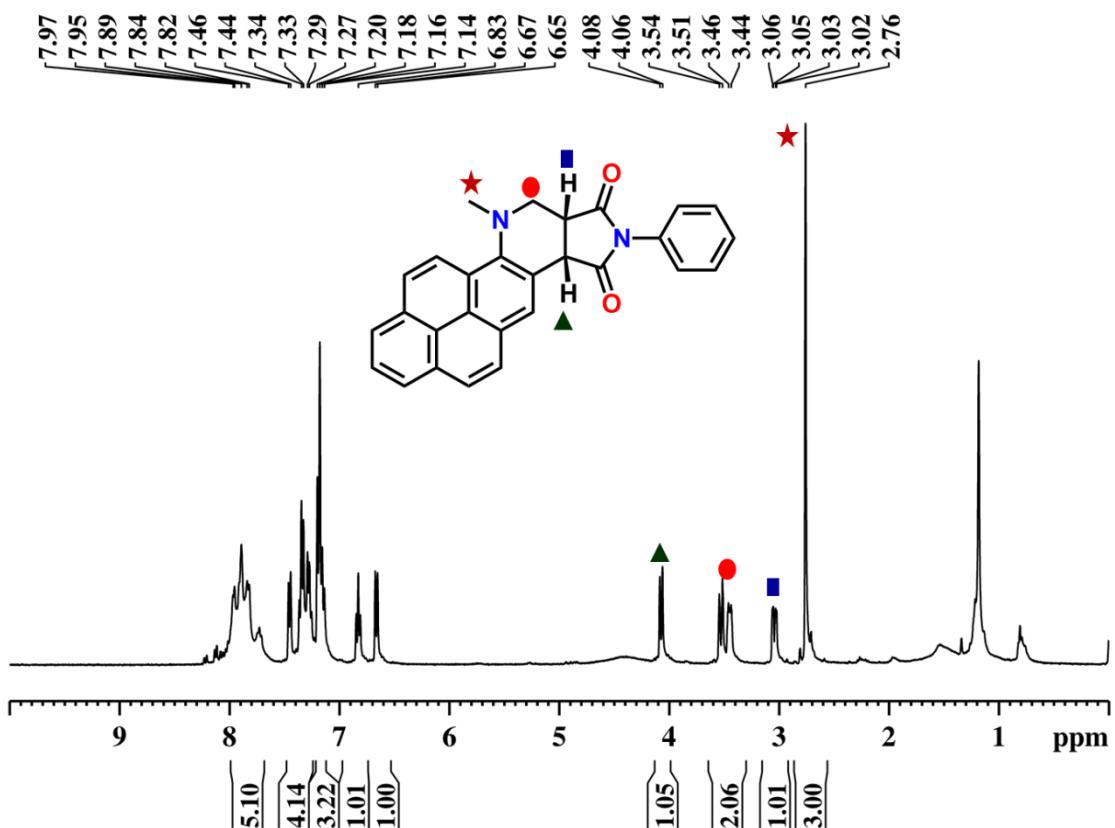


Fig. S85 ^{13}C NMR (CD_3CN , 100 MHz) of **6f**.

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Coordinate of L from Computational studies

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Coordinate of 1 from Computational studies

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| H | -3.48791300 | 3.25778800 | 6.38706200 |
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| H | -4.53057700 | 0.75316800 | 3.04198800 |
| C | -1.50488400 | 1.14425700 | 4.57442500 |
| H | -1.18067000 | 2.45815700 | 6.26026800 |
| H | -2.20654200 | -0.01671000 | 2.89506500 |
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| C | -3.30156500 | 2.75607100 | -5.56180100 |
| C | -2.63031200 | 0.81883900 | -3.68043400 |
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| C | -1.99903500 | 2.26184900 | -5.49601400 |
| H | -3.54637400 | 3.49604000 | -6.31943400 |
| C | -1.63664400 | 1.26283000 | -4.57190400 |
| H | -2.38795900 | 0.05656200 | -2.94651200 |
| H | -1.26144100 | 2.63576200 | -6.19900100 |
| N | 4.65720800 | 6.74520200 | 2.09989900 |
| C | 4.06279500 | 5.75054000 | 2.76880200 |
| C | 5.10214300 | 7.65302500 | 3.04180500 |

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| H | 3.61576800 | 4.87809800 | 2.32313700 |
| C | 4.75404000 | 7.19426400 | 4.28332700 |
| H | 5.62479100 | 8.55762900 | 2.77083900 |
| H | 4.92194000 | 7.61202700 | 5.26561600 |
| N | 4.61104200 | 6.74198700 | -2.04447500 |
| C | 4.06974700 | 5.71285200 | -2.70522300 |
| C | 5.01206100 | 7.66297300 | -2.99349400 |
| H | 3.66635200 | 4.82250900 | -2.25317400 |
| C | 4.68596700 | 7.17890800 | -4.23108000 |
| H | 5.49818100 | 8.58956800 | -2.72969800 |
| H | 4.83345000 | 7.59697900 | -5.21640600 |
| C | 3.64565100 | 5.08681200 | -5.16489200 |
| H | 3.17677700 | 5.76871100 | -5.88349300 |
| H | 4.54998800 | 4.69791400 | -5.64260100 |
| C | 3.58696200 | 5.17445900 | 5.23205100 |
| H | 4.46160200 | 4.84266300 | 5.79862200 |
| H | 3.03779100 | 5.87263500 | 5.87436100 |
| C | 2.70730100 | 3.97679100 | 4.91444200 |
| C | 2.87324000 | 2.82019900 | 5.69180100 |
| C | 1.63264900 | 4.00688700 | 4.01323900 |
| C | 1.99539200 | 1.74069600 | 5.58832700 |
| H | 3.67344900 | 2.77453000 | 6.42613500 |
| C | 0.77416300 | 2.91383700 | 3.88771700 |
| H | 1.43268300 | 4.89950200 | 3.42555200 |
| C | 0.92876000 | 1.75381200 | 4.67256000 |
| H | 2.13471200 | 0.88901400 | 6.24496000 |
| H | -0.05566900 | 2.97629800 | 3.18979800 |
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| C | 0.72629900 | 2.93272300 | -3.85536100 |
| H | 1.48218000 | 4.87130100 | -3.34120900 |
| C | 0.82023300 | 1.78948900 | -4.67257500 |
| H | 1.96952700 | 0.91684900 | -6.28298500 |
| H | -0.09205200 | 3.01219400 | -3.14554300 |
| N | -4.60860400 | -6.78339600 | 2.08877100 |
| C | -3.93307400 | -5.82609600 | 2.73711500 |
| C | -5.09395800 | -7.65054800 | 3.05056400 |
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| C | -3.79932400 | -5.02843600 | -5.15325400 |
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| C | -3.34932900 | -5.28083100 | 5.19032700 |

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| C | -1.83346800 | -1.81243100 | 5.55352300 |
| H | -3.48809300 | -2.88107000 | 6.39447000 |
| C | -0.60902700 | -2.94853700 | 3.83046200 |
| H | -1.23852300 | -4.93958100 | 3.35486100 |
| C | -0.76996200 | -1.80185600 | 4.63416600 |
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| C | -1.00652100 | -1.70161700 | -4.67535100 |
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| N | 7.01571600 | -4.41998600 | 1.99545000 |
| C | 6.25148300 | -3.47302200 | 2.54617500 |
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| H | 5.61849900 | -2.78926800 | 2.00563000 |
| C | 7.26024200 | -4.49723600 | 4.21271600 |
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| H | 7.54165100 | -4.71333100 | 5.23311500 |
| N | 6.80931700 | -4.55652700 | -2.12623800 |
| C | 6.11375600 | -3.55509700 | -2.67204300 |
| C | 7.21944100 | -5.37068400 | -3.16587400 |
| H | 5.65942800 | -2.74345800 | -2.12873300 |
| C | 6.75682900 | -4.83661400 | -4.34113800 |
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| C | 5.52520500 | -2.68857800 | -4.97831700 |
| H | 6.20648400 | -1.83184300 | -4.94903900 |
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| C | 5.81850000 | -2.48752900 | 4.84322900 |
| H | 5.96737400 | -2.91245400 | 5.83767100 |
| H | 6.45521800 | -1.59921100 | 4.77293100 |
| C | 4.35938800 | -2.10451200 | 4.65763700 |
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| C | 2.06811000 | -2.15270000 | 5.47709600 |
| H | 3.66502000 | -3.32024600 | 6.30353300 |
| C | 2.63112800 | -0.71870600 | 3.63165100 |
| H | 4.68783500 | -0.72507900 | 3.02270000 |
| C | 1.66288500 | -1.18247500 | 4.54014800 |
| H | 1.35065100 | -2.53918300 | 6.19415800 |
| H | 2.35504600 | 0.02372100 | 2.88908700 |
| C | 4.09113300 | -2.23083100 | -4.76778200 |
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| C | 2.44998400 | -0.76256200 | -3.71421300 |
| H | 4.51219200 | -0.86754400 | -3.13925900 |
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| H | 3.31210600 | -3.40956400 | -6.40231200 |
| C | 1.44520100 | -1.17891600 | -4.60616700 |
| H | 2.22270200 | -0.00845400 | -2.96707100 |
| H | 1.04096900 | -2.51696400 | -6.25494800 |
| C | -0.23329600 | 0.71746400 | -4.59035300 |
| C | 0.04444900 | -0.62652000 | -4.59936700 |
| C | 0.24017300 | -0.68832500 | 4.55890300 |
| C | -0.08451900 | 0.64495900 | 4.57682100 |
| Pt | 7.05812900 | -4.64491600 | -0.06437500 |
| Pt | -4.70455900 | -6.91286300 | 0.01484300 |
| Pt | 4.69273000 | 6.86200800 | 0.02711700 |
| Pt | -7.13613400 | 4.61943300 | 0.05303700 |
| N | -4.11112400 | -5.96072300 | -4.04086100 |
| N | 6.05535200 | -3.69211600 | -4.01277800 |
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| N | 6.36855800 | -3.49163100 | 3.88997800 |
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| C | -5.64653400 | 2.48512500 | 4.90302700 |
| H | -6.29340200 | 1.60596400 | 4.81694000 |
| H | -5.79211700 | 2.89236500 | 5.90511800 |
| P | -9.18574400 | 3.29132000 | 0.07966000 |
| P | -5.56236700 | 6.46482000 | 0.08752900 |
| P | 2.77478200 | 8.40500500 | 0.07213700 |
| P | 6.93489800 | 5.94577300 | 0.04537100 |
| P | 9.15573700 | -3.41404100 | -0.22792600 |
| P | 5.33434300 | -6.34151500 | 0.03902500 |
| P | -2.94739800 | -8.61501300 | 0.06391700 |
| P | -6.94554100 | -5.98887400 | -0.01913800 |
| C | 2.06318200 | 8.59105200 | 1.78773700 |
| H | 2.03567900 | 7.58736700 | 2.22698500 |
| H | 2.81285800 | 9.15067400 | 2.35765900 |
| C | 3.48843700 | 10.05653700 | -0.40004000 |
| H | 3.86191000 | 9.94045000 | -1.42406900 |
| H | 4.37563500 | 10.19097900 | 0.23095800 |
| C | 1.28687800 | 8.13838500 | -1.01618800 |
| H | 0.91722700 | 7.12636100 | -0.80522200 |
| H | 0.52170400 | 8.83263200 | -0.65366400 |
| C | 0.68509500 | 9.25611500 | 1.93849200 |
| H | -0.11385900 | 8.63924500 | 1.51415000 |
| H | 0.46852000 | 9.38894300 | 3.00365600 |
| H | 0.63754600 | 10.24338100 | 1.47441300 |
| C | 2.57830000 | 11.29248000 | -0.30435300 |
| H | 2.31054600 | 11.52517200 | 0.72947800 |
| H | 3.11452300 | 12.16027600 | -0.70098400 |
| H | 1.65897000 | 11.18285000 | -0.88820700 |
| C | 1.47635000 | 8.34876400 | -2.52386800 |
| H | 2.19693400 | 7.65190100 | -2.95580900 |
| H | 0.51901900 | 8.20203700 | -3.03515900 |
| H | 1.80686200 | 9.36542900 | -2.75446900 |

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| C | 7.21642000 | 4.45776100 | 1.13852900 |
| H | 7.99951700 | 3.86236000 | 0.65577100 |
| H | 6.29682600 | 3.86085800 | 1.10195200 |
| C | 8.10986000 | 7.25597700 | 0.62623300 |
| H | 9.10799200 | 6.80417400 | 0.66970200 |
| H | 7.83607700 | 7.50362900 | 1.65729200 |
| C | 7.54757300 | 5.41665900 | -1.62591000 |
| H | 6.93994700 | 4.54945500 | -1.91636500 |
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| C | 9.04763800 | 5.09237600 | -1.72115200 |
| H | 9.35519300 | 4.29876600 | -1.03241800 |
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| C | 7.62146600 | 4.74564100 | 2.59255600 |
| H | 6.89091800 | 5.36741400 | 3.11739000 |
| H | 7.71468200 | 3.80215200 | 3.14049900 |
| H | 8.59102300 | 5.24730200 | 2.65015900 |
| C | 8.12846000 | 8.52139800 | -0.24438200 |
| H | 8.43087200 | 8.31039000 | -1.27501200 |
| H | 7.14848200 | 9.01216400 | -0.26424800 |
| H | 8.84936600 | 9.23616400 | 0.16342600 |
| C | 10.50501300 | -4.60929100 | -0.66205200 |
| H | 11.42357800 | -4.02800500 | -0.80683200 |
| H | 10.25344100 | -5.04278200 | -1.63628100 |
| C | 9.22581300 | -2.04959600 | -1.49874700 |
| H | 8.23698300 | -1.57411000 | -1.50632300 |
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| C | 9.68166500 | -2.58718100 | 1.35066300 |
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| H | 10.67716400 | -2.82522000 | -2.94306300 |
| C | 10.72962900 | -5.71799400 | 0.37699100 |
| H | 11.03245300 | -5.31826900 | 1.34995000 |
| H | 9.83090700 | -6.32980200 | 0.51626400 |
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| C | 11.12635200 | -2.05992200 | 1.38202200 |
| H | 11.33392900 | -1.33789600 | 0.58610100 |
| H | 11.30593900 | -1.55374500 | 2.33581200 |
| H | 11.85806300 | -2.86867600 | 1.30498800 |
| C | 4.90012900 | -6.89153200 | 1.75728600 |
| H | 4.53237600 | -6.01050300 | 2.29632300 |
| H | 5.84480000 | -7.16538100 | 2.23866600 |
| C | 5.87637100 | -7.86864900 | -0.86047900 |
| H | 5.05497700 | -8.59251200 | -0.79971600 |
| H | 5.96842100 | -7.59607600 | -1.91798500 |
| C | 7.18221600 | -8.48927600 | -0.34235200 |
| H | 8.02111300 | -7.78883500 | -0.41964700 |
| H | 7.10134000 | -8.81073800 | 0.70096000 |
| H | 7.43135100 | -9.37540200 | -0.93372700 |
| C | 3.90009600 | -8.05239400 | 1.86531700 |
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| H | 2.92667300 | -7.80098100 | 1.42979100 |

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| H | 4.26820400 | -8.96109800 | 1.38056500 |
| C | 3.73392700 | -5.89676800 | -0.78725200 |
| H | 3.08798900 | -6.78260300 | -0.76967900 |
| H | 3.97170000 | -5.70513000 | -1.83984400 |
| C | 3.01763600 | -4.68861100 | -0.17238500 |
| H | 3.64842600 | -3.79299500 | -0.20571600 |
| H | 2.09855200 | -4.46872700 | -0.72682300 |
| H | 2.74105000 | -4.86650300 | 0.87253000 |
| C | -1.78535300 | -8.73898500 | -1.37909400 |
| H | -1.09847300 | -9.56701200 | -1.16864300 |
| H | -2.39525300 | -9.05587100 | -2.23216000 |
| C | -3.90672100 | -10.21202800 | 0.02807000 |
| H | -4.50173700 | -10.22928500 | 0.94968900 |
| H | -4.62687900 | -10.12880800 | -0.79444600 |
| C | -1.92157300 | -8.76784100 | 1.60383100 |
| H | -1.47262000 | -9.76735700 | 1.58368300 |
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| C | -1.00755200 | -7.46773800 | -1.74222000 |
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| C | -3.09464500 | -11.51144100 | -0.10950100 |
| H | -2.54256800 | -11.55642100 | -1.05274100 |
| H | -2.39014600 | -11.65500000 | 0.71507600 |
| H | -3.78275600 | -12.36233900 | -0.09511500 |
| C | -8.13377800 | -7.39720400 | -0.25002200 |
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| C | -7.49625900 | -5.16835400 | 1.54857800 |
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| C | -7.40533100 | -4.75552800 | -1.34263500 |
| H | -8.24319400 | -4.17790300 | -0.93207000 |
| H | -6.56424300 | -4.05979600 | -1.44783600 |
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| C | -6.87205600 | -3.79082600 | 1.80563500 |
| H | -5.77831500 | -3.84358200 | 1.84550200 |
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| C | -9.66616300 | 2.49920400 | -1.52899000 |
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| H | -8.39112500 | 1.34596800 | 1.30034100 |

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| C | -10.61012800 | 4.42011100 | 0.46204900 |
| H | -11.48702700 | 3.77460300 | 0.60249800 |
| H | -10.40656600 | 4.88925000 | 1.43081400 |
| C | -8.90463800 | 1.21797900 | -1.89357200 |
| H | -7.82454000 | 1.38994200 | -1.96852100 |
| H | -9.07185500 | 0.42216800 | -1.16095900 |
| H | -9.25615900 | 0.84711200 | -2.86174800 |
| C | -9.73400700 | 2.28158000 | 2.74439600 |
| H | -9.77058500 | 1.37964200 | 3.36406200 |
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| H | -10.72913500 | 2.73183500 | 2.78336400 |
| C | -10.90748800 | 5.48868200 | -0.59963200 |
| H | -10.06222600 | 6.17130500 | -0.73813400 |
| H | -11.16687100 | 5.05060300 | -1.56818500 |
| H | -11.76432900 | 6.08855900 | -0.27868700 |
| C | -4.56299100 | 6.74041400 | -1.45080400 |
| H | -4.17416300 | 7.76470300 | -1.40525700 |
| H | -5.25821100 | 6.71214400 | -2.29547000 |
| C | -4.33913000 | 6.42577900 | 1.48627200 |
| H | -3.77150600 | 5.49244700 | 1.38652400 |
| H | -4.92690800 | 6.33303600 | 2.40595800 |
| C | -6.50704500 | 8.04581400 | 0.32396700 |
| H | -5.77208200 | 8.85695700 | 0.38754800 |
| H | -6.99121900 | 7.98373100 | 1.30582600 |
| C | -3.41905800 | 5.74082300 | -1.66469400 |
| H | -2.91699700 | 5.94944700 | -2.61515000 |
| H | -2.66873300 | 5.80724700 | -0.86937400 |
| H | -3.78028800 | 4.70777700 | -1.70199800 |
| C | -3.39200200 | 7.63135400 | 1.58878600 |
| H | -2.71094900 | 7.49006900 | 2.43499500 |
| H | -2.78445600 | 7.75730100 | 0.68615900 |
| H | -3.93208500 | 8.56534300 | 1.76560200 |
| C | -7.54257800 | 8.35930900 | -0.76488000 |
| H | -7.08321400 | 8.47169400 | -1.75213300 |
| H | -8.31209000 | 7.58285800 | -0.82115100 |
| H | -8.04347300 | 9.30369000 | -0.53232700 |

Coordinate of 2 from Computational studies

| | | | |
|---|--------------|-------------|-------------|
| N | 7.83955500 | 7.56676000 | 4.22611400 |
| C | 7.85048500 | 6.39233600 | 4.84980200 |
| C | 9.16080200 | 7.92412600 | 4.04450700 |
| H | 6.97518700 | 5.84144000 | 5.15835600 |
| C | 9.96332100 | 6.94343800 | 4.56736600 |
| H | 9.43931400 | 8.85551200 | 3.57565100 |
| H | 11.03748700 | 6.86397900 | 4.63953300 |
| N | -7.21908400 | 9.08184300 | -0.80689200 |
| C | -7.71984800 | 7.86824900 | -0.59346000 |
| C | -8.21693500 | 9.81662100 | -1.41705200 |
| H | -7.19574500 | 7.05092800 | -0.12238000 |
| C | -9.32507800 | 9.02395800 | -1.56223500 |
| H | -8.07544600 | 10.85023500 | -1.69431800 |
| H | -10.30281700 | 9.23295300 | -1.96975100 |

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|---|--------------|-------------|--------------|
| C | -9.92931300 | 6.65669100 | -0.83151100 |
| H | -9.96321300 | 6.45675400 | 0.24386100 |
| H | -10.91501500 | 7.03308900 | -1.11619000 |
| C | 9.59305000 | 3.47499600 | 4.98393200 |
| C | 10.82865700 | 2.98495600 | 4.54169300 |
| C | 8.44767100 | 2.70753200 | 4.72891600 |
| C | 10.91857000 | 1.75803100 | 3.88478900 |
| H | 11.73754900 | 3.54978200 | 4.73436700 |
| C | 8.53642800 | 1.47647400 | 4.07950800 |
| H | 7.47375800 | 3.05840100 | 5.06500000 |
| C | 9.77854800 | 0.96307300 | 3.66785000 |
| H | 11.89206500 | 1.39782400 | 3.56595600 |
| H | 7.63654200 | 0.89219800 | 3.91389700 |
| C | -9.62917000 | 5.37180900 | -1.58387000 |
| C | -9.09814900 | 4.26110000 | -0.91388000 |
| C | -9.99157600 | 5.22038500 | -2.93014200 |
| C | -8.97926200 | 3.02392800 | -1.54909400 |
| H | -8.80697700 | 4.35004900 | 0.13091100 |
| C | -9.86550500 | 3.98836500 | -3.56855800 |
| H | -10.41179200 | 6.06033500 | -3.47813000 |
| C | -9.39809200 | 2.85184700 | -2.87898100 |
| H | -8.59191600 | 2.17348900 | -0.99665800 |
| H | -10.17974200 | 3.89352900 | -4.60349600 |
| N | 11.42193500 | 0.87045200 | -4.84726500 |
| C | 11.46698900 | 0.32907800 | -3.63082800 |
| C | 12.67350700 | 1.40131800 | -5.08814100 |
| H | 10.65098600 | -0.17461400 | -3.13766900 |
| C | 13.46665500 | 1.18218600 | -3.99454800 |
| H | 12.91213100 | 1.89646200 | -6.01699800 |
| H | 14.49913300 | 1.43153800 | -3.80020900 |
| N | -3.78670800 | 2.67955900 | -9.62667100 |
| C | -4.66043000 | 1.75574100 | -9.23892100 |
| C | -4.52489700 | 3.80822700 | -9.93159200 |
| H | -4.41646700 | 0.74535800 | -8.94759600 |
| C | -5.85164500 | 3.54806200 | -9.71438300 |
| H | -4.05867100 | 4.70936400 | -10.29874000 |
| H | -6.73211300 | 4.15727600 | -9.85259700 |
| C | -7.15127700 | 1.48239500 | -8.98665100 |
| H | -7.90741300 | 1.80885000 | -9.70694900 |
| H | -6.93256800 | 0.43576700 | -9.22698000 |
| C | 13.22125000 | -0.05705300 | -1.81389500 |
| H | 13.64164200 | -1.04361900 | -2.03647300 |
| H | 14.06272500 | 0.58750700 | -1.53617300 |
| C | 12.25808800 | -0.16737700 | -0.64392900 |
| C | 12.47114000 | -1.19616700 | 0.28545600 |
| C | 11.25365400 | 0.76915500 | -0.36989800 |
| C | 11.71876900 | -1.28172200 | 1.45495400 |
| H | 13.26017200 | -1.92409900 | 0.11233600 |
| C | 10.48607300 | 0.67033600 | 0.79141000 |
| H | 11.07797100 | 1.59744900 | -1.05009300 |
| C | 10.69673900 | -0.35590000 | 1.73148200 |
| H | 11.93926000 | -2.07013300 | 2.16630000 |
| H | 9.72133100 | 1.41769700 | 0.98198200 |
| C | -7.70086800 | 1.58241700 | -7.56841600 |
| C | -8.99875400 | 1.10223900 | -7.34035900 |

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|---|--------------|--------------|-------------|
| C | -6.97383700 | 2.07147200 | -6.47952200 |
| C | -9.53727000 | 1.07379500 | -6.05687400 |
| H | -9.59922500 | 0.74493400 | -8.17395400 |
| C | -7.52367700 | 2.06330300 | -5.19445300 |
| H | -5.97471800 | 2.47278900 | -6.62718700 |
| C | -8.80255400 | 1.53616300 | -4.95026600 |
| H | -10.54330700 | 0.69402800 | -5.91135600 |
| H | -6.94379000 | 2.46124400 | -4.36588600 |
| N | 3.77991000 | -2.60665100 | 9.62940200 |
| C | 4.69022700 | -1.70645000 | 9.27268000 |
| C | 4.46751000 | -3.78112000 | 9.87180000 |
| H | 4.48960700 | -0.67396200 | 9.02886100 |
| C | 5.80330200 | -3.57038600 | 9.65388500 |
| H | 3.96174500 | -4.67768600 | 10.19614800 |
| H | 6.65701600 | -4.22331000 | 9.75573000 |
| N | -11.45024300 | -0.94793500 | 4.82037800 |
| C | -11.49219900 | -0.38920700 | 3.61177700 |
| C | -12.70176700 | -1.48394500 | 5.04966400 |
| H | -10.67544600 | 0.12278700 | 3.12850500 |
| C | -13.49183800 | -1.25001700 | 3.95678800 |
| H | -12.94249900 | -1.99264700 | 5.97063100 |
| H | -14.52332000 | -1.49799900 | 3.75554800 |
| C | -13.23812900 | 0.02001100 | 1.79353100 |
| H | -14.08027600 | -0.61865900 | 1.50455800 |
| H | -13.65630400 | 1.00529800 | 2.02571300 |
| C | 7.19030300 | -1.53480300 | 9.01047600 |
| H | 7.02227900 | -0.49071900 | 9.29683500 |
| H | 7.93327700 | -1.92676200 | 9.71197100 |
| C | 7.72847500 | -1.60051200 | 7.58558100 |
| C | 9.00975100 | -1.07936600 | 7.35177700 |
| C | 7.01414700 | -2.11515300 | 6.50066300 |
| C | 9.54534200 | -1.04242600 | 6.06748500 |
| H | 9.60107900 | -0.70004900 | 8.18225300 |
| C | 7.56019600 | -2.09372200 | 5.21385800 |
| H | 6.03074600 | -2.55065200 | 6.65351500 |
| C | 8.82332400 | -1.53281100 | 4.96406400 |
| H | 10.54006400 | -0.63517600 | 5.91913900 |
| H | 6.99044400 | -2.51241500 | 4.38845300 |
| C | -12.26806600 | 0.14010700 | 0.63029300 |
| C | -12.46759800 | 1.18255100 | -0.28671300 |
| C | -11.26862700 | -0.80009800 | 0.35054000 |
| C | -11.70739400 | 1.27739900 | -1.45052900 |
| H | -13.25215700 | 1.91418300 | -0.10890700 |
| C | -10.49334500 | -0.69224700 | -0.80462100 |
| H | -11.10318500 | -1.63814400 | 1.02128600 |
| C | -10.69114400 | 0.34705100 | -1.73312100 |
| H | -11.91776000 | 2.07634000 | -2.15315800 |
| H | -9.73304600 | -1.44281100 | -1.00012800 |
| N | 7.28733300 | -9.07309500 | 0.78579300 |
| C | 7.78453400 | -7.84665800 | 0.65356100 |
| C | 8.29870800 | -9.85245300 | 1.31280500 |
| H | 7.24853200 | -6.99464700 | 0.26480100 |
| C | 9.41227400 | -9.07380400 | 1.48754400 |
| H | 8.15912900 | -10.90202900 | 1.52216500 |
| H | 10.39926400 | -9.31328700 | 1.85396800 |

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|---|--------------|--------------|-------------|
| N | -7.80044700 | -7.54123500 | -4.25589700 |
| C | -7.82336000 | -6.36749900 | -4.88064300 |
| C | -9.11808100 | -7.90959700 | -4.06985100 |
| H | -6.95380500 | -5.80924300 | -5.19216900 |
| C | -9.93050800 | -6.93605900 | -4.59080500 |
| H | -9.38724300 | -8.84268700 | -3.59895200 |
| H | -11.00553900 | -6.86560900 | -4.65942900 |
| C | -9.50552700 | -4.73932100 | -5.82845200 |
| H | -8.79345900 | -4.61328100 | -6.64954800 |
| H | -10.47601300 | -4.95885000 | -6.27948000 |
| C | 10.01571400 | -6.67228000 | 0.89305900 |
| H | 10.98882300 | -7.05063200 | 1.21536700 |
| H | 10.08954400 | -6.47502600 | -0.18106900 |
| C | 9.69318600 | -5.38562900 | 1.63170400 |
| C | 10.05460000 | -5.21709200 | 2.97618400 |
| C | 9.14554300 | -4.28852400 | 0.95232000 |
| C | 9.91358700 | -3.98100700 | 3.60330500 |
| H | 10.48722800 | -6.04645700 | 3.53059600 |
| C | 9.00994900 | -3.04750500 | 1.57691900 |
| H | 8.85627200 | -4.39044300 | -0.09185400 |
| C | 9.42980200 | -2.85737700 | 2.90405300 |
| H | 10.22933700 | -3.87215500 | 4.63638400 |
| H | 8.61084000 | -2.20731500 | 1.01717800 |
| C | -9.58445900 | -3.46501800 | -5.00425300 |
| C | -8.43841400 | -2.70204300 | -4.73896700 |
| C | -10.82132900 | -2.97304600 | -4.56793000 |
| C | -8.52747500 | -1.47423400 | -4.08371400 |
| H | -7.46336100 | -3.05403000 | -5.07057500 |
| C | -10.91163700 | -1.74887000 | -3.90576700 |
| H | -11.73064600 | -3.53434700 | -4.76870100 |
| C | -9.77051700 | -0.95912800 | -3.67674400 |
| H | -7.62672000 | -0.89407300 | -3.90890200 |
| H | -11.88602100 | -1.38740500 | -3.59106300 |
| C | -9.38093000 | 1.51883800 | -3.56447700 |
| C | -9.90196200 | 0.38034800 | -3.00818000 |
| C | 9.40035900 | -1.51818900 | 3.57779900 |
| C | 9.91263900 | -0.38130300 | 3.01007200 |
| N | -12.71334100 | -0.56042400 | 3.04622400 |
| N | -9.09672700 | -5.96153600 | -5.10199900 |
| N | -8.99706400 | 7.78802000 | -1.03870900 |
| N | -5.92698700 | 2.24097600 | -9.27329200 |
| N | 5.93397300 | -2.24918500 | 9.27177100 |
| N | 9.07328000 | -7.80083200 | 1.07015300 |
| N | 12.69021700 | 0.50687700 | -3.07155500 |
| N | 9.11969000 | 5.97550400 | 5.07504900 |
| C | 9.51562600 | 4.75130700 | 5.80523200 |
| H | 8.79705200 | 4.63044600 | 6.62136600 |
| H | 10.48421300 | 4.96546100 | 6.26297000 |
| P | 9.29549800 | 3.30624900 | -5.69821900 |
| P | 10.07050200 | -1.18307100 | -7.08088000 |
| P | 5.91885400 | -10.44152100 | -1.95570100 |
| P | 4.45388500 | -9.29753000 | 2.42645100 |
| P | 6.25974400 | 7.90146700 | 1.31644300 |
| P | 5.72170900 | 9.68472500 | 5.70242100 |
| P | 1.40858900 | -2.94550700 | 7.36284000 |

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|----|-------------|--------------|--------------|
| P | 1.52618700 | -1.80305600 | 11.99768600 |
| Pt | 9.68306400 | 0.97848100 | -6.12139600 |
| Pt | 5.28800300 | -9.62204600 | 0.20440000 |
| Pt | 6.02885000 | 8.56079200 | 3.60611700 |
| Pt | 1.63951300 | -2.31471600 | 9.66052900 |
| C | 7.99414500 | 1.07439100 | -7.13161200 |
| C | 6.88527800 | 1.17217400 | -7.64638300 |
| C | 3.43644300 | -9.91113400 | -0.39580800 |
| C | 2.28074200 | -9.94729800 | -0.80391200 |
| C | 4.27443300 | 9.24884400 | 3.03569800 |
| C | 3.14149500 | 9.51964400 | 2.65333700 |
| C | -0.30732700 | -2.03139300 | 9.54424400 |
| C | -1.50237100 | -1.86873900 | 9.32217200 |
| C | 5.55835700 | 1.30215900 | -8.16641500 |
| C | 5.19814000 | 2.36596300 | -9.02156800 |
| C | 4.54649900 | 0.39232100 | -7.79016000 |
| C | 3.88426700 | 2.53802500 | -9.44290600 |
| H | 5.96115300 | 3.06637400 | -9.34746700 |
| C | 3.23405600 | 0.56380100 | -8.21029000 |
| H | 4.80305100 | -0.44602800 | -7.14920200 |
| C | 2.86572500 | 1.65415800 | -9.02813300 |
| H | 3.63212900 | 3.37236700 | -10.09039400 |
| H | 2.47108300 | -0.14486400 | -7.90050900 |
| C | 0.93698700 | -9.87367800 | -1.29053100 |
| C | 0.45877400 | -8.65735600 | -1.82548500 |
| C | 0.04928000 | -10.96896300 | -1.25008100 |
| C | -0.84496600 | -8.53931600 | -2.28353400 |
| H | 1.13017700 | -7.80470300 | -1.87423900 |
| C | -1.25899600 | -10.85068400 | -1.71035900 |
| H | 0.39410400 | -11.91834800 | -0.85189900 |
| C | -1.73957300 | -9.63117600 | -2.23079900 |
| H | -1.19226700 | -7.59470700 | -2.69255800 |
| H | -1.92314800 | -11.70844700 | -1.66586400 |
| C | 1.79354300 | 9.70033400 | 2.20879800 |
| C | 0.89431400 | 8.61279800 | 2.27154700 |
| C | 1.31586500 | 10.91936700 | 1.68463600 |
| C | -0.41134000 | 8.73473600 | 1.82046700 |
| H | 1.23959500 | 7.66862700 | 2.68326400 |
| C | 0.00559200 | 11.04144200 | 1.23090600 |
| H | 1.98354500 | 11.77395200 | 1.63257900 |
| C | -0.88714200 | 9.95070400 | 1.28236700 |
| H | -1.08638700 | 7.88556300 | 1.87747500 |
| H | -0.33731000 | 11.99068400 | 0.83074800 |
| C | -2.88038300 | -1.67991700 | 8.98394500 |
| C | -3.86170700 | -2.63948900 | 9.31147600 |
| C | -3.29137900 | -0.54212100 | 8.25602800 |
| C | -5.17906300 | -2.48996900 | 8.89270800 |
| H | -3.57737100 | -3.51275200 | 9.89082000 |
| C | -4.60741500 | -0.39294600 | 7.83893900 |
| H | -2.55940700 | 0.22370500 | 8.01544000 |
| C | -5.58081200 | -1.37396300 | 8.12743400 |
| H | -5.91277500 | -3.24713300 | 9.15238600 |
| H | -4.89657300 | 0.48515700 | 7.26906800 |
| C | -3.08664800 | -9.45541100 | -2.68003800 |
| C | -4.22056300 | -9.19124900 | -3.06415100 |

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|----|--------------|-------------|--------------|
| C | 1.49129800 | 1.87907700 | -9.36102600 |
| C | 0.29901000 | 2.08752600 | -9.55744000 |
| C | -2.23432600 | 10.02747700 | 0.80647700 |
| C | -3.39684500 | 9.99195500 | 0.41872100 |
| C | -6.91024100 | -1.25645500 | 7.61123200 |
| C | -8.02174000 | -1.16321600 | 7.10130400 |
| Pt | -1.64362400 | 2.41686800 | -9.64846800 |
| Pt | -5.98030500 | -8.51748200 | -3.63589700 |
| Pt | -9.71256400 | -1.06549800 | 6.09479900 |
| Pt | -5.24273700 | 9.67981200 | -0.19136900 |
| P | -6.21433400 | -7.85013400 | -1.34865100 |
| P | -5.66777200 | -9.64811700 | -5.72729800 |
| P | -1.52613100 | 1.59838200 | -11.88700600 |
| P | -1.34331100 | 3.24450500 | -7.41941500 |
| P | -4.31120000 | 9.57205900 | -2.38651600 |
| P | -5.99374100 | 10.32720300 | 1.98635600 |
| P | -10.11184400 | 1.08341600 | 7.07771800 |
| P | -9.31834800 | -3.38787700 | 5.65084900 |
| C | -9.62393900 | 1.10582700 | 8.86379500 |
| H | -8.55524300 | 0.87778300 | 8.90463200 |
| H | -9.76475000 | 2.13420600 | 9.22171700 |
| C | -11.89154200 | 1.63704700 | 7.12879000 |
| H | -12.49440700 | 0.75115200 | 7.35418800 |
| H | -11.97978000 | 2.30191900 | 7.99728300 |
| C | -9.20572400 | 2.52044300 | 6.32716300 |
| H | -9.53246600 | 3.42381300 | 6.85886500 |
| H | -9.55859800 | 2.61500000 | 5.29357200 |
| C | -7.67641000 | 2.40301000 | 6.35616200 |
| H | -7.33668700 | 1.49482400 | 5.84928800 |
| H | -7.22761800 | 3.26999600 | 5.85822500 |
| H | -7.29376400 | 2.37609100 | 7.38087100 |
| C | -10.40445300 | 0.11522500 | 9.73916600 |
| H | -11.47913200 | 0.32379700 | 9.74590800 |
| H | -10.25165600 | -0.91419000 | 9.39963300 |
| H | -10.05364700 | 0.18220800 | 10.77363400 |
| C | -12.43764600 | 2.34793400 | 5.88391900 |
| H | -12.36684600 | 1.72410200 | 4.98796600 |
| H | -13.49369000 | 2.59137800 | 6.03871900 |
| H | -11.91278500 | 3.28840300 | 5.68867800 |
| C | -9.45728200 | -4.32479000 | 7.24341900 |
| H | -9.20224000 | -5.37354900 | 7.05032100 |
| H | -8.68609900 | -3.90906100 | 7.90069200 |
| C | -10.47336600 | -4.28198700 | 4.50201100 |
| H | -10.34185200 | -5.35801600 | 4.66981900 |
| H | -11.49359200 | -4.04116000 | 4.81582400 |
| C | -7.61769700 | -3.74841400 | 4.99991500 |
| H | -7.53996700 | -3.22802100 | 4.03748700 |
| H | -6.93325400 | -3.23356600 | 5.68083100 |
| C | -10.83648500 | -4.22890900 | 7.91266300 |
| H | -10.82930800 | -4.78136000 | 8.85732400 |
| H | -11.09958300 | -3.18952600 | 8.13638100 |
| H | -11.62770900 | -4.66163700 | 7.29104800 |
| C | -10.28555500 | -3.94443700 | 3.01797900 |
| H | -11.06287600 | -4.43157700 | 2.41960100 |
| H | -10.34980300 | -2.86522100 | 2.84571100 |

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|---|-------------|-------------|-------------|
| H | -9.31481200 | -4.28658200 | 2.64336900 |
| C | -7.23947600 | -5.22832400 | 4.85045500 |
| H | -7.91742700 | -5.76776300 | 4.17988800 |
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| C | -7.71100400 | 9.75098400 | 2.41206500 |
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| C | -4.91934200 | 9.77781000 | 3.38719000 |
| H | -3.92250800 | 10.17676800 | 3.17979000 |
| H | -5.28309100 | 10.25539200 | 4.30474100 |
| C | -6.08763300 | 12.17575000 | 2.11952300 |
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| C | -4.85038000 | 8.25417200 | 3.54706500 |
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| H | -4.17079700 | 7.99381600 | 4.36532400 |
| C | -8.24259400 | 10.14004000 | 3.80018400 |
| H | -8.29000600 | 11.22420700 | 3.93536300 |
| H | -9.26053400 | 9.75602600 | 3.92675900 |
| H | -7.63134200 | 9.72401000 | 4.60712500 |
| C | -3.64763700 | 11.24568200 | -2.82424400 |
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| H | -3.18059600 | 11.18616000 | -3.81451900 |
| C | -5.44030400 | 9.14955900 | -3.80206800 |
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| C | -2.87203300 | 8.41007900 | -2.53581700 |
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| C | -2.10375700 | 8.43744600 | -3.86377900 |
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| H | 0.77138200 | 4.21015300 | -7.94662200 |
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| H | -0.52594900 | 2.34383100 | -5.30388200 |
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| C | 0.36259500 | 5.10604100 | -6.00235200 |
| H | 1.08691900 | 5.91844100 | -6.12580400 |
| H | -0.47251900 | 5.49978700 | -5.41209300 |
| H | 0.84985700 | 4.31870600 | -5.41814500 |
| C | -1.56961900 | 0.67229100 | -6.23099400 |
| H | -1.11766200 | -0.07921700 | -5.57422300 |
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| H | -1.68977800 | 0.22391700 | -7.22275400 |
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| H | 0.07861600 | -0.12741300 | -11.44484700 |
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| H | -7.56118200 | -11.16371100 | -0.04439700 |
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| H | -6.83043800 | -4.82449500 | -0.77021900 |
| C | -4.57901400 | -8.78319400 | -6.95703100 |
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| C | 2.99271600 | -3.46134400 | 6.53417200 |
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| H | 0.05802900 | -1.00904400 | 7.04051300 |
| C | -0.08453800 | -1.90432300 | 5.07569300 |
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| H | 0.51028600 | -2.45789500 | 4.34294300 |
| H | -0.97253300 | -2.49881900 | 5.31085500 |
| C | 0.68564500 | -5.62561000 | 7.96036900 |
| H | 0.75947700 | -5.40786700 | 9.03053500 |
| H | -0.05213500 | -6.42436700 | 7.83265800 |
| H | 1.65315200 | -6.01500500 | 7.62293500 |
| C | 2.91949600 | -3.99223900 | 5.09612300 |
| H | 2.57888800 | -3.22566800 | 4.39381900 |
| H | 3.91356000 | -4.32021800 | 4.76942600 |
| H | 2.24679600 | -4.85204100 | 5.01140000 |
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| H | 2.08723600 | 0.54281900 | 11.96614300 |
| C | 0.13329200 | -2.71296600 | 12.80793000 |
| H | 0.07195700 | -2.35640400 | 13.84421900 |
| H | -0.78315400 | -2.40652000 | 12.29524000 |
| C | 3.00928500 | -2.27838600 | 13.01734400 |
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| C | -0.08555200 | 0.57862800 | 11.95355200 |
| H | -0.12418600 | 1.63876600 | 12.22490900 |
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| H | -0.93287000 | 0.08474500 | 12.43817500 |

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| C | 0.27633600 | -4.24054700 | 12.76742800 |
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| H | -0.59020700 | -4.70604100 | 13.24722100 |
| C | 4.19553500 | -1.30542400 | 12.98071400 |
| H | 5.01855900 | -1.70832800 | 13.57949500 |
| H | 4.56596500 | -1.14729000 | 11.96273900 |
| H | 3.93471800 | -0.33058300 | 13.40302300 |
| C | 4.63119000 | 8.81786100 | 6.92923500 |
| H | 4.64818600 | 9.41238500 | 7.85212000 |
| H | 5.11184000 | 7.86031500 | 7.16276100 |
| C | 7.27310700 | 10.07335800 | 6.65869200 |
| H | 8.02271700 | 10.40858700 | 5.93399700 |
| H | 7.03349300 | 10.94376400 | 7.28264900 |
| C | 4.94686900 | 11.34924100 | 5.46762700 |
| H | 4.74774200 | 11.75493900 | 6.46802000 |
| H | 3.98523200 | 11.18261400 | 4.97434400 |
| C | 3.18675700 | 8.58950200 | 6.46535100 |
| H | 2.63774500 | 8.03153900 | 7.23160700 |
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| H | 3.14971900 | 8.02577700 | 5.52833200 |
| C | 7.84375800 | 8.95488300 | 7.54023200 |
| H | 8.09656400 | 8.06172400 | 6.96131700 |
| H | 8.75896100 | 9.30699100 | 8.02675800 |
| H | 7.14658700 | 8.66510100 | 8.33240600 |
| C | 5.79806500 | 12.32630600 | 4.64498400 |
| H | 6.76216700 | 12.53726300 | 5.11854000 |
| H | 5.98303500 | 11.93653600 | 3.63860900 |
| H | 5.27046800 | 13.27982000 | 4.54397500 |
| C | 6.40996400 | 9.43024500 | 0.27975700 |
| H | 6.46272200 | 9.13551300 | -0.77520500 |
| H | 5.47294400 | 9.97918300 | 0.42489200 |
| C | 7.74240300 | 6.88245000 | 0.84112900 |
| H | 7.87119200 | 6.96936700 | -0.24504400 |
| H | 8.61569700 | 7.35713600 | 1.29965600 |
| C | 4.80272100 | 6.97436100 | 0.63674100 |
| H | 4.73851500 | 6.03974200 | 1.20720600 |
| H | 3.92725500 | 7.56590500 | 0.92036100 |
| C | 7.66974200 | 5.40670800 | 1.25372400 |
| H | 8.61308100 | 4.90210200 | 1.01755200 |
| H | 7.49588900 | 5.29594500 | 2.32832200 |
| H | 6.86908200 | 4.87622800 | 0.72724200 |
| C | 7.60749600 | 10.31868600 | 0.64743400 |
| H | 7.61209300 | 11.21611700 | 0.02097800 |
| H | 7.55427600 | 10.64125700 | 1.69257700 |
| H | 8.56410400 | 9.80787200 | 0.49152800 |
| C | 4.81056600 | 6.69109600 | -0.87142700 |
| H | 5.68961800 | 6.11598600 | -1.18391300 |
| H | 3.92237400 | 6.10956600 | -1.14395800 |
| H | 4.78705700 | 7.61483400 | -1.45728400 |
| C | 10.45513800 | 4.20868300 | -4.56039600 |
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| H | 11.47419800 | 3.96253900 | -4.87391500 |
| C | 7.59717400 | 3.67459700 | -5.04574700 |
| H | 7.52134700 | 3.16218300 | -4.07888700 |

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| H | 6.91024300 | 3.15526900 | -5.72070300 |
| C | 9.43178200 | 4.22959200 | -7.29901400 |
| H | 9.18113500 | 5.28083300 | -7.11367000 |
| H | 8.65671400 | 3.81137000 | -7.95006700 |
| C | 10.80829300 | 4.12317700 | -7.97207600 |
| H | 11.06706500 | 3.08092400 | -8.18728900 |
| H | 10.79982100 | 4.66724200 | -8.92157900 |
| H | 11.60306600 | 4.55869900 | -7.35698500 |
| C | 10.26996000 | 3.88694000 | -3.07254200 |
| H | 10.33504400 | 2.80971100 | -2.88864600 |
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| H | 9.29980300 | 4.23278100 | -2.69987100 |
| C | 7.22141400 | 5.15617300 | -4.90753100 |
| H | 6.21180500 | 5.24512700 | -4.49003200 |
| H | 7.90199600 | 5.70027300 | -4.24343800 |
| H | 7.21844900 | 5.66804300 | -5.87437300 |
| C | 9.14950200 | -2.60471900 | -6.31911000 |
| H | 9.47190300 | -3.51622400 | -6.83948300 |
| H | 9.49684100 | -2.69080500 | -5.28290500 |
| C | 9.58861700 | -1.21948600 | -8.86842100 |
| H | 9.72127600 | -2.25271800 | -9.21529700 |
| H | 8.52208700 | -0.98248800 | -8.91503500 |
| C | 11.84529700 | -1.75261600 | -7.11978700 |
| H | 12.45647000 | -0.87517300 | -7.35564400 |
| H | 11.92979600 | -2.43005400 | -7.97890300 |
| C | 7.62121600 | -2.47641400 | -6.35649900 |
| H | 7.16407800 | -3.33465400 | -5.85107600 |
| H | 7.28585800 | -1.56035700 | -5.86107500 |
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| C | 12.38201100 | -2.45096300 | -5.86378300 |
| H | 13.43630200 | -2.70566400 | -6.01235500 |
| H | 12.31430100 | -1.81411100 | -4.97677000 |
| H | 11.84845600 | -3.38403600 | -5.65684700 |
| C | 10.38076400 | -0.24510900 | -9.75147800 |
| H | 10.23687600 | 0.78910700 | -9.42279900 |
| H | 11.45344100 | -0.46379800 | -9.75322200 |
| H | 10.03213300 | -0.31920000 | -10.78620000 |
| C | 5.64458700 | -8.38735600 | 3.53053100 |
| H | 5.86092400 | -7.43691600 | 3.02665500 |
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| C | 2.84063300 | -8.37327700 | 2.51029900 |
| H | 2.32487900 | -8.61359700 | 1.57610600 |
| H | 3.10374100 | -7.30819500 | 2.45441500 |
| C | 4.20822500 | -10.93199300 | 3.27214100 |
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| H | 3.82323500 | -10.73732600 | 4.28008400 |
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| H | 2.38640400 | -8.41917400 | 4.66929900 |
| C | 5.23820500 | -8.13331700 | 4.98879700 |
| H | 6.06783500 | -7.65796600 | 5.52445800 |
| H | 4.37272800 | -7.46686500 | 5.05961600 |
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| C | 3.30311800 | -11.93085700 | 2.53762200 |

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| H | 2.29100000 | -11.54052300 | 2.39281700 |
| H | 3.70140900 | -12.18248200 | 1.55154700 |
| H | 3.22736400 | -12.85246100 | 3.12339500 |
| C | 7.72717600 | -10.46051600 | -2.38339400 |
| H | 7.85701100 | -11.17983000 | -3.20118100 |
| H | 8.25867000 | -10.87220200 | -1.51906500 |
| C | 5.07490500 | -9.58005600 | -3.36438100 |
| H | 5.40709300 | -8.53499700 | -3.33283000 |
| H | 4.01189200 | -9.57261300 | -3.10297000 |
| C | 5.41092700 | -12.21924600 | -2.07361900 |
| H | 4.31915400 | -12.22799400 | -1.98398800 |
| H | 5.66372100 | -12.57850900 | -3.07809500 |
| C | 6.04500600 | -13.12613100 | -1.00928700 |
| H | 7.13623200 | -13.16119500 | -1.09524400 |
| H | 5.78841100 | -12.79165100 | 0.00204200 |
| H | 5.67784600 | -14.15018700 | -1.12813500 |
| C | 8.32427700 | -9.10398100 | -2.77933300 |
| H | 7.87648700 | -8.71711000 | -3.70015300 |
| H | 8.18289600 | -8.35375700 | -1.99388900 |
| H | 9.39957500 | -9.20945400 | -2.95730600 |
| C | 5.29633900 | -10.18038800 | -4.76061100 |
| H | 4.89857100 | -11.19662300 | -4.83542300 |
| H | 4.77649500 | -9.57292700 | -5.50929400 |
| H | 6.35438000 | -10.21088400 | -5.04129800 |

Coordinate of 3 from Computational studies

| | | | |
|---|------------|-------------|--------------|
| N | 6.78212000 | -2.39727700 | -8.60925900 |
| C | 5.50105900 | -2.09794100 | -8.79969300 |
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| H | 4.66576500 | -2.60568600 | -8.34176200 |
| C | 6.63894600 | -0.70568700 | -10.07101900 |
| H | 8.58433300 | -1.56677500 | -9.44984100 |
| H | 6.81314800 | 0.07721300 | -10.79342000 |
| N | 5.83255700 | -8.81957100 | 4.02139000 |
| C | 4.53669500 | -8.61634000 | 4.23799600 |
| C | 6.37821100 | -9.18603100 | 5.23704700 |
| H | 3.81337800 | -8.33661800 | 3.48736500 |
| C | 5.38786400 | -9.20091500 | 6.18339600 |
| H | 7.42490600 | -9.42784300 | 5.34075900 |
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| C | 2.86165200 | -8.83543400 | 6.11961100 |
| H | 2.20151700 | -9.28560200 | 5.37274800 |
| H | 2.89822000 | -9.52452200 | 6.96737900 |
| C | 3.48632400 | 0.64620300 | -9.50294800 |
| C | 3.80715400 | 1.95505100 | -9.88837100 |
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| C | 3.14628700 | 3.04784400 | -9.32940100 |
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| C | 2.11357000 | 2.87140100 | -8.38941800 |
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| H | 1.05350400 | 1.39190100 | -7.23058100 |

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| C | 2.56088100 | -6.98535300 | 7.84107300 |
| C | 0.74686700 | -5.65219600 | 6.20441200 |
| H | 1.17468700 | -7.16921400 | 4.74719900 |
| C | 1.92048100 | -5.83461900 | 8.29750800 |
| H | 3.24602300 | -7.50745600 | 8.50476600 |
| C | 0.96718300 | -5.16747800 | 7.50460700 |
| H | 0.03417400 | -5.14841000 | 5.55921000 |
| H | 2.12849800 | -5.47473500 | 9.30070000 |
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| C | 6.00885900 | 8.27472300 | -3.92695200 |
| C | 7.98601500 | 8.31644100 | -4.81943700 |
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| C | 5.13135600 | 1.52407100 | 9.28153400 |
| C | 6.99686100 | 0.42317800 | 9.41095900 |
| H | 4.38895500 | 2.27779900 | 9.06632100 |
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| H | 8.04558000 | 0.21708700 | 9.26233700 |
| H | 6.12866800 | -1.23454300 | 10.63614000 |
| C | 3.59554700 | 0.05492400 | 10.63183800 |
| H | 3.80635600 | -0.23690700 | 11.66553300 |
| H | 3.01537200 | 0.98294000 | 10.68664500 |
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| C | 3.82816500 | 7.34703300 | -6.49827000 |
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| H | 1.55779500 | -1.34823400 | 11.69022600 |
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| H | -4.15584100 | -2.30390000 | -8.87357900 |
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| C | -2.50437200 | 1.06596800 | -9.70721800 |
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| H | -1.37725400 | 1.47853400 | -11.50372400 |
| C | -1.89282100 | 2.43410000 | -7.79649500 |
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| C | -4.52564900 | 8.59456400 | -4.16827100 |
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| H | -3.88408000 | 8.19453700 | -3.39817200 |
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| H | -5.10610900 | 9.77619900 | -7.11759600 |
| N | -6.70583300 | 2.38932600 | 8.53287800 |
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| C | -7.37527900 | 1.55407300 | 9.40660100 |
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| C | -6.45874700 | 0.82667700 | 10.11941600 |
| H | -8.45262600 | 1.54658100 | 9.47243800 |
| H | -6.58351800 | 0.09745300 | 10.90544500 |
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| C | -0.51772700 | 5.77769500 | -6.02039200 |
| H | -0.92705100 | 7.29871500 | -4.56133700 |
| C | -0.77548100 | 5.27521500 | -7.30648800 |
| H | -2.01784500 | 5.53336000 | -9.05592300 |
| H | 0.23201800 | 5.29860900 | -5.39887900 |
| C | -3.27919800 | -0.43708900 | 9.53550300 |
| C | -2.24526600 | -0.28264400 | 8.60245700 |
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| C | -2.97542700 | -2.84497300 | 9.38675500 |
| H | -4.43143900 | -1.89552000 | 10.64102200 |
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| H | -3.26779300 | -3.84036600 | 9.70753100 |
| C | 0.22013400 | -3.99173300 | 8.06301700 |
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| C | -0.01357800 | 4.12064900 | -7.88708400 |
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| N | -5.66623300 | -8.11000300 | 5.34364300 |
| N | -5.21306200 | 1.22055200 | 9.67298200 |
| N | 4.22218600 | -8.83590000 | 5.53815400 |
| N | 4.87494900 | 0.40296800 | 10.00231800 |
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| N | 5.82862400 | 8.36306800 | -5.26989200 |
| N | 5.36741900 | -1.07479700 | -9.67935800 |
| C | 4.09316500 | -0.55019300 | -10.21706600 |
| H | 3.38771800 | -1.38566500 | -10.20758100 |
| H | 4.28173800 | -0.30521600 | -11.26572100 |
| P | 8.90913100 | 5.84678600 | -1.89973800 |
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| Pt | -7.17648200 | -3.07631400 | -7.61708700 |
| C | 8.68176500 | 7.83930900 | 0.25538700 |
| C | 9.01676800 | 7.63098000 | 1.41556000 |
| C | -7.98987000 | 8.11624400 | -0.60083800 |
| C | -8.57028900 | 7.86521900 | 0.44871700 |
| C | 8.13913400 | -5.30773700 | -6.01502800 |
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| C | -8.61457900 | -5.14705300 | -5.65587500 |

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| C | 10.99611800 | 7.94440000 | 4.57389200 |
| C | 9.45335700 | 7.42358900 | 2.76617400 |
| C | 10.35760800 | 7.02426400 | 5.40162600 |
| H | 11.84629800 | 8.50661200 | 4.94838100 |
| C | 8.81169400 | 6.49781200 | 3.61079800 |
| C | 9.25394800 | 6.28358900 | 4.93049900 |
| H | 10.71187500 | 6.86651800 | 6.41521400 |
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| C | 10.59918500 | -8.78583500 | -3.58733300 |
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| C | 8.83684400 | -8.16752600 | -2.02942400 |
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| C | -10.67673100 | -7.78183000 | -3.03483500 |
| H | -12.04295200 | -8.06932700 | -4.66869700 |
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| C | -8.82685900 | 5.66321500 | 4.87102300 |
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| C | 8.12863200 | 4.48792700 | 6.53856400 |
| C | 8.19944100 | -8.32796000 | -0.75476200 |
| C | 7.68334000 | -8.49342000 | 0.34401200 |
| C | -9.04384800 | -7.35324300 | -1.24013500 |
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| Pt | 7.32735100 | 3.09529000 | 7.68345500 |
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| P | 6.68843500 | 2.09726200 | 5.60858300 |
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| H | -9.07238800 | -10.21491500 | -0.77133500 |
| H | -8.98275900 | -11.81493900 | -0.01836000 |

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| C | -6.28077300 | -10.69981200 | 0.52717600 |
| H | -6.32060600 | -11.79305500 | 0.43576500 |
| H | -5.47445000 | -10.47109100 | 1.23430100 |
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| H | -5.01717000 | -10.39583400 | -1.20512100 |
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| H | -10.78557700 | -11.10602700 | 1.64565100 |
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| C | -6.83251100 | -11.57042800 | 3.63473200 |
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| C | -8.09592400 | -4.37689900 | 0.71741100 |
| H | -7.00259300 | -4.38115800 | 0.80452500 |
| H | -8.32901500 | -4.87360400 | -0.22938300 |
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| C | -6.88161300 | -4.29963400 | 3.82767600 |
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| H | 5.08148300 | -11.59275500 | 3.50206000 |
| C | 5.81291600 | -11.14756100 | -0.28903500 |
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| C | 7.62080200 | -12.09207000 | 1.84749400 |
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| C | 8.92536200 | -11.81850300 | 1.08682900 |
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| C | 4.56846100 | -10.37366000 | -0.74154800 |
| H | 3.66441700 | -10.70292900 | -0.21651200 |
| H | 4.69660900 | -9.29877900 | -0.57482200 |

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| C | 4.33517200 | -13.03226800 | 2.05233200 |
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| H | 3.49746600 | -13.34067000 | 2.68696300 |
| H | 3.99557100 | -13.08112500 | 1.01325900 |
| C | 9.72779900 | -6.84482200 | 2.62792800 |
| H | 9.99909100 | -7.15063200 | 1.61156500 |
| H | 10.20577900 | -5.87754300 | 2.82400600 |
| C | 7.51746700 | -5.79480500 | 4.23758700 |
| H | 8.29086400 | -5.03909500 | 4.42344700 |
| H | 7.64036000 | -6.56360800 | 5.00728300 |
| C | 7.57963800 | -5.28963200 | 1.32841700 |
| H | 6.49854600 | -5.10395200 | 1.33198100 |
| H | 7.80320200 | -5.77117500 | 0.37114800 |
| C | 6.12058700 | -5.16922600 | 4.33872100 |
| H | 5.33620300 | -5.90112300 | 4.12175100 |
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| H | 5.99993700 | -4.33072500 | 3.64399900 |
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| H | 5.33005300 | 0.34512400 | 4.61031900 |
| C | 8.15547800 | 1.84063500 | 4.50262000 |
| H | 8.82513300 | 1.15283400 | 5.03200000 |
| H | 8.66999100 | 2.80627000 | 4.48749100 |
| C | 5.55390100 | 3.22666200 | 4.67171800 |
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| H | 5.32750600 | 2.77798400 | 3.69670300 |
| C | 6.65017800 | -0.75345200 | 5.94312400 |
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| H | 7.44527600 | -0.90581900 | 5.20635000 |
| C | 7.87687700 | 1.33914200 | 3.08043200 |
| H | 8.82328000 | 1.22405300 | 2.54050100 |
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| H | 7.25838000 | 2.04417000 | 2.51456900 |
| C | 4.26161400 | 3.56537900 | 5.42630300 |
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| H | 10.20933000 | 5.22815200 | 10.39195500 |
| C | 7.28928400 | 6.06437000 | 9.51881400 |
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| C | 5.77061400 | 6.02456300 | 9.72570900 |
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| H | 8.45877300 | 2.37037800 | 12.75921500 |
| H | 8.77702100 | 1.80155700 | 11.11562400 |
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| C | -10.59236800 | 1.47737100 | 6.59893000 |
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| C | -5.35764900 | 0.37874500 | -4.45453000 |
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| H | -6.27416200 | 0.67414500 | -3.93317300 |
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| H | 8.46153200 | -0.02229700 | -5.15932800 |
| H | 8.16996400 | -0.34526300 | -6.86263400 |
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| H | 5.70083900 | -0.73590400 | -6.35713800 |
| H | 6.00279100 | -0.32456300 | -4.66218800 |
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| C | 7.93376900 | -1.94541200 | -2.73349200 |
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| C | 8.29788200 | 4.63624600 | -0.63196600 |
| H | 7.20920100 | 4.58057600 | -0.75372600 |
| H | 8.47355300 | 5.12435200 | 0.33166500 |
| C | 10.75223500 | 5.87404300 | -1.71073200 |
| H | 11.12831100 | 4.84739400 | -1.79400500 |
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| C | 11.47048500 | 6.79062600 | -2.71184100 |
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| C | 8.92292900 | 3.23538100 | -0.66480900 |
| H | 8.47239000 | 2.60892600 | 0.11367300 |
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| H | 9.99972600 | 3.26591900 | -0.47354600 |
| C | 6.19388900 | 10.89024300 | -0.36996700 |
| H | 6.19088300 | 11.98297700 | -0.26512200 |
| H | 5.40835200 | 10.63998600 | -1.09301500 |
| C | 9.09555200 | 11.05187100 | 0.03360300 |
| H | 8.84187600 | 12.10130300 | 0.23279300 |

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| H | 8.98158900 | 10.49687000 | 0.96825100 |
| C | 8.00747700 | 11.55236700 | -2.60446200 |
| H | 8.80622700 | 11.13622700 | -3.22773200 |
| H | 8.38835800 | 12.49895900 | -2.20151900 |
| C | 5.90676900 | 10.22070800 | 0.98105100 |
| H | 4.91608400 | 10.52110600 | 1.33883200 |
| H | 5.93338000 | 9.12921500 | 0.90303300 |
| H | 6.63429300 | 10.51731200 | 1.74199900 |
| C | 6.75790300 | 11.82875700 | -3.45011500 |
| H | 7.01982500 | 12.49743000 | -4.27644100 |
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| H | 5.97440900 | 12.32401400 | -2.86859900 |
| C | 10.53720100 | 10.93062000 | -0.47901000 |
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| C | -6.66280000 | 5.70341400 | -4.46903900 |
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| C | -10.46573700 | -6.70615700 | -5.19148700 |
| H | -10.83880400 | -6.53823500 | -6.19665400 |
| C | -10.56650600 | 8.12058900 | 1.87315800 |
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| H | 11.06182100 | 8.85923500 | 2.62501700 |
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