Electronic Supplementary Information for:

Tuning the Photophysical Properties of *N^N* Pt(II) Bisacetylide Complexes with Fluorene Moiety and Its Applications for Triplet-triplet-annihilation based Upconversion

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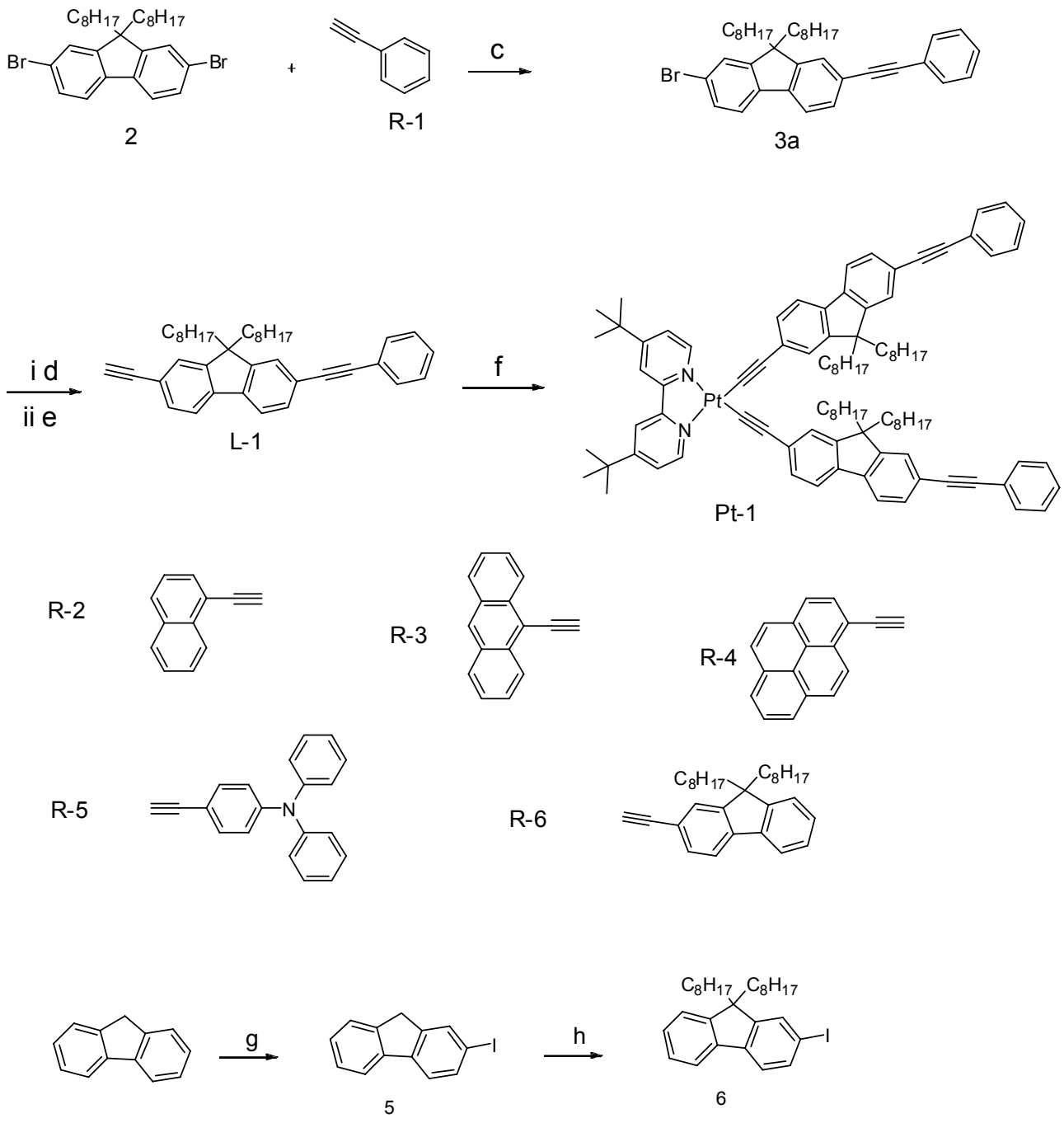
Experimental Section

General

All the chemicals are analytical pure and were used as received. Solvents were dried and distilled for synthesis. NMR spectra were recorded on a 400 MHz Varian Unity Inova NMR spectrophotometer. Mass spectra were recorded with Q-TOF Micro MS spectrometer. UV-Vis absorption spectra were measured with a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Fluorescence lifetimes were measured on a Horiba Jobin Yvon Fluoro Max-4 (TCSPC) instrument. Emission curves were generated using the Origin 5.0 (Microcal software). The binding constants were calculated using custom-written nonlinear least-square curve-fitting programs implemented within SigmaPlot 2000 (SPSS Inc.).

All these calculations were performed in Gaussian 09 suit.

Synthesis :



Scheme S1. Synthesis of the ligands of the complexes. (c) $Pd(PPh_3)_2Cl_2$, CuI, PPh_3, NEt_3, reflux, 8 h; (d) 3-methyl-1-butyn-3-ol, $Pd(PPh_3)Cl_2$, PPh_3, CuI, NEt_3, reflux, 12 h; (e) 2-propanol, KOH, reflux, 4 h; (f) CH_2Cl_2, CuI, $(i\text{-}Pr)_2NH$, r.t., 24 h; (g) I_2, H_2SO_4, KIO_3, H_2O, 8 h; reflux, 1 h; (h) octylpyridinium bromide, TBAB, NaOH (w= 50 %) , toluene, reflux, 4 h.

1-(2-(2-Ethynyl-9,9-dioctyl-9H-fluoren-7-yl)ethynyl)-naphthalene (3b)

3b was prepared with the similar method of **3a** and obtained as cream solid 320.0 mg, yield: 51.8 %.^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.51 (d, 1H, *J* = 8.0 Hz), δ 7.90–7.85 (m, 2H), δ 7.81 (d, 1H, *J* = 8.0 Hz), δ 7.70 (d, 1H, *J* = 8.0 Hz), δ 7.65–7.62 (m, 2H), δ 7.58–7.54 (m, 3H), δ 7.50–7.46 (m, 3H), δ 2.01–1.95 (m, 4H), δ 1.25–1.07 (m, 20H), δ 0.83–0.79 (m, 6H), δ 0.63–0.62 (m, 4H). ESI-MS $C_{41}H_{47}Br$ Calculated *m/z* = 618.2861, found *m/z* = 618.2859.

1-(7-Ethynyl-9,9-dioctyl-9H-fluoren-2-yl)-ethynylnaphthalene (L-2)

L-2 was prepared with the similar method of **L-1** and obtained as yellow solid 214.0 mg, yield: 75.9 %.^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, 1H, *J* = 8.0 Hz), δ 7.88–7.83 (m, 2H), δ 7.81 (d, 1H, *J* = 8.0 Hz), δ 7.71 (d, 1H, *J* = 8.0 Hz), δ 7.66–7.63 (m, 3H), δ7. 61 (s, 1H), δ 7.56 (t, 1H, *J* = 8.0 Hz), δ 7.49–7.45 (m, 3H), δ 3.16(s, 1H), δ 2.00–1.97 (m, 4H), δ 1.22–1.05 (m, 20H), δ 0.82–0.79 (m, 6H), δ 0.63–0.60 (m, 4H). ^{13}C NMR(100MHz, $CDCl_3$) , δ 151.3, 141.2, 140.7,133.3, 131.3, 130.4, 128.8, 128.4 , 126.8, 126.6 , 126.5, 126.3, 126.0, 125.4, 122.3, 121.0 , 120.7, 120.2, 120.0, 95.3, 88.0, 84.6, 55.3, 40.3, 31.8, 30.0, 29.3, 23.7, 22.6, 14.1. HR-MALDI-MS: $C_{43}H_{48}$ Calculated *m/z* = 564.3756, found *m/z* = 574.3724.

1-(2-(2-Ethynyl-9,9-dioctyl-9H-fluoren-7-yl)ethynyl)-anthracene (3c)

3c was prepared with the similar method of **3a** and obtained as yellow solid 300.0 mg, yield: 44.9 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, 2H, *J* = 8.0 Hz), δ 8.46 (s, 1H), δ 8.05 (d, 2H, *J* = 8.0 Hz), δ 7.78–7.72 (m, 2H), δ 7.68–7.59 (m, 4H), δ 7.56–7.48 (m, 4H), δ 2.06–1.98 (m, 4H) , δ 1.20–1.09 (m, 20H), δ 0.83–0.78 (m, 6H), δ 0.69–0.63 (m, 4H). HR-MALDI-MS: $C_{45}H_{49}Br$ Calculated *m/z* = 668.3018, found *m/z* = 668.3685.

1-(7-Ethynyl-9,9-dioctyl-9H-fluoren-2-yl)-ethynyl-anthracene (L-3)

L-3 was prepared with the similar method of **L-1** and obtained as yellow solid 190.0 mg, yield: 69.0 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73(d, 2H, *J* = 8.0 Hz), δ 8.46 (s, 1H), δ 8.06 (d, 2H, *J* = 12.0 Hz), δ 7.76 (s, 2H), δ 7.69–7.62 (m, 4H), δ 7.54–7.50 (m, 4H), δ 3.18 (s, 1H), δ 2.05–2.00 (m, 4H), δ 1.25–1.07 (m, 20H), δ 0.86–0.78 (m, 6H), δ 0.66–0.60 (m, 4H). ^{13}C NMR(100MHz, $CDCl_3$): δ 151.54, 151.25, 141.38. 141.98, 132.8, 131.4, 131.1, 128.9, 127.9, 127.0, 126.8, 125.9, 120.4, 120.1, 117.6, 102.0, 87.0, 84.8, 55.5, 40.5, 39.6, 32.1, 29.9, 29.4, 23.9, 22.8, 14.3. HR-MALDI-MS: $C_{47}H_{50}$: Calculated *m/z* = 614.3913, found *m/z* = 614.3868.

1-(2-(2-Ethynyl-9,9-dioctyl-9H-fluoren-7-yl)ethynylpyrene (3d)

3d was prepared with the similar method of **3a** and obtained as yellow solid 400.0 mg, yield: 57.6 %.^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, 1H, *J* = 8.0 Hz), δ 8.26 (s, 1H), δ 8.24–8.21 (m, 3H), δ 8.17 (d, 1H, *J* = 8.0 Hz), δ 8.08–8.04 (m, 2H), δ 7.72 (s, 2H), δ 7.66 (s, 1H), δ 7.60 (s, 1H), δ 7.49 (d, 2H, *J* = 4.0 Hz), δ 2.04–1.97 (m, 4H), δ 1.24–1.08 (m, 20H), δ 0.83–0.80 (m, 6H), δ 0.67–0.63 (m, 4H). HR-MALDI-MS: $C_{47}H_{49}Br$ Calculated *m/z* = 692.3018, found *m/z* = 692.3815.

1-(7-Ethynyl-9,9-dioctyl-9H-fluoren-2-ylethynyl)pyrene (L-4)

L-4 was prepared with the similar method of **L-1**. Yellow solid 235.0 mg, yield:74.6 %.^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, 1H, *J* = 8.0 Hz), δ 8.28–8.22 (m, 4H), δ 8.18 (d, 1H, *J* = 8.0 Hz), δ 8.14 (d, 1H, *J* = 8.0 Hz), δ 8.09–8.04 (m, 2H), δ 7.76 (s, 2H), δ 7.71 (d, 2H, *J* = 8.0 Hz), δ 7.55 (d, 2H, *J* = 8.0 Hz), δ 3.20 (s, 1H), δ 2.06–2.03 (m, 4H), δ 1.24–1.09 (m, 20H), δ 0.86–0.82 (m, 6H), δ 0.69–0.64 (m, 4H). ^{13}C NMR(100MHz, $CDCl_3$): δ 151.5, 151.3, 141.4, 140.8, 132.0, 131.5, 131.3, 131.1, 129.8, 128.5, 128.3, 127.5, 126.7, 126.4, 126.1, 125.8, 125.8, 124.8, 124.7, 124.6, 122.6, 120.9, 120.4, 120.1, 118.1, 96.3, 89.3, 84.8, 55.5, 40.5, 32.0, 30.2, 29.9, 29.4, 23.9, 22.8, 14.3. HR-MALDI-MS: $C_{49}H_{50}$ Calculated *m/z* = 638.3913, found *m/z* = 638.3969.

1-(2-(2-Ethynyl-9,9-dioctyl-9H-fluoren-7-yl)ethynyl)-triphenylamine (3e)

3e was prepared with the similar method of **3a** and obtained green yellow oily 190.0 mg, yield: 51.7 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, 1H, *J* = 8.0 Hz), δ 7.52 (d, 1H, *J* = 8.0 Hz), δ 7.49–7.44 (m, 4H), δ 7.41 (d, 2H, *J* = 8.0 Hz), δ

7.30–7.25 (m, 4H), δ 7.13 (d, 4H, *J* = 8.0 Hz), δ 7.08 (t, 2H, J = 8.0 Hz), δ 7.03 (d, 2H, *J* = 8.0 Hz), δ 1.94–1.92 (m, 4H), δ 1.22–1.05 (m, 20H), δ 0.84–0.80 (m, 6H), δ 0.62–0.59 (m, 4H). HR-MALDI-MS: $C_{49}H_{54}NBr$ Calculated *m/z* = 735.3440, found *m/z* = 735.4805.

1-(7-Ethynyl-9,9-dioctyl-9H-fluoren-2-yl)ethynyl-triphenylamine (L-5)

L-5 was prepared with the similar method of **L-1** and obtained yellow oil 130.0 mg, yield: 82.3 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (t, 2H, *J* = 8.0 Hz), δ 7.48–7.44 (m, 4H), δ 7.39 (d, 2H, *J* = 8.0 Hz), δ 7.28–7.23 (m, 4H), δ 7.11–7.09 (d, 4H, *J* = 8.0 Hz), δ 7.06–6.99 (m, 4H), δ 3.12 (s, 1H), δ 1.95–1.91 (m, 4H), δ 1.08–1.02 (m, 20H), δ 0.85–0.78 (m, 6H), δ 0.60–0.55 (m, 4H). ^{13}C NMR (100MHz, $CDCl_3$): δ 151.3, 121.2, 148.1, 147.4, 141.4, 140.3, 132.7, 131.4, 130.8, 129.6, 126.7, 126.0, 89.8, 84.8, 55.4, 40.5, 39.6, 32.1, 32.0, 30.2, 29.9, 29.6, 29.4, 23.9, 22.8, 14.3. HR-MALDI-MS: $C_{51}H_{55}N$ Calculated *m/z* = 681.4335, found *m/z* = 681.4288.

1-(2-(2-Ethynyl-9,9-dioctyl-9H-fluoren-7-yl)ethynyl)-9,9-dioctylfluorene(3f)

3f was prepared with the similar method of 3a and obtained as yellow solid 215.0 mg, yield: 48.86 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70–7.64 (m, 3H), δ 7.56–7.52 (m, 5H), δ 7.47 (s, 2H), δ 7.33 (s, 3H), δ 1.99–1.95 (m, 8H), δ 1.21–1.03 (m, 40H), δ 0.84–0.80 (m, 12H), δ 0.62–0.59 (m, 8H). HR–MALDI–MS: $C_{60}H_{81}Br$ Calculated *m/z* = 880.5522, found *m/z* = 880.7422.

1-(7-Ethynyl-9,9-dioctyl-9H-fluoren-2-ylethynyl)-9,9-dioctyl-fluoren (L-6)

L-6 was prepared with the similar method of **L-1** and obtained as yellow solid 95.4 mg, yield: 70.7 %. 1H NMR (400 MHz, $CDCl_3$): δ 7.71–7.69(m, 2H), δ 7.68(d, 1H, *J* = 8.0 Hz), δ 7.65(d, 1H, *J* = 8.0 Hz), δ 7.57–7.53 (m, 4H), δ 7.50–7.47 (m, 2H), δ7.35–7.33 (m, 3H), δ 3.15 (s, 1H), δ 2.00–1.95 (m, 8H), δ 1.14–1.05 (m, 40H), δ 0.84–0.80 (m, 12H), δ 0.61–0.58 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 151.0, 150.8, 141.5, 141.3, 140.4, 131.3, 130.7, 130.6, 127.5, 126.9, 126.5, 125.9, 122.9, 122.3, 121.4, 120.6,120.1, 120.0, 119.9, 119.7, 91.0, 90.3, 84.8, 55.3, 55.2, 40.4, 40.4, 32.8, 32.0, 31.8, 30.1, 29.7, 29.4, 29.3, 23.7, 22.6, 14.1. HR-MALDI-MS: $C_{62}H_{82}$ Calculated *m/z* = 826.6417, found *m/z* = 826.6438.

Naphthalene-acetylene (compound R-2)

Under argon atmosphere, 1-bromonaphthalene(1.0 g, 4.83 mmol), $Pd(PPh_3)_2Cl_2$ (67.6 mg, 0.09 mmol), triphenylphosphine (50.6 mg, 0.201 mmol), cuprous iodide (36.7 mg, 0.18 mmol) and dry triethylamine (10 mL) were mixed together, The mixture was purged with Ar and then the trimethylsilyl acetylene was added. The mixture was stirred and refluxed for about 8 h. The reaction mixture was cooled to room temperature and the solvent was removed under reduced pressure. The product was purified by column chromatography (silica gel, hexane) obtained canary oily 0.57 g, yield 77.0 %. Then **P-2**, K_2CO_3 (1.05 g, 7.61 mmol), methanol (15 mL) was mixed together. The mixture was stirred at room temperature for 3h. The product R-2 of was obtained canary oily 379.0 mg, yield: 96.0 %.(*J. Mater. Chem.,* 2010, **20**, 9775–9786).

9-ethynylanthracene (compound R-3)

R-3 was prepared with the similar method of **R-2**. **P-3** was obtained as yellow oily 620.0 mg, yield: 59.0 %. **R-3** was obtained as yellow solid 380.0 mg, yield: 77.4 %. (*J*. Am. Chem. Soc. 2010, **132**, 2646–2654).

Pyrene alkyne (compound R-4)

R-4 was prepared with the similar method of **R-2**. **P-4** was obtained as yellow oily 730.0 mg, yield: 68.9 %. R-4 was obtained as yellow solid 440.0 mg, yield: 79.3 %.(*Organic Electronics*, 2009, **10**, 256–265.)

4-ethynyl-N,N-diphenylaniline (compound R-5)

R-5 was prepared with the similar method of **R-2**. **R-5** was obtained as yellow solid 210.0 mg, yield: 85.9%.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34(d, 2H, *J* = 8.0 Hz), δ 7.29–7.25 (m, 4H), δ 7.11–7.08(m, 6H), δ 6.98(d, 2H, *J* = 8.0 Hz), δ (s, 2H).

2-Iodofluorene (compound 5)

Fluorene (0.850 g, 5 mmol) was dissolved in acetic acid (10 mL) at 40℃ in a 100 mL flask. To this solution, I_2 (5.040 g, 2.0 mmol), H_2SO_4 (0.5 mL, 9.5 mmol), and a solution of iodic acid (0.300 g, 1.5mmol) in water (1 mL) were added. The mixture was heated to 70 ℃ for 1 h. At the end of this period, the solution was cooled to room temperature and poured into water (100 mL). The resulting precipitate was collected by vacuum filtration, washed with a solution of 2% $NaHCO_3$ (aq), water, and dried under reduced pressure. The crude product was re-crystallized from methanol, and dried under vacuum to obtain a white solid 1.15 g, yield: 78.0 %.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (s, 1H), δ 7.77 (d, 1H, *J* = 8.0 Hz), δ 7.71 (d, 1H, *J* = 8.0 Hz), δ 7.54 (d, 2H, *J* = 8.0 Hz), δ 7.40–7.31 (m, 2H), δ 3.87 (s, 2H).(*Chem. Mater.* **2010**, *22*, 3472–3481)

9,9-dioctyl-2-Iodofluorene (compound 6)

Compound **6** was prepared with the similar method compound **2** obtained white solid 560.0 mg, yield: 29.5%. (*Polym. Adv. Technol.* 2004; **15**: 266–269)

9,9-dioctyl-9H-fluorene-2-acetylene (compound R-6)

R-6 was prepared with the similar method of R-2. P-6 was obtained as yellow oily 380 mg, yield: 78.2 %. R-6 was obtained as yellow solid 180.0 mg, yield: 65.0 %.^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (d, 2H, *J* = 8.0 Hz), δ 7.69–7.68 (m, 1H), δ 7.65 (d, 1H, *J* = 8.0 Hz), δ 7.48 (d, 2H, *J* = 8.0 Hz), δ 7.48 (s, 3H), δ 3.13(s, 1H), δ 1.96–1.92 (m, 4H), δ 1.21–1.03 (m, 20H), δ 0.83–0.80 (m, 6H), δ 0.59–0.53 (m, 4H).

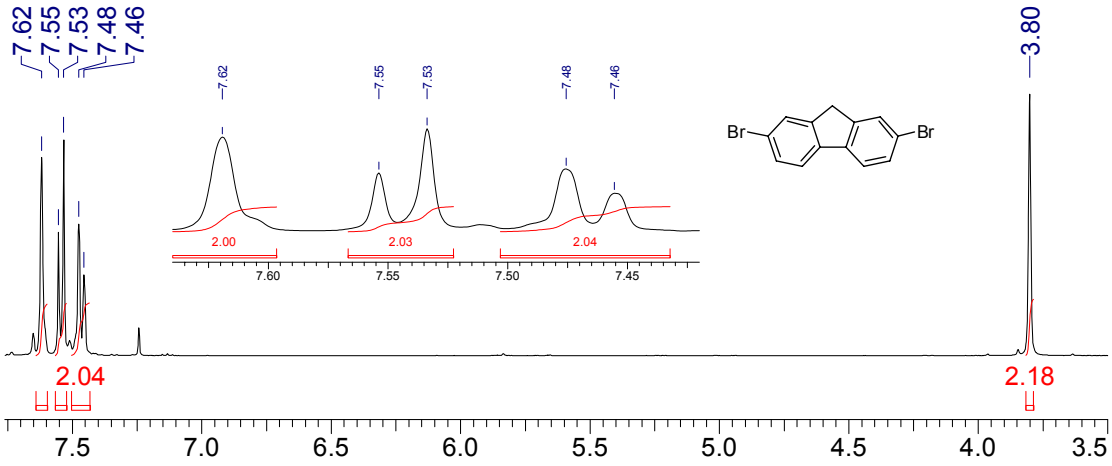


Fig . S1 ^{1}H NMR of compound **1** (400 MHz, $CDCl_3$).

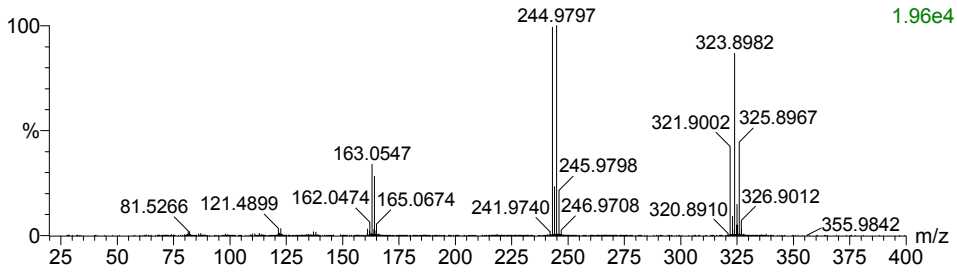


Fig. S2 ESI-HRMS compound **1**.

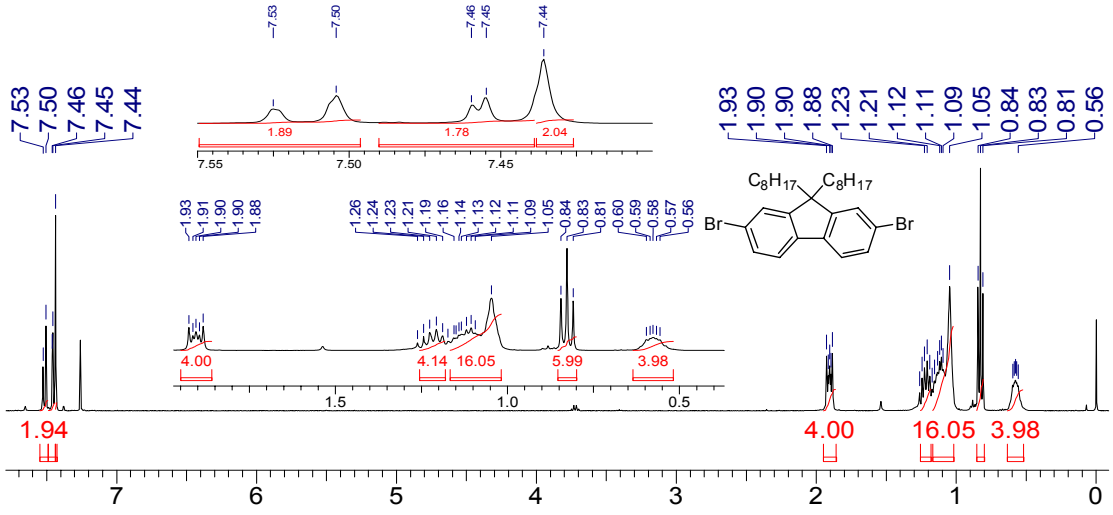


Fig. S3 ^{1}H NMR of compound **2** (400 MHz, $CDCl_3$).

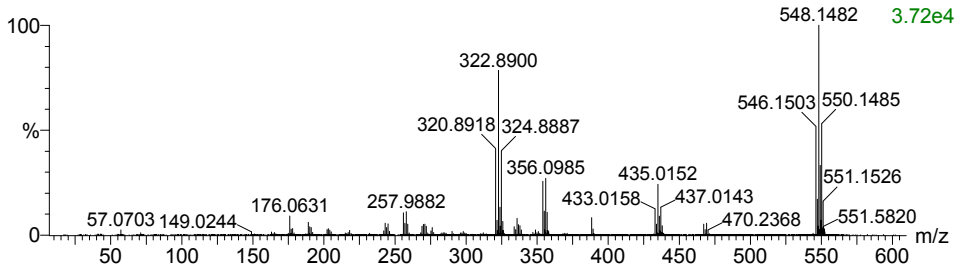


Fig. S4 ESI-MS compound **2**.

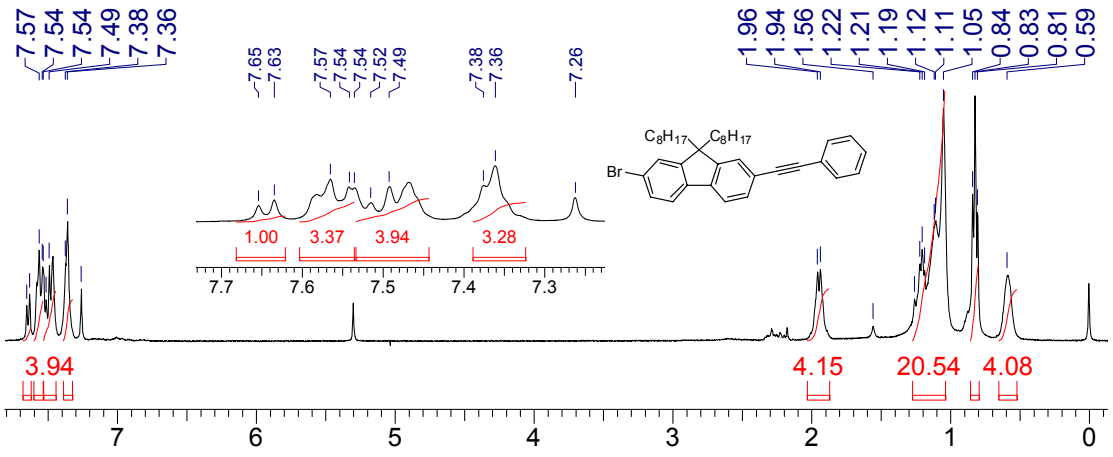


Fig. S5 ^{1}H NMR of compound **3a** (400 MHz, $CDCl_3$).

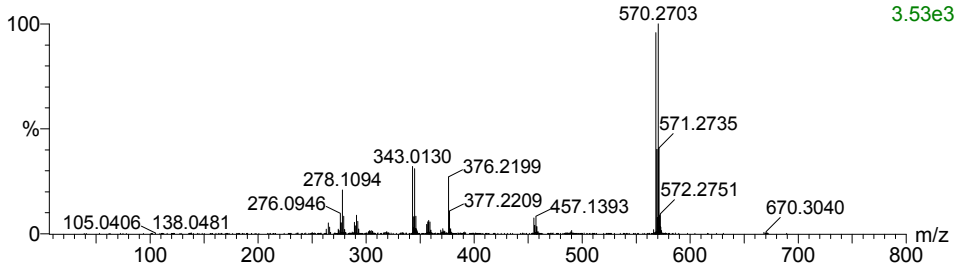


Fig. S6 ESI-MS compound **3a**.

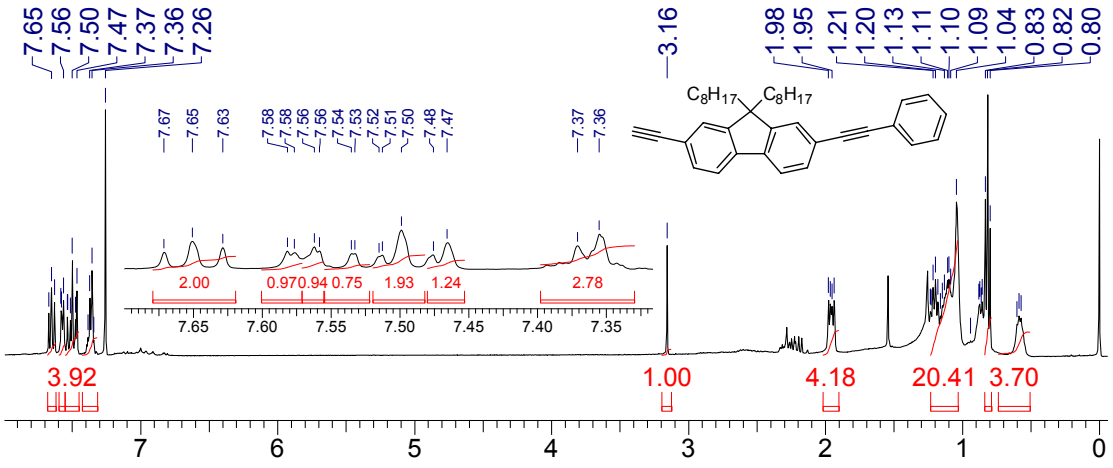


Fig. S7 ^{1}H NMR of compound **L-1** (400 MHz, $CDCl_3$).

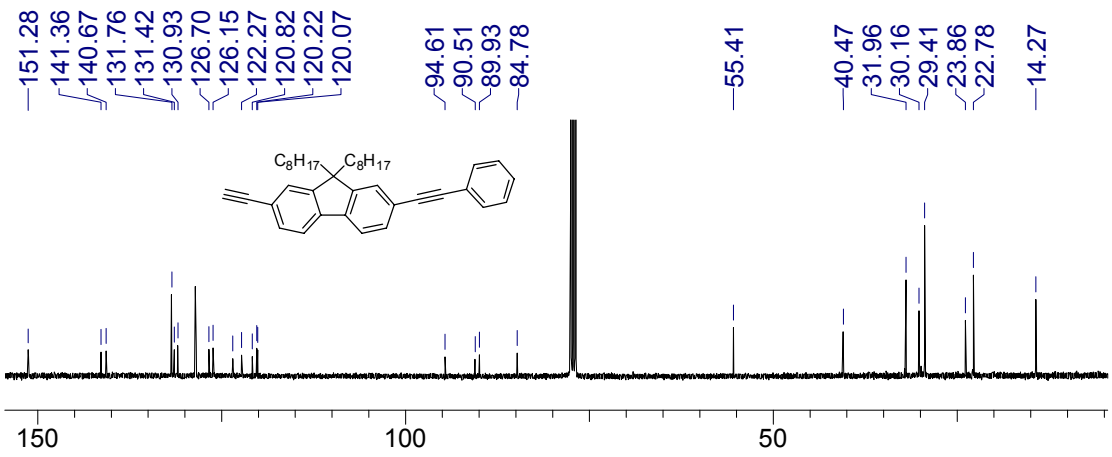


Fig. S8 ^{13}C NMR of compound **L-1** (100 MHz ,$CDCl_3$).

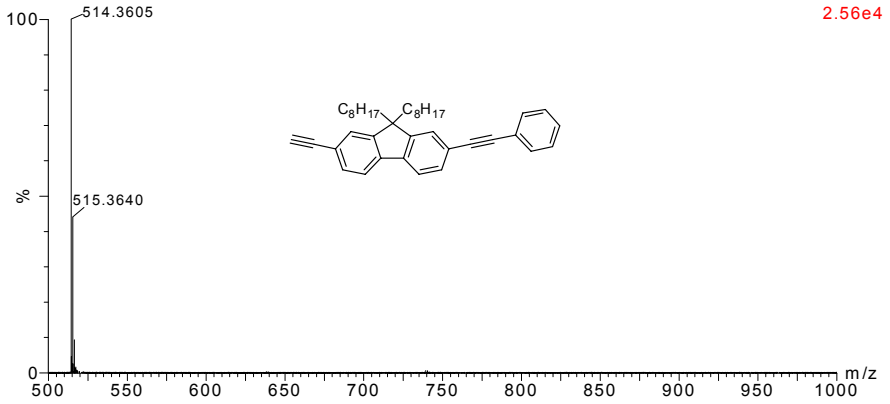


Fig. S9 HR-MALDI-MS of **L-1**.

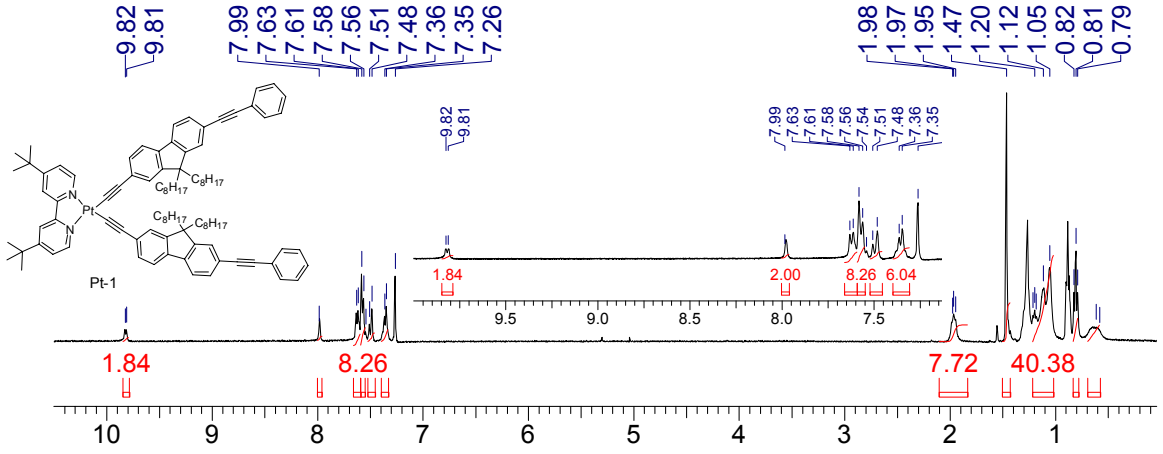


Fig. S10 ^{1}H NMR of compound **Pt-1** ($CDCl_3$, 400 MHz).

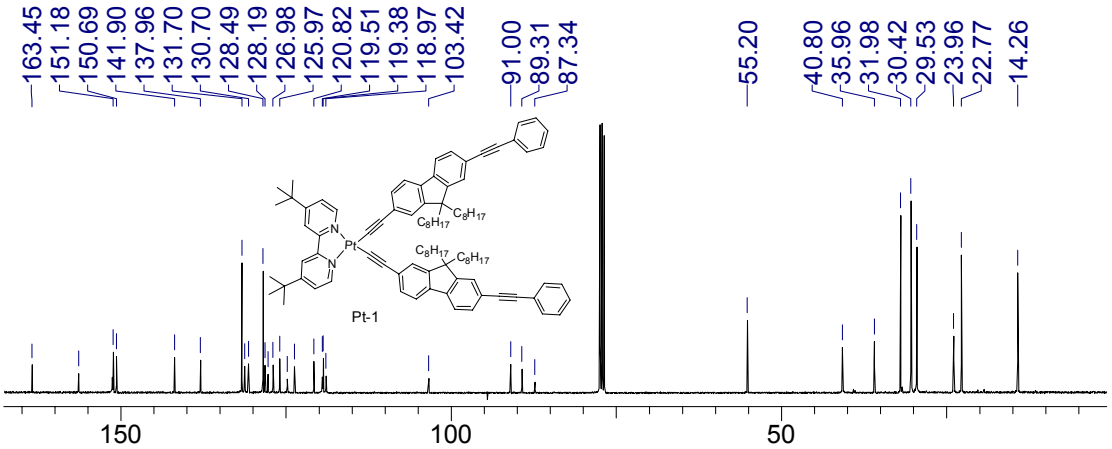


Fig. S11 ^{13}C NMR of compound **Pt-1** (100 MHz, $CDCl_3$).

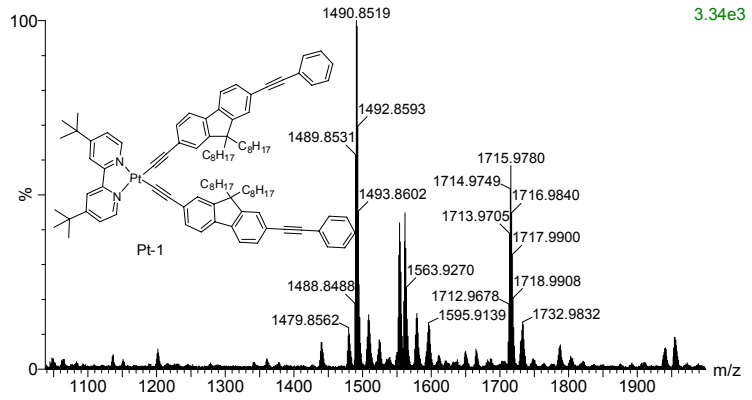


Fig. S12 HR-MALDI-MS of **Pt-1**.

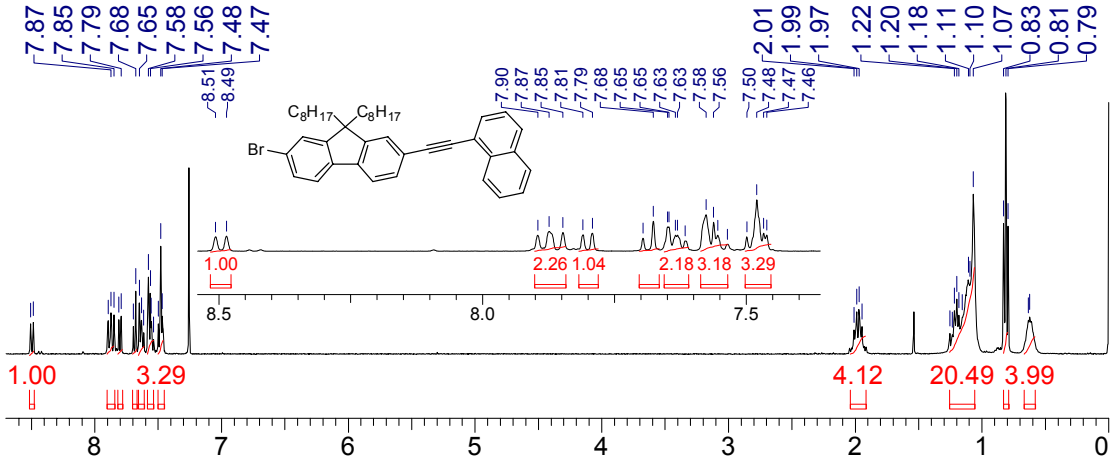


Fig. S13 ^{1}H NMR of compound **3b** (400 MHz, $CDCl_3$).

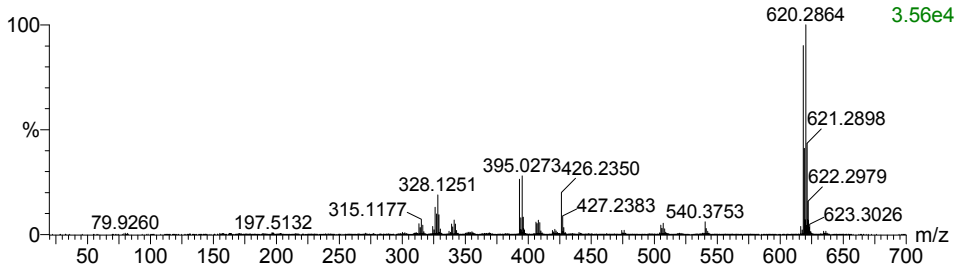


Fig. S14 ESI-HRMS compound **3b**.

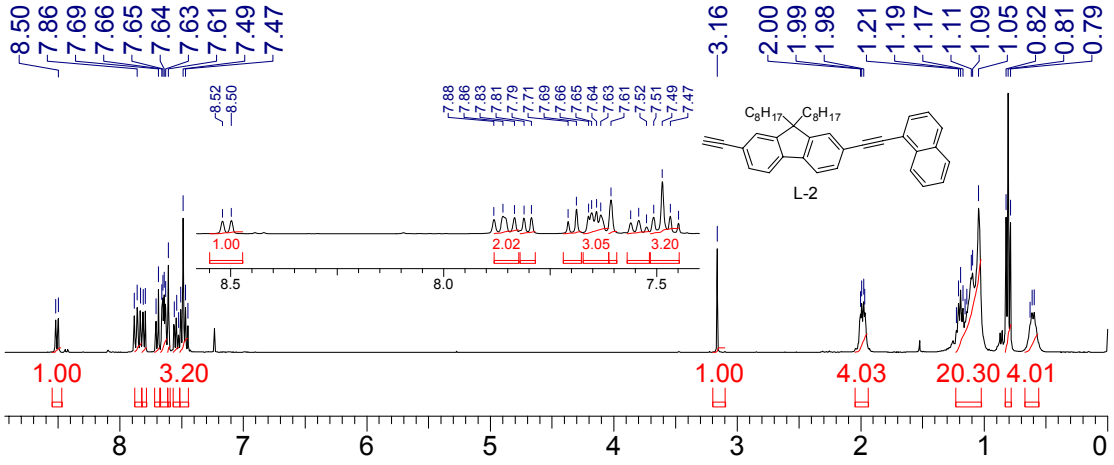


Fig. S15 ^{1}H NMR of compound **L-2** (400 MHz, $CDCl_3$).

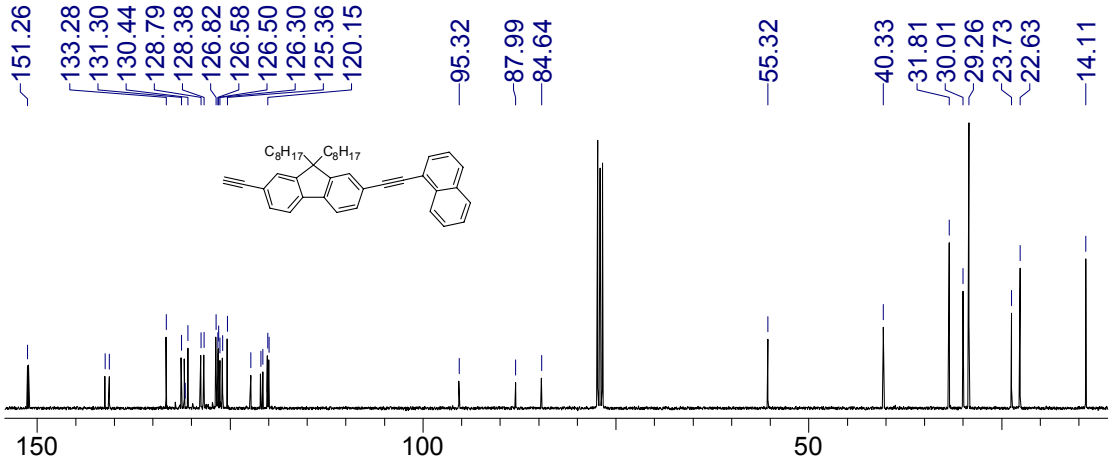


Fig. S16 ^{13}C NMR of compound **L-2** (100 MHz, $CDCl_3$).

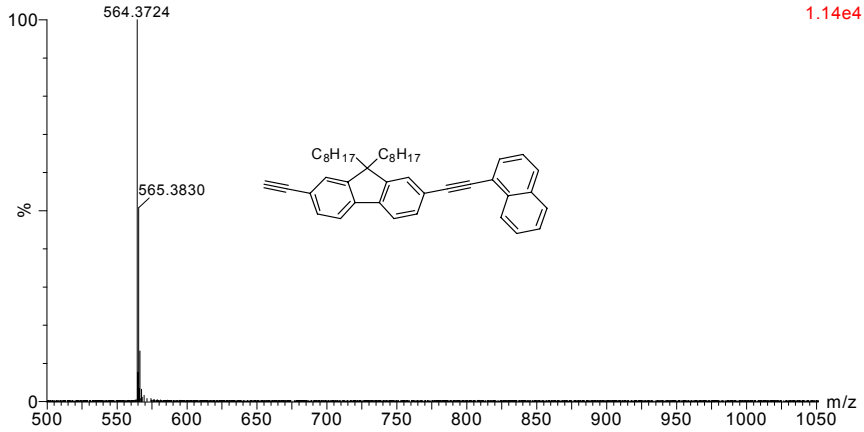


Fig. S17 HR-MALDI-MS of **L-2**.

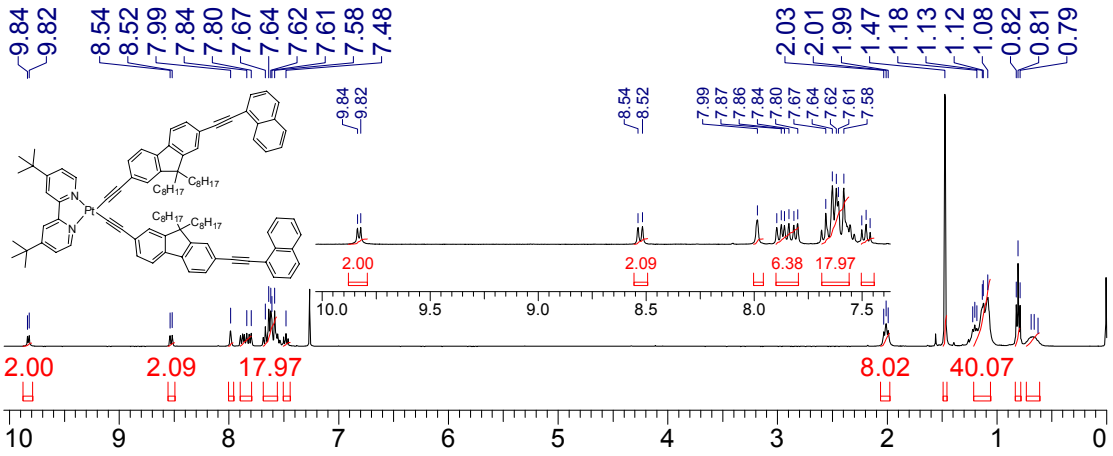


Fig. S18 ^{1}H NMR of compound **Pt-2** (400 MHz, $CDCl_3$).

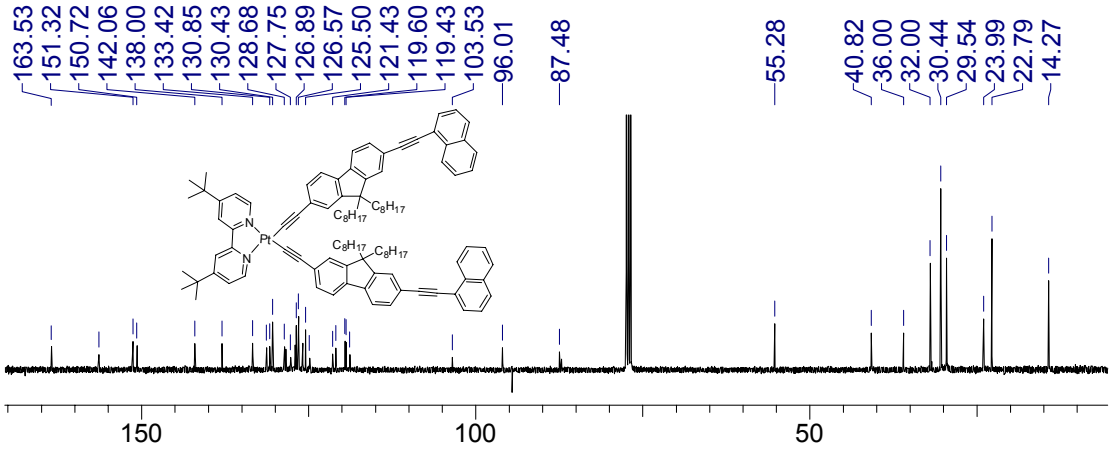


Fig. S19 ^{13}C NMR of compound **Pt-2** (100 MHz, $CDCl_3$).

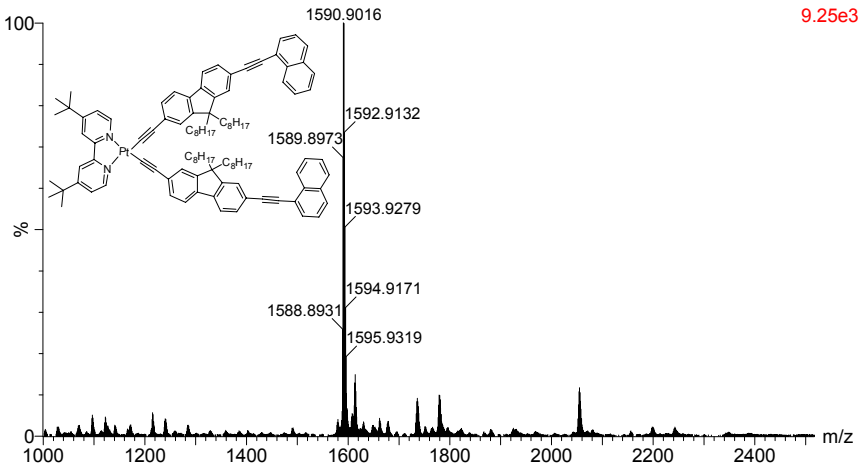


Fig. S20 HR-MALDI-MS of **Pt-2**.

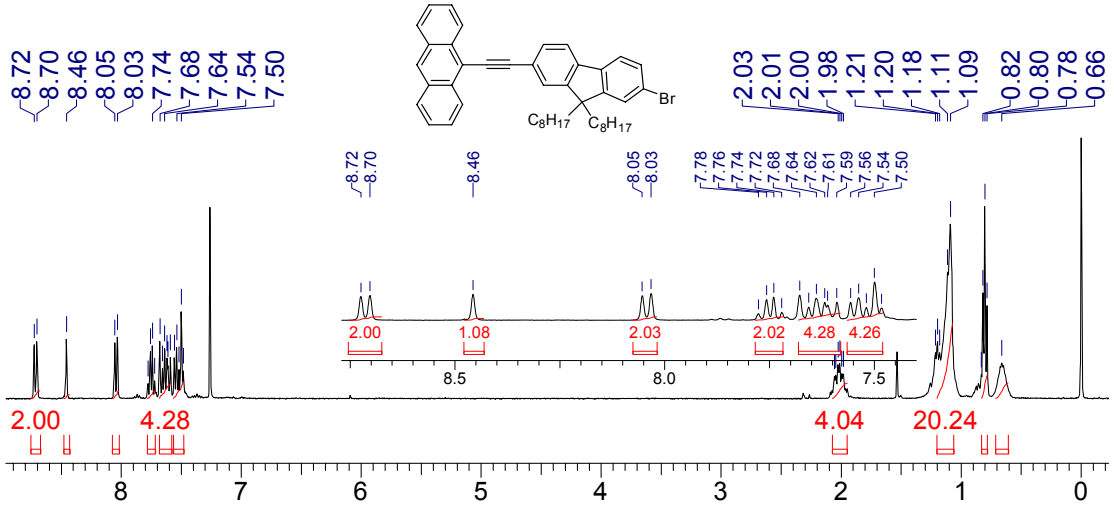


Fig. S21 ^{1}H NMR of compound **3c** (400 MHz, $CDCl_3$).

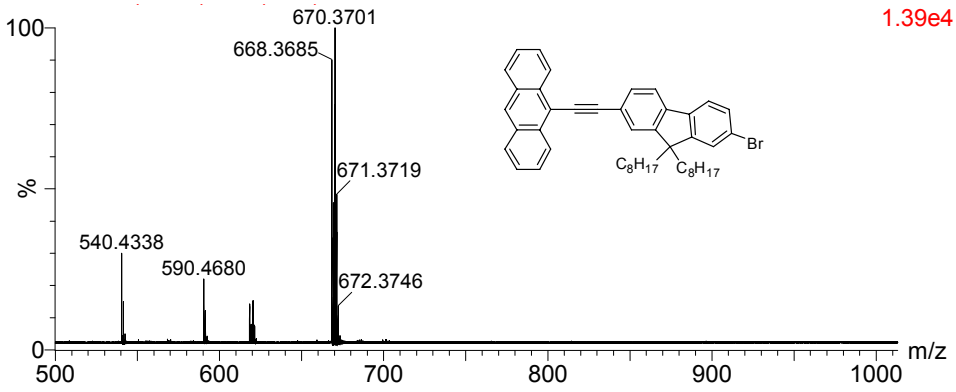


Fig. S22 MALDI-MS compound **3c**.

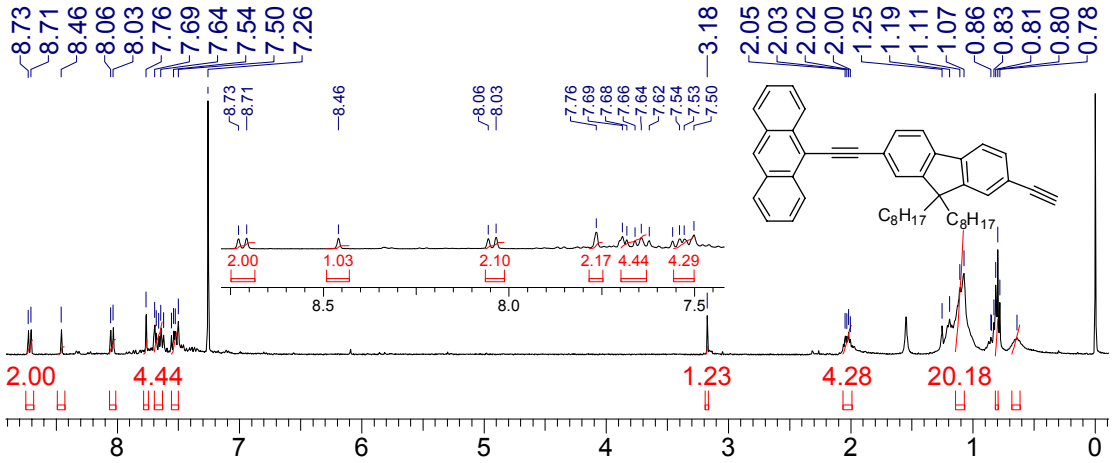


Fig. S23 ^{1}H NMR of compound **L-3** (400 MHz, $CDCl_3$).

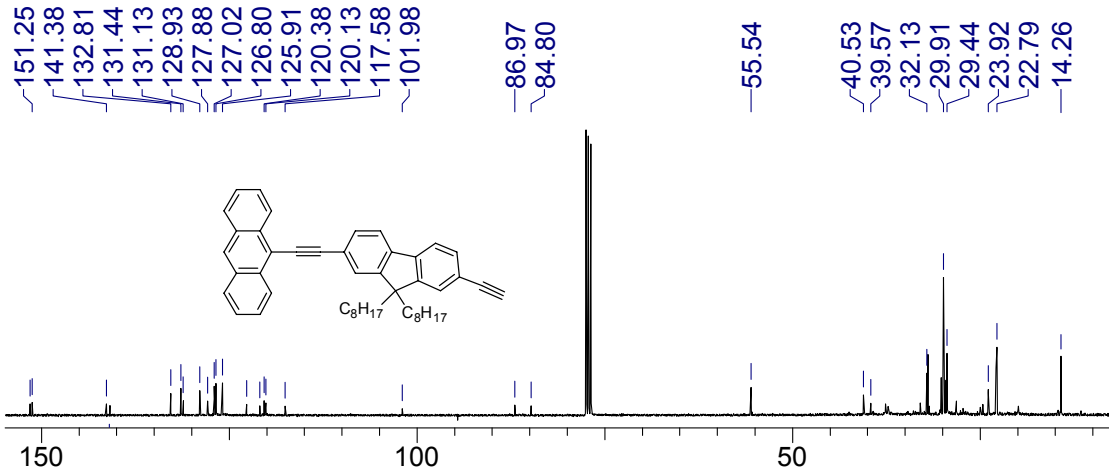


Fig. S24 ^{13}C NMR of compound **L-3** (100 MHz, $CDCl_3$).

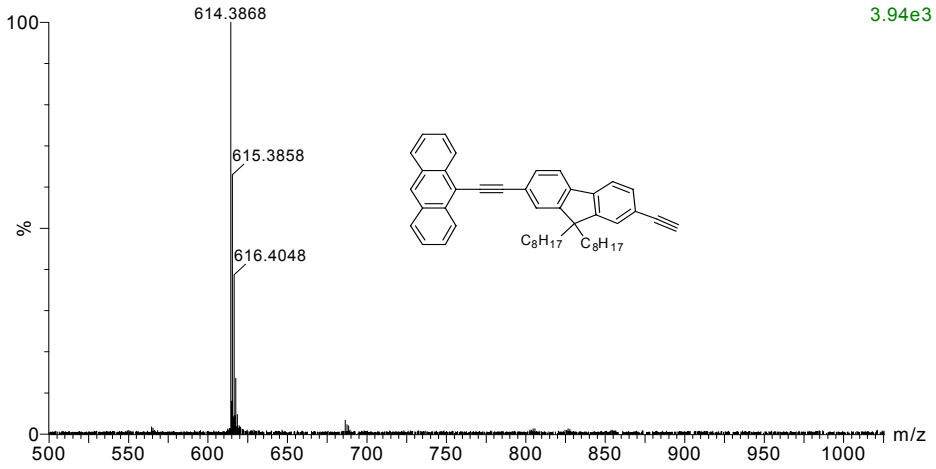


Fig. S25 HR-MALDI-MS of **L-3**.

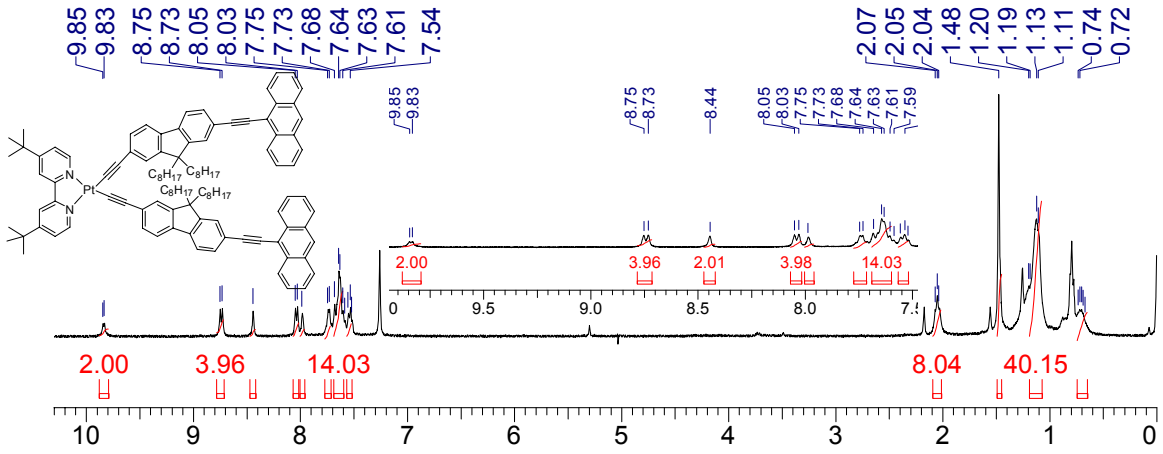


Fig. S26 ^{1}H NMR of compound **Pt-3** (400 MHz, $CDCl_3$).

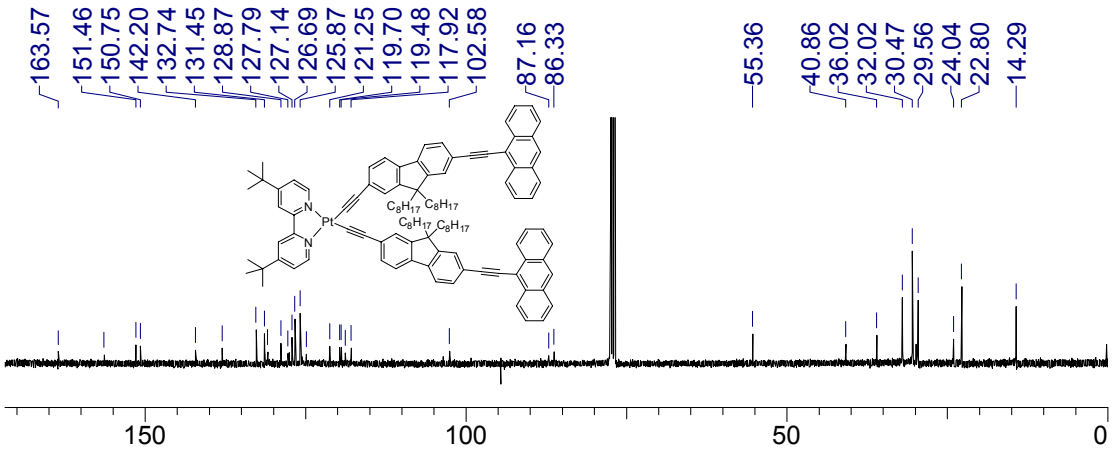


Fig. S27 ^{13}C NMR of compound **Pt-3** (100 MHz, $CDCl_3$).

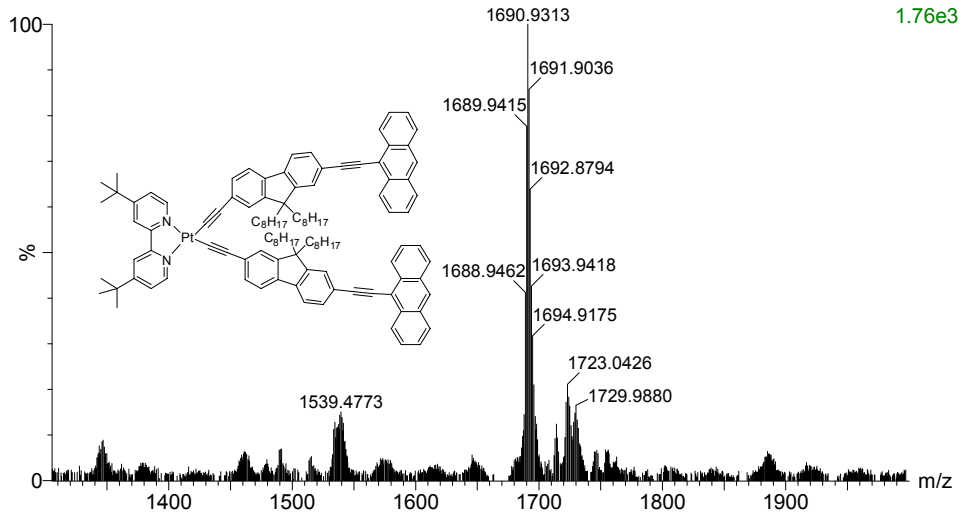


Fig. S28 HR-MALDI-MS of **Pt-3**.

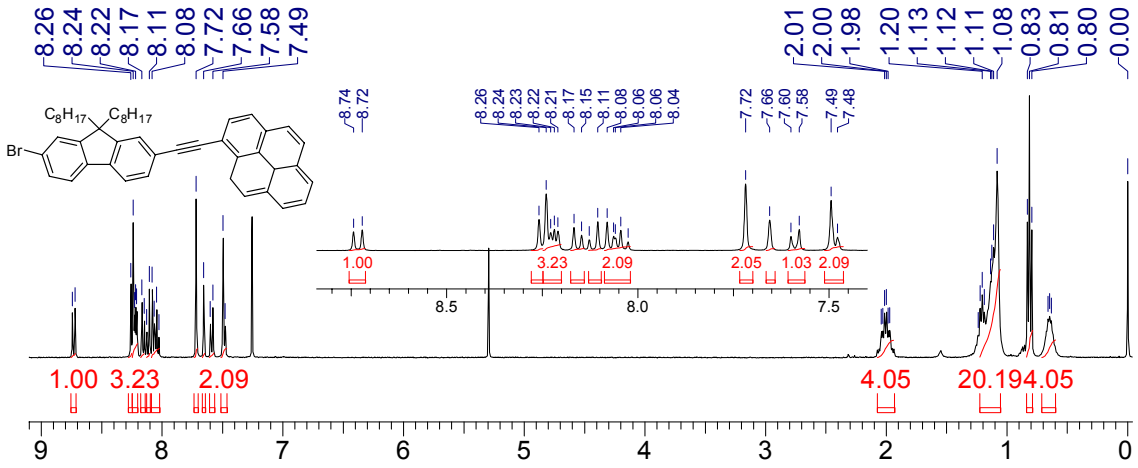


Fig. S29 ^{1}H NMR of compound **3d** (400 MHz, $CDCl_3$).

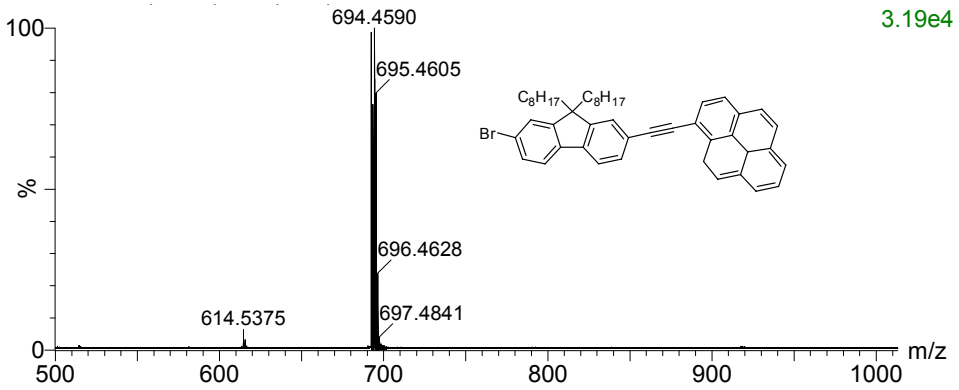


Fig. S30 MALDI-MS compound **3d**.

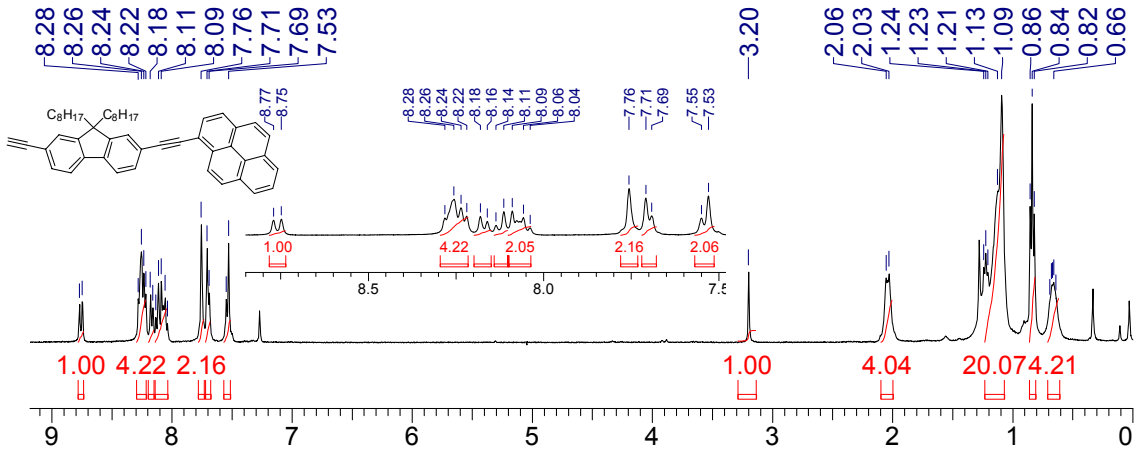


Fig. S31 ^{1}H NMR of compound **L-4** (400 MHz, $CDCl_3$).

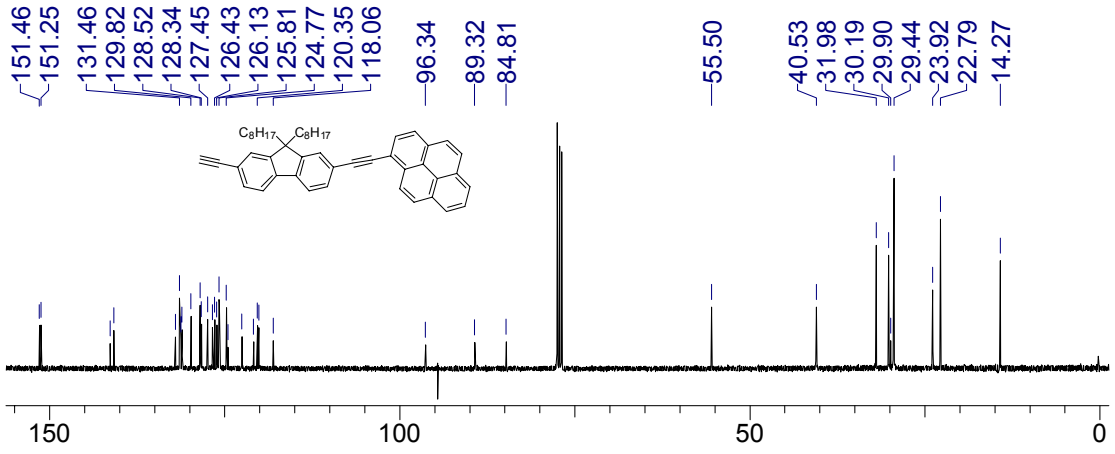


Fig. S32 ^{13}C NMR of compound **L-4** (100 MHz, $CDCl_3$).

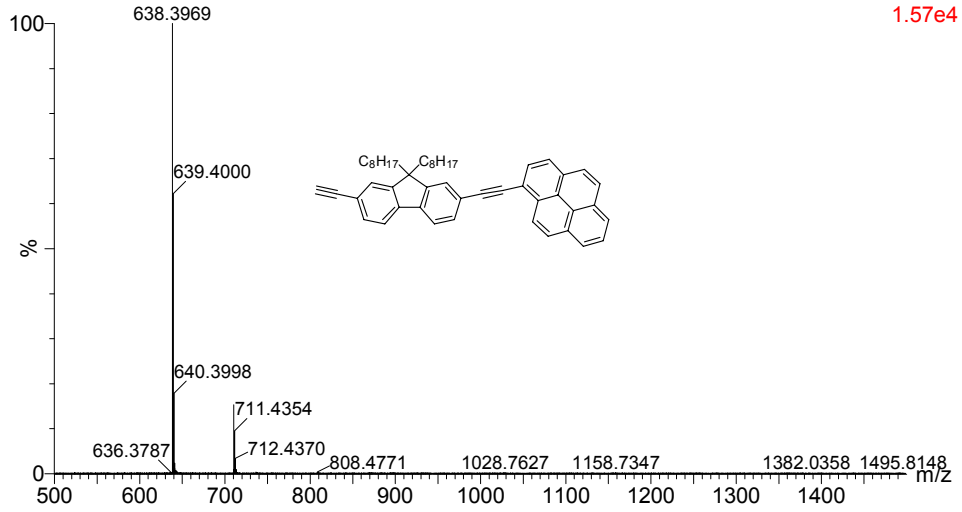


Fig. S33 HR-MALDI-MS of **L-4**.

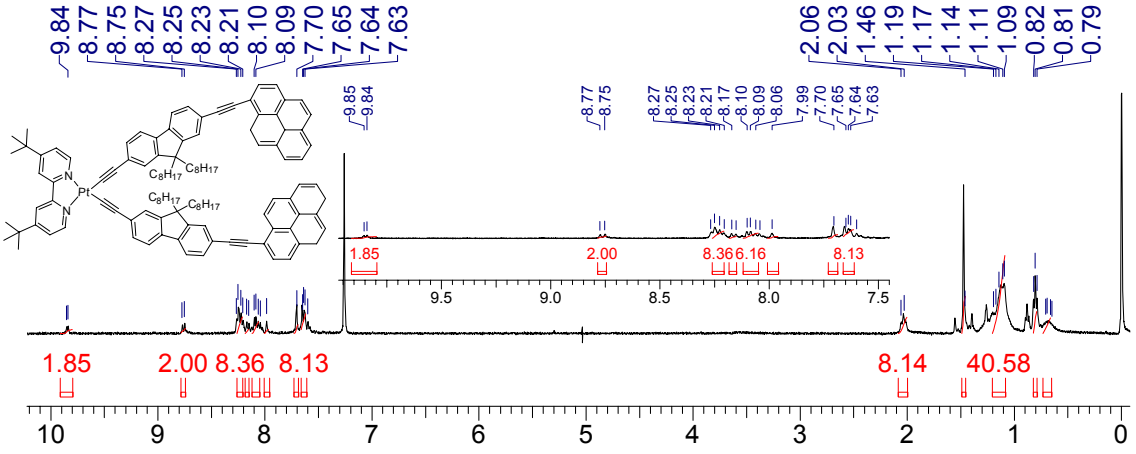


Fig. S34 ^{1}H NMR of compound **Pt-4** (400 MHz, $CDCl_3$).

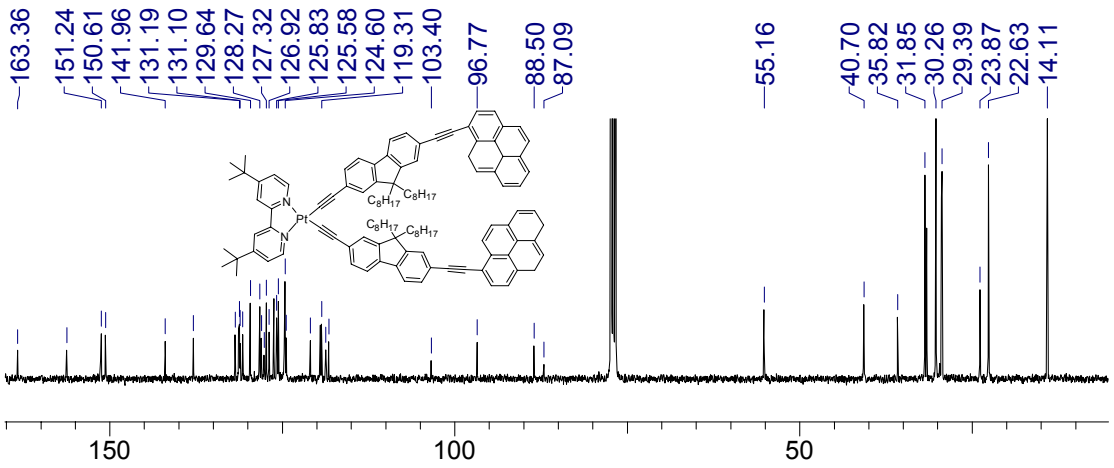


Fig. S35 ^{13}C NMR of compound **Pt-4** (100 MHz, $CDCl_3$).

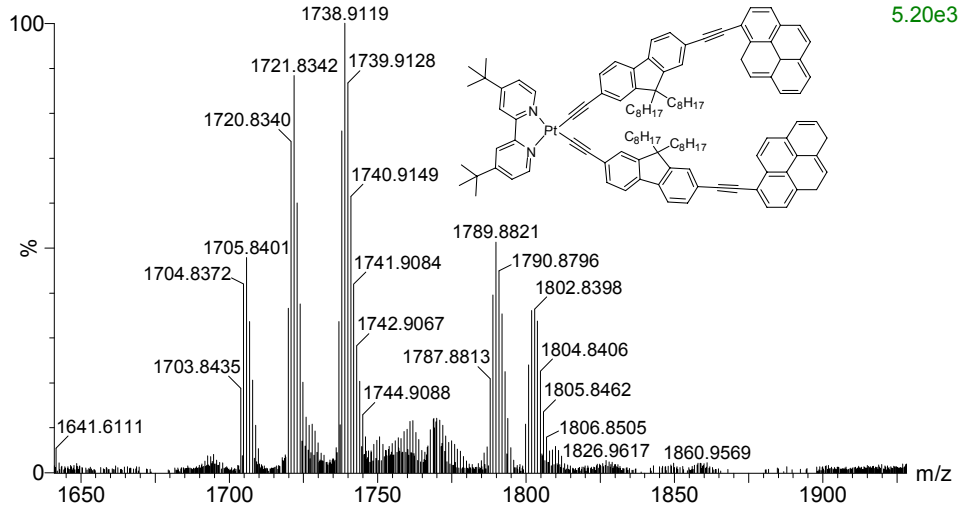


Fig. S36 HR-MALDI-MS of **Pt-4**.

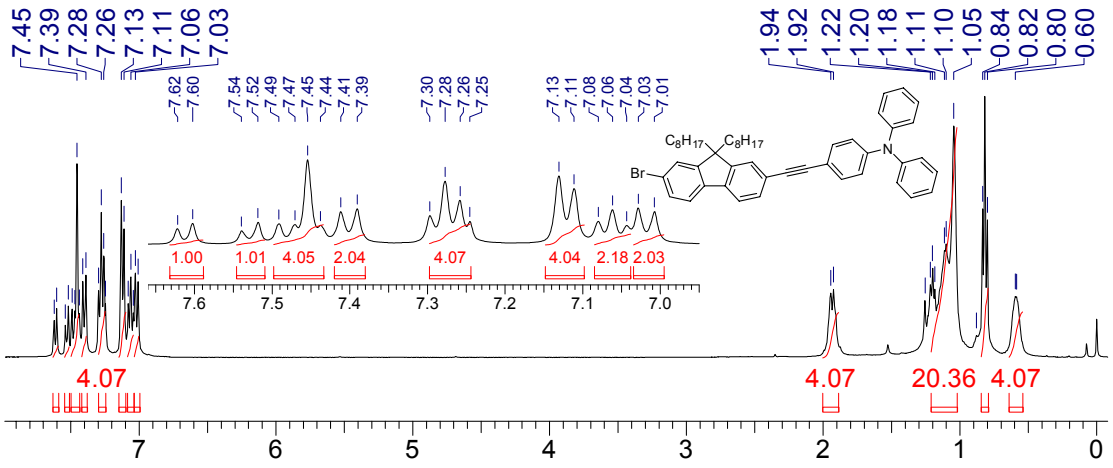


Fig. S37 ^{1}H NMR of compound **3e** (400 MHz, $CDCl_3$).

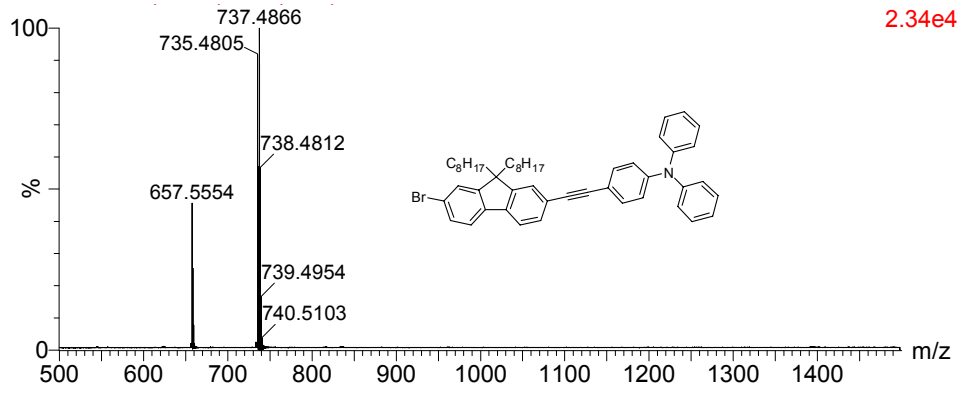


Fig. S38 MALDI-MS of **3e**.

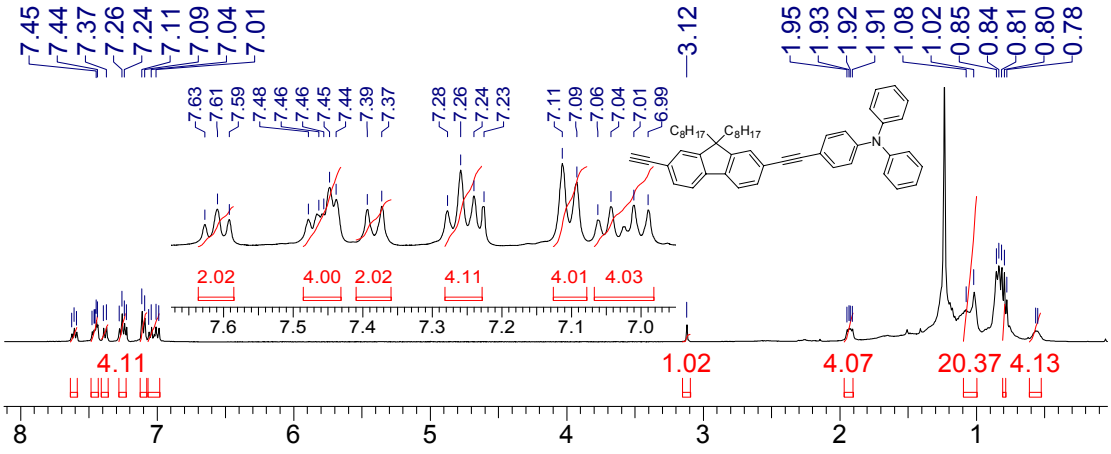


Fig. S39 ^{1}H NMR of compound **L-5** (400 MHz ,$CDCl_3$).

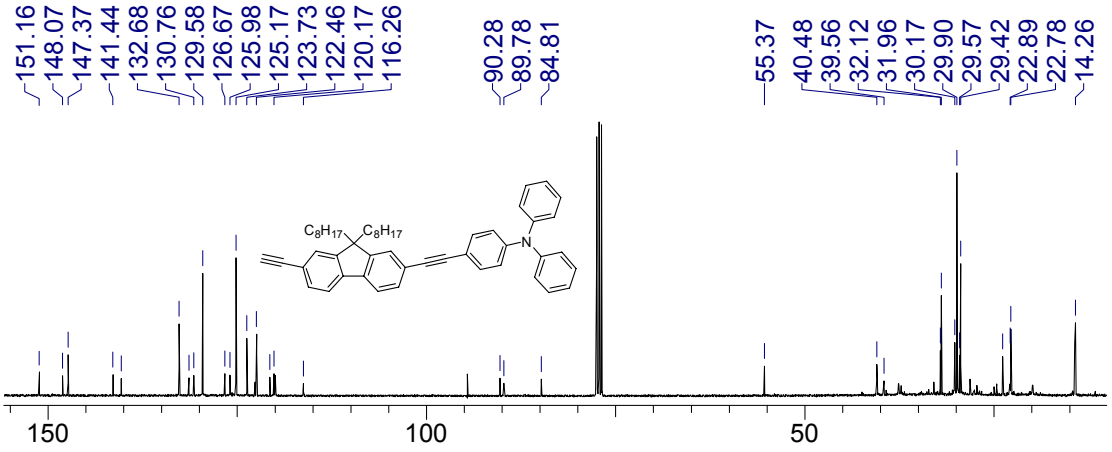


Fig. S40 ^{13}C NMR of compound **L-5** (100 MHz, $CDCl_3$).

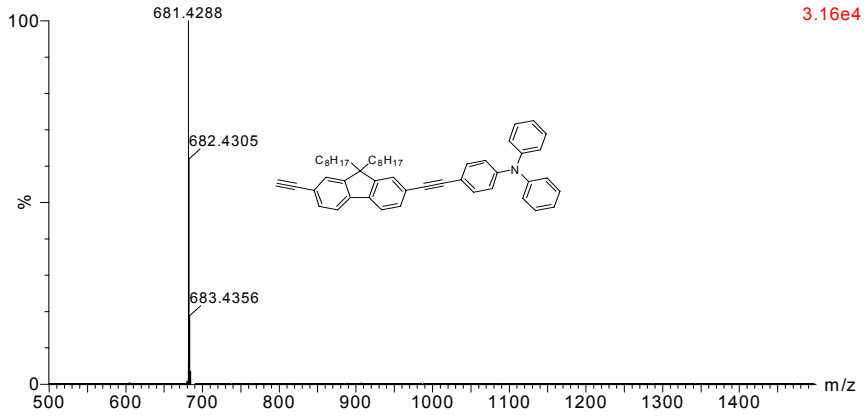


Fig. S41 HR-MALDI-MS of **L-5**.

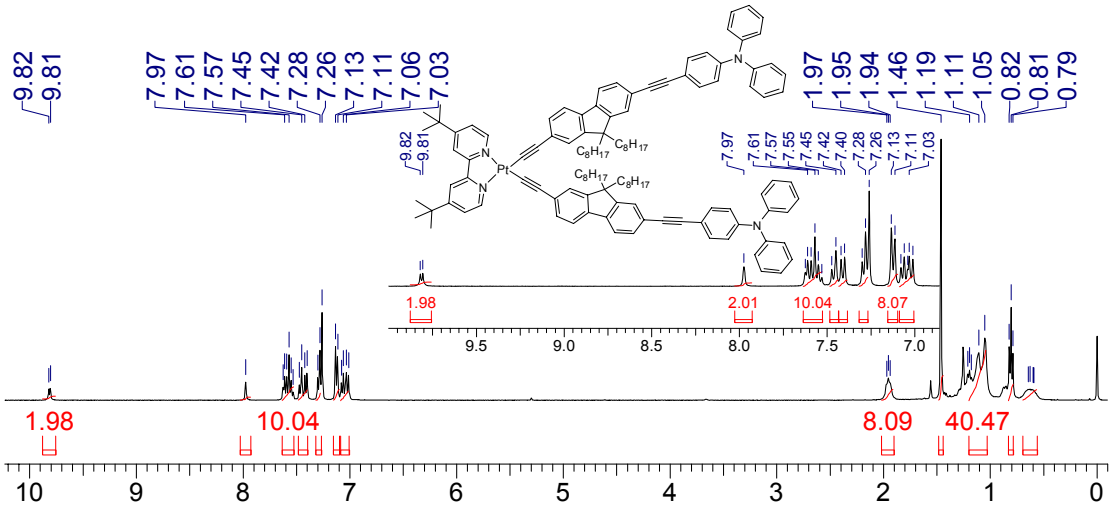


Fig. S42 ^{1}H NMR of compound **Pt-5** (400 MHz, $CDCl_3$).

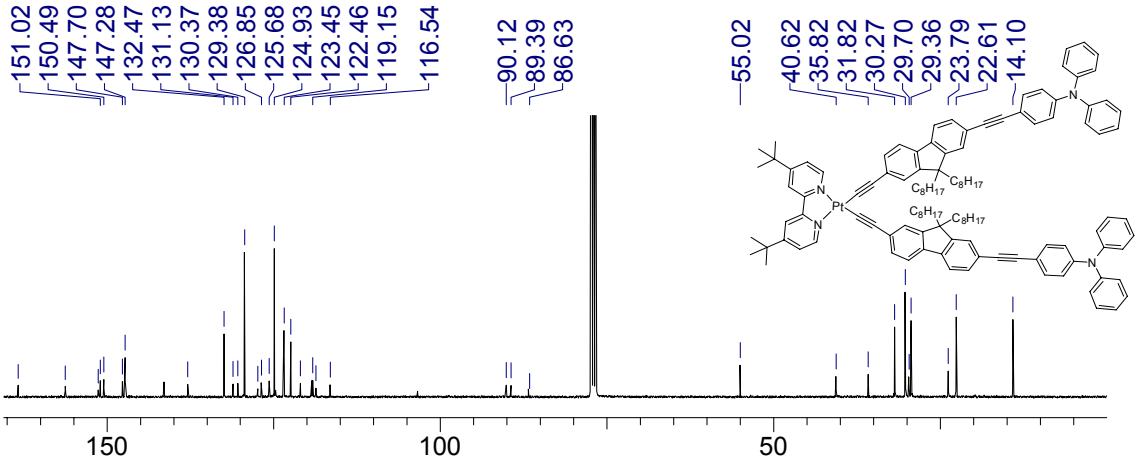


Fig. S43 ^{13}C NMR of compound **Pt-5** (100 MHz, $CDCl_3$).

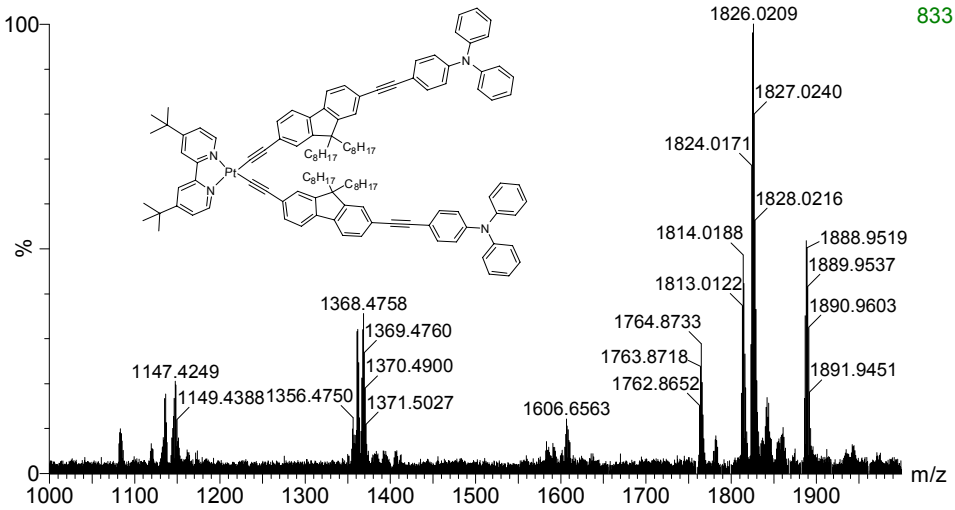


Fig. S44 HR-MALDI-MS of **Pt-5**.

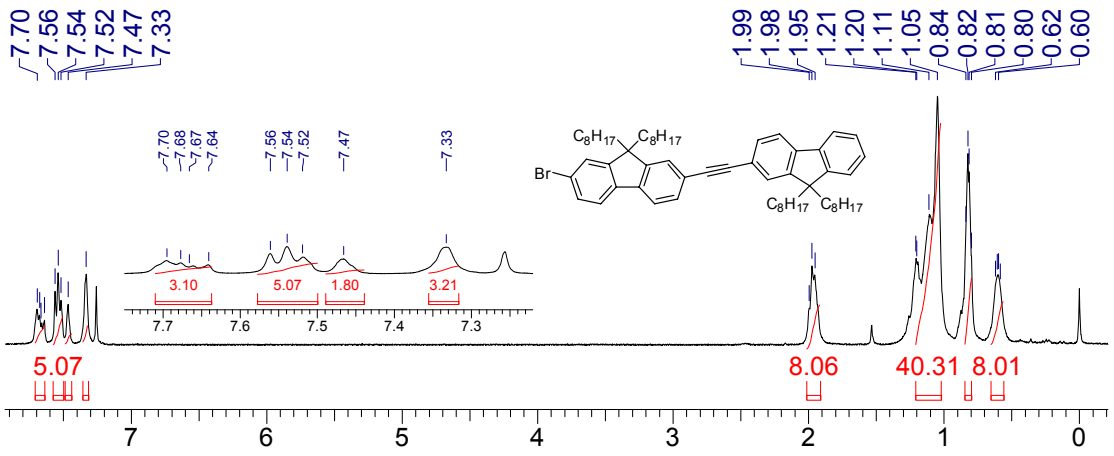


Fig. S45 ^{1}H NMR of compound **3f** (400 MHz, $CDCl_3$).

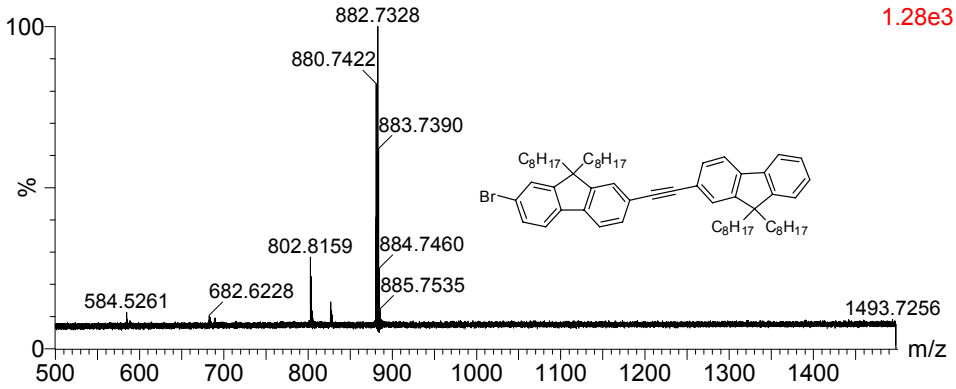


Fig. S46 MALDI-MS of **3f**.

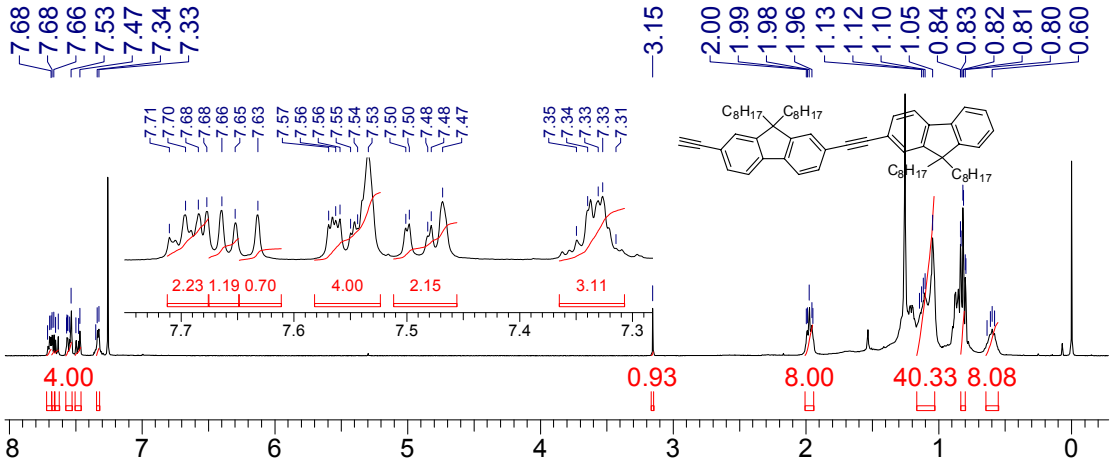


Fig. S47 ^{1}H NMR of compound **L-6** (400 MHz, $CDCl_3$).

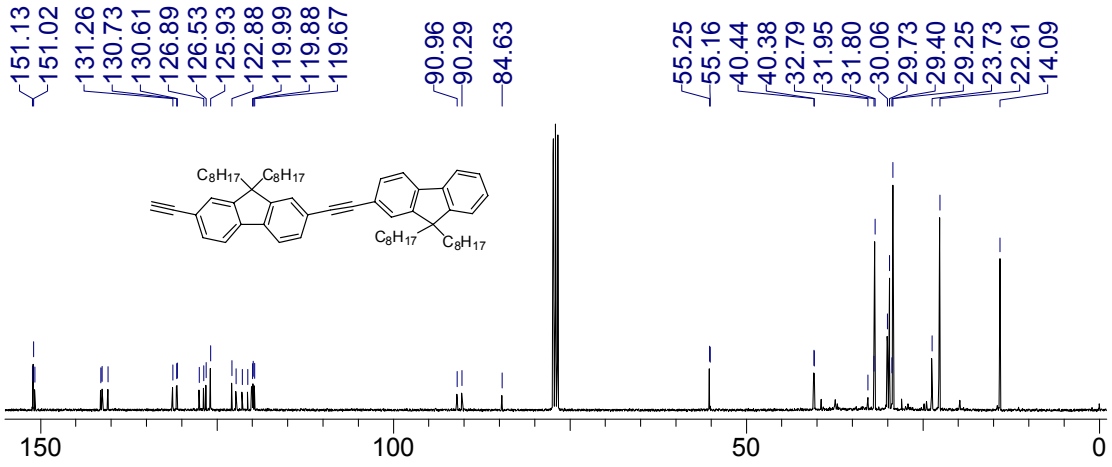


Fig. S48 ^{13}C NMR of compound **L-6** (100 MHz, $CDCl_3$).

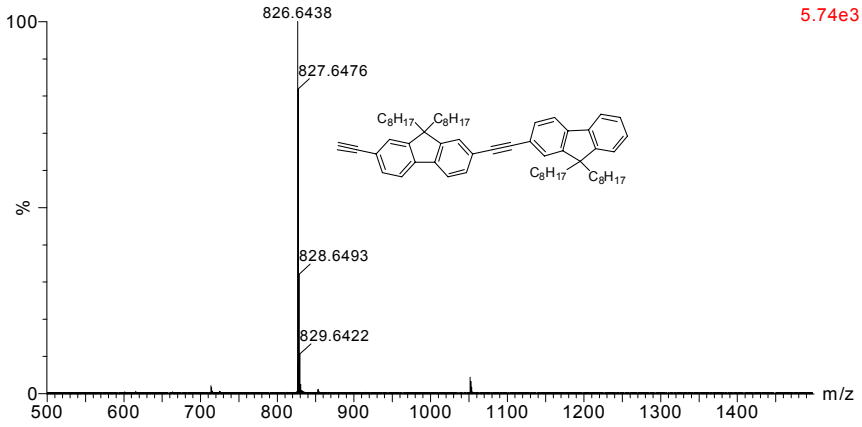


Fig. S49 HR-MALDI-MS of **L-6**.

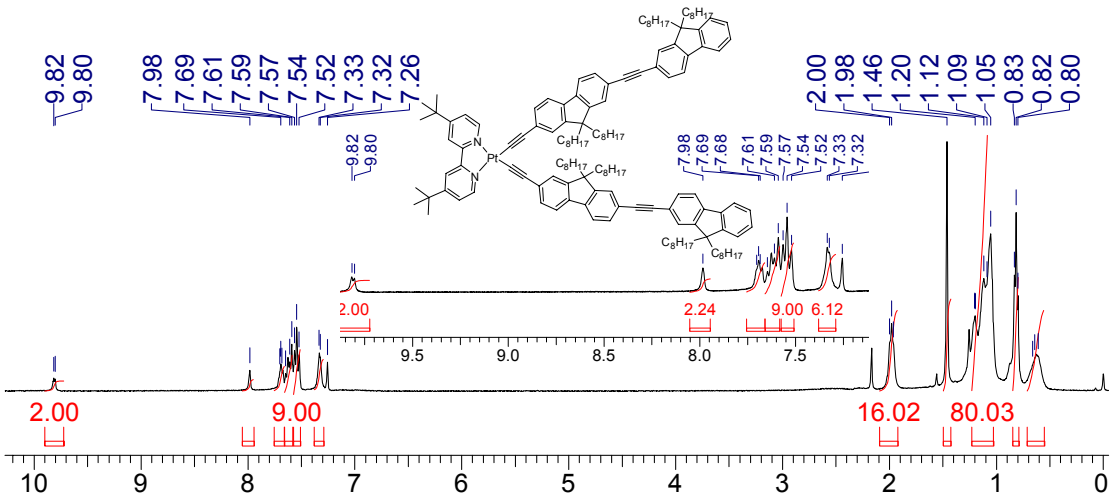


Fig. S50 ^{1}H NMR of compound **Pt-6** (400 MHz, $CDCl_3$).

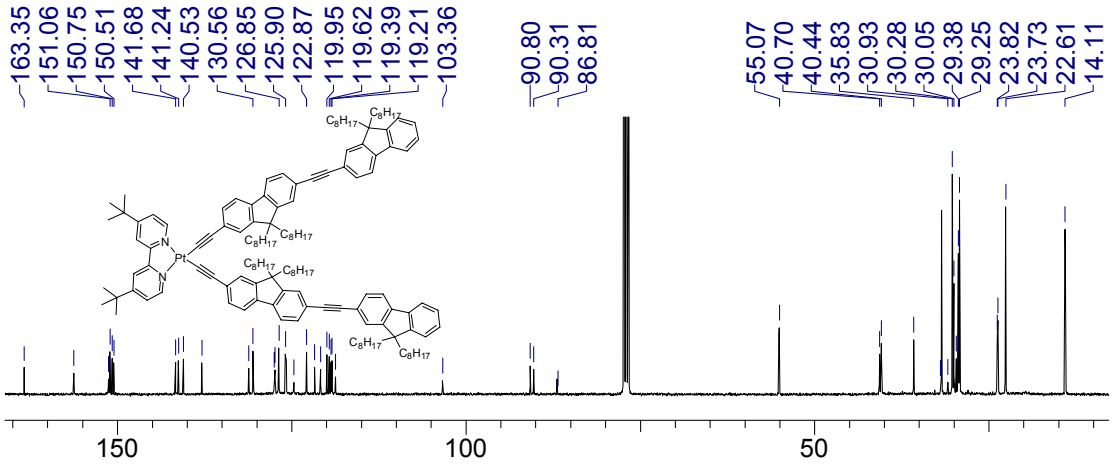


Fig. S51 ^{13}C NMR of compound **Pt-6** (100 MHz, $CDCl_3$).

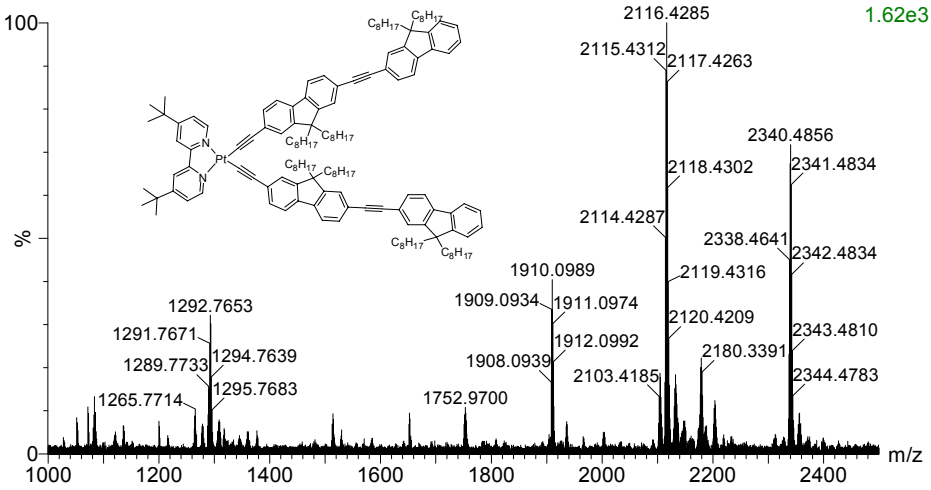


Fig. S52 HR-MALDI-MS of **Pt-6**.

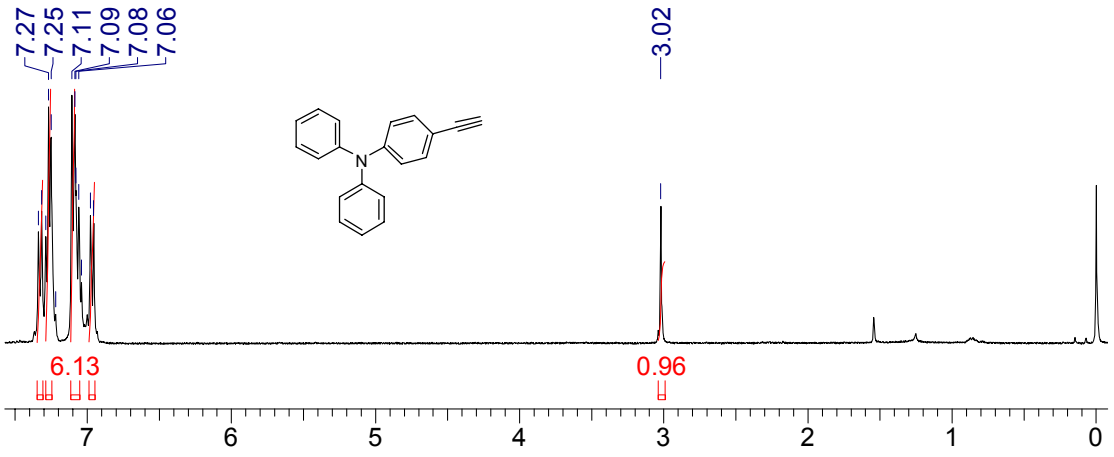


Fig. S53 ^{1}H NMR of compound **R-5** (400 MHz, $CDCl_3$).

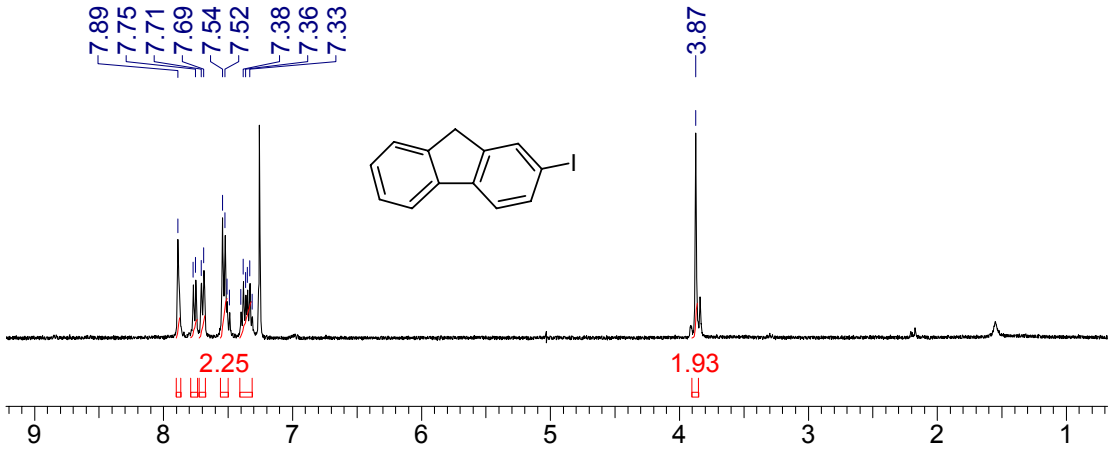


Fig. S54 ^{1}H NMR of compound **5** (400 MHz, $CDCl_3$).

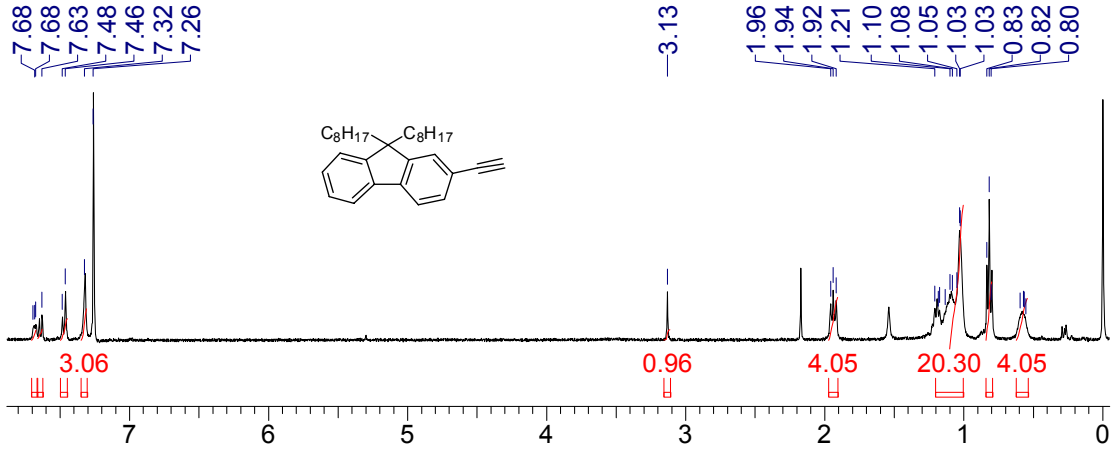


Fig. S55 ^{1}H NMR of compound **R-6** (400 MHz, $CDCl_3$).

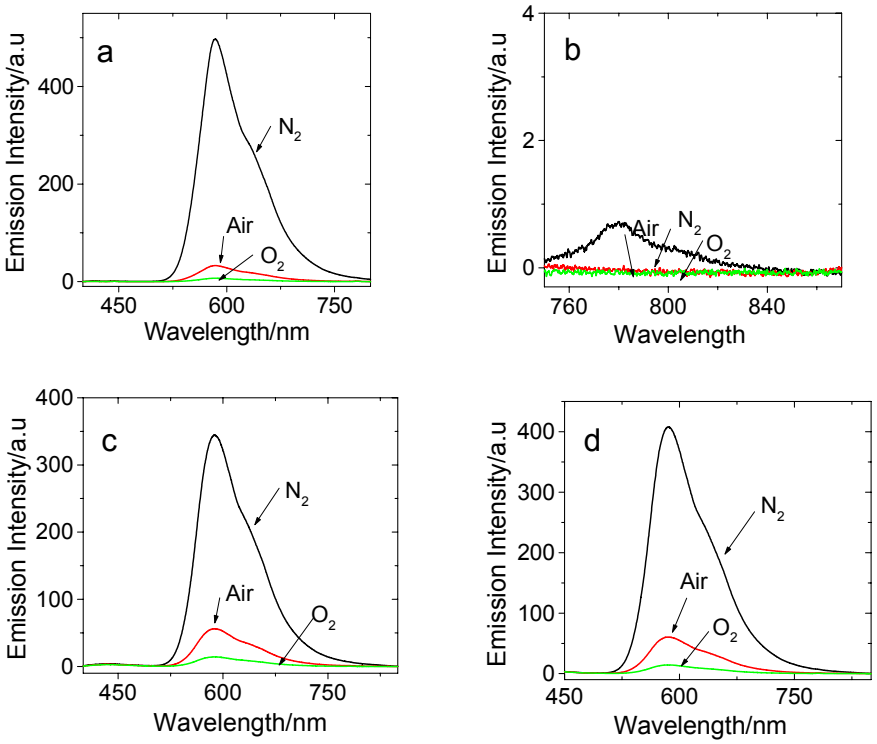


Fig. S56 Emission spectra of (a) **Pt-2** (λ_{ex} = 390 nm), (b) **Pt-3** (λ_{ex} = 445 nm), (c) **Pt-5** (λ_{ex} = 390 nm) and (d) **Pt-6** (λ_{ex} = 390 nm) (c = 1.0×10^{-5} M) under different atmosphere in toluene at 298 K.

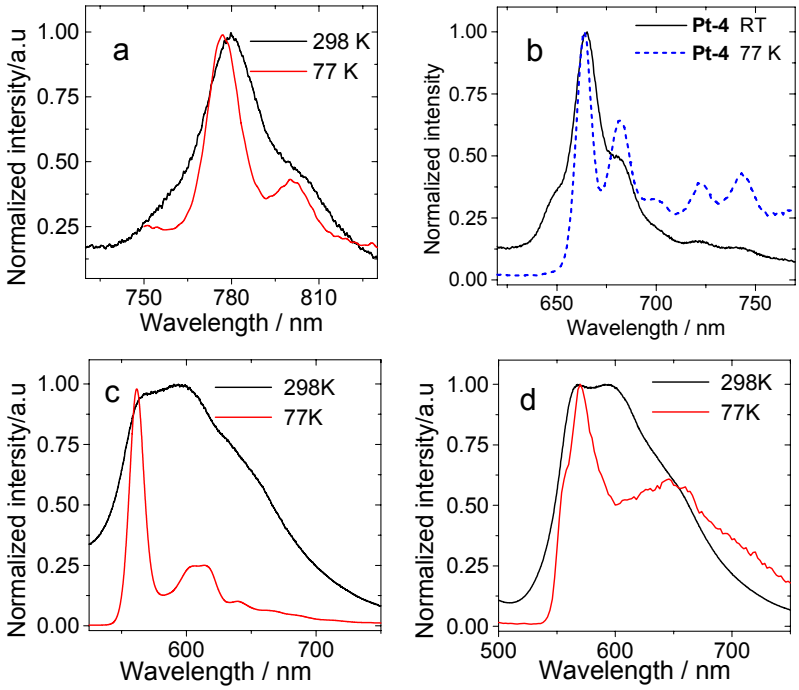


Fig. S57 The normalization of emission emission spectra of (a) **Pt-3** (λex = 445 nm; (b) **Pt–4**, λ_{ex} = 420 nm; (c) **Pt-5** (λex = 390 nm) and (d) **Pt-6** (λ_{ex} = 390 nm) in EtOH : MeOH = 4:1 v/v at 298 K and 77 K.

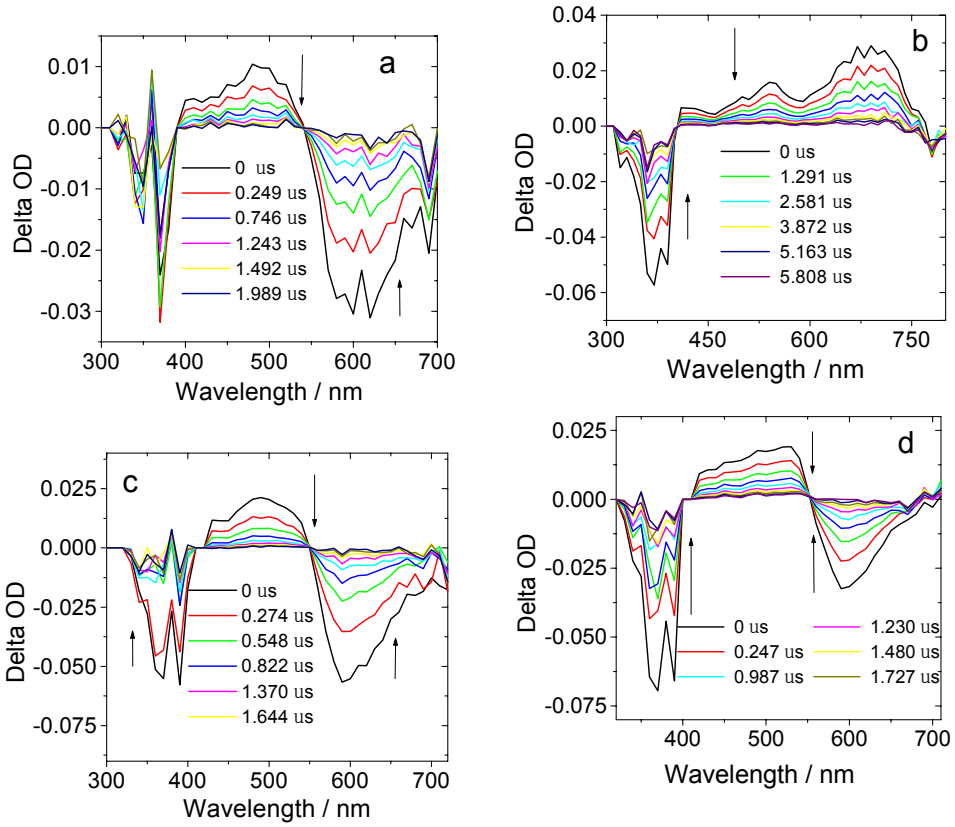


Fig. S58 Nanosecond transient absorption difference spectra of (a) **Pt-1**, (b) **Pt-2**, (c) **Pt-5** and (d) **Pt-6** ($c = 1.0\times10^{-5}$ M) intoluene measured as a function of the delay times indicated following 355 nm pulsed-laser excitation at 25°C.

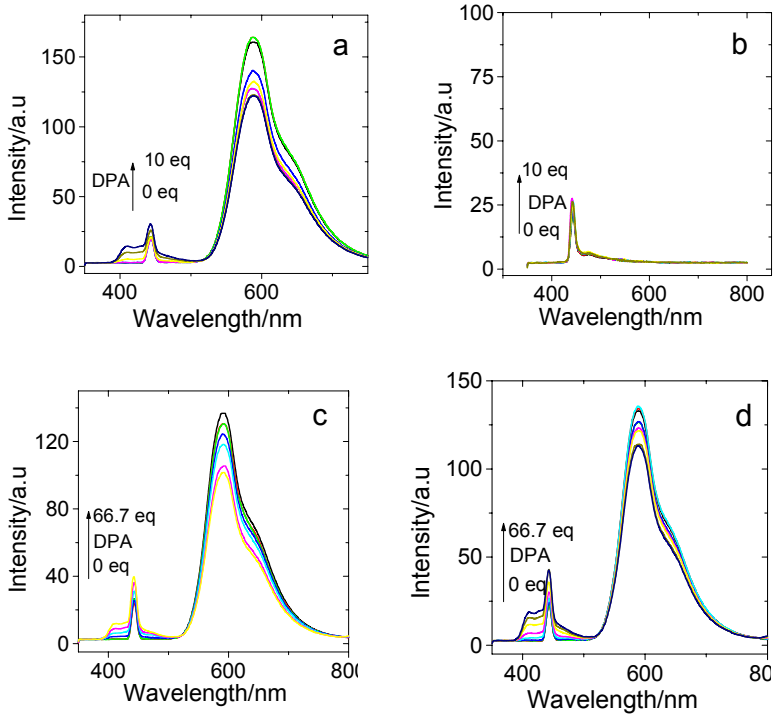


Fig. S59 The difference upconversion spectra of (a) **Pt-1**, (b) **Pt-3**, (c) **Pt-5** and (d) **Pt-6** ($c = 1.0 \times 10^{-5}$ M) with added diffent DPA with 445 nm laser excitation in toluenen at 25°C.

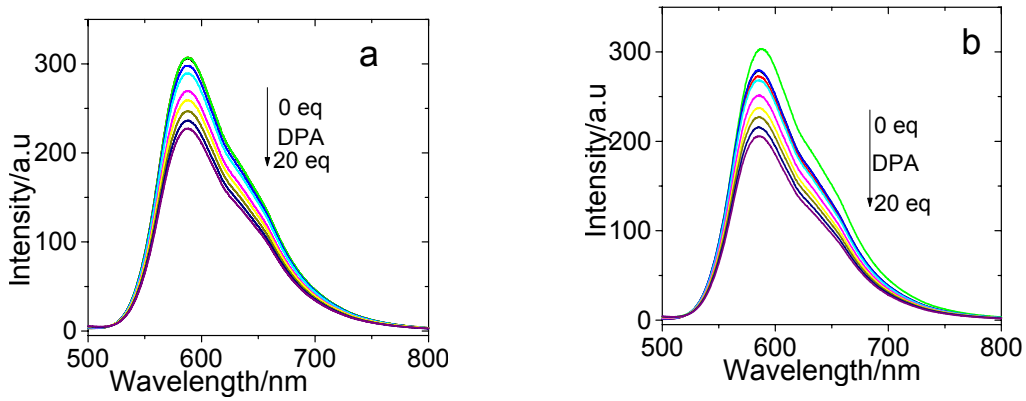


Fig. S60 Phosphorescence emission spectra of complex (a) **Pt-5** (λex = 390 nm) and (b) **Pt-6** (λex = 390 nm) with increasing DPA concentration in toluene (c =1.0 × 10^{-5} M).

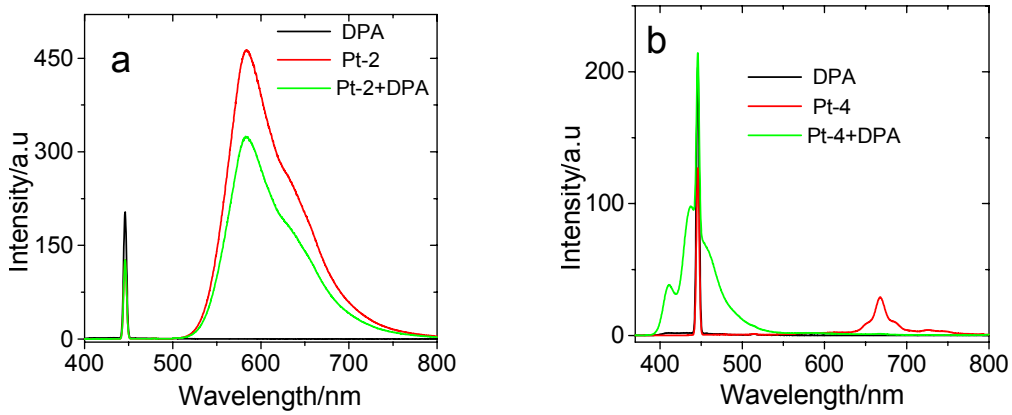


Fig. S61 Upconverted of (a) **Pt-2** and (b) **Pt-4** (1.0 × 10^{-5}M) and residual phosphorescence of mixtures of **DPA** (4.3 × 10^{-5}M) use fluorescence Instruments 445 nm in toluene at 298 K. Note the upconversions were carried out with the spectrofluorometer as the excitation source.

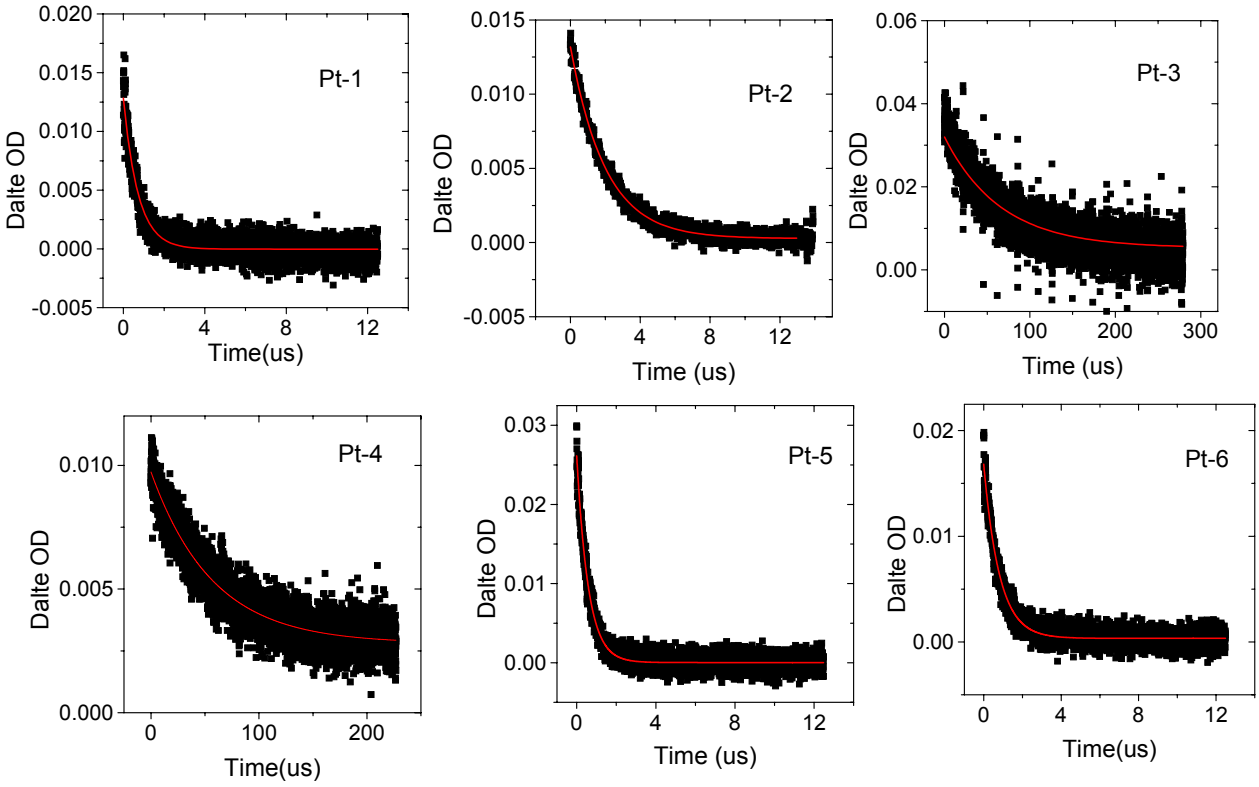


Fig. S62 The triplet lifetime of **Pt-1** (λex = 450 nm), **Pt-2** (λex = 500 nm), **Pt-3** (λex = 600 nm), **Pt-4** (λex = 600 nm), **Pt-5** (λex = 450 nm) and **Pt-6** (λex = 450 nm) in toluene measured as a function of the delay times indicated following 355 nm pulsed-laser excitation at 25°C.

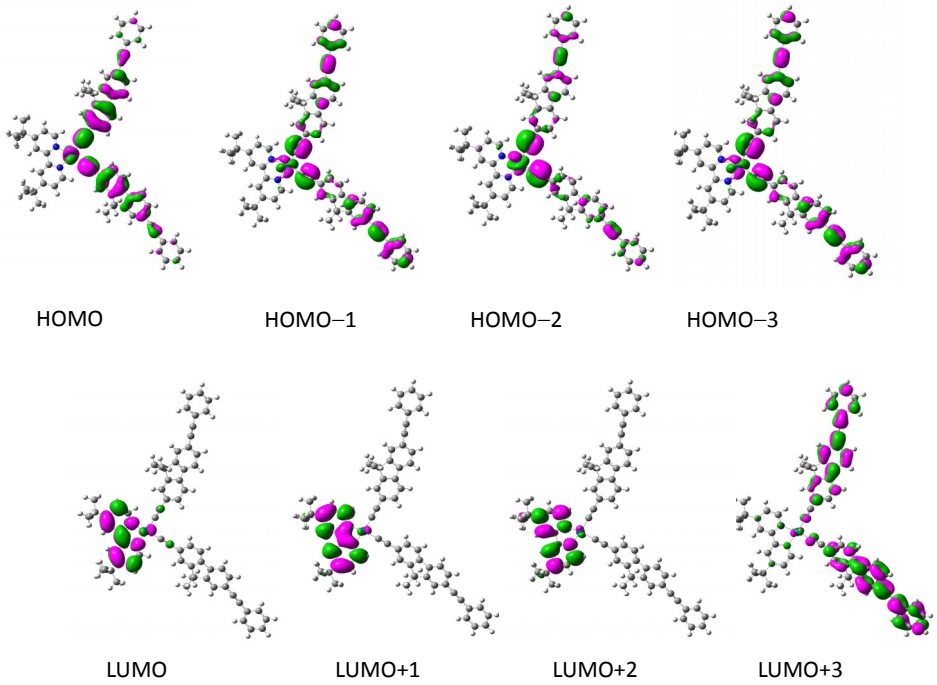


Fig. S63 Selected frontier molecular orbitals of **Pt-1** without solvent. Calculated by DFT at the B3LYP/6-31G((d)/LanL2DZ level. The alkyl groups were simplified in the calculation to reduce computation time. Calculated with Gaussian 09W.

Table S1. Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-1** without solvent, calculated byTDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6−31G(d)				
		Energy [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.69 eV 732 nm	0.1029	HOMO→LUMO	0.6965	LLCT/MLCT
	$S_0 \rightarrow S_9$	2.86 eV 433 nm	0.3252	HOMO−4→LUMO	0.2666	MLCT/LLCT
				HOMO−1→LUMO+1	0.4425	LLCT/MLCT
				HOMO→LUMO+2	0.4654	LLCT/MLCT
	$S_0 \rightarrow S_{12}$	3.140 eV 394 nm	1.4659	HOMO−1→LUMO+4	0.1420	ILCT/MLCT
				HOMO→LUMO+3	0.6802	ILCT
	$S_0 \rightarrow S_{15}$	3.39eV 366 nm	0.6048	HOMO−2→LUMO+2	0.1267	ILCT/MLCT
				HOMO−1→LUMO+3	0.5568	ILCT/MLCT
				HOMO−1→LUMO+4	0.3683	MLCT
Triplet	$S_0 \rightarrow T_1$	1.60eV 775 nm	0.0000[e]	HOMO→LUMO	0.6861	LLCT/MLCT
	$S_0 \rightarrow T_3$	2.28ev 542nm	0.0000[e]	HOMO−3→LUMO	0.3376	MLCT/LLCT
				HOMO−2→LUMO	0.6025	MLCT/LLCT

a Only the selected low−lying excited states are presented. b Oscillator strength. c Only the main configurations are presented. d The CI coefficients are in absolute values. e No spin−orbital coupling effect was considered, thus the f values are zero.

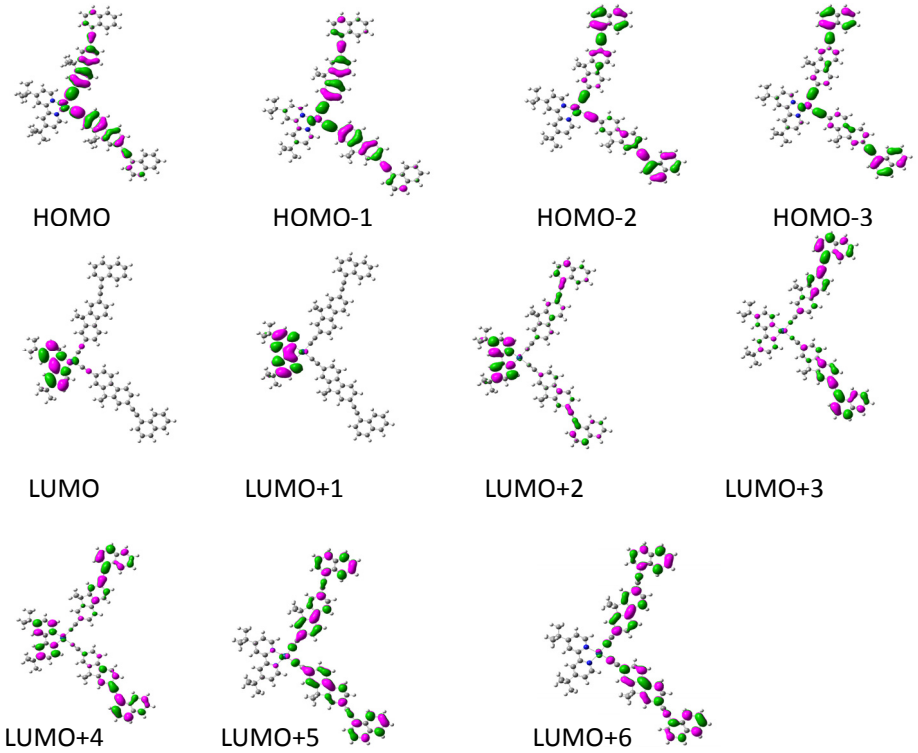


Fig. S64 Selected frontier molecular orbitals of complex **Pt-2** without solvent, calculated by DFT at the B3LYP/6-31G((d)/LanL2DZ level. The octyl group was simplified as methy in the calculation to reduce computation time. Calculated with Gaussian 09W.

Table S2 Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-2** without solvent, calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy [a]	*f* [b]	Compositi[c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.69 eV 733 nm	0.1381	HOMO-2→LUMO	0.1096	ILCT LLCT MLCT
				HOMO→LUMO	0.6946	ILCT MLCT
	$S_0 \rightarrow S_{10}$	2.92 eV 424 nm	1.6158	HOMO−1→LUMO+2	0.4228	ILCT LLCT MLCT
				HOMO→LUMO+3	0.5442	LLCT MLCT
	$S_0 \rightarrow S_{15}$	3.18 eV 389 nm	0.3752	HOMO−1→LUMO+2	0.2379	LLCT MLCT
				HOMO−1→LUMO+4	0.6361	ILCT LLCT MLCT
				HOMO→LUMO+3	0.1654	ILCT LLCT MLCT
	$S_0 \rightarrow S_{24}$	3.65 eV 339nm	0.6458	HOMO−3→LUMO+2	0.3477	LLCT MLCT
				HOMO−3→LUMO+4	0.1371	LLCT MLCT
				HOMO-2→LUMO+3	0.2830	LLCT MLCT
				HOMO-1→LUMO+6	0.1253	ILCT LLCT MLCT
				HOMO →LUMO+5	0.4967	ILCT MLCT
Triplet	$S_0 \rightarrow T_1$	1.59eV 780 nm	0.000[e]	HOMO-2→LUMO	0.1348	LLCT MLCT
				HOMO→LUMO	0.6830	ILCT LLCT MLCT
	$S_0 \rightarrow T_3$	2.17 eV 571nm	0.000[e]	HOMO-3→LUMO+2	0.1209	ILCT LLCT MLCT
				HOMO-3→LUMO+4	0.2025	ILCT MLCT
				HOMO-2→LUMO+3	0.2564	ILCT MLCT
				HOMO-1→LUMO+2	0.2224	LLCT MLCT
				HOMO-1→LUMO+4	0.2984	ILCT MLCT
				HOMO→LUMO+1	0.1582	LLCT MLCT
				HOMO→LUMO+3	0.3774	ILCT MLCT

a :Only the selected low-lying excited states are presented. b: Oscillator strength. c :Only the mainconfigurations are presented. d: The CI coefficients are in absolute values. e:No spin-orbital coupling effect wasconsidered, thus the f values are zero.

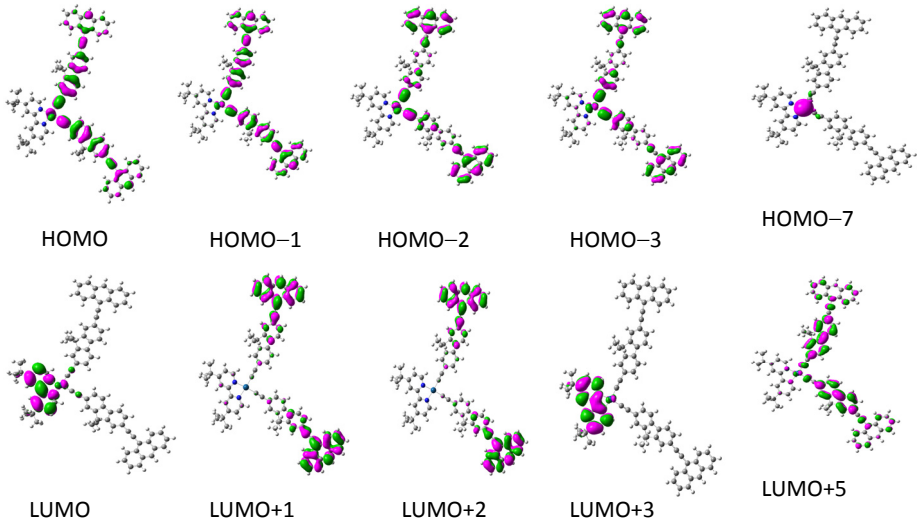


Fig. S65 Selected frontier molecular orbitals of **Pt−3** without solvent calculated by DFT at the B3LYP/6−31G((d)/LanL2DZ level. The alkyl groups were simplified in the calculation to reduce computation time. Calculated with Gaussian 09W.

Table S3. Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-3** without solvent, calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6—31G(d)					
		Energy [a]		*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.67 eV	740 nm	0.1406	HOMO−2→LUMO	0.1843	ILCT MLCT LLCT
					HOMO→LUMO	0.6780	ILCT MLCT LLCT
	$S_0 \rightarrow S_6$	2.52 eV	490 nm	1.1400	HOMO−1→LUMO+2	0.2086	ILCT MLCT
					HOMO→LUMO+1	0.6190	ILCT MLCT
					HOMO→LUMO+3	0.2415	ILCT LLCT MLCT
	$S_0 \rightarrow S_{11}$	2.72 eV	456 nm	0.2500	HOMO−7→LUMO	0.1116	MLCT
					HOMO−1→LUMO+2	0.6407	ILCT MLCT
					HOMO→LUMO+1	0.2516	ILCT MLCT
	$S_0 \rightarrow S_{16}$	3.06 eV	405 nm	0.1397	HOMO−3→LUMO+2	0.2750	ILCT MLCT
					HOMO−2→LUMO+1	0.6337	MLCT
	$S_0 \rightarrow S_{27}$	3.44ev	360nm	0.6765	HOMO−3→LUMO+2	0.1245	ILCT MLCT
					HOMO−1→LUMO+6	0.1784	ILCT
					HOMO→LUMO+5	0.6472	ILCT MLCT
Triplet	$S_0 \rightarrow T_1$	1.54eV	805 nm	0.0000[e]	HOMO−3→LUMO+2	0.2295	ILCT MLCT
					HOMO−2→LUMO+1	0.2893	ILCT MLCT
					HOMO−1→LUMO+2	0.3646	ILCT MLCT
					HOMO→LUMO	0.3176	LLCT MLCT
					HOMO→LUMO+1	0.3205	ILCT MLCT
	$S_0 \rightarrow T_3$	1.60ev	775nm	0.0000[e]	HOMO−3→LUMO+2	0.1302	ILCT MLCT
					HOMO−2→LUMO	0.2197	LLCT MLCT
					HOMO−2→LUMO+1	0.1549	ILCT MLCT
					HOMO−1→LUMO+2	0.1793	ILCT MLCT
					HOMO→LUMO	0.5784	LLCT MLCT
					HOMO→LUMO+1	0.1608	ILCT MLCT

a :Only the selected low-lying excited states are presented. b: Oscillator strength. c :Only the mainconfigurations are presented. d: The CI coefficients are in absolute values. e:No spin-orbital coupling effect wasconsidered, thus the f values are zero.

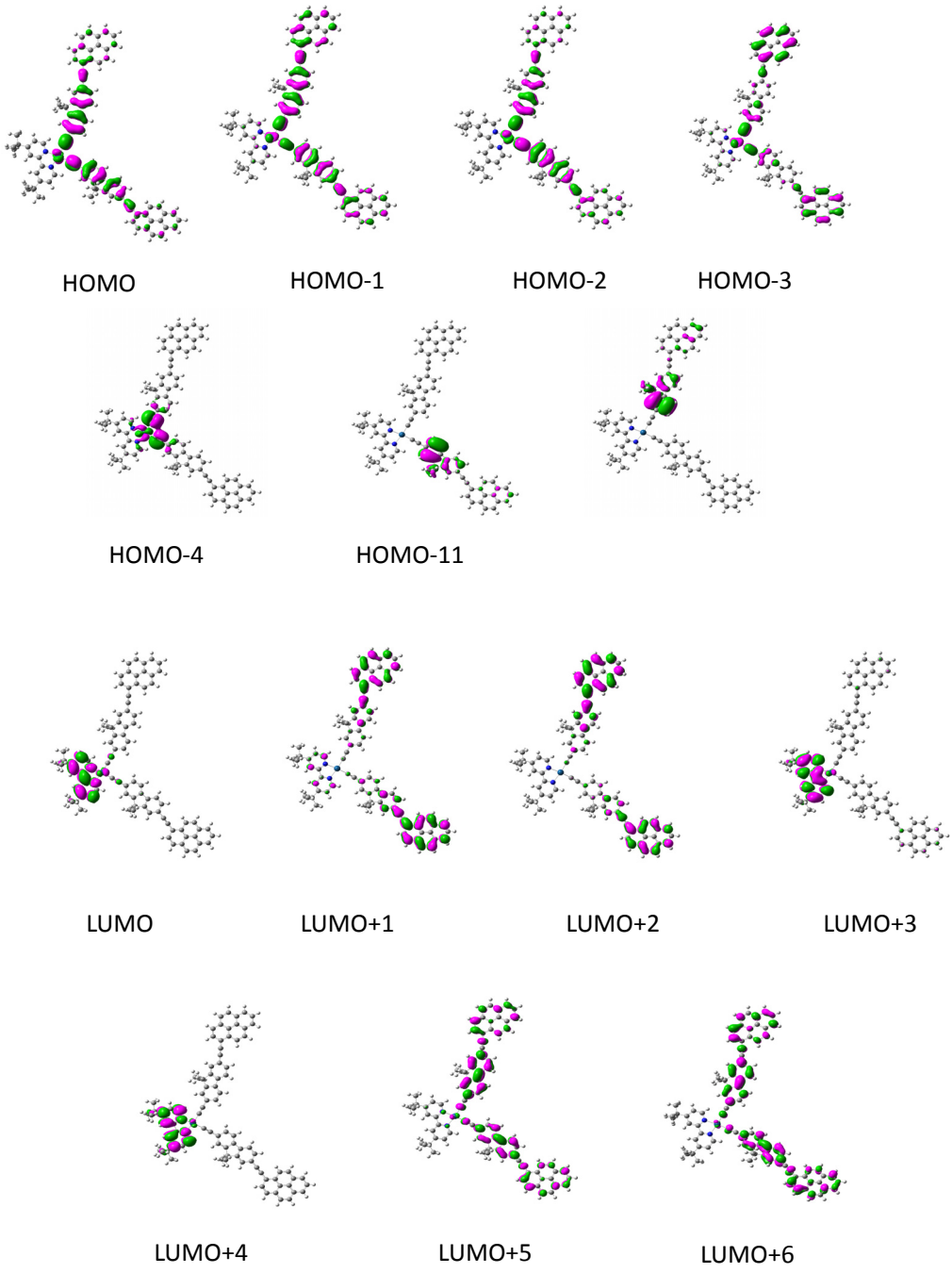


Fig. S66 Selected frontier molecular orbitals of complex **Pt-4** wihtout solvent calculated by DFT at the B3LYP/6-31G((d)/LanL2DZ level. The octyl group was simplified as methy in the calculation to reduce computation time. Calculated with Gaussian 09W.

Table S4. Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-4** without solvent, calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.69eV 733 nm	0.1516	HOMO-2→LUMO	0.1533	ILCT MLCT
				HOMO→LUMO	0.6848	LLCT MLCT
	$S_0 \rightarrow S_7$	2.69 eV 461 nm	1.1049	HOMO−1→LUMO+2	0.2226	ILCT LLCT MLCT
				HOMO→LUMO+1	0.4883	ILCT MLCT
				HOMO→LUMO+3	0.4215	LLCT MLCT
	$S_0 \rightarrow S_{12}$	2.85 eV 434 nm	0.3744	HOMO−1→LUMO+2	0.6330	ILCT LLCT MLCT
				HOMO−1→LUMO+4	0.1245	LLCT MLCT
				HOMO→LUMO+1	0.2296	ILCT MLCT
				HOMO →LUMO+3	0.1110	LLCT MLCT
	$S_0 \rightarrow S_{18}$	3.25 eV 380 nm	0.4136	HOMO−3→LUMO+2	0.1802	ILCT MLCT
				HOMO−2→LUMO+1	0.5972	ILCT MLCT
				HOMO-2→LUMO+3	0.1763	LLCT MLCT
				HOMO-1→LUMO+6	0.1179	ILCT MLCT
				HOMO →LUMO+5	0.1876	ILCT MLCT
	$S_0 \rightarrow S_{26}$	3.50 eV 355nm	0.1190	HOMO-12 →LUMO	0.1027	LLCT MLCT
				HOMO-11 →LUMO	0.1009	LLCT MLCT
				HOMO-4→LUMO+4	0.1922	MLCT
				HOMO-3→LUMO+2	0.1748	ILCT MLCT
				HOMO-3→LUMO+4	0.3079	LLCT MLCT
				HOMO-2→LUMO+4	0.2997	LLCT MLCT
				HOMO →LUMO+5	0.3786	ILCT MLCT
Triplet	$S_0 \rightarrow T_1$	1.60eV 776 nm	0.0000[e]	HOMO-2→LUMO	0.1817	ILCT MLCT
				HOMO→LUMO	0.6677	LLCT MLCT
	$S_0 \rightarrow T_3$	1.86 eV 666nm	0.0000[e]	HOMO-3→LUMO+1	0.1166	ILCT MLCT
				HOMO-3→LUMO+2	0.2308	ILCT MLCT
				HOMO-2→LUMO+1	0.3081	ILCT MLCT
				HOMO-2→LUMO+2	0.1261	ILCT MLCT
				HOMO-1→LUMO+1	0.1685	ILCT MLCT
				HOMO-1→LUMO+2	0.3153	ILCT LLCT MLCT
				HOMO→LUMO+1	0.3311	ILCT MLCT
				HOMO→LUMO+2	0.1280	ILCT MLCT

a :Only the selected low-lying excited states are presented. b: Oscillator strength. c :Only the mainconfigurations are presented. d: The CI coefficients are in absolute values. e:No spin-orbital coupling effect wasconsidered, thus the f values are zero.

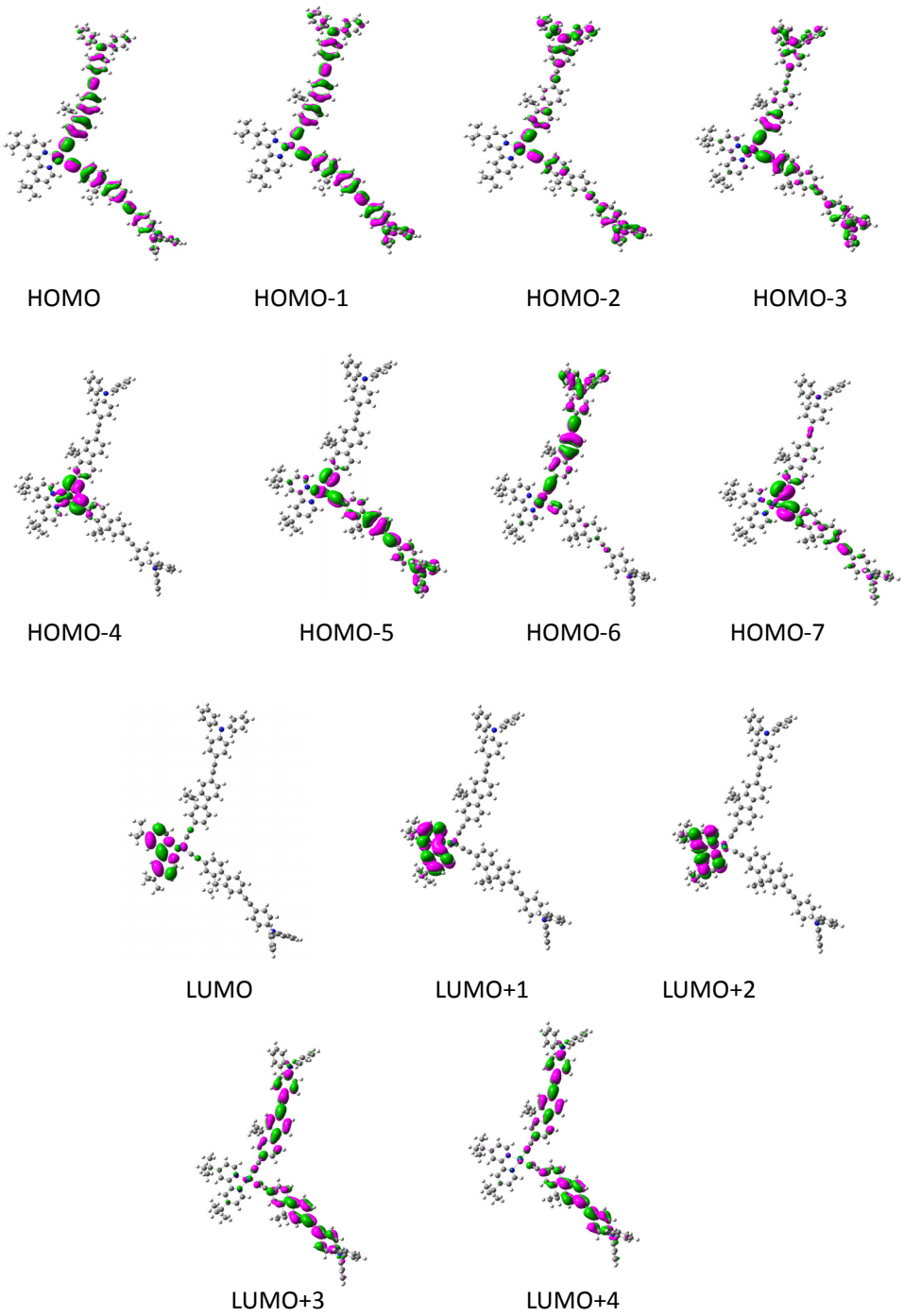


Fig. S67 Selected frontier molecular orbitals of complex **Pt-5** without solvent calculated by DFT at the B3LYP/6-31G((d)/LanL2DZ level. The octyl group was simplified as methy in the calculation to reduce computation time. Calculated with Gaussian 09W.

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Table S5. Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-5** without solvent, calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.65 eV 753nm	0.1257	HOMO-2→LUMO	0.2116	ILCT LLC MLCT
				HOMO→LUMO	0.6689	LLCT MLCT
	$S_0 \rightarrow S_9$	2.76 eV 449nm	0.1186	HOMO−7→LUMO	0.1566	ILCT LLCT MLCT
				HOMO−5→LUMO	0.2031	ILCT LLCT MLCT
				HOMO−3→LUMO+1	0.1262	ILCT LLCT MLCT
				HOMO−2→LUMO+2	0.1319	LLCT MLCT
				HOMO−1→LUMO+1	0.4160	ILCT LLCT MLCT
				HOMO→LUMO+2	0.4597	ILCT LLCT MLCT
	$S_0 \rightarrow S_{13}$	3.02 eV 411 nm	2.5341	HOMO-1→LUMO+2	0.1315	ILCT LLCT MLCT
				HOMO-1→LUMO+4	0.2918	ILCT
				HOMO→LUMO+3	0.6155	ILCT MLCT
	$S_0 \rightarrow S_{17}$	3.17 eV 391 nm	0.4224	HOMO−6→LUMO	0.1154	ILCT LLCT MLCT
				HOMO−5→LUMO	0.1623	ILCT LLCT MLCT
				HOMO-3→LUMO+1	0.3536	ILCT LLCT MLCT
				HOMO-1→LUMO+1	0.1007	ILCT LLCT MLCT
				HOMO-1→LUMO+3	0.2716	ILCT MLCT
				HOMO→LUMO+4	0.4520	ILCT
Triplet	$S_0 \rightarrow T_1$	1.56eV 793 nm	0.0000e	HOMO−2→ LUMO	0.2479	ILCT LLCT MLCT
				HOMO→LUMO	0.6480	ILCT LLCT MLCT
	$S_0 \rightarrow T_3$	2.17ev 272nm	0.0000[e]	HOMO-4→LUMO	0.1736	LLCT MLCT
				HOMO-2→LUMO	0.6158	ILCT LLCT MLCT
				HOMO→LUMO	0.2591	ILCT LLCT MLCT

a :Only the selected low-lying excited states are presented. b: Oscillator strength. c :Only the mainconfigurations are presented. d: The CI coefficients are in absolute values. e:No spin-orbital coupling effect wasconsidered, thus the f values are zero.

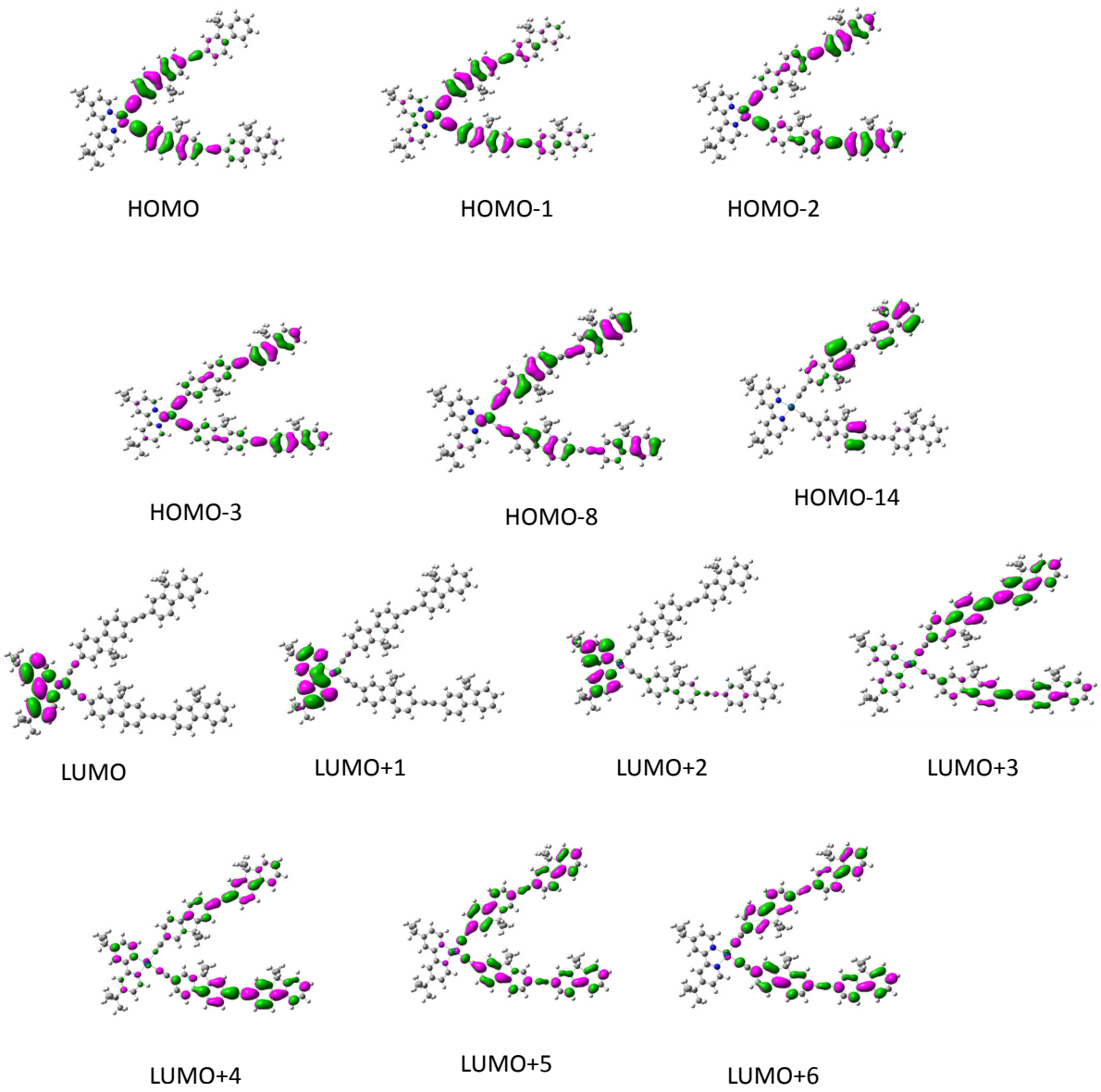

Fig. S68 Selected frontier molecular orbitals of complex **Pt-6** without solvent calculated by DFT at the B3LYP/6-31G((d)/LanL2DZ level. The octyl group was simplified as methy in the calculation to reduce computation time. Calculated with Gaussian 09W.

Table S6. Selected vertical electronic excitation energies (ev) and corresponding oscillator strengths (f), main configurations and ci coefficients of the lowlying electronically excited states of complex **Pt-6** without solvent, calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries.

	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy [a]	*f* [b]	Composition [c]	CI [d]	Character
Singlet	$S_0 \rightarrow S_1$	1.63ev 761nm	0.0660	HOMO−2→ LUMO	0.1174	LLCT MLCT
				HOMO→ LUMO	0.6934	LLCT MLCT
	$S_0 \rightarrow S_9$	2.85ev 435nm	0.6493	HOMO−1→LUMO+1	0.4753	LLCT MLCT
				HOMO→LUMO+2	0.4921	LLCT MLCT
	$S_0 \rightarrow S_{14}$	3.22ev 385nm	1.0681	HOMO−8→LUMO	0.1442	ILCT LLCT MLCT
				HOMO−1→LUMO+3	0.6356	ILCT MLCT
				HOMO−1→LUMO+4	0.2297	ILCT MLCT
	$S_0 \rightarrow S_{30}$	3.79 ev 327nm	1.1191	HOMO−14→LUMO+3	0.1304	ILCT MLCT
				HOMO−3→LUMO+3	0.3515	MLCT
				HOMO−2→LUMO+4	0.5007	ILCT MLCT
				HOMO−1→LUMO+5	0.1785	ILCT
				HOMO →LUMO+6	0.2027	ILCT MLCT
Triplet	$S_0 \rightarrow T_1$	1.53 eV 811nm	0.0000[e]	HOMO−2→ LUMO	0.1463	ILCT MLCT
				HOMO→LUMO	0.6817	LLCT MLCT
	$S_0 \rightarrow T_3$	2.27 eV 547nm	0.0000[e]	HOMO-3→LUMO+4	0.1442	ILCT MLCT
				HOMO-2→LUMO	0.1169	ILCT LLCT MLCT
				HOMO-2→LUMO+3	0.1779	ILCT MLCT
				HOMO-1→LUMO+2	0.1425	LLCT MLCT
				HOMO-1→LUMO+3	0.1018	ILCT MLCT
				HOMO-1→LUMO+4	0.3363	ILCT MLCT
				HOMO-1→LUMO+6	0.1050	ILCT
				HOMO→LUMO+1	0.1850	LLCT MLCT
				HOMO→LUMO+3	0.4137	ILCT MLCT
				HOMO→LUMO+5	0.1245	ILCT

a :Only the selected low-lying excited states are presented. b: Oscillator strength. c :Only the mainconfigurations are presented. d: The CI coefficients are in absolute values. e:No spin-orbital coupling effect wasconsidered, thus the f values are zero.

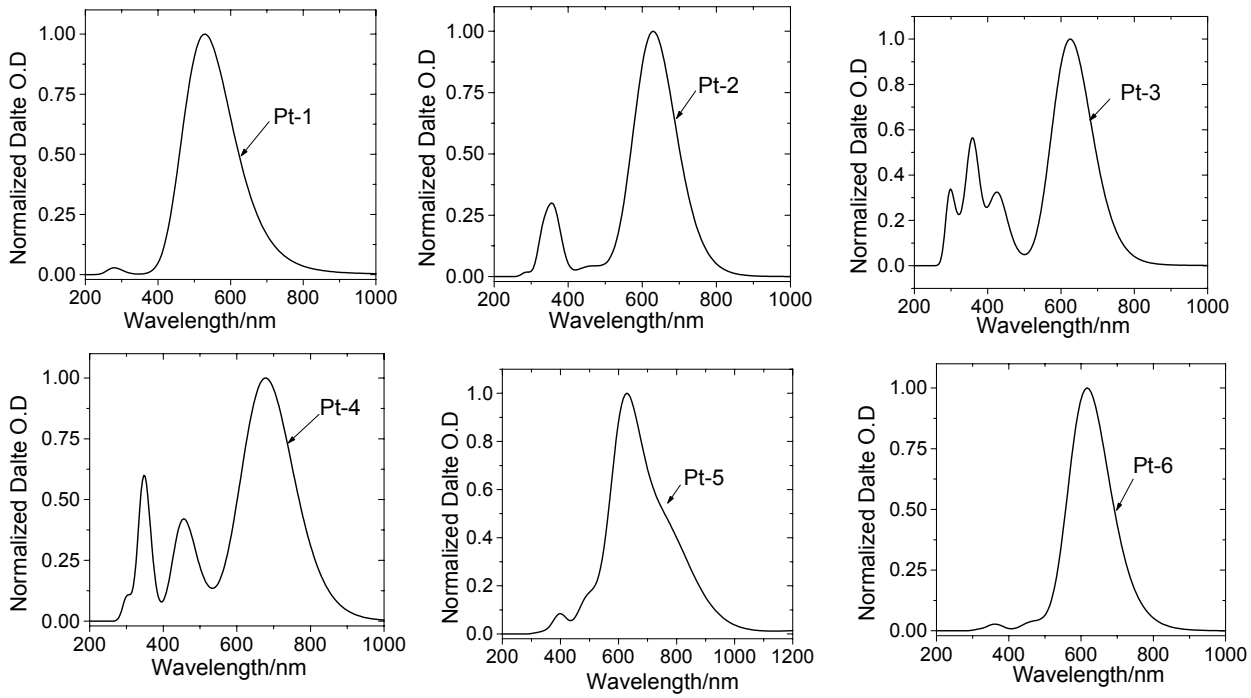

Fig. S69 The calculated transient absorption spectra of the ligands T_1 state, please note that the information of bleaching is not included in the calculated transient absorption spectra). Calculated at B3LYP/6-31G(d) level with Gaussian 09W.

The coordinates of the singlet optimized geometries of complexes:

complex Pt-1 （DFT//B3LYP/6-31G(d)/ LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.48222400	5.28676400	-0.22536000
C	2.92064500	6.57086200	-0.17058800
C	1.52306400	6.64685700	-0.08136000
C	0.73963900	5.49649600	-0.04566700
C	2.66652800	4.16278700	-0.19046700
C	-0.73134500	5.49818800	0.05008700
C	-1.50987900	6.65019300	0.12275400
C	-2.90782900	6.57737100	0.20796100
C	-3.47504700	5.29463200	0.21950300
C	-2.66413200	4.16891100	0.14829300
H	4.55071400	5.14765800	-0.29633300
H	3.05795600	3.15509000	-0.23322000
H	-4.54424200	5.15806600	0.28433400
H	-3.05966200	3.16197600	0.15657700

N	-1.31688700	4.25927600	0.06386600
N	1.31963400	4.25611300	-0.10081800
Pt	-0.00210200	2.62944400	-0.04459700
C	-1.37775000	1.23480800	0.01928400
C	-2.26634500	0.39285500	0.06757400
C	1.37029800	1.23393800	-0.15466900
C	2.26155100	0.39709700	-0.23186400
H	-1.02306400	7.61487400	0.11342000
H	1.04029000	7.61272800	-0.04011200
C	-3.74301500	7.86502900	0.28954400
C	3.76102600	7.85708900	-0.21207600
C	-3.34738600	8.64048600	1.57610100
H	-2.28644000	8.91090600	1.56647200
H	-3.93684000	9.56169000	1.64349600
H	-3.54347100	8.03214200	2.46513500
C	-3.45451800	8.74045200	-0.96048700
H	-4.04358100	9.66270200	-0.90440000
H	-2.39613100	9.01409600	-1.02072200
H	-3.72833300	8.20431500	-1.87513600
C	-5.25992900	7.56966000	0.34015200
H	-5.59108200	7.03495700	-0.55700300
H	-5.52329900	6.98141000	1.22611000
H	-5.80448900	8.51836400	0.38992300
C	3.37132000	8.67063000	-1.47669900
H	2.31080700	8.94249000	-1.46262500
H	3.96273200	9.59224800	-1.51569100
H	3.56916300	8.08781800	-2.38230700
C	3.47294600	8.69680500	1.06221600
H	4.06784000	9.61661500	1.03586000
H	2.41609300	8.97531900	1.12668600
H	3.73984400	8.13206300	1.96156400
C	5.27693500	7.55745000	-0.26792800
H	5.60390700	6.99434200	0.61325600
H	5.54032600	6.99557700	-1.17081400
H	5.82512800	8.50517800	-0.28762900
C	7.90820400	-5.29932700	-0.99620200
C	8.94259000	-4.63529000	-0.29915200
C	8.69742100	-3.35312900	0.25110600
C	7.45204700	-2.77253400	0.09650100
C	6.42307900	-3.44611900	-0.60472000
C	6.65501900	-4.71152200	-1.15003800
H	8.10672500	-6.27926800	-1.41197400
H	9.49376600	-2.84834300	0.78539200
H	5.87236400	-5.23409400	-1.68799200

C	5.51425900	-1.40006400	0.08019300
C	4.55280900	-0.41387100	0.21408100
C	3.26595800	-0.60264000	-0.34811500
C	2.99248900	-1.80903600	-1.03712500
C	3.96116000	-2.79962300	-1.17214800
C	5.22643900	-2.59751900	-0.61452000
H	4.75955400	0.50638000	0.74855300
H	2.00568000	-1.94482500	-1.46148300
H	3.73057600	-3.71517100	-1.70563700
C	10.21647100	-5.24917600	-0.15282900
C	11.30541500	-5.77295600	-0.02828600
C	6.95941500	-1.40806100	0.59914500
C	6.99479200	-1.34333600	2.14618700
H	8.02782800	-1.41481100	2.50551900
H	6.56900300	-0.39551700	2.49427000
H	6.41442300	-2.16681600	2.57157100
C	7.78162500	-0.25632100	-0.02888300
H	8.82650700	-0.31379100	0.29708800
H	7.74732700	-0.31924900	-1.12026600
H	7.37263700	0.71147700	0.28313200
C	12.57907300	-6.39123500	0.11326400
C	-7.78498600	-5.45548800	0.56521400
C	-8.91141800	-4.68595100	0.19669300
C	-8.74451500	-3.31300600	-0.11007500
C	-7.48398700	-2.74861700	-0.04307700
C	-6.36233700	-3.52867100	0.32815900
C	-6.51677200	-4.88382300	0.63149900
H	-7.92453200	-6.50395200	0.79713800
H	-9.61136300	-2.72783400	-0.39376000
H	-5.66293400	-5.48794600	0.91606200
C	-5.55243400	-1.36725700	-0.06255400
C	-4.61298700	-0.35493500	-0.14936100
C	-3.25354900	-0.62719400	0.14274900
C	-2.88651300	-1.94253600	0.51819500
C	-3.83265500	-2.95953000	0.60573500
C	-5.16976400	-2.67455600	0.31614200
H	-4.89421700	0.65039500	-0.44206500
H	-1.84520600	-2.14057100	0.73893700
H	-3.52964900	-3.95930200	0.89663700
C	-10.19886700	-5.28579000	0.13553500
C	-11.29849700	-5.79950800	0.08469000
C	-7.06340100	-1.29950800	-0.32744800
C	-7.35140800	-0.91717500	-1.80008100
H	-8.43027900	-0.93063100	-1.99307000

H	-6.97213500	0.08970700	-2.00827300
H	-6.86184000	-1.62398000	-2.47585900
C	-7.75500800	-0.32001900	0.65221700
H	-8.84071100	-0.33588200	0.50273700
H	-7.53568700	-0.60257500	1.68574600
H	-7.39507700	0.70099500	0.48076600
C	-12.58262600	-6.40985000	0.02951300
C	-13.72643800	-5.65288700	-0.30071700
H	-13.61460300	-4.59704000	-0.51363100
C	-14.98023900	-6.25702900	-0.35100700
H	-15.85136500	-5.66451900	-0.60595800
C	-15.11918500	-7.62043500	-0.07488900
H	-16.09652200	-8.08684500	-0.11509900
C	-13.99207800	-8.37974500	0.25301300
H	-14.09506100	-9.43722700	0.46750500
C	-12.73400700	-7.78514500	0.30608200
H	-11.85845300	-8.36963800	0.55977700
C	12.82107800	-7.66820800	-0.43584400
H	12.02278600	-8.17210600	-0.96632300
C	14.06931700	-8.26954500	-0.29621600
H	14.24256900	-9.25096200	-0.72248600
C	15.09652200	-7.61454800	0.38957300
H	16.06646800	-8.08597800	0.49597300
C	14.86717000	-6.34914000	0.93779700
H	15.66056000	-5.83778800	1.47068200
C	13.62243800	-5.73919900	0.80369200
H	13.44067000	-4.75911000	1.22682500

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 22 1.0
8 9 1.5 24 1.0
9 10 1.5 13 1.0
10 14 1.0 15 1.5
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15 17 1.0
16 17 1.0

17 18 1.0 20 1.0

18 19 3.0

19 91 1.5

20 21 3.0

21 61 1.5

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83 84 1.5 100 1.0

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89 90 2.0 94 1.5 100 1.0

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109 110 1.5 118 1.5
110 111 1.0 112 1.5
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112 113 1.0 114 1.5
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114 115 1.0 116 1.5
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116 117 1.0 118 1.5
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118 119 1.0
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120 121 1.0 122 1.5
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122 123 1.0 124 1.5
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124 125 1.0 126 1.5
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126 127 1.0 128 1.5
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128 129 1.0
129

complex Pt-2 （DFT//B3LYP/6-31G(d)/ LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.48543800	5.86721500	0.00060800
C	-2.91915000	7.15048500	0.00075100
C	-1.51877600	7.22346600	0.00077300
C	-0.73680100	6.07156000	0.00066200
C	-2.67119800	4.74167600	0.00049600
C	0.73686600	6.07154600	0.00068800
C	1.51886500	7.22343600	0.00082500
C	2.91923700	7.15042600	0.00083800
C	3.48549900	5.86714500	0.00070500
C	2.67123600	4.74162200	0.00057100
H	-4.55658600	5.73053800	0.00058200
H	-3.06588400	3.73444900	0.00038300
H	4.55664400	5.73044500	0.00070500
H	3.06590100	3.73438700	0.00046500

N	1.32128100	4.83201100	0.00056400
N	-1.32124200	4.83203700	0.00052000
Pt	0.00000400	3.20283900	0.00037000
C	1.38068100	1.81219500	0.00023800
C	2.28547900	0.98599500	0.00017900
C	-1.38070100	1.81222200	0.00017800
C	-2.28550900	0.98603200	0.00004700
H	1.03251700	8.18830800	0.00092100
H	-1.03240900	8.18832800	0.00087600
C	3.75768100	8.43866000	0.00098600
C	-3.75756700	8.43873700	0.00087800
C	3.41698300	9.26448800	-1.26960300
H	2.35699400	9.53744600	-1.29494900
H	4.00898200	10.18651300	-1.27615800
H	3.65046500	8.69105600	-2.17271400
C	3.41693100	9.26423700	1.27172300
H	4.00894200	10.18625300	1.27848800
H	2.35694400	9.53720600	1.29707200
H	3.65036200	8.69062300	2.17473100
C	5.27525200	8.14246300	0.00098800
H	5.57195200	7.58070100	0.89363200
H	5.57198000	7.58084200	-0.89173600
H	5.82155400	9.09148000	0.00107100
C	-3.41681200	9.26431700	1.27161200
H	-2.35682100	9.53727000	1.29696500
H	-4.00880800	10.18634200	1.27836900
H	-3.65025600	8.69071200	2.17462300
C	-3.41684000	9.26454700	-1.26971400
H	-4.00881600	10.18658700	-1.27627800
H	-2.35684300	9.53747900	-1.29505500
H	-3.65033000	8.69111500	-2.17282300
C	-5.27514400	8.14257200	0.00086600
H	-5.57187600	7.58095800	-0.89186000
H	-5.57186400	7.58081600	0.89350800
H	-5.82142500	9.09160100	0.00094500
C	-8.06989900	-4.62764600	-0.00085900
C	-9.17892600	-3.75197800	-0.00094500
C	-8.95776700	-2.35227600	-0.00085000
C	-7.66386500	-1.86690500	-0.00067600
C	-6.55905500	-2.75270000	-0.00059300
C	-6.76709200	-4.13473700	-0.00068400
H	-8.24899000	-5.69567600	-0.00093300
H	-9.81178600	-1.68530100	-0.00091700
H	-5.92771700	-4.82061100	-0.00062100

C	-5.66368400	-0.58959000	-0.00040000
C	-4.67953700	0.38214600	-0.00025200
C	-3.31371000	0.00497400	-0.00011000
C	-2.98887800	-1.37341200	-0.00012700
C	-3.98035700	-2.35067300	-0.00028000
C	-5.32285200	-1.96199800	-0.00041600
H	-4.93186100	1.43651200	-0.00024100
H	-1.94303600	-1.65327500	-0.00001900
H	-3.70746400	-3.40021500	-0.00029200
C	-10.50479400	-4.26294500	-0.00112300
C	-11.64872800	-4.67456700	-0.00127200
C	-12.99522900	-5.12982400	-0.00143500
C	-13.29399700	-6.54085300	-0.00154900
C	-14.03975100	-4.20957100	-0.00148100
C	-12.27688700	-7.53142300	-0.00151600
C	-14.66602200	-6.95728900	-0.00170000
C	-15.38449200	-4.63440600	-0.00163300
H	-13.80718600	-3.15213900	-0.00139500
C	-12.59709300	-8.87098600	-0.00162300
H	-11.24341800	-7.20741900	-0.00140400
C	-14.96089800	-8.34959800	-0.00180800
C	-15.69510600	-5.97621600	-0.00173900
H	-16.17372800	-3.89181100	-0.00166500
C	-13.95212500	-9.28515800	-0.00177000
H	-11.81074700	-9.61678400	-0.00159600
H	-16.00082100	-8.65875400	-0.00192100
H	-16.72873400	-6.30494100	-0.00185400
H	-14.18859900	-10.34283200	-0.00185300
C	-7.18796400	-0.40790200	-0.00055500
C	-7.65988700	0.32758500	-1.27881500
H	-8.75405100	0.38835900	-1.30026400
H	-7.25395800	1.34543100	-1.30033400
H	-7.31761600	-0.20676500	-2.16947400
C	-7.66014600	0.32745000	1.27769100
H	-8.75431300	0.38823500	1.29891900
H	-7.31806700	-0.20700500	2.16836100
H	-7.25420700	1.34528800	1.29940700
C	8.06990400	-4.62764800	-0.00006000
C	9.17892500	-3.75197300	0.00008000
C	8.95775800	-2.35227200	0.00019100
C	7.66385300	-1.86690900	0.00016200
C	6.55904800	-2.75271000	0.00002500
C	6.76709300	-4.13474600	-0.00008700
H	8.24900100	-5.69567600	-0.00014500

H	9.81177300	-1.68529200	0.00029900
H	5.92772300	-4.82062500	-0.00019200
C	5.66366400	-0.58960600	0.00017600
C	4.67951100	0.38212500	0.00022300
C	3.31368700	0.00494300	0.00012400
C	2.98886300	-1.37344400	-0.00002400
C	3.98034800	-2.35069900	-0.00006700
C	5.32284000	-1.96201600	0.00003400
H	4.93182900	1.43649200	0.00033600
H	1.94302300	-1.65331300	-0.00009900
H	3.70746200	-3.40024300	-0.00017700
C	10.50479700	-4.26293200	0.00011200
C	11.64873000	-4.67455500	0.00014100
C	12.99521400	-5.12986300	0.00017900
C	13.29392900	-6.54090300	0.00018200
C	14.03977000	-4.20964800	0.00021400
C	12.27678200	-7.53143400	0.00015100
C	14.66593800	-6.95739000	0.00022100
C	15.38449500	-4.63453400	0.00025200
H	13.80724400	-3.15220700	0.00021100
C	12.59693700	-8.87100900	0.00015600
H	11.24332500	-7.20739100	0.00012400
C	14.96076200	-8.34971000	0.00022400
C	15.69505900	-5.97635600	0.00025500
H	16.17375900	-3.89196800	0.00028000
C	13.95195400	-9.28523300	0.00019200
H	11.81056300	-9.61677700	0.00013200
H	16.00067300	-8.65890500	0.00025300
H	16.72867500	-6.30511900	0.00028400
H	14.18838800	-10.34291600	0.00019500
C	7.18794300	-0.40790900	0.00025500
C	7.65994400	0.32742500	1.27857500
H	8.75410900	0.38820700	1.29995900
H	7.25400600	1.34526500	1.30024700
H	7.31773800	-0.20703800	2.16919100
C	7.66003800	0.32760200	-1.27793100
H	8.75420400	0.38839200	-1.29922400
H	7.31790200	-0.20674400	-2.16864400
H	7.25409500	1.34544200	-1.29949400

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
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19 107 1.5

20 21 3.0

21 61 1.5

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51 52 1.5 68 1.5
52 53 2.0 57 1.0
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54 55 1.5 64 1.0
55 58 1.0
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59 60 2.0 64 1.5 87 1.0
60 61 1.5 65 1.0
61 62 1.5
62 63 1.5 66 1.0
63 64 1.5 67 1.0
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68 69 3.0
69 70 1.5
70 71 1.5 72 1.5
71 73 1.5 74 1.5
72 75 1.5 76 1.0
73 77 2.0 78 1.0
74 79 1.5 80 1.5
75 80 2.0 81 1.0
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77 82 1.5 83 1.0
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88 89 1.0 90 1.0 91 1.0
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96 97 1.5 101 1.5 102 1.0

97 98 1.5 114 1.5

98 99 2.0 103 1.0

99 100 1.5 133 1.0

100 101 1.5 110 1.0

101 104 1.0

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105 106 2.0 110 1.5 133 1.0

106 107 1.5 111 1.0

107 108 1.5

108 109 1.5 112 1.0

109 110 1.5 113 1.0

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114 115 3.0

115 116 1.5

116 117 1.5 118 1.5

117 119 1.5 120 1.5

118 121 1.5 122 1.0

119 123 2.0 124 1.0

120 125 1.5 126 1.5

121 126 2.0 127 1.0

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123 128 1.5 129 1.0

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125 128 2.0 130 1.0

126 131 1.0

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128 132 1.0

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133 134 1.0 138 1.0

134 135 1.0 136 1.0 137 1.0

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138 139 1.0 140 1.0 141 1.0

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complex Pt-3 （DFT//B3LYP/6-31G(d)/ LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.48108400	6.44260700	-0.17905100
C	2.91618300	7.72618000	-0.15228700
C	1.51747200	7.80035700	-0.08223600
C	0.73598200	6.64896600	-0.03864900
C	2.66727800	5.31753200	-0.13654500
C	-0.73598300	6.64897800	0.03858100
C	-1.51745800	7.80038100	0.08208300
C	-2.91617200	7.72622700	0.15212500
C	-3.48108700	6.44266200	0.17897700
C	-2.66729400	5.31757300	0.13656400
H	4.55072800	6.30506700	-0.23362700
H	3.06112400	4.31014500	-0.15714800
H	-4.55073400	6.30514000	0.23354800
H	-3.06115300	4.31019300	0.15724200
N	-1.31922500	5.40919100	0.06653700
N	1.31921000	5.40917100	-0.06651900
Pt	-0.00001800	3.78097600	0.00005300
C	-1.37245000	2.38349600	0.07114800
C	-2.25718800	1.53762100	0.12238100
C	1.37240200	2.38347800	-0.07093400
C	2.25713700	1.53759700	-0.12213000
H	-1.03225800	8.76568000	0.06181000
H	1.03228700	8.76566500	-0.06202300
C	-3.75437100	9.01360100	0.20150900
C	3.75440200	9.01353400	-0.20180500
C	-3.37268200	9.81370900	1.47706700
H	-2.31205900	10.08546600	1.47310100
H	-3.96388000	10.73519500	1.52134700
H	-3.57698700	9.22188900	2.37535900
C	-3.45504000	9.86550900	-1.06214100
H	-4.04703100	10.78701900	-1.03023200
H	-2.39677300	10.14081500	-1.11661400
H	-3.71780200	9.31094700	-1.96900400
C	-5.27119700	8.71639000	0.24313400

H	-5.59330400	8.16521800	-0.64733400
H	-5.54183500	8.14373700	1.13709100
H	-5.81763500	9.66491500	0.27089300
C	3.37259300	9.81359700	-1.47736200
H	2.31197500	10.08537300	-1.47329000
H	3.96380400	10.73507100	-1.52173700
H	3.57679300	9.22173800	-2.37565200
C	3.45523400	9.86551100	1.06183100
H	4.04724300	10.78700600	1.02980600
H	2.39698100	10.14085100	1.11641200
H	3.71808400	9.31099700	1.96869900
C	5.27121500	8.71627900	-0.24358600
H	5.59339200	8.16508600	0.64684400
H	5.54174600	8.14362700	-1.13757500
H	5.81767900	9.66478700	-0.27139000
C	7.73696500	-4.34571300	-0.61943100
C	8.86571200	-3.58920600	-0.22856800
C	8.70518500	-2.21741500	0.09020400
C	7.45050600	-1.64257300	0.01307300
C	6.32727800	-2.40977900	-0.38080100
C	6.47488300	-3.76323100	-0.69611100
H	7.87031100	-5.39295300	-0.86089300
H	9.57239900	-1.64134000	0.39124700
H	5.62005500	-4.35746500	-0.99783500
C	5.52935500	-0.24682200	0.02372300
C	4.59631200	0.77125800	0.11130700
C	3.23841100	0.51230800	-0.19972300
C	2.86669800	-0.79585600	-0.59570000
C	3.80618600	-1.81867900	-0.68384900
C	5.14176900	-1.54694700	-0.37450500
H	4.88120400	1.77098000	0.41914600
H	1.82685000	-0.98338100	-0.83186900
H	3.49957200	-2.81268900	-0.99028600
C	10.14546000	-4.19995200	-0.15794400
C	11.24132400	-4.72647300	-0.10007800
C	7.03745700	-0.19321700	0.30730500
C	7.31104600	0.17221900	1.78697500
H	8.38750400	0.14963400	1.99219400
H	6.93623700	1.17953600	2.00085100
H	6.80911200	-0.53779400	2.45018300
C	7.74781300	0.79067100	-0.65444500
H	8.83143100	0.76636700	-0.49141200
H	7.53979700	0.51939500	-1.69330400
H	7.39233200	1.81232500	-0.47783900

C	12.51454700	-5.34844200	-0.03839200
C	12.63749000	-6.74135300	-0.30941800
C	13.66728800	-4.58046100	0.29204200
C	11.51050900	-7.55315400	-0.64276300
C	13.93811600	-7.36466700	-0.24753600
C	14.95783700	-5.22478500	0.34836400
C	13.59406200	-3.18165300	0.57218200
C	11.65449700	-8.89224200	-0.89922000
H	10.53689500	-7.08170600	-0.68710200
C	14.04425200	-8.76630400	-0.52305000
C	15.06097200	-6.59456900	0.07803900
C	16.10711200	-4.43768500	0.68174000
H	12.62405900	-2.70252000	0.52849700
C	14.71860900	-2.46359900	0.88768400
C	12.93833000	-9.50876400	-0.83914800
H	10.78845000	-9.49340900	-1.15039300
H	15.02580100	-9.22564600	-0.47412600
H	16.03519300	-7.07129000	0.12235500
C	15.99351600	-3.09875400	0.94370700
H	17.07237700	-4.93108900	0.72151500
H	14.64478200	-1.40285300	1.09747800
H	13.03041800	-10.56869700	-1.04529600
H	16.87002700	-2.51312000	1.19515400
C	-7.73691500	-4.34579000	0.61927100
C	-8.86567900	-3.58925800	0.22850200
C	-8.70518100	-2.21742700	-0.09010700
C	-7.45051300	-1.64256800	-0.01291100
C	-6.32726400	-2.40980400	0.38084300
C	-6.47484000	-3.76329800	0.69599200
H	-7.87024100	-5.39305900	0.86061500
H	-9.57241100	-1.64132600	-0.39105400
H	-5.61999600	-4.35755100	0.99763000
C	-5.52938600	-0.24678500	-0.02344400
C	-4.59636000	0.77131300	-0.11096600
C	-3.23843400	0.51233300	0.19993000
C	-2.86668000	-0.79588000	0.59570800
C	-3.80615500	-1.81872000	0.68380000
C	-5.14176500	-1.54695700	0.37459600
H	-4.88128400	1.77106900	-0.41866700
H	-1.82681100	-0.98342700	0.83176600
H	-3.49951000	-2.81276800	0.99008300
C	-10.14542200	-4.20001300	0.15784500
C	-11.24128300	-4.72653500	0.09994500
C	-7.03751500	-0.19314700	-0.30687900

C	-7.31131400	0.17266900	-1.78639300
H	-8.38780300	0.15016500	-1.99145500
H	-6.93651600	1.18003300	-2.00007600
H	-6.80950200	-0.53718600	-2.44986500
C	-7.74776300	0.79047900	0.65525300
H	-8.83139900	0.76624700	0.49232500
H	-7.53964400	0.51886900	1.69400400
H	-7.39226700	1.81217600	0.47893400
C	-12.51451200	-5.34848900	0.03824600
C	-12.63746900	-6.74141000	0.30921900
C	-13.66725200	-4.58047700	-0.29212000
C	-11.51049100	-7.55324000	0.64250100
C	-13.93810700	-7.36470100	0.24736000
C	-14.95781300	-5.22478000	-0.34842900
C	-13.59401200	-3.18165900	-0.57220300
C	-11.65449500	-8.89233500	0.89892000
H	-10.53686700	-7.08181300	0.68682200
C	-14.04426000	-8.76634400	0.52283300
C	-15.06096200	-6.59457200	-0.07815200
C	-16.10708400	-4.43764900	-0.68174200
H	-12.62400100	-2.70254300	-0.52852200
C	-14.71855700	-2.46357600	-0.88764900
C	-12.93834000	-9.50883300	0.83887200
H	-10.78845100	-9.49352400	1.15005000
H	-15.02581900	-9.22566600	0.47392800
H	-16.03519200	-7.07127500	-0.12246000
C	-15.99347500	-3.09871000	-0.94366300
H	-17.07235900	-4.93103700	-0.72151100
H	-14.64472100	-1.40282200	-1.09740100
H	-13.03044000	-10.56877100	1.04499100
H	-16.86998300	-2.51305300	-1.19506800

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 22 1.0
8 9 1.5 24 1.0
9 10 1.5 13 1.0
10 14 1.0 15 1.5
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15 17 1.0

16 17 1.0

17 18 1.0 20 1.0

18 19 3.0

19 113 1.5

20 21 3.0

21 61 1.5

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24 26 1.0 30 1.0 34 1.0

25 38 1.0 42 1.0 46 1.0

26 27 1.0 28 1.0 29 1.0

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50 51 1.5 55 1.5 56 1.0

51 52 1.5 68 1.5

52 53 2.0 57 1.0

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59 60 2.0 64 1.5 70 1.0

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69 79 1.5

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86 93 1.5 94 1.0

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93 100 1.0

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102 103 1.5 107 1.5 108 1.0

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104 105 2.0 109 1.0

105 106 1.5 122 1.0

106 107 1.5 116 1.0

107 110 1.0

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111 112 2.0 116 1.5 122 1.0

112 113 1.5 117 1.0

113 114 1.5

114 115 1.5 118 1.0

115 116 1.5 119 1.0

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120 121 3.0

121 131 1.5

122 123 1.0 127 1.0

123 124 1.0 125 1.0 126 1.0

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127 128 1.0 129 1.0 130 1.0

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131 132 1.5 133 1.5

132 134 1.5 135 1.5

133 136 1.5 137 1.5

134 138 2.0 139 1.0

135 140 1.5 141 1.5

136 141 1.5 142 1.5

137 143 1.0 144 2.0

138 145 1.5 146 1.0

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140 145 2.0 147 1.0

141 148 1.0

142 149 2.0 150 1.0

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144 149 1.5 151 1.0

145 152 1.0
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149 153 1.0
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complex Pt-4 （DFT//B3LYP/6-31G(d)/ LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.48139300	6.86833300	-0.19129600
C	-2.91695400	8.15124800	-0.13838300
C	-1.51786400	8.22440300	-0.07559000
C	-0.73566800	7.07273500	-0.06355000
C	-2.66689100	5.74301500	-0.17948700
C	0.73681000	7.07250800	0.00102400
C	1.51732000	8.22378500	0.06284100
C	2.91667300	8.15021600	0.11756900
C	3.48331900	6.86721300	0.10889200
C	2.67042100	5.74229300	0.04857100
H	-4.55126700	6.73133800	-0.24289300
H	-3.06057400	4.73619700	-0.22092500
H	4.55365200	6.73010600	0.14902100
H	3.06540100	4.73520100	0.04115600
N	1.32171100	5.83325600	-0.00491800
N	-1.31836300	5.83351400	-0.11531500
Pt	0.00271300	4.20442000	-0.09451900
C	1.38289900	2.81349900	-0.06884200
C	2.28691400	1.98669800	-0.04929800
C	-1.37862700	2.81668300	-0.18119600
C	-2.28788400	1.99763100	-0.23886200
H	1.03083400	9.18860000	0.06860100
H	-1.03282000	9.18918200	-0.03672800
C	3.75381300	9.43735500	0.18653600
C	-3.75578200	9.43911600	-0.15278400
C	3.44926300	10.30959100	-1.06198000
H	2.38992900	10.58209800	-1.10950600
H	4.03849100	11.23228600	-1.01579700
H	3.71179800	9.77113000	-1.97856200
C	3.37599900	10.21631200	1.47626000

H	3.96836800	11.13626300	1.53417500
H	2.31578400	10.48965800	1.47962800
H	3.58191100	9.60953000	2.36413700
C	5.27101800	9.14091900	0.21816700
H	5.54459800	8.55144500	1.10024500
H	5.59115500	8.60727600	-0.68359300
H	5.81669500	10.08925000	0.26235500
C	-3.44887000	10.26143200	1.12849600
H	-2.39088100	10.53806000	1.18158100
H	-4.04329300	11.18188000	1.12302100
H	-3.70342400	9.68473400	2.02381600
C	-3.38212300	10.26848100	-1.41189100
H	-3.97202200	11.19170400	-1.43046700
H	-2.32103300	10.53836900	-1.40937500
H	-3.59397500	9.69811000	-2.32224200
C	-5.27272700	9.14232000	-0.19228500
H	-5.54833100	8.59050600	-1.09773900
H	-5.58962400	8.57048900	0.68696100
H	-5.81952200	10.09104900	-0.19496700
C	8.06622800	-3.63047300	0.08061700
C	9.17615500	-2.75599900	0.05037600
C	8.95570800	-1.35631300	0.01268900
C	7.66238800	-0.87019600	0.00597300
C	6.55675500	-1.75472100	0.03623500
C	6.76394400	-3.13653300	0.07366000
H	8.24443500	-4.69824900	0.10962700
H	9.81012600	-0.69025200	-0.01059500
H	5.92406900	-3.82137800	0.09725900
C	5.66335500	0.40835700	-0.01951300
C	4.68008700	1.38062500	-0.04240800
C	3.31399500	1.00482000	-0.02579000
C	2.98769700	-0.37268800	0.01513900
C	3.97841800	-1.35045700	0.03796600
C	5.32133600	-0.96325300	0.02034800
H	4.93322600	2.43431500	-0.07442900
H	1.94159400	-0.65130800	0.02968700
H	3.70457600	-2.39926600	0.06963700
C	10.50143600	-3.26603600	0.05725000
C	11.64675100	-3.67572200	0.06199700
C	7.18767000	0.58867500	-0.03064300
C	7.66505100	1.35600800	1.22677700
H	8.75932300	1.41650500	1.24253200
H	7.25986400	2.37438300	1.22371900
H	7.32582900	0.84468000	2.13199900

C	7.65546800	1.29091900	-1.32888300
H	8.74957800	1.35071100	-1.35561600
H	7.30998600	0.73412300	-2.20442800
H	7.24977300	2.30801400	-1.37530500
C	12.99627000	-4.11338200	0.06642100
C	13.32574600	-5.49865100	0.07400300
C	14.03376000	-3.15617300	0.06245300
C	14.70060000	-5.88626500	0.07706100
C	12.32018700	-6.52509100	0.07805300
C	15.36602300	-3.53692800	0.06579600
H	13.76687700	-2.10691300	0.05679600
C	15.05103500	-7.27197200	0.08381400
C	15.73121700	-4.89550400	0.07299300
C	12.65470000	-7.84497800	0.08459300
H	11.28263100	-6.21501900	0.07552800
H	16.14435100	-2.78172200	0.06274100
C	14.02868100	-8.27026900	0.08762400
C	16.42614400	-7.66467400	0.08650600
C	17.10397100	-5.31994700	0.07611500
H	11.88275300	-8.60700100	0.08751100
C	14.39677200	-9.62668400	0.09395500
C	16.74537200	-9.03316500	0.09283200
C	17.43688500	-6.64025300	0.08253100
H	17.87482400	-4.55680900	0.07306800
C	15.74003700	-9.99924000	0.09647700
H	13.62048300	-10.38401900	0.09681300
H	17.78805500	-9.33179200	0.09482100
H	18.47726800	-6.94705800	0.08471800
H	16.00572300	-11.04994500	0.10131900
C	-8.18347600	-3.46898500	-0.79918000
C	-9.20074100	-2.71029100	-0.17719800
C	-8.90367500	-1.40785300	0.29650700
C	-7.62735500	-0.90125100	0.14224100
C	-6.61586600	-1.66822700	-0.48541900
C	-6.89860200	-2.95410700	-0.95446700
H	-8.41996900	-4.46297600	-1.15808300
H	-9.68670200	-0.83103300	0.77443100
H	-6.13072400	-3.54873700	-1.43589200
C	-5.62561300	0.37294000	0.09265500
C	-4.62149900	1.31921300	0.19167700
C	-3.09943100	-0.22427500	-0.92455600
C	-4.11101100	-1.17568400	-1.02356000
C	-5.37908800	-0.87948800	-0.51620700
H	-4.79773500	2.27991200	0.66223000

H	-2.11035700	-0.43283800	-1.31240800
H	-3.91148500	-2.13353500	-1.49118500
C	-10.50998400	-3.23900200	-0.02450300
C	-11.64007700	-3.66519900	0.11967100
C	-7.08026900	0.46601600	0.57400800
C	-7.83200400	1.61542900	-0.14044400
H	-8.88569100	1.62553000	0.16103300
H	-7.38519700	2.58017600	0.12579400
H	-7.77539500	1.48682000	-1.22508500
C	-7.14392800	0.62497500	2.11332500
H	-8.18607200	0.62322900	2.45287400
H	-6.61176800	-0.19762700	2.59907700
H	-6.67996500	1.57118800	2.41400100
C	-12.97070600	-4.12181900	0.30425800
C	-13.33708600	-5.46955200	0.02722200
C	-13.95110500	-3.22195800	0.77496700
C	-14.69008800	-5.87872500	0.23361800
C	-12.38942000	-6.43793700	-0.45110900
C	-15.26271800	-3.62296300	0.97204600
H	-13.65680800	-2.20059300	0.98088600
C	-15.07596600	-7.22863700	-0.03495300
C	-15.66295500	-4.94598800	0.71009700
C	-12.75775900	-7.72361200	-0.70695100
H	-11.36754600	-6.11248000	-0.60120000
H	-15.99696200	-2.91167400	1.33415600
C	-14.11093400	-8.16943300	-0.50947800
C	-16.42902900	-7.64309700	0.17170600
C	-17.01502900	-5.39079600	0.90698300
H	-12.02929800	-8.44198300	-1.06735300
C	-14.51279400	-9.49177100	-0.76526700
C	-16.78363800	-8.97589400	-0.09793000
C	-17.38180800	-6.67681200	0.65058800
H	-17.74205600	-4.67168000	1.26880400
C	-15.83409200	-9.88602700	-0.56043500
H	-13.78013600	-10.20568700	-1.12548200
H	-17.80955500	-9.29106300	0.05863200
H	-18.40588900	-6.99969100	0.80390100
H	-16.12623000	-10.90991700	-0.76267400
C	-3.33120800	1.03552700	-0.32111200

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5

5 12 1.0 16 1.5

6 7 1.5 15 1.5

7 8 1.5 22 1.0

8 9 1.5 24 1.0

9 10 1.5 13 1.0

10 14 1.0 15 1.5

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15 17 1.0

16 17 1.0

17 18 1.0 20 1.0

18 19 3.0

19 61 1.5

20 21 3.0

21 157 1.5

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24 26 1.0 30 1.0 34 1.0

25 38 1.0 42 1.0 46 1.0

26 27 1.0 28 1.0 29 1.0

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46 47 1.0 48 1.0 49 1.0

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50 51 1.5 55 1.5 56 1.0

51 52 1.5 68 1.5

52 53 2.0 57 1.0

53 54 1.5 70 1.0

54 55 1.5 64 1.0

55 58 1.0

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59 60 2.0 64 1.5 70 1.0

60 61 1.5 65 1.0

61 62 1.5

62 63 1.5 66 1.0

63 64 1.5 67 1.0

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81 84 2.0 85 1.0

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83 88 2.0 89 1.0

84 87 1.5 90 1.0

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91 95 1.5

92 96 1.5 97 1.5

93 97 2.0 98 1.0
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95 99 1.5 100 1.0
96 99 1.5 101 1.0
97 102 1.0
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99 103 1.0
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104 105 1.5 109 1.5 110 1.0
105 106 1.5 121 1.5
106 107 2.0 111 1.0
107 108 1.5 123 1.0
108 109 1.5 117 1.0
109 112 1.0
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113 114 2.0 117 1.5 123 1.0
114 118 1.0 157 1.5
115 116 1.5 119 1.0 157 1.5
116 117 1.5 120 1.0
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121 122 3.0
122 132 1.5
123 124 1.0 128 1.0
124 125 1.0 126 1.0 127 1.0
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128 129 1.0 130 1.0 131 1.0
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132 133 1.5 134 1.5
133 135 1.5 136 1.5
134 137 2.0 138 1.0
135 139 1.5 140 1.5
136 141 2.0 142 1.0

137 140 1.5 143 1.0
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139 144 1.5 145 1.5
140 146 1.5
141 144 1.5 147 1.0
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144 148 1.5
145 149 1.5 150 1.5
146 150 2.0 151 1.0
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148 152 1.5 153 1.0
149 152 1.5 154 1.0
150 155 1.0
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152 156 1.0
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The coordinates of complex Pt-5（DFT//B3LYP/6-31G(d)/ LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.47490700	7.36820600	-0.34552400
C	2.91420500	8.65280200	-0.29268200
C	1.51748600	8.72979000	-0.19206600
C	0.73399200	7.57986700	-0.14372600
C	2.65923000	6.24473400	-0.29795800
C	-0.73607100	7.58240300	-0.03558100
C	-1.51395600	8.73490100	0.03726400
C	-2.91117700	8.66265900	0.13379700
C	-3.47837800	7.38004100	0.15670200
C	-2.66815800	6.25388400	0.08535600
H	4.54271500	7.22832200	-0.42475700
H	3.04989500	5.23664700	-0.33879800
H	-4.54705000	7.24390400	0.23051400
H	-3.06361100	5.24701100	0.10236500
N	-1.32158500	6.34361300	-0.01028300
N	1.31314200	6.33896700	-0.19741500
Pt	-0.00823200	4.71295800	-0.12098400
C	-1.38404600	3.31961700	-0.03633000
C	-2.27375900	2.47973800	0.02595200

C	1.36342900	3.31712100	-0.23590300
C	2.25527500	2.48125200	-0.31709200
H	-1.02713500	9.69947400	0.01904000
H	1.03539300	9.69606700	-0.15180500
C	-3.74567700	9.95073900	0.21585900
C	3.75469700	9.93838700	-0.34871800
C	-3.34374200	10.72886200	1.49885800
H	-2.28251800	10.99795600	1.48387200
H	-3.93195800	11.65083800	1.56677100
H	-3.53650100	10.12269900	2.39011300
C	-3.46299900	10.82347100	-1.03733800
H	-4.05217900	11.74562000	-0.98067600
H	-2.40504100	11.09753700	-1.10284000
H	-3.74059800	10.28522700	-1.94960400
C	-5.26242100	9.65585300	0.27416700
H	-5.59747100	9.11795200	-0.61962600
H	-5.52204800	9.07078300	1.16332000
H	-5.80662400	10.60481900	0.32300100
C	3.35702700	10.74278700	-1.61673300
H	2.29672300	11.01518500	-1.59755300
H	3.94863100	11.66377400	-1.66642600
H	3.54852900	10.15316600	-2.51929200
C	3.47529300	10.78780300	0.92105600
H	4.06996500	11.70738900	0.88357900
H	2.41892200	11.06691400	0.99059900
H	3.74832200	10.22996600	1.82287200
C	5.27014300	9.63780900	-0.41205300
H	5.60219800	9.08020700	0.47072800
H	5.52779100	9.06995100	-1.31284200
H	5.81860700	10.58514100	-0.44126200
C	7.91587200	-3.19862400	-1.10936300
C	8.96252900	-2.51697800	-0.44774100
C	8.72082300	-1.22728300	0.08701700
C	7.46841200	-0.65718600	-0.04841700
C	6.42770600	-1.34836000	-0.71421600
C	6.65563500	-2.62127500	-1.24352300
H	8.11102700	-4.18400100	-1.51376800
H	9.52586200	-0.70831900	0.59409100
H	5.86436600	-3.15763800	-1.75475500
C	5.52303600	0.70496200	-0.04514800
C	4.55964500	1.68866900	0.09243100
C	3.26146000	1.48364700	-0.43719500
C	2.97898700	0.26354400	-1.09765300
C	3.94970200	-0.72465500	-1.23655700

C	5.22622900	-0.50640900	-0.71159800
H	4.77341400	2.61953800	0.60536800
H	1.98368100	0.11524300	-1.49729100
H	3.71205700	-1.65083700	-1.74814900
C	10.24361300	-3.11915900	-0.32294300
C	11.34035600	-3.63234900	-0.21813900
C	6.97925500	0.71290000	0.44222600
C	7.04678100	0.80315100	1.98683000
H	8.08746300	0.74304800	2.32568000
H	6.62274000	1.75417700	2.32829800
H	6.48000800	-0.01649100	2.43720400
C	7.78153600	1.85822000	-0.22206700
H	8.83416900	1.80927800	0.07930100
H	7.72122600	1.77876400	-1.31124200
H	7.37635500	2.82913300	0.08531500
C	12.62090300	-4.23472800	-0.10149800
C	-7.80551300	-3.34830000	0.61602600
C	-8.93565500	-2.57481100	0.26609900
C	-8.76765500	-1.20265400	-0.04488000
C	-7.50382300	-0.64350200	0.00035700
C	-6.37908200	-1.42744300	0.35340200
C	-6.53415800	-2.78173700	0.66030400
H	-7.94521000	-4.39598400	0.85143400
H	-9.63666500	-0.61398200	-0.31443900
H	-5.67815400	-3.38918100	0.93115200
C	-5.56765000	0.73095300	-0.05122700
C	-4.62609900	1.73984200	-0.15327000
C	-3.26304600	1.46291000	0.11704700
C	-2.89481000	0.14640500	0.48681900
C	-3.84309600	-0.86725700	0.58974400
C	-5.18369700	-0.57778600	0.32152300
H	-4.90835600	2.74621000	-0.44146000
H	-1.85082800	-0.05533300	0.69102400
H	-3.53902200	-1.86802200	0.87610800
C	-10.22577400	-3.16944700	0.22853300
C	-11.32821800	-3.68026000	0.19897000
C	-7.08251000	0.80380200	-0.29213700
C	-7.39176800	1.18564800	-1.76056500
H	-8.47348900	1.17589700	-1.93715600
H	-7.01197400	2.19090000	-1.97564100
H	-6.91507800	0.47626000	-2.44281100
C	-7.75526000	1.78675200	0.69705600
H	-8.84335900	1.77291800	0.56598000
H	-7.51923200	1.50548200	1.72725600

H	-7.39610800	2.80671100	0.51775200
C	-12.61142300	-4.28763000	0.16982900
C	-13.76680800	-3.53851600	-0.13874900
H	-13.66512900	-2.48466600	-0.36636700
C	-15.01873300	-4.13665100	-0.17066100
H	-15.89269700	-3.54897700	-0.41916800
C	-15.17067600	-5.50556000	0.11800400
C	-14.02236300	-6.25586200	0.43223900
H	-14.12535700	-7.30857600	0.66019600
C	-12.76862400	-5.66169400	0.45112800
H	-11.89447900	-6.25104100	0.69852800
C	12.87236400	-5.51608400	-0.63686600
H	12.06843200	-6.04592000	-1.13251600
C	14.12283600	-6.10623600	-0.52069300
H	14.29448700	-7.09358100	-0.92866700
C	15.17945900	-5.43551800	0.12313300
C	14.93527800	-4.15535700	0.65446300
H	15.73940600	-3.62677300	1.14914200
C	13.68139000	-3.57016800	0.55048100
H	13.51011900	-2.58263500	0.96060800
N	16.46295100	-6.03638700	0.23501200
N	-16.45413600	-6.11758500	0.09176200
C	-16.59972100	-7.45980200	-0.38177900
C	-17.43972700	-8.36380400	0.28823400
C	-15.90705000	-7.89156600	-1.52452500
C	-17.58690000	-9.66768700	-0.18157400
H	-17.97228800	-8.03571700	1.17152000
C	-16.04598700	-9.20204400	-1.97799400
H	-15.26188300	-7.19639200	-2.04600700
C	-16.88875000	-10.09670600	-1.31329300
H	-18.23874000	-10.35387800	0.34689300
H	-15.50423100	-9.52013500	-2.86134200
H	-16.99969400	-11.11290100	-1.67196900
C	-17.60628000	-5.39887300	0.53920000
C	-17.54249700	-4.58726900	1.68382500
C	-18.82182900	-5.49915000	-0.15708200
C	-18.66758600	-3.88542500	2.11238100
H	-16.60941900	-4.51079600	2.22690700
C	-19.94701300	-4.80768800	0.28789500
H	-18.87483800	-6.12137200	-1.04108100
C	-19.87717300	-3.99348400	1.42121600
H	-18.60164300	-3.26354000	2.99780800
H	-20.87758400	-4.89571900	-0.26107400
H	-20.75179000	-3.45188700	1.76080700

C	16.96863100	-6.86060200	-0.81890800
C	16.79466300	-6.48963200	-2.16231300
C	17.65142500	-8.05179900	-0.52399500
C	17.28216300	-7.30115300	-3.18498000
H	16.27430700	-5.56926400	-2.39392600
C	18.15123400	-8.84906800	-1.55195300
H	17.78606200	-8.34161900	0.51003600
C	17.96600000	-8.48291100	-2.88756800
H	17.13883900	-7.00144800	-4.21679000
H	18.67520900	-9.76612100	-1.30801000
H	18.34925000	-9.10860800	-3.68458100
C	17.25963900	-5.82207100	1.40384900
C	16.67733600	-5.85514300	2.68144000
C	18.63818900	-5.58091300	1.28937600
C	17.45783200	-5.64028500	3.81592800
H	15.61596700	-6.04593500	2.77468900
C	19.41510000	-5.38420800	2.42962500
H	19.08990900	-5.55193000	0.30619500
C	18.83065100	-5.40773600	3.69856400
H	16.99345500	-5.66905300	4.79497200
H	20.47796300	-5.19890200	2.32459200
H	19.43587600	-5.24773900	4.58271600

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 22 1.0
8 9 1.5 24 1.0
9 10 1.5 13 1.0
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168 170 1.5 172 1.0
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complex Pt-6（DFT//B3LYP/6-31G(d)/LanL2DZ）

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	11.05047000	2.28449600	0.00678600
C	11.02253500	0.88200200	0.00657300
C	9.81600600	0.18637100	0.00479300
N	8.62253200	0.86084700	0.00318400
C	8.63006400	2.21368800	0.00329800
C	9.81197900	2.94307500	0.00506200
C	9.70343900	-1.28246500	0.00454900
C	10.79287200	-2.15527400	0.00550200
C	10.60083000	-3.53916200	0.00517900
C	9.27751000	-4.01019000	0.00385900
C	8.22240800	-3.11193300	0.00291100
N	8.42452900	-1.76981200	0.00324200
C	12.39534500	3.02995800	0.00885300
C	11.78599600	-4.49540800	0.00612500
C	12.20578900	4.56390200	0.00900500
C	13.19649100	2.63212700	-1.26089100
C	13.19304000	2.63144200	1.28054900
C	11.78193200	-5.37581400	1.28119000

C	11.78435500	-5.37521700	-1.26938000
Pt	6.90177700	-0.33151300	0.00138000
C	5.38363400	-1.57077100	0.00036000
C	5.59534100	1.12879300	-0.00067000
C	4.42111700	-2.32828300	0.00003900
C	4.77179800	2.03545400	-0.00201500
C	3.22558800	-3.09606600	-0.00114400
C	1.64883900	4.89013000	-0.00388000
C	1.97013200	-2.43611400	-0.01542500
C	0.80354800	-3.17733800	-0.01672600
C	0.84663300	-4.59154500	-0.00368900
C	2.07523200	-5.25626000	0.01066200
C	3.25150800	-4.51015500	0.01183100
C	-0.64801400	-2.67780500	-0.03086600
C	-1.42126200	-4.00448100	-0.02661200
C	-0.52835800	-5.10319200	-0.00927100
C	-2.78875700	-4.20713100	-0.03580200
C	-3.29948900	-5.52869900	-0.02698500
C	-2.39950800	-6.61828700	-0.00890600
C	-1.02243700	-6.41042000	-0.00035200
C	-0.94518600	-1.86606300	-1.31550700
C	-0.96308300	-1.85021100	1.23959100
C	-4.70229600	-5.75533300	-0.03577400
C	-5.90356700	-5.93924200	-0.04304000
C	3.72812600	2.99954600	-0.00313700
C	4.00199800	4.38727800	-0.00246500
C	2.97523000	5.32856300	-0.00280600
C	1.35823600	3.50502800	-0.00486400
C	2.37647300	2.57035700	-0.00448900
C	0.38462300	5.63503100	-0.00354100
C	-0.68666000	4.70926600	-0.00432900
C	-0.15846400	3.26805400	-0.00579200
C	0.12650900	7.00867300	-0.00206800
C	-1.19309800	7.45380800	-0.00112300
C	-2.26959000	6.53809200	-0.00162700
C	-1.99764300	5.14760700	-0.00340500
C	-3.61146900	7.00558600	0.00016100
C	-4.76201700	7.39683200	0.00218000
C	-0.60580300	2.51413400	1.27068200
C	-0.60469200	2.51728200	-1.28454700
C	-7.30770100	-6.15781300	-0.05021300
C	-6.11121300	7.84293900	0.00487800
C	-7.82890100	-7.47232100	0.02838000
C	-9.19893100	-7.66378300	0.02166300

C	-10.08071700	-6.56149200	-0.06438200
C	-9.57765900	-5.26119900	-0.14260400
C	-8.19890900	-5.06377500	-0.13489700
C	-6.40845800	9.22493200	0.00508100
C	-7.72680200	9.67449300	0.00788400
C	-8.76542500	8.74103900	0.01051200
C	-8.48019600	7.35597500	0.01033500
C	-7.17250900	6.90514600	0.00755500
C	-9.98308900	-8.98110700	0.09897300
C	-11.42966800	-8.47290100	0.04148400
C	-11.46376800	-7.06312100	-0.05268900
C	-10.22573600	8.92034500	0.01375300
C	-10.83539100	7.64498700	0.01552600
C	-9.77671200	6.53465000	0.01352000
C	-12.61114800	-9.20181600	0.07156800
C	-13.83472000	-8.52050000	0.00761400
C	-13.86778300	-7.12462000	-0.08529100
C	-12.68191300	-6.38467400	-0.11608600
C	-11.00313900	10.07956600	0.01520000
C	-12.39583000	9.95715500	0.01844600
C	-13.00009800	8.69501800	0.02019300
C	-12.21924300	7.53061100	0.01873200
C	-9.70626900	-9.71420800	1.43492800
C	-9.66433700	-9.88923900	-1.11446600
C	-9.87940900	5.66617300	1.29195500
C	-9.88514600	5.66535800	-1.26388900
H	11.95030000	0.32750800	0.00790500
H	7.65486700	2.68194300	0.00195800
H	9.75323500	4.02125100	0.00512300
H	11.79952300	-1.75909800	0.00645000
H	9.06609000	-5.07129900	0.00352100
H	7.18602400	-3.42171400	0.00184200
H	12.70137400	-3.89033000	0.00713300
H	11.66433500	4.89797400	0.90094400
H	11.66683000	4.89845200	-0.88425800
H	13.18996300	5.04401200	0.01050100
H	12.64391600	2.90978500	-2.16457500
H	13.39030900	1.55496300	-1.28839600
H	14.15971400	3.15445500	-1.26387600
H	12.63790800	2.90836400	2.18288800
H	14.15613000	3.15398000	1.28654700
H	13.38704900	1.55430600	1.30787600
H	12.66219100	-6.02774900	1.28657800
H	11.79743100	-4.75760000	2.18434100

H	10.88759200	-6.00748000	1.30825600
H	12.66466500	-6.02709200	-1.27345000
H	11.80148400	-4.75656300	-2.17219900
H	10.89010200	-6.00692200	-1.29840200
H	1.95539000	-1.35258700	-0.02524400
H	2.11834500	-6.33987700	0.02066900
H	4.21271900	-5.00941100	0.02297000
H	-3.48279800	-3.37503500	-0.04872700
H	-2.80026900	-7.62424300	-0.00229300
H	-0.34619800	-7.25761800	0.01305000
H	-2.00424000	-1.58608900	-1.35085400
H	-0.34460300	-0.94924800	-1.33079000
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H	-2.02237900	-1.56939000	1.25640000
H	5.03604200	4.70997100	-0.00146900
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H	2.17200300	1.50616100	-0.00487600
H	0.94047700	7.72466900	-0.00145900
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H	-0.27150000	3.04940900	2.16381000
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H	-0.17709400	1.50823800	-1.29995100
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H	-12.71201100	-5.30326700	-0.18811900
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H	-13.01381300	10.84765100	0.01962100
H	-14.08121100	8.61720200	0.02270800
H	-12.69632400	6.55649000	0.02012900
H	-10.32788600	-10.61390900	1.50707800
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H	-9.93349900	-9.05848200	2.28017300
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