Electronic Supporting Information

Different structural preference of Ag(I) and Au(I) in neutral and cationic luminescent heteropolynuclear platinum(II) complexes: Z (U)-shaped Pt_2M_2 type vs. trinuclear PtM_2 type

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Experimental section

Materials. $[Pt(N^C)(\mu\text{-}Cl)]_2$ (N^C = ppy (2-phenylpyridinate), bzq (benzo[*h*]quinolinate)),[1] [PtCl(dfppy)(Hdfppy)] (dfppy = 2-(2,4-difluorophenyl)pyridinate),[2] $[PtCl_2(bpy)]$[3] and [AuCl(tht)] (tht = tetrahydrothiophene)[4] were prepared by the literature methods. All other commercially available reagents were used as purchased.

Physical Measurement and Instrumentation. The ^{1}H NMR spectra were obtained at 300 MHz with a Varian Gemini 300 spectrometer. UV/Vis spectra were recorded on a Jasco V-560 spectrophotometer at 20°C. Corrected emission spectra were obtained by using a Jasco FP-6500 spectrofluorometer (λ_{ex} = 350 nm). Lifetime measurements were conducted by using a streak camera (Hamamatsu C4334) as a detector and the third-harmonic generation of an Nd:YAG Laser (Continuum Minilite) at 355 nm excitation. Emission quantum yields in the solid state were determined by using a Hamamatsu Photonic Absolute PL Quantum Yield Measurement System C9920-02. Powder X-ray diffraction patterns were measured on Rigaku RINT-2200VL and Rigaku SmartLab diffractometer with Cu Kα (λ = 1.5418 Å) radiation at 296 K.

Preparation of Complexes. $[Pt(ppy)(Me_2pzH)_2]Cl$ (1a). To a solution of $[Pt(ppy)(\mu\text{-}Cl)]_2$ (40 mg, 0.052 mmol) in dichloromethane (5 mL) was added a solution of Me_2pzH (20 mg, 0.21 mmol) in dichloromethane (5 mL). The solution was refluxed for 3 h with stirring under air and concentrated to dryness. The pale yellow-brown solid was dissolved into methanol, and the solution was filtered. The filtrate was again concentrated to dryness, and the solid was extracted with dichloromethane. The extract was concentrated, and *n*-hexane was added to the solution. The resulted pale yellow-brown precipitate was collected, washed with diethyl ether, and dried in vacuum. Yield 48 mg (80%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{21}H_{24}ClN_5Pt$: C, 43.71; H, 4.19; N, 12.14. Found: C, 43.60; H, 4.04; N, 12.36. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.83 (ddd, *J* = 7.5, 7.4, 1.5 Hz, 1H), 7.68 (d, *J* = 7.7 Hz, 1H), 7.43 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.37 (dd, *J* = 5.8, 0.8 Hz, 1H), 7.06 (ddd, *J* = 7.5, 7.4, 1.2 Hz, 1H), 6.96 (m, 2H), 6.15 (dd, *J* = 7.5, 0.8 Hz, 1H), 5.99 (s, 1H), 5.98 (s, 1H), 2.43 (s, 3H), 2.42 (s, 6H), 2.36 ppm (s, 3H). ESIMS: *m*/*z* 541.3 $[M–Cl]^+$.

$[Pt(dfppy)(Me_2pzH)_2]Cl$ (1b). To a solution of [PtCl(dfppy)(Hdfppy)] (90 mg, 0.15 mmol) in dichloromethane (5 mL) was added a solution of Me_2pzH (41 mg, 0.42 mmol) in dichloromethane

(5 mL). The solution was refluxed for 3 h with stirring under an argon atmosphere and concentrated to dryness. The yellow solid was dissolved into methanol, and the solution was filtered. The filtrate was again concentrated to dryness, and the solid was extracted with dichloromethane. The extract was concentrated, and *n*-hexane was added to the solution. The resulted yellow precipitate was collected, washed with diethyl ether, and dried in vacuum. Yield 60 mg (66%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{21}H_{22}ClF_2N_5Pt$: C, 41.15; H, 3.62; N, 11.43. Found: C, 41.11; H, 3.49; N, 11.55. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 8.07 (d, *J* = 8.4 Hz, 1H), 7.87 (t, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 5.0 Hz, 1H), 7.00 (ddd, *J* = 6.7, 6.7, 1.2 Hz, 1H), 6.56 (ddd, 12.4, 9.3, 2.3 Hz, 1H), 6.00 (s, 2H), 5.98 (s, 1H), 5.60 (dd, *J* = 8.7, 2.3 Hz, 1H), 2.43 (s, 3H), 2.42 (s, 3H), 2.41 (s, 3H), 2.40 ppm (s, 3H). ESIMS: *m*/*z* 577.2 $[M–Cl]^+$.

[Pt(bzq)(Me$_2$pzH)$_2$]Cl (1c). To a solution of $[Pt(bzq)(\mu\text{-}Cl)]_2$ (60 mg, 0.073 mmol) in dichloromethane (5 mL) was added a solution of Me_2pzH (28 mg, 0.29 mmol) in dichloromethane (5 mL). The solution was refluxed for 3 h with stirring under air and concentrated to dryness. The brown solid was dissolved into methanol, and the solution was filtered. The filtrate was again concentrated to dryness, and the solid was extracted with dichloromethane. The extract was concentrated, and *n*-hexane was added to the solution. The resulted yellow precipitate was collected, washed with diethyl ether, and dried in vacuum. Yield 64 mg (73%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{23}H_{24}ClN_5Pt$: C, 45.96; H, 4.03; N, 11.65. Found: C, 46.10; H, 3.76; N, 11.72. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 8.31 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.62 (d, *J* = 5.3 Hz, 1H), 7.57 (d, *J* = 6.4 Hz, 1H), 7.54 (d, *J* = 7.3 Hz, 1H), 7.37 (d, *J* = 7.3 Hz, 1H), 7.31 (dd, *J* = 9.3, 3.7 Hz, 1H), 6.47 (d, *J* = 7.2 Hz, 1H), 6.05 (s, 1H), 6.04 (s, 1H), 2.47 (s, 6H), 2.46 (s, 3H), 2.42 ppm (s, 3H). ESIMS: *m*/*z* 565.3 $[M–Cl]^+$.

[Pt(bpy)(Me$_2$pzH)$_2$](PF$_6$)$_2$ (1d). To a suspension of $[PtCl_2(bpy)]$ (80 mg, 0.19 mmol) in acetonitrile (5 mL) was added a solution of $AgPF_6$ (96 mg, 0.38 mmol) in acetonitrile (5 mL). The suspension was stirred for 2 h at 80 °C in the dark, and resulted precipitate (AgCl) was filtered off. To the filtrate was added a solution of Me_2pzH (37 mg, 0.38 mmol) in acetonitrile (5 mL), and the solution was stirred for 2 h at 80 °C under air and filtered. The filtrate was concentrated to dryness, and the residue was dissolved into small amount of dichloromethane. The addition of

n-hexane to the dichloromethane solution resulted white precipitate. It was collected, washed with *n*-hexane, and dried in vacuum. Yield 127 mg (80%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{20}H_{24}F_{12}N_6P_2Pt$: C, 28.82; H, 2.90; N, 10.08. Found: C, 29.30; H, 3.01; N, 9.95. ^{1}H NMR (300 MHz, acetone-d_6, 25°C, TMS): δ = 8.76 (d, *J* = 8.4 Hz, 2H), 8.60 (ddd, *J* = 7.9, 7.9, 1.2 Hz, 2H), 7.96 (d, *J* = 5.5 Hz, 2H), 7.88 (ddd, *J* = 7.5, 5.9, 1.3 Hz, 2H), 6.42 (s, 2H), 2.57 (s, 6H), 2.44 ppm (s, 6H). ESIMS: *m*/*z* 688.1 $[M–PF_6]^+$.

$[Pt_2Ag_2(ppy)_2(\mu\text{-}Me_2pz)_4]$ (2a). To a solution of **1a** (60 mg, 0.10 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (26 mg, 0.10 mmol) in methanol (5 mL). The solution was stirred for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. A solution of $AgBF_4$ (20 mg, 0.10 mmol) in methanol (5 mL) and Et_3N (28 μL, 0.20 mmol) were added to the solution, and the mixture was stirred for 3 h in the dark. The resulted yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 36 mg (53%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{34}H_{34}Ag_2Cl_4N_6Pt_2$: C, 36.08; H, 3.30; N, 9.56. Found: C, 36.40; H, 3.42; N, 9.68. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.57 (dd, *J* = 7.6, 7.5 Hz, 1H), 7.50 (ddd, *J* = 7.6, 7.5, 1.1 Hz, 1H), 7.39-7.20 (m, 5H), 7.01-6.97 (m, 2H), 6.95-6.85 (m, 2H), 6.78 (t, *J* = 7.0 Hz, 1H), 6.63 (t, *J* = 6.0 Hz, 1H), 6.53-6.44 (m, 2H), 6.11 (d, *J* = 7.0 Hz, 1H), 5.89 (s, 2H), 5.82 (s, 1H), 5.81 (s, 1H), 2.22 (s, 3H), 2.18 (s, 3H), 2.16 (s, 3H), 2.12 (s, 3H), 2.07 (s, 3H), 1.99 (s, 3H), 1.90 (s, 3H), 1.74 ppm (s, 3H). ESIMS: *m*/*z* 1294.2 $[M]^+$.

$[Pt_2Ag_2(dfppy)_2(\mu\text{-}Me_2pz)_4]$ (2b). To a solution of **1b** (40 mg, 0.065 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (17 mg, 0.065 mmol) in methanol (5 mL). The solution was stirred for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. A solution of $AgBF_4$ (13 mg, 0.065 mmol) in methanol (5 mL) and Et_3N (36 μL, 0.26 mmol) were added to the solution, and the mixture was stirred for 3 h in the dark. The resulted pale yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 27 mg (61%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{42}H_{40}Ag_2F_4N_{10}Pt_2$: C, 36.91; H, 32.95; N, 10.25. Found: C, 37.11; H, 3.15; N, 10.33. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.80 (d, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 5.7 Hz, 1H), 7.18 (d, *J* = 5.7 Hz, 1H), 6.75 (t, *J* = 6.8 Hz, 1H), 6.68 (t, *J* = 6.8 Hz, 1H), 6.41 (ddd, *J* = 12.1, 9.6, 2.5 Hz, 1H), 6.37 (ddd, *J* = 12.1, 9.6, 2.5 Hz, 1H), 5.91 (s, 1H), 5.90 (s, 1H), 5.88 (s, 1H), 5.86 (s, 1H), 5.85 (dd, *J* = 7.7, 2.4 Hz, 1H), 5.61 (d, *J* = 7.9 Hz, 1H), 2.17 (s, 3H), 2.14 (s, 3H), 2.13

(s, 3H), 2.10 (s, 3H), 2.09 (s, 3H), 2.02 (s, 6H), 2.00 ppm (s, 3H). ESIMS: *m/z* 1366.2 [*M*]$^+$.

[$Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4$] (2c). To a solution of **1c** (60 mg, 0.10 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (25 mg, 0.10 mmol) in methanol (5 mL). The solution was stirred for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. A solution of $AgBF_4$ (19 mg, 0.10 mmol) in methanol (5 mL) and Et_3N (60 μL, 0.40 mmol) were added to the solution, and the mixture was stirred for 3 h in the dark. The resulted yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 40 mg (60%). It was recrystallized from chloroform/*n*-hexane. Anal. Calcd for $C_{46}H_{44}Ag_2N_{10}Pt_2$: C, 41.14; H, 3.30; N, 10.43. Found: C, 41.18; H, 3.33; N, 10.49. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.97 (d, *J* = 8.0 Hz, 1H), 7.81 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.66 (d, *J* = 6.3 Hz, 1H), 7.64 (d, *J* = 6.3 Hz, 1H), 7.47 (d, *J* = 7.3 Hz, 1H), 7.40 (dd, *J* = 8.9, 1.4 Hz, 1H), 7.37 (d, *J* = 8.9 Hz, 4H), 7.03 (t, *J* = 7.3 Hz, 1H), 6.97 (dd, *J* = 6.9, 0.7 Hz, 1H), 6.75 (t, *J* = 6.2 Hz, 1H), 6.51 (d, *J* = 5.5 Hz, 1H), 6.39 (dd, *J* = 7.9, 5.4 Hz, 1H), 6.16 (d, *J* = 6.2 Hz, 1H) 5.92 (s, 1H), 5.89 (s, 1H), 5.80 (s, 1H), 5.77 (s, 1H), 2.25 (s, 3H), 2.12 (s, 3H), 2.11 (s, 3H), 2.06 (s, 9H), 1.97 (s, 3H), 1.86 ppm (s, 3H). ESIMS: *m/z* 1343.2 [*M*]$^+$.

[$PtAu_2(ppy)(\mu\text{-}Me_2pz)_3$] (3a). To a solution of **1a** (60 mg, 0.10 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (26 mg, 0.10 mmol) in methanol (5 mL). The solution was stirred for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. The filtrate was concentrated to dryness and the yellow residue was dissolved into dichloromethane (5 mL). To this dichloromethane solution was added solutions of AuCl(tht) (67 mg, 0.21 mmol) in dichloromethane (5 mL) and Me_2pzH (10 mg, 0.10 mmol) in dichloromethane (5 mL) and Et_3N (43 μL, 0.31 mmol) were added to the solution, and the mixture was stirred for 1 h at 25 °C under an argon atmosphere. The yellow solution was filtered and the filtrate was concentrated to dryness. The resulted yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 48 mg (45%). It was recrystallized from chloroform/*n*-pentane. Anal. Calcd for $C_{26}H_{29}Au_2N_7Pt$: C, 30.36; H, 2.84; N, 9.53. Found: C, 30.60; H, 2.52; N, 9.65. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.70 (ddd, *J* = 7.7, 7.7, 1.5 Hz, 1H), 7.57 (m, 1H), 7.36 (m, 1H), 7.03-6.96 (m, 2H), 6.94-6.82 (m, 2H), 6.12 (s, 2H), 6.06 (s, 1H), 5.83 (m, 1H), 2.47 (s, 3H), 2.43 (s, 3H), 2.37 (s, 3H), 2.36 (s, 3H), 2.14 (s, 3H), 2.13 ppm (s, 3H). ESIMS: *m/z* 1028.2 [*M*]$^+$.

[$PtAu_2(dfppy)(\mu\text{-}Me_2pz)_3$] (3b). To a solution of **1b** (40 mg, 0.065 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (17 mg, 0.10 mmol) in methanol (5 mL). The solution was stirred

for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. The filtrate was concentrated to dryness and the yellow residue was dissolved into dichloromethane (5 mL). To this dichloromethane solution was added solutions of AuCl(tht) (42 mg, 0.13 mmol) in dichloromethane (5 mL) and Me_2pzH (6.3 mg, 0.065 mmol) in dichloromethane (5 mL) and Et_3N (32 μL, 0.23 mmol) were added to the solution, and the mixture was stirred for 1 h at 25 °C under an argon atmosphere. The yellow solution was filtered and the filtrate was concentrated to dryness. The resulted yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 23 mg (33%). It was recrystallized from dichloromethane/*n*-hexane. Anal. Calcd for $C_{26}H_{27}Au_2F_2N_7Pt$: C, 29.33; H, 2.56; N, 9.21. Found: C, 29.70; H, 2.27; N, 9.34. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 8.01 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.76 (ddd, *J* = 8.5, 7.2, 1.1 Hz, 1H), 6.94 (ddd, *J* = 7.8, 5.3, 1.4 Hz, 1H), 6.88 (dd, *J* = 5.9, 1.1 Hz, 1H), 6.49 (ddd, *J* = 12.6, 9.2, 2.4 Hz, 1H), 6.13 (s, 2H), 6.10 (s, 1H), 5.26 (dd, *J* = 9.2, 2.4 Hz, 1H), 2.46 (s, 3H), 2.41 (s, 3H), 2.37 (s, 3H), 2.36 (s, 3H), 2.16 (s, 3H), 2.14 ppm (s, 3H). ESIMS: *m*/*z* 10.64.2 [*M*]$^+$.

[$PtAu_2$(bzq)(μ-Me_2pz)$_3$] (3c). To a solution of **1c** (80 mg, 0.13 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (34 mg, 0.13 mmol) in methanol (5 mL). The solution was stirred for 1 h at 25 °C in the dark, and resulted precipitate (AgCl) was filtered off. The filtrate was concentrated to dryness and the yellow residue was dissolved into dichloromethane (5 mL). To this dichloromethane solution was added solutions of AuCl(tht) (85 mg, 0.27 mmol) in dichloromethane (5 mL) and Me_2pzH (13 mg, 0.13 mmol) in dichloromethane (5 mL) and Et_3N (56 μL, 0.40 mmol) were added to the solution, and the mixture was stirred for 1 h at 25 °C under an argon atmosphere. The yellow solution was filtered and the filtrate was concentrated to dryness. The resulted yellow precipitate was collected, washed with methanol, and dried in vacuum. Yield 53 mg (38%). It was recrystallized from acetone/methanol. Anal. Calcd for $C_{28}H_{29}Au_2N_7Pt$: C, 31.95; H, 2.78; N, 9.32. Found: C, 32.06; H, 2.85; N, 9.28. ^{1}H NMR (300 MHz, CD_2Cl_2, 25°C): δ = 8.23 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.51 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.30 (m, 2H), 7.15 (dd, *J* = 5.5, 1.4 Hz, 1H), 6.18 (s, 2H), 6.14 (dd, *J* = 7.2, 0.9 Hz, 1H), 6.01 (s, 1H), 2.45 (s, 3H), 2.42 (s, 3H), 2.39 (s, 3H), 2.37 (s, 3H), 2.04 ppm (s, 6H). ESIMS: *m*/*z* 1052.2 [*M*]$^+$.

[Pt_2Ag_2(bpy)$_2$(μ-Me_2pz)$_4$](PF_6)$_2$ (4d). To a solution of **1d** (40 mg, 0.048 mmol) in methanol (5 mL) was added a solution of $AgPF_6$ (12 mg, 0.048 mmol) in methanol (5 mL) and Et_3N (13 μL,

0.096 mmol). The mixture was stirred for 3 h at 25 °C in the dark. After filtration, the filtrate was concentrated. The resulted yellow precipitate was collected, washed with methanol and diethyl ether, and dried in vacuum. Yield 28 mg (74%). It was recrystallized from acetone/*n*-hexane. Anal. Calcd for $C_{40}H_{44}Ag_2F_{12}N_{12}P_2Pt_2$: C, 30.24; H, 2.79; N, 10.58. Found: C, 30.44; H, 2.64; N, 10.65. ^{1}H NMR (300 MHz, acetone-d_6, 25°C): δ = 8.55-8.47 (m, 8H), 7.77 (ddd, *J* = 7.3, 5.6, 1.9 Hz, 4H), 7.56 (d, *J* = 5.2 Hz, 4H), 6.10 (s, 4H), 2.23 (s, 12H), 2.10 ppm (s, 12H). ESIMS: *m*/*z* 1442.9 $[M–PF_6]^+$.

$[Pt_2Au_2(bpy)_2(\mu\text{-}Me_2pz)_4](PF_6)_2$ (5d). To a solution of **1d** (60 mg, 0.072 mmol) in dichloromethane (5 mL) was added a solution of AuCl(tht) (23 mg, 0.072 mmol) in dichloromethane (5 mL) and Et_3N (20 μL, 0.144 mmol). The mixture was stirred for 1 h at 25 °C under an argon atmosphere. The resulted yellow precipitate was collected, washed with dichloromethane and *n*-hexane, and dried in vacuum. Yield 34 mg (54%). It was recrystallized from acetonitrile/diethyl ether. Anal. Calcd for $C_{40}H_{44}Au_2F_{12}N_{12}P_2Pt_2$: C, 27.19; H, 2.51; N, 9.51. Found: C, 27.35; H, 2.43; N, 9.78. ^{1}H NMR (300 MHz, acetone-d_6, 25°C): δ = 8.81 (d, *J* = 7.7 Hz, 4H), 8.61 (ddd, *J* = 7.9, 7.9, 1.5 Hz, 4H), 8.24 (dd, *J* = 5.7, 0.8 Hz, 4H), 7.98 (ddd, *J* = 7.5, 5.9, 1.3 Hz, 4H), 6.04 (s, 4H), 2.46 (s, 12H), 1.59 ppm (s, 12H). ESIMS: *m*/*z* 1621.2 $[M–PF_6]^+$.

X-ray Structural Determinations. Crystals suitable for X-ray structural analysis were obtained by recrystallization from dichloromethane/*n*-hexane (**2a**·$2CH_2Cl_2$, **2b**·$2CH_2Cl_2$, **3b**·$0.5CH_2Cl_2$), chloroform/*n*-hexane (**2c**), acetone/methanol (**3c**), acetone/*n*-hexane (**4d**·$(CH_3)_2CO$) and acetonitrile/diethyl ether (**5d**·$2CH_3CN$), respectively. Intensity data were collected on a Rigaku Saturn724 diffractometer using multi-layer mirror monochromated Mo Kα (λ = 0.71075 Å) radiation at 93 K. The data were corrected for Lorentz and polarization effects. An empirical absorption correction was applied.

The crystal structures were solved by direct method (SIR2008[5] for **2b**·$2CH_2Cl_2$, **2c**, **3b**·$0.5CH_2Cl_2$, **4d**·$(CH_3)_2CO$ and **5d**·$2CH_3CN$ and SIR92[6] for **2a**·$2CH_2Cl_2$) or heavy-atom method by using DIRDIF[7] (**3c**). The positional and thermal parameters of non-H atoms were refined anisotropically by the full-matrix least-squares method except for dichloromethane molecule in **3b**·$0.5CH_2Cl_2$. Disorder of C^N chelate ligands (ppy, dfppy and bzq) was observed for **2a**·$2CH_2Cl_2$, **2b**·$2CH_2Cl_2$, **2c** and **3c**. Among them, the site occupancy factors of C^N chelate were refined for **2b**·$2CH_2Cl_2$ and **3c**. The minimized function was $\Sigma w(F_o^2\text{-}F_c^2)^2$. Hydrogen atoms

were included at calculated positions with fixed displacement parameters. In the final cycle of the refinement, parameter shifts were less than 0.1σ. No correction was made for secondary extinction.

All calculations were performed using the CrystalStructure[8] crystallographic software package except for refinement, which was performed using SHELXL-97.[9] Listings of the selected bond distances and angles are summarized in Tables S2-S8.

Computational methods. The geometries of **2a**, **2b**, **2c**, **3b**, **3c**, **4d** and **5d** were optimized with the DFT method, where B3LYP functional was employed.[10] X-ray structures were used as initial geometries without any geometrical constraints. Since the ^{1}H NMR spectra of **2a**, **2b** and **2c** indicate that the crystals of these complexes contain two geometrical isomers, the geometries of possible isomers were optimized individually by using disordered X-ray structures as initial geometries. The structures of geometrical isomers are shown in Fig. S22. In these calculations, for all metals, basis sets with ECPs proposed by Christiansen et al were employed.[11] In details, for Ag, Au, and Pt atoms, (541/541/211), (541/551/211), and (541/5511/211) basis sets were used, respectively. For F, C, N, and H atoms, cc-pVDZ basis sets were used.[12] All calculations were carried out using the Gaussian 09 package.[13] Molecular orbitals with the isovalue of 0.02 were drawn by the Gauss View 5.[14]

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Table S1 Crystallographic Information

	2a·2CH_2Cl_2	**2b**·2CH_2Cl_2	**2c**
Empirical formula	$C_{44}H_{48}Ag_2Cl_4N_{10}Pt_2$	$C_{44}H_{44}Ag_2Cl_4F_4N_{10}Pt_2$	$C_{46}H_{44}Ag_2N_{10}Pt_2$
Formula weight	1464.66	1536.62	1342.84
Temperature (K)	93(1)	93(1)	93(1)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P*–1	*P*–1	$P2_1/n$
Unit cell dimensions			
a (Å)	9.481(2)	9.841(3)	11.740(2)
b (Å)	11.831(3)	11.774(3)	16.500(2)
c (Å)	12.311(4)	12.813(2)	21.910(3)
α (deg)	114.544(2)	59.90(2)	
β (deg)	103.778(3)	67.36(2)	92.460(2)
γ (deg)	100.725(2)	79.67(3)	
V (Å^3)	1154.8(5)	1185.4(6)	4240.3(9)
Z	1	1	4
ρ_{calcd} (g/cm^3)	2.106	2.152	2.103
μ(Mo Kα) (mm^{-1})	7.123	6.956	7.506
F(000)	700	732	2560
Index ranges	-11<=h<=12	-11<=h<=12	-15<=h<=15
	-15<=k<=15	-15<=k<=15	-20<=k<=21
	-15<=l<=15	-16<=l<=16	-28<=l<=26
Reflections collected	14397	9923	34852
Independent reflections	5272 [R_{int} = 0.0329]	5363 [R_{int} = 0.0204]	9717 [R_{int} = 0.0380]
Data / restraints / parameters	5272 / 12 / 284	5363 / 159 / 321	9717 / 0 / 549
Goodness-of-fit on F^2	0.909	1.073	1.130
Final *R* index [$I>2\sigma(I)$][a]	R_1 = 0.0181	R_1 = 0.0268	R_1 = 0.0374
R indices (all data)[a,b]	R_1 = 0.0205, wR_2 = 0.0355	R_1 = 0.0324, wR_2 = 0.0642	R_1 = 0.0440, wR_2 = 0.0676
Largest diff. peak and hole (e.Å^{-3})	0.860 and –0.690	1.51 and –1.12	2.13 and –1.14
CCDC number	1438721	1438722	1438723

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Table S1 Crystallographic Information (continued)

3b·0.5CH_2Cl_2	**3c**	**4d**·$(CH_3)_2CO$	**5d**·2CH_3CN
$C_{26.5}H_{28}Au_2ClF_2N_7Pt$	$C_{28}H_{29}Au_2N_7Pt$	$C_{43}H_{50}Ag_2F_{12}N_{12}OP_2Pt_2$	$C_{44}H_{50}Au_2F_{12}N_{14}P_2Pt_2$
1107.03	1052.61	1646.79	1849.01
293(1)	93(1)	93(1)	93(1)
0.71073	0.71073	0.71073	0.71073
Triclinic	Monoclinic	Monoclinic	Triclinic
P–1	$P2_1/c$	$P2_1/n$	*P*–1
11.388(2)	10.832(2)	13.979(2)	10.2943(13)
11.5678(19)	16.340(3)	17.286(3)	11.4915(15)
12.457(3)	16.739(3)	21.804(3)	12.268(2)
72.169(10)			86.513(5)
77.301(10)	105.934(4)	94.440(3)	88.377(5)
68.929(9)			65.233(4)
1446.5(5)	2848.8(9)	5252.9(13)	1315.3(3)
2	4	4	1
2.541	2.454	2.082	2.334
15.092	15.220	6.171	11.011
1014	1928	3152	864
-14<=h<=14	-14<=h<=14	-18<=h<=17	-13<=h<=13
-15<=k<=14	-21<=k<=16	-22<=k<=22	-13<=k<=14
-16<=l<=16	-19<=l<=21	-28<=l<=23	-15<=l<=15
12150	23136	43379	10943
6546 [R_{int} = 0.0384]	6465 [R_{int} = 0.0351]	12021 [R_{int} = 0.0422]	5394 [R_{int} = 0.0210]
6545 / 177 / 361	6465 / 0 / 350	12021 / 36 / 677	5394 / 0 / 348
1.004	0.971	1.104	0.933
R_1 = 0.0435	R_1 = 0.0206	R_1 = 0.0416	R_1 = 0.0183
R_1 = 0.0666, wR_2 = 0.0995	R_1 = 0.0260, wR_2 = 0.0436	R_1 = 0.0512, wR_2 = 0.0793	R_1 = 0.0252, wR_2 = 0.0381
2.55 and –2.23	1.48 and –1.92	1.92 and –0.87	1.39 and –1.06
1438724	1438725	1438726	1438727

a $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. *b* $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Table S2 Selected Bond Lengths [Å] and Angles [°] for $[Pt_2Ag_2(ppy)_2(\mu\text{-}Me_2pz)_4]\cdot 2CH_2Cl_2$ (**2a**$\cdot 2CH_2Cl_2$)

Pt1	···	Pt1'	5.9137(15)	Pt1	–	N21/C21	2.003(3)
Pt1	···	Ag1	3.2815(7)	Pt1	–	N31	2.053(3)
Pt1	···	Ag1'	3.4301(8)	Pt1	–	N41	2.043(3)
Ag1	···	Ag1'	3.1772(7)	Ag1	–	N32	2.0926(19)
Pt1	–	N11/C11	1.998(4)	Ag1	–	N42'	2.0971(18)
N32	–	Ag1	– N42' 161.89(11)				

Table S3 Selected Bond Lengths [Å] and Angles [°] for $[Pt_2Ag_2(dfppy)_2(\mu\text{-}Me_2pz)_4]\cdot 2CH_2Cl_2$ (**2b**$\cdot 2CH_2Cl_2$)

Pt1	···	Pt1'	5.9228(15)	Pt1	–	N21/C21	2.015(5)
Pt1	···	Ag1	3.3606(11)	Pt1	–	N31	2.051(4)
Pt1	···	Ag1'	3.3683(8)	Pt1	–	N41	2.041(5)
Ag1	···	Ag1'	3.1936(11)	Ag1	–	N32	2.090(4)
Pt1	–	N11/C11	2.005(4)	Ag1	–	N42'	2.095(4)
N32	–	Ag1	– N42' 161.81(19)				

Table S4 Selected Bond Lengths [Å] and Angles [°] for $[Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4]$ (**2c**)

Pt1	···	Pt2	5.9174(6)	Pt1	–	N51	2.019(5)
Pt1	···	Ag1	3.6814(7)	Pt2	–	N21/C21	1.989(6)
Pt1	···	Ag2	3.4574(5)	Pt2	–	N30/C30	2.036(5)
Pt2	···	Ag1	3.3546(6)	Pt2	–	N61	2.093(5)
Pt2	···	Ag2	3.6686(6)	Pt2	–	N71	2.002(5)
Ag1	···	Ag2	3.1023(6)	Ag1	–	N42	2.097(5)
Pt1	–	N1/C1	1.987(5)	Ag1	–	N72	2.094(5)
Pt1	–	N10/C10	2.038(5)	Ag2	–	N52	2.072(5)
Pt1	–	N41	2.097(5)	Ag2	–	N62	2.077(5)
N42	–	Ag1	– N72 169.05(17)	N52	–	Ag2	– N62 170.91(17)

Table S5 Selected Bond Lengths [Å] and Angles [°] for $[PtAu_2(dfppy)(\mu\text{-}Me_2pz)_3]\cdot 0.5CH_2Cl_2$ (**3b**·$0.5CH_2Cl_2$)

Pt1	···	Au1	3.4026(7)	Pt1	–	N41	2.095(9)
Pt1	···	Au2	3.3979(9)	Au1	–	N32	1.998(11)
Au1	···	Au2	3.0070(9)	Au1	–	N51	2.007(12)
Pt1	–	N11	2.026(8)	Au2	–	N42	1.980(8)
Pt1	–	C21	1.980(9)	Au2	–	N52	1.990(9)
Pt1	–	N31	2.036(10)				
N32	–	Au1	– N51 175.7(4)	N42	–	Au2	– N52 176.3(5)

Table S6 Selected Bond Lengths [Å] and Angles [°] for $[PtAu_2(bzq)(\mu\text{-}Me_2pz)_3]$ (**3c**)

Pt1	···	Au1	3.3712(6)	Pt1	–	N31	2.098(4)
Pt1	···	Au2	3.4630(5)	Au1	–	N22	1.991(4)
Au1	···	Au2	2.9917(5)	Au1	–	N41	1.994(4)
Pt1	–	N1/C1	2.005(4)	Au2	–	N32	1.985(4)
Pt1	–	N10/C10	2.014(4)	Au2	–	N42	2.004(4)
Pt1	–	N21	2.042(4)				
N22	–	Au1	– N41 175.81(14)	N32	–	Au2	– N42 174.28(13)

Table S7 Selected Bond Lengths [Å] and Angles [°] for $[Pt_2Ag_2(bpy)_2(\mu\text{-}Me_2pz)_4](PF_6)_2\cdot(CH_3)_2CO$ (**4d**·$(CH_3)_2CO$)

Pt1	···	Pt2	5.0943(7)	Pt1	–	N41	2.000(5)
Pt1	···	Ag1	3.4323(6)	Pt2	–	N51	2.014(5)
Pt1	···	Ag2	3.5202(6)	Pt2	–	N61	2.021(5)
Pt2	···	Ag1	3.5124(5)	Pt2	–	N71	2.007(5)
Pt2	···	Ag2	3.4232(6)	Pt2	–	N81	1.999(5)
Ag1	···	Ag2	3.1490(7)	Ag1	–	N32	2.078(5)
Pt1	–	N11	2.013(5)	Ag1	–	N72	2.070(5)
Pt1	–	N21	2.016(5)	Ag2	–	N42	2.092(5)
Pt1	–	N31	2.005(4)	Ag2	–	N82	2.094(4)
N32	–	Ag1	– N72 166.00(18)	N42	–	Ag2	– N82 173.70(18)

Table S8 Selected Bond Lengths [Å] and Angles [°] for $[Pt_2Au_2(bpy)_2(\mu\text{-}Me_2pz)_4](PF_6)_2 \cdot 2CH_3CN$ (**5d**·$2CH_3CN$)

Pt1	···	Pt1'	6.1628(9)	Pt1	–	N21	2.013(3)
Pt1	···	Au1	3.5534(5)	Pt1	–	N31	2.022(3)
Pt1	···	Au1'	3.3449(5)	Pt1	–	N41	2.005(3)
Au1	···	Au1'	3.1064(4)	Au1	–	N32	1.997(4)
Pt1	–	N11	2.016(3)	Au1	–	N42'	1.995(3)

N32 – Au1 – N42' 171.50(11)

Table S9 Photophysical Data for **2a**, **2b**, **2c**, **3a**, **3b**, **3c**, **4d** and **5d**

Complex	Absorption λ_{max} [nm] (ε_{max} [$dm^3mol^{-1}cm^{-1}$])	Emission λ_{max} [nm] (τ [μs])	Φ_{em}
2a	259 (42900), 332 sh, 370 (7200), 409 sh[a]	491, 525 (τ = 0.43)[a]	0.04[f]
		497, 531 (τ_1 = 0.69 (A_1 = 0.52), τ_2 = 3.93 (A_2 = 0.48))[c,d]	0.34[g]
2b	255 sh, 316 (7400), 326 (7800), 365 (4700)[a]	471, 504 (τ_1 = 0.08 (A_1 = 0.81), τ_2 = 0.22 (A_2 = 0.19))[a,d]	0.01[f]
		478, 509 (τ_1 = 0.69 (A_1 = 0.54), τ_2 = 4.07 (A_2 = 0.46))[c,d]	0.69[g]
2c	261 sh, 298 (22100), 315 sh, 378 sh, 425 (4000)[a]	493, 523 (τ_1 = 0.77 (A_1 = 0.54), τ_2 = 2.01 (A_2 = 0.46))[a,d]	0.01[f]
		581 (τ_1 = 0.30 (A_1 = 0.79), τ_2 = 2.38 (A_2 = 0.21))[c,d]	0.04[g]
3a	257 sh, 319 (5900), 330 (6000), 364 (4100), 402 sh[a]	486, 522 (τ = 1.48)[a]	0.14[f]
		489, 524 (τ_1 = 1.08 (A_1 = 0.70), τ_2 = 4.92 (A_2 = 0.30))[c,d]	0.51[g]
3b	253 sh, 324 (7000), 360 (4100), 399 sh[a]	468, 501 (τ = 0.23)[a]	0.03[f]
		474, 499 (τ_1 = 0.98 (A_1 = 0.85), τ_2 = 4.25 (A_2 = 0.15))[c,d]	0.55[g]
3c	258 sh, 294 (11000), 311 (10700), 358 (3800), 420 (2000)[a]	504 (τ = 1.54)[a]	0.02[f]
		501, 522 (τ_1 = 13.55 (A_1 = 0.33), τ_2 = 53.24 (A_2 = 0.67))[c,d]	0.52[g]
4d	250 sh, 313 (14900), 322 (16000), 362 (3000)[b]	553 (τ = 0.049)[a]	0.03[f]
		463, 494, 520 (τ_1 = 0.14 (A_1 = 0.79), τ_2 = 0.64 (A_2 = 0.21))[c,d]	0.11[g]
5d	250 sh, 310 (20000), 320 (21500), 366 (4300)[b]	580 (τ = 0.16)[a]	0.10[f]
		460, 493, 524 (τ_1 = 0.72 (A_1 = 0.60), τ_2 = 3.46 (A_2 = 0.40))[c,d]	0.17[g]
		555 (τ_1 = 0.26 (A_1 = 0.69), τ_2 = 0.87 (A_2 = 0.31))[c,d,e]	0.10[e,g]

[a] In CH_2Cl_2 at 298 K. [b] In CH_3CN at 298 K. [c] In the solid state at 298 K. [d] Emission decay curve was analyzed by the equation ($I(t) = A_1\exp(-t/\tau_1) + A_2\exp(-t/\tau_2)$) using the nonlinear least-squares method. [e] Ground sample. [f] Emission quantum yield in CH_2Cl_2. [g] Emission quantum yield in the solid state.

Table S10 Emission Energies (eV) of **2a$_1$**, **2a$_2$**, **2b$_1$**, **2b$_2$**, **2c$_1$**, **2c$_2$**, **2c$_3$**, **3b**, **3c**, **4d** and **5d** by the B3LYP method.

Compound	**2a$_1$**	**2a$_2$**	**2b$_1$**	**2b$_2$**	**2c$_1$**	**2c$_2$**	**2c$_3$**	**3b**	**3c**	**4d**	**5d**
Emission E	2.23	2.23	2.34	2.35	2.16	2.16	2.17	2.35	2.18	2.16	2.51

Table S11 Excitation Energies of **2a$_1$**, **2a$_2$**, **2b$_1$** and **2b$_2$** by the TD-B3LYP method.

Compound	State	Excitation Energy (eV)	Excitation Energy (nm)	Oscillator Strength	Contribution (%)		
2a$_1$	1	3.02	410	0.0009	HOMO-1	→ LUMO	24 %
					HOMO	→ LUMO+1	23 %
	2	3.02	410	0.0009	HOMO	→ LUMO	25 %
					HOMO-1	→ LUMO+1	21 %
	3	3.13	396	0.0472	HOMO-2	→ LUMO+1	22 %
					HOMO-4	→ LUMO	19 %
2a$_2$	1	3.00	414	0.0013	HOMO-1	→ LUMO	33 %
					HOMO	→ LUMO+1	10 %
	2	3.00	414	0.0001	HOMO	→ LUMO+1	32 %
	3	3.09	402	0.0465	HOMO-2	→ LUMO	18 %
					HOMO-3	→ LUMO+1	13 %
2b$_1$	1	3.07	404	0.0004	HOMO-1	→ LUMO	47 %
	2	3.07	403	0.0004	HOMO	→ LUMO+1	47 %
	3	3.25	382	0.0329	HOMO-3	→ LUMO	17 %
	4	3.26	381	0.0112	HOMO-3	→ LUMO+1	34 %
2b$_2$	1	3.05	407	0.0001	HOMO	→ LUMO+1	48 %
	2	3.05	407	0.0001	HOMO-1	→ LUMO	48 %
	3	3.22	385	0.0422	HOMO-3	→ LUMO	22 %
					HOMO-3	→ LUMO+1	11 %

Table S12 Excitation Energies of **2c$_1$**, **2c$_2$**, **2c$_3$**, **3b**, **3c**, **4d** and **5d** by the TD-B3LYP method.

Compound	State	Excitation Energy (eV)	Excitation Energy (nm)	Oscillator Strength	Contribution (%)			
2c$_1$	1	2.89	430	0.0224	HOMO	→	LUMO	29 %
					HOMO-1	→	LUMO+1	15 %
	2	2.90	428	0.0012	HOMO-1	→	LUMO	23 %
					HOMO	→	LUMO+1	22 %
	3	3.04	408	0.0001	HOMO-3	→	LUMO	24 %
					HOMO-2	→	LUMO+1	14 %
	4	3.04	408	0.0406	HOMO-2	→	LUMO	26 %
					HOMO-3	→	LUMO+1	13 %
2c$_2$	1	2.84	437	0.0020	HOMO	→	LUMO	20 %
					HOMO	→	LUMO+1	15 %
	2	2.84	436	0.0025	HOMO-1	→	LUMO	19 %
					HOMO-1	→	LUMO+1	14 %
					HOMO	→	LUMO	10 %
	3	2.96	419	0.0223	HOMO-2	→	LUMO	16 %
					HOMO-2	→	LUMO+1	11 %
					HOMO-3	→	LUMO	10 %
	4	2.96	419	0.0229	HOMO-2	→	LUMO	16 %
					HOMO-2	→	LUMO+1	10 %
					HOMO-3	→	LUMO	10 %
2c$_3$	1	2.85	435	0.0017	HOMO	→	LUMO	41 %
	2	2.95	421	0.0104	HOMO-1	→	LUMO+1	46 %
	3	2.98	416	0.0309	HOMO-3	→	LUMO	35 %
	4	3.07	404	0.0165	HOMO-2	→	LUMO+1	41 %
3b	1	3.25	381	0.0145	HOMO	→	LUMO	31 %
					HOMO-2	→	LUMO	10 %
3c	1	2.97	418	0.0254	HOMO	→	LUMO	45 %
4d	1	2.39	518	0.0008	HOMO	→	LUMO	29 %
					HOMO-1	→	LUMO+1	12 %
	2	2.40	518	0.0028	HOMO	→	LUMO+1	30 %
					HOMO-1	→	LUMO	14 %
5d	1	2.58	481	0.0024	HOMO-1	→	LUMO	22 %
					HOMO-2	→	LUMO+1	13 %
	2	2.58	481	0.0000	HOMO-1	→	LUMO+1	23 %
					HOMO-2	→	LUMO	14 %
					HOMO-3	→	LUMO	10 %

Table S13 Orbital Composition Percentages of Selected Orbitals in **2a$_1$**, **2a$_2$**, **2b$_1$**, **2b$_2$**, **2c$_1$**, **2c$_2$**, **2c$_3$**, **3b**, **3c**, **4d** and **5d** by the B3LYP method.

	2a$_1$				**2a$_2$**				**2b$_1$**				**2b$_2$**			
	Pt	Ag	ppy	Me_2pz	Pt	Ag	ppy	Me_2pz	Pt	Ag	dfppy	Me_2pz	Pt	Ag	dfppy	Me_2pz
LUMO+1	0.04	0.01	0.94	0.01	0.03	0.02	0.93	0.02	0.04	0.01	0.93	0.02	0.04	0.01	0.93	0.02
LUMO	0.03	0.02	0.92	0.02	0.04	0.01	0.94	0.02	0.04	0.01	0.93	0.02	0.04	0.01	0.93	0.02
HOMO	0.25	0.00	0.04	0.72	0.22	0.00	0.02	0.75	0.23	0.00	0.02	0.75	0.21	0.00	0.02	0.77
HOMO−1	0.24	0.00	0.03	0.73	0.23	0.00	0.03	0.75	0.23	0.00	0.02	0.75	0.21	0.00	0.02	0.77
HOMO−2	0.37	0.03	0.50	0.10	0.46	0.12	0.28	0.14	0.07	0.07	0.01	0.85	0.05	0.07	0.01	0.86
HOMO−3	0.15	0.07	0.02	0.76	0.33	0.00	0.54	0.13	0.45	0.11	0.19	0.25	0.50	0.17	0.10	0.23
HOMO−4	0.35	0.00	0.61	0.04												

	2c$_1$				**2c$_2$**				**2c$_3$**				**3b**			
	Pt	Ag	bzq	Me_2pz	Pt	Ag	bzq	Me_2pz	Pt	Ag	bzq	Me_2pz	Pt	Au	dfppy	Me_2pz
LUMO+1	0.02	0.00	0.97	0.01	0.02	0.00	0.97	0.01	0.02	0.01	0.96	0.01	0.00	0.01	0.97	0.02
LUMO	0.03	0.01	0.95	0.01	0.02	0.01	0.96	0.01	0.02	0.01	0.96	0.01	0.04	0.01	0.93	0.02
HOMO	0.25	0.00	0.63	0.11	0.25	0.00	0.10	0.64	0.25	0.00	0.06	0.69	0.25	0.01	0.32	0.42
HOMO−1	0.28	0.00	0.34	0.38	0.25	0.01	0.10	0.65	0.27	0.01	0.46	0.27	0.11	0.19	0.31	0.39
HOMO−2	0.24	0.00	0.08	0.67	0.24	0.03	0.50	0.23	0.22	0.01	0.21	0.56	0.31	0.12	0.38	0.19
HOMO−3	0.23	0.00	0.32	0.45	0.23	0.00	0.55	0.21	0.24	0.01	0.56	0.19				

	3c				**4d**				**5d**			
	Pt	Au	bzq	Me_2pz	Pt	Ag	bpy	Me_2pz	Pt	Au	bpy	Me_2pz
LUMO+1	0.02	0.01	0.96	0.02	0.03	0.00	0.96	0.01	0.03	0.00	0.96	0.01
LUMO	0.02	0.01	0.96	0.01	0.03	0.01	0.95	0.01	0.03	0.00	0.96	0.01
HOMO	0.26	0.02	0.65	0.07	0.15	0.00	0.01	0.84	0.00	0.14	0.00	0.86
HOMO−1	0.26	0.01	0.08	0.66	0.15	0.00	0.01	0.83	0.16	0.00	0.01	0.83
HOMO−2									0.11	0.03	0.01	0.85
HOMO−3									0.08	0.10	0.00	0.82

Table S14 Optimized Geometries of $[Pt_2Ag_2(ppy)_2(\mu\text{-}Me_2pz)_4]$ (**2a$_1$**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	0.270122	3.058989	0.972026	Pt	3.151886	-0.032673	-0.536679
Pt	-0.270122	-3.058989	-0.972026	Pt	-3.168248	-0.069288	0.534370
Ag	-1.455521	0.019089	0.688174	Ag	0.042536	-1.411241	0.012493
Ag	1.455521	-0.019089	-0.688174	Ag	-0.077061	1.829609	-0.002837
N	1.060442	3.963529	-0.698648	N	4.024415	0.918799	1.065637
N	-0.629803	2.230269	2.607275	N	2.276257	-1.107750	-2.035203
N	-1.024989	0.926865	2.569221	N	0.992007	-1.539766	-1.885379
N	2.097662	2.064749	1.524780	N	2.601178	1.774986	-1.570067
N	2.408180	0.840677	1.006131	N	1.310884	2.218190	-1.574868
N	-1.060442	-3.963529	0.698648	N	-3.685581	-1.737398	-0.506308
N	0.629803	-2.230269	-2.607275	N	-2.746284	1.665766	1.549785
N	1.024989	-0.926865	-2.569221	N	-1.476530	2.159315	1.581821
N	-2.097662	-2.064749	-1.524780	N	-2.185901	-1.166334	2.108348
N	-2.408180	-0.840677	-1.006131	N	-0.916221	-1.623035	1.896655
C	0.186588	4.745733	-1.406226	C	4.597528	0.090048	1.993393
C	0.632950	5.418995	-2.554023	C	5.212578	0.641768	3.127990
C	1.955493	5.296783	-2.967175	C	5.235510	2.020258	3.311090
C	2.830598	4.496031	-2.227117	C	4.637700	2.846428	2.354455
C	2.341221	3.845741	-1.099557	C	4.041977	2.253382	1.246770
C	-1.365087	4.030749	0.337180	C	3.787092	-1.641806	0.475760
C	-1.168631	4.793234	-0.850397	C	4.488587	-1.337061	1.678176
C	-2.215390	5.534962	-1.425335	C	5.028868	-2.352492	2.486977
C	-3.476102	5.536607	-0.832197	C	4.884684	-3.687993	2.117218
C	-3.688096	4.793924	0.336590	C	4.200425	-4.006332	0.936432
C	-2.649332	4.051732	0.909321	C	3.660136	-2.998960	0.130137
C	-1.488277	0.592616	3.795037	C	0.621438	-2.166118	-3.024371
C	-1.382916	1.703495	4.637596	C	1.695066	-2.142129	-3.920521
C	-0.837453	2.726197	3.846950	C	2.726608	-1.461878	-3.257505
C	-2.034020	-0.771770	4.083768	C	-0.748327	-2.743558	-3.199983
C	-0.516977	4.139175	4.222795	C	4.106047	-1.142292	-3.739024
C	3.545760	0.398416	1.591442	C	1.207481	3.235899	-2.461156
C	3.978366	1.358127	2.511566	C	2.458544	3.450505	-3.048679
C	3.036291	2.394794	2.438938	C	3.312784	2.509325	-2.455997
C	4.174168	-0.909156	1.218562	C	-0.083120	3.963988	-2.683084
C	2.995881	3.677430	3.210467	C	4.780039	2.300309	-2.679872
C	-0.186588	-4.745733	1.406226	C	-4.368946	-1.479465	-1.729866

C	-0.632950	-5.418995	2.554023
C	-1.955493	-5.296783	2.967175
C	-2.830598	-4.496031	2.227117
C	-2.341221	-3.845741	1.099557
C	1.365087	-4.030749	-0.337180
C	1.168631	-4.793234	0.850397
C	2.215390	-5.534962	1.425335
C	3.476102	-5.536607	0.832197
C	3.688096	-4.793924	-0.336590
C	2.649332	-4.051732	-0.909321
C	1.488277	-0.592616	-3.795037
C	1.382916	-1.703495	-4.637596
C	0.837453	-2.726197	-3.846950
C	2.034020	0.771770	-4.083768
C	0.516977	-4.139175	-4.222795
C	-3.545760	-0.398416	-1.591442
C	-3.978366	-1.358127	-2.511566
C	-3.036291	-2.394794	-2.438938
C	-4.174168	0.909156	-1.218562
C	-2.995881	-3.677430	-3.210467
H	-0.064214	6.039657	-3.115880
H	2.302428	5.822355	-3.859387
H	3.875586	4.371083	-2.511772
H	2.968616	3.204742	-0.480925
H	-2.053158	6.114667	-2.337176
H	-4.290061	6.112915	-1.276849
H	-4.675864	4.792988	0.805781
H	-2.841620	3.478813	1.818506
H	-1.662074	1.766631	5.686496
H	-1.457110	-1.548187	3.557243
H	-3.087540	-0.867474	3.767377
H	-1.991275	-0.985191	5.162455
H	-0.388936	4.760715	3.324916
H	0.410668	4.204372	4.815099
H	-1.326670	4.569470	4.833235
H	4.856592	1.310384	3.151078
H	4.806387	-1.282061	2.038400
H	4.814256	-0.815406	0.323591
H	3.413253	-1.674050	0.999366
C	-4.801302	-2.584480	-2.528150
C	-4.573043	-3.876343	-2.127840
C	-3.889076	-4.101318	-0.892418
C	-3.473811	-3.012136	-0.135764
C	-4.014277	0.831569	-0.993818
C	-4.547812	-0.117219	-2.013920
C	-5.193228	0.405411	-3.185363
C	-5.301817	1.761750	-3.356579
C	-4.783599	2.686695	-2.385372
C	-4.158905	2.211579	-1.238033
C	-1.453659	3.202450	2.442732
C	-2.733245	3.378625	2.977900
C	-3.528715	2.387947	2.384492
C	-0.206592	3.996461	2.684566
C	-4.988487	2.116793	2.577901
C	-0.488919	-2.246627	3.018225
C	-1.507386	-2.189629	3.976148
C	-2.561334	-1.497795	3.362292
C	0.858264	-2.894306	3.105293
C	-3.896715	-1.130419	3.930328
H	5.668383	-0.018953	3.864663
H	5.713263	2.448338	4.194889
H	4.628341	3.931782	2.457503
H	3.556925	2.837087	0.464482
H	5.566340	-2.107235	3.406172
H	5.305170	-4.477968	2.742923
H	4.087956	-5.053307	0.641494
H	3.130257	-3.273051	-0.783781
H	1.728598	-2.562997	-4.922330
H	-1.507744	-1.953150	-3.323528
H	-1.048562	-3.350824	-2.330928
H	-0.783348	-3.385294	-4.092661
H	4.816411	-1.105625	-2.899798
H	4.140857	-0.166245	-4.250776
H	4.448550	-1.905102	-4.454675
H	2.714337	4.186073	-3.807736
H	-0.136812	4.355992	-3.710286
H	-0.194468	4.821477	-1.996336
H	-0.946064	3.297806	-2.525902

H	2.287281	4.385525	2.757202	H	5.131706	1.403170	-2.150620
H	3.991250	4.149319	3.240519	H	5.365735	3.163453	-2.318724
H	2.683053	3.509234	4.254853	H	5.009994	2.180668	-3.750911
H	0.064214	-6.039657	3.115880	H	-5.322664	-2.380321	-3.464169
H	-2.302428	-5.822355	3.859387	H	-4.906810	-4.717569	-2.737048
H	-3.875586	-4.371083	2.511772	H	-3.689342	-5.109373	-0.528714
H	-2.968616	-3.204742	0.480925	H	-2.947858	-3.145858	0.809524
H	2.053158	-6.114667	2.337176	H	-5.593479	-0.271839	-3.941646
H	4.290061	-6.112915	1.276849	H	-5.791316	2.153522	-4.252007
H	4.675864	-4.792988	-0.805781	H	-4.886635	3.759546	-2.558996
H	2.841620	-3.478813	-1.818506	H	-3.768701	2.918555	-0.503921
H	1.662074	-1.766631	-5.686496	H	-3.050731	4.126468	3.700435
H	1.457110	1.548187	-3.557243	H	0.681974	3.345343	2.687481
H	3.087540	0.867474	-3.767377	H	-0.053488	4.766397	1.908236
H	1.991275	0.985191	-5.162455	H	-0.257861	4.510604	3.656135
H	0.388936	-4.760715	-3.324916	H	-5.371545	1.459433	1.784653
H	-0.410668	-4.204372	-4.815099	H	-5.188742	1.630760	3.546937
H	1.326670	-4.569470	-4.833235	H	-5.561081	3.057755	2.558939
H	-4.856592	-1.310384	-3.151078	H	-1.487699	-2.596121	4.984539
H	-4.806387	1.282061	-2.038400	H	1.187013	-2.963226	4.153121
H	-4.814256	0.815406	-0.323591	H	0.845128	-3.918816	2.694589
H	-3.413253	1.674050	-0.999366	H	1.616526	-2.328500	2.543314
H	-2.287281	-4.385525	-2.757202	H	-4.642272	-0.989461	3.134065
H	-3.991250	-4.149319	-3.240519	H	-4.258883	-1.916247	4.611215
H	-2.683053	-3.509234	-4.254853	H	-3.842226	-0.191891	4.507796

Table S15 Optimized Geometries of $[Pt_2Ag_2(ppy)_2(\mu\text{-}Me_2pz)_4]$ (**2a₂**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	3.164020	-0.055066	0.545639	Pt	-3.169926	-0.046388	-0.554369
Pt	-3.167787	-0.135000	-0.523806	Pt	3.174638	-0.141640	0.514140
Ag	0.035130	1.899454	-0.196274	Ag	-0.032315	1.883054	0.202414
Ag	-0.015900	-1.301825	0.139239	Ag	-0.001335	-1.316620	-0.135966
N	2.749118	1.918998	1.304702	N	-2.733031	1.919202	-1.321494
N	1.488458	2.438614	1.269917	N	-1.467777	2.427366	-1.278179
N	2.209783	-0.841999	2.169033	N	-2.220156	-0.852489	-2.171278
N	0.914648	-1.251623	2.053121	N	-0.929068	-1.272179	-2.048684
N	4.106602	0.586117	-1.168063	N	-4.111490	0.614794	1.152110
N	-4.076091	0.926596	0.987648	N	4.076445	0.935816	-0.954292
N	-2.255206	-1.316263	-1.915911	N	2.248513	-1.321634	1.915594
N	-0.951518	-1.672211	-1.737466	N	0.945285	-1.681747	1.737096
N	-2.670001	1.593136	-1.714132	N	2.672472	1.582856	1.713991
N	-1.400932	2.092025	-1.761859	N	1.393802	2.054173	1.782753
C	3.675343	-1.835932	-0.217337	C	-3.695236	-1.817758	0.221166
C	4.398343	-1.763117	-1.442572	C	-4.419132	-1.730301	1.444930
C	4.860158	-2.923290	-2.089168	C	-4.888463	-2.882261	2.100700
C	4.612683	-4.176121	-1.532187	C	-4.647785	-4.141209	1.554530
C	3.902550	-4.266755	-0.327455	C	-3.937083	-4.246233	0.351324
C	3.441335	-3.114848	0.318801	C	-3.468420	-3.102495	-0.304080
C	4.613307	-0.409564	-1.960756	C	-4.627068	-0.371072	1.951292
C	5.264096	-0.076603	-3.159209	C	-5.279912	-0.024146	3.144650
C	5.389647	1.254695	-3.541298	C	-5.398870	1.311113	3.514972
C	4.858497	2.253829	-2.719914	C	-4.858835	2.300032	2.687039
C	4.223658	1.874651	-1.542390	C	-4.222053	1.907171	1.515067
C	1.478332	3.589597	1.982726	C	-1.439882	3.574619	-1.996493
C	2.759361	3.815540	2.494941	C	-2.714380	3.809897	-2.521082
C	3.534538	2.737664	2.041131	C	-3.503864	2.741907	-2.068992
C	0.242186	4.425233	2.122012	C	-0.194691	4.398106	-2.127267
C	4.991468	2.466838	2.266826	C	-4.961369	2.484269	-2.306202
C	0.506714	-1.711387	3.256730	C	-0.519145	-1.737694	-3.249319
C	1.568396	-1.601093	4.162484	C	-1.575345	-1.621463	-4.159993
C	2.630275	-1.045619	3.435902	C	-2.636527	-1.055835	-3.439342
C	-0.884309	-2.215522	3.482549	C	0.868678	-2.255559	-3.464893
C	4.012016	-0.705923	3.896620	C	-4.013108	-0.706070	-3.907728
C	-4.626540	0.165023	1.984189	C	4.658962	0.148817	-1.988657

C	-5.260736	0.795083	3.066472	C	5.316348	0.808536	-3.073305
C	-5.326159	2.182933	3.128267	C	5.386459	2.177314	-3.128658
C	-4.751561	2.940071	2.102778	C	4.785239	2.938795	-2.078317
C	-4.135248	2.270609	1.051397	C	4.153740	2.275534	-1.033974
C	-3.758017	-1.666825	0.625555	C	3.755557	-1.655577	-0.594367
C	-4.473346	-1.279951	1.795288	C	4.507069	-1.235416	-1.813835
C	-4.984584	-2.236763	2.689952	C	5.009978	-2.241478	-2.705797
C	-4.794977	-3.594309	2.440806	C	4.799590	-3.567786	-2.426123
C	-4.093604	-3.993335	1.295079	C	4.078819	-3.985506	-1.253719
C	-3.583129	-3.044313	0.402733	C	3.575813	-3.036088	-0.372503
C	-0.567142	-2.416951	-2.797839	C	0.556774	-2.410639	2.806103
C	-1.653310	-2.547189	-3.671861	C	1.639310	-2.527298	3.687231
C	-2.704833	-1.835752	-3.078755	C	2.692511	-1.823762	3.089116
C	0.825697	-2.948629	-2.929622	C	-0.836332	-2.941328	2.939455
C	-4.104181	-1.638077	-3.568931	C	4.087718	-1.616330	3.587205
C	-1.346336	3.034905	-2.731975	C	1.333116	2.984013	2.764571
C	-2.605638	3.143611	-3.328745	C	2.597548	3.109308	3.348739
C	-3.415162	2.217347	-2.654568	C	3.417575	2.209943	2.652947
C	-0.090485	3.796960	-3.028736	C	0.067992	3.721725	3.081538
C	-4.871396	1.924081	-2.853673	C	4.882905	1.948215	2.827687
H	5.415891	-2.855610	-3.027504	H	-5.444743	-2.803525	3.037840
H	4.971725	-5.078310	-2.031685	H	-5.012826	-5.036977	2.061186
H	3.707431	-5.248288	0.113304	H	-3.747732	-5.232602	-0.081095
H	2.889066	-3.212358	1.255180	H	-2.916213	-3.210851	-1.239340
H	5.666957	-0.869927	-3.787989	H	-5.689901	-0.809676	3.778583
H	5.895225	1.512422	-4.474352	H	-5.906306	1.579836	4.443899
H	4.929724	3.310205	-2.980145	H	-4.924764	3.358995	2.937985
H	3.785550	2.600993	-0.858181	H	-3.777074	2.624918	0.826216
H	3.084646	4.645258	3.118171	H	-3.026277	4.639470	-3.151291
H	0.308368	5.068039	3.012787	H	-0.225906	5.004130	-3.045394
H	-0.654188	3.792575	2.222872	H	0.700879	3.758057	-2.170994
H	0.087299	5.083496	1.249185	H	-0.066910	5.091515	-1.277484
H	5.295005	1.533793	1.770336	H	-5.281109	1.562242	-1.799341
H	5.224538	2.372431	3.340161	H	-5.184615	2.376548	-3.380381
H	5.613801	3.288145	1.872704	H	-5.577925	3.318582	-1.930916
H	1.575443	-1.890074	5.210551	H	-1.579380	-1.912215	-5.207547
H	-0.902034	-2.953522	4.298811	H	0.906413	-2.899721	-4.356099
H	-1.294004	-2.690501	2.578289	H	1.219879	-2.841155	-2.601094
H	-1.571413	-1.397561	3.758740	H	1.589730	-1.433999	-3.615249

H	4.749214	-0.881785	3.098734	H	-4.754752	-0.867623	-3.110978
H	4.285999	-1.319291	4.768137	H	-4.290413	-1.324004	-4.774963
H	4.089053	0.352576	4.195420	H	-4.078121	0.350490	-4.215954
H	-5.698311	0.187725	3.858105	H	5.761931	0.200650	-3.861712
H	-5.818819	2.671931	3.971364	H	5.887507	2.678047	-3.958363
H	-4.775458	4.030067	2.110287	H	4.810616	4.028605	-2.080337
H	-3.665770	2.798002	0.221235	H	3.680519	2.820310	-0.216333
H	-5.534193	-1.928539	3.582640	H	5.561757	-1.955760	-3.602921
H	-5.192527	-4.339236	3.133222	H	5.188106	-4.329203	-3.107525
H	-3.944319	-5.058027	1.095273	H	3.933737	-5.050929	-1.065281
H	-3.039836	-3.380955	-0.482070	H	3.027542	-3.360111	0.513436
H	-1.682503	-3.089596	-4.613665	H	1.664271	-3.054787	4.637586
H	1.460715	-2.271293	-3.526284	H	-1.468021	-2.266141	3.541884
H	1.306663	-3.065739	-1.947176	H	-1.320442	-3.052269	1.957827
H	0.824984	-3.927965	-3.432551	H	-0.835789	-3.923312	3.437296
H	-4.817128	-1.617712	-2.730776	H	4.812258	-1.636104	2.758899
H	-4.211336	-0.690028	-4.121554	H	4.195208	-0.646712	4.100713
H	-4.388575	-2.454178	-4.250070	H	4.356782	-2.405343	4.305299
H	-2.894740	3.799869	-4.146241	H	2.883881	3.760010	4.171569
H	-0.138365	4.242583	-4.033718	H	0.048483	4.021325	4.140577
H	0.074689	4.617806	-2.309010	H	-0.037016	4.639447	2.476630
H	0.792502	3.139007	-2.988696	H	-0.814814	3.092142	2.887652
H	-5.497144	2.779659	-2.545321	H	5.486511	2.793240	2.453215
H	-5.098590	1.724032	-3.913254	H	5.139534	1.812959	3.890472
H	-5.176642	1.047943	-2.264043	H	5.189294	1.046127	2.279573

Table S16 Optimized Geometries of $[Pt_2Ag_2(dfppy)_2(\mu\text{-}Me_2pz)_4]$ (**2b$_1$**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	3.097389	0.668033	-0.599960	Pt	3.092912	0.671066	-0.600876
Pt	-3.063558	-0.703687	0.650766	Pt	-3.063990	-0.707661	0.648124
Ag	-0.211157	1.606850	0.865435	Ag	-0.211120	1.606516	0.868865
Ag	0.187162	-1.222983	-0.596734	Ag	0.181574	-1.224365	-0.590792
N	2.273222	2.648319	-0.652611	N	2.272483	2.653346	-0.647515
N	0.945198	2.857298	-0.418122	N	0.946154	2.865515	-0.407274
N	2.157381	0.287956	-2.373097	N	2.144610	0.294007	-2.369990
N	0.941178	-0.327953	-2.368550	N	0.927124	-0.319328	-2.360184
N	4.050130	0.892154	1.207141	N	4.054253	0.891082	1.202472
N	-3.639408	-1.699292	-1.056054	N	-3.603844	-1.690265	-1.039289
N	-1.857272	-2.309777	1.402366	N	-1.863832	-2.324390	1.397299
N	-0.560423	-2.414884	0.988462	N	-0.563557	-2.421139	0.993109
N	-2.628580	0.366183	2.333689	N	-2.622055	0.352790	2.348372
N	-1.404815	0.940370	2.507491	N	-1.401460	0.936709	2.514791
C	3.970601	-1.128639	-0.482537	C	3.962747	-1.127624	-0.489204
C	4.761960	-1.314553	0.695063	C	4.758669	-1.316686	0.684818
C	5.438647	-2.532042	0.866346	C	5.433257	-2.535974	0.851791
C	5.372870	-3.565249	-0.057940	C	5.361103	-3.567949	-0.073354
C	4.595773	-3.351408	-1.194355	C	4.579636	-3.351018	-1.206197
C	3.901480	-2.167411	-1.422177	C	3.887143	-2.165126	-1.429718
C	4.786465	-0.186082	1.628421	C	4.789902	-0.189389	1.619261
C	5.461328	-0.121818	2.859873	C	5.470530	-0.128044	2.847745
C	5.374384	1.025294	3.642968	C	5.390025	1.018433	3.632400
C	4.611764	2.107514	3.197273	C	4.628110	2.103050	3.191270
C	3.964574	1.997056	1.971910	C	3.975090	1.995409	1.968776
C	0.648388	4.138397	-0.737146	C	0.652679	4.149252	-0.718537
C	1.810084	4.769356	-1.196497	C	1.814762	4.778786	-1.178734
C	2.815385	3.795388	-1.124095	C	2.816956	3.800964	-1.114965
C	-0.731444	4.697097	-0.569206	C	-0.724713	4.711677	-0.543011
C	4.272204	3.919487	-1.454352	C	4.272896	3.921602	-1.450264
C	0.502051	-0.404018	-3.644126	C	0.480356	-0.391820	-3.633496
C	1.460286	0.169963	-4.485654	C	1.434719	0.183635	-4.478641
C	2.495682	0.598419	-3.642894	C	2.475926	0.607752	-3.640918
C	-0.819250	-1.017935	-3.987576	C	-0.837673	-1.015209	-3.971876
C	3.775120	1.285991	-3.999673	C	3.753565	1.296145	-4.002607
C	-4.162954	0.737691	-0.196229	C	-4.143103	0.732853	-0.161371

C	-4.749423	0.364087	-1.446603
C	-5.531255	1.306360	-2.132501
C	-5.756572	2.589014	-1.653024
C	-5.167095	2.923500	-0.436224
C	-4.383952	2.033518	0.292812
C	-4.461508	-0.998093	-1.901741
C	-4.937366	-1.615622	-3.071690
C	-4.577953	-2.928344	-3.362203
C	-3.741771	-3.623199	-2.485236
C	-3.294782	-2.969366	-1.342701
C	0.015579	-3.458465	1.627623
C	-0.932050	-4.039459	2.477252
C	-2.101485	-3.284739	2.305095
C	1.433280	-3.864234	1.367333
C	-3.430810	-3.451529	2.972966
C	-1.357674	1.455540	3.758049
C	-2.573819	1.202288	4.399957
C	-3.357255	0.513434	3.463869
C	-0.154721	2.191696	4.263153
C	-4.755687	-0.000821	3.609544
F	6.200115	-2.748336	1.970712
F	4.514817	-4.346620	-2.102451
F	-6.107888	0.989617	-3.321446
F	-5.369371	4.168027	0.045272
H	6.044960	-0.976094	3.190080
H	4.513549	3.023431	3.780464
H	-5.587879	-1.057655	-3.738630
H	-3.435832	-4.652643	-2.673277
H	5.910163	-4.498430	0.103683
H	3.311735	-2.067909	-2.333279
H	5.899020	1.071253	4.599651
H	3.351260	2.799365	1.562534
H	1.911568	5.795308	-1.542275
H	-0.849042	5.220113	0.395776
H	-1.488352	3.898391	-0.610258
H	-0.958186	5.423194	-1.365096
H	4.420881	4.399042	-2.434936
H	4.754442	2.931659	-1.475958
H	4.799780	4.540004	-0.709026

C	-4.734765	0.348577	-1.473220
C	-5.541164	1.337567	-2.143640
C	-5.757133	2.581775	-1.627134
C	-5.164772	2.911422	-0.375801
C	-4.381711	2.017375	0.340223
C	-4.447712	-0.943022	-1.932531
C	-4.894322	-1.569891	-3.145971
C	-4.534422	-2.856305	-3.448768
C	-3.698051	-3.572505	-2.533061
C	-3.269959	-2.947744	-1.365688
C	0.008557	-3.472136	1.623036
C	-0.945655	-4.066713	2.455958
C	-2.115203	-3.312745	2.283568
C	1.429698	-3.870509	1.370603
C	-3.450855	-3.495878	2.934172
C	-1.343804	1.438385	3.769672
C	-2.550647	1.167890	4.423047
C	-3.338548	0.482263	3.489113
C	-0.141366	2.179147	4.269051
C	-4.730953	-0.044574	3.648402
F	6.198928	-2.755274	1.952653
F	4.492443	-4.344922	-2.114955
F	-6.110162	1.034002	-3.337337
F	-5.392624	4.150800	0.102342
H	6.053652	-0.984043	3.174379
H	4.534972	3.018661	3.775779
H	-5.529200	-0.997340	-3.817340
H	-3.389386	-4.599693	-2.728440
H	5.896885	-4.502577	0.084890
H	3.293828	-2.063300	-2.338231
H	5.919178	1.062103	4.586702
H	3.362132	2.799783	1.562941
H	1.918603	5.806106	-1.519728
H	-0.834172	5.239732	0.420202
H	-1.483020	3.913788	-0.574270
H	-0.956327	5.434189	-1.340856
H	4.419378	4.403800	-2.429878
H	4.751749	2.932274	-1.476942
H	4.805271	4.537978	-0.704927

H	1.417643	0.265034	-5.567678	H	1.385412	0.282553	-5.560043
H	-1.656872	-0.408046	-3.609761	H	-1.668399	-0.504183	-3.458204
H	-0.922796	-2.025448	-3.552471	H	-0.874234	-2.077291	-3.676959
H	-0.930360	-1.105474	-5.078185	H	-1.022075	-0.958856	-5.054434
H	4.601490	0.947960	-3.356147	H	4.583134	0.956288	-3.364145
H	3.690902	2.379277	-3.888046	H	3.670311	2.389236	-3.887885
H	4.040586	1.076616	-5.046620	H	4.013711	1.089270	-5.051383
H	-6.366605	3.298016	-2.210457	H	-6.368957	3.308527	-2.161283
H	-3.956528	2.361604	1.240437	H	-3.960417	2.329603	1.295925
H	-4.951215	-3.405918	-4.270616	H	-4.877995	-3.328286	-4.369943
H	-2.639812	-3.452030	-0.618262	H	-2.630246	-3.464771	-0.650099
H	-0.792850	-4.894944	3.133937	H	-0.810919	-4.931048	3.101864
H	1.500824	-4.617962	0.563553	H	1.503968	-4.632612	0.575472
H	2.045214	-3.001858	1.062308	H	2.035554	-3.006843	1.057340
H	1.884158	-4.304376	2.269778	H	1.882136	-4.297430	2.278694
H	-3.426811	-3.023061	3.989662	H	-3.458591	-3.088034	3.959272
H	-4.224249	-2.949629	2.400161	H	-4.240713	-2.986718	2.362896
H	-3.689605	-4.517808	3.068469	H	-3.706614	-4.564696	3.005954
H	-2.859085	1.479802	5.411609	H	-2.826580	1.431958	5.440881
H	0.766544	1.804470	3.800196	H	0.771541	1.836483	3.757272
H	-0.211430	3.272401	4.044736	H	-0.230662	3.267083	4.104149
H	-0.062174	2.080331	5.354337	H	-0.008007	2.019589	5.350101
H	-5.286022	0.015340	2.646105	H	-5.287172	0.007935	2.700910
H	-4.775785	-1.037980	3.981481	H	-4.737638	-1.096279	3.976752
H	-5.314082	0.618686	4.327623	H	-5.272489	0.542020	4.405799

Table S17 Optimized Geometries of $[Pt_2Ag_2(dfppy)_2(\mu\text{-}Me_2pz)_4]$ (**2b₂**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	-3.106053	-0.071158	0.794252	Pt	-3.110089	-0.075452	0.797445
Pt	3.108722	-0.134752	-0.772768	Pt	3.116030	-0.132725	-0.773033
Ag	0.013612	1.160837	-0.040281	Ag	-0.003063	1.172115	-0.049254
Ag	0.016693	-2.054156	0.081919	Ag	0.024104	-2.044218	0.096756
N	-4.114171	-1.104848	-0.669974	N	-4.118368	-1.105686	-0.668811
N	-2.109550	1.087400	2.147419	N	-2.112219	1.080121	2.152652
N	-0.816423	1.441969	1.901181	N	-0.826940	1.453580	1.894214
N	-2.502066	-1.815270	1.892527	N	-2.505846	-1.820976	1.892095
N	-1.239970	-2.321192	1.783554	N	-1.237928	-2.314482	1.793955
N	4.142931	-0.948034	0.807434	N	4.146947	-0.948936	0.765993
N	2.572842	-2.010442	-1.666250	N	2.575189	-2.013227	-1.659398
N	1.305154	-2.502899	-1.557309	N	1.302842	-2.493833	-1.552015
N	2.076091	0.814730	-2.256578	N	2.064126	0.805126	-2.265553
N	0.800977	1.234746	-2.017384	N	0.792562	1.236904	-2.024275
C	-4.743604	-0.332550	-1.613382	C	-4.748452	-0.331406	-1.610174
C	-5.454519	-0.956665	-2.653464	C	-5.460070	-0.953378	-2.650988
C	-5.510553	-2.345208	-2.723719	C	-5.515839	-2.341818	-2.724233
C	-4.854946	-3.110960	-1.756556	C	-4.859291	-3.109559	-1.759320
C	-4.166938	-2.448204	-0.746604	C	-4.170763	-2.448870	-0.748330
C	-3.779064	1.480110	-0.274115	C	-3.783204	1.478328	-0.267557
C	-4.575524	1.106888	-1.402430	C	-4.580208	1.107621	-1.396317
C	-5.120954	2.119749	-2.206292	C	-5.125496	2.122229	-2.197982
C	-4.919811	3.469569	-1.955036	C	-4.923353	3.471537	-1.944467
C	-4.140023	3.799504	-0.848594	C	-4.143133	3.799009	-0.837635
C	-3.571706	2.842450	-0.013234	C	-3.575374	2.840101	-0.004032
C	-0.367942	2.162747	2.952959	C	-0.373543	2.166584	2.948901
C	-1.400699	2.279133	3.890924	C	-1.395168	2.259802	3.901223
C	-2.488482	1.585397	3.345284	C	-2.481506	1.559115	3.361224
C	1.032475	2.687143	3.014163	C	1.022191	2.704502	2.997776
C	-3.858467	1.388363	3.912722	C	-3.840857	1.337574	3.944757
C	-1.092679	-3.307106	2.699715	C	-1.087865	-3.297874	2.712257
C	-2.283605	-3.436818	3.419685	C	-2.283396	-3.438596	3.422844
C	-3.151467	-2.477505	2.876561	C	-3.156469	-2.488728	2.871814
C	0.180458	-4.087107	2.827626	C	0.191449	-4.066129	2.849414
C	-4.576275	-2.188132	3.239399	C	-4.587210	-2.213731	3.222519
C	3.723756	1.556733	0.100161	C	3.712222	1.551092	0.063924

C	4.528515	1.350430	1.264823	C	4.555051	1.331327	1.272442
C	5.037391	2.471585	1.938432	C	5.056061	2.504210	1.943407
C	4.792280	3.773100	1.524158	C	4.785586	3.769273	1.509982
C	4.006344	3.939391	0.385654	C	3.977424	3.934069	0.349022
C	3.473069	2.869129	-0.326249	C	3.452642	2.861081	-0.355884
C	4.743284	-0.046212	1.649535	C	4.777997	-0.001189	1.643897
C	5.470834	-0.515219	2.757420	C	5.532558	-0.493078	2.762062
C	5.571667	-1.882221	2.996697	C	5.648883	-1.837494	2.998235
C	4.943974	-2.781258	2.130962	C	4.999243	-2.752756	2.108733
C	4.238395	-2.269475	1.048120	C	4.274938	-2.258445	1.029280
C	1.191381	-3.578044	-2.371287	C	1.184233	-3.573527	-2.358956
C	2.410224	-3.780696	-3.025941	C	2.404027	-3.789902	-3.007890
C	3.259154	-2.770537	-2.549932	C	3.259821	-2.784592	-2.534754
C	-0.077538	-4.369349	-2.465647	C	-0.089705	-4.356775	-2.451521
C	4.699300	-2.519344	-2.880393	C	4.704304	-2.550883	-2.859085
C	0.324633	1.805206	-3.146208	C	0.309448	1.787441	-3.159594
C	1.320503	1.754768	-4.129165	C	1.296536	1.712730	-4.150237
C	2.415020	1.119915	-3.528385	C	2.392498	1.083937	-3.546719
C	-1.064034	2.356771	-3.230112	C	-1.076831	2.345372	-3.242018
C	3.753437	0.797120	-4.112447	C	3.722257	0.741391	-4.139274
F	-5.884154	1.806963	-3.286313	F	-5.889421	1.811870	-3.278181
F	-3.931035	5.106541	-0.588798	F	-3.932812	5.105516	-0.575734
F	5.806663	2.318605	3.048182	F	5.827649	2.358745	3.050060
F	3.754856	5.197233	-0.031421	F	3.730389	5.197068	-0.049067
H	-5.953809	-0.342748	-3.397224	H	-5.960312	-0.337990	-3.392895
H	-4.870570	-4.200958	-1.775621	H	-4.874528	-4.199512	-1.780877
H	-6.062960	-2.826592	-3.533512	H	-6.068798	-2.821527	-3.534641
H	-3.632336	-2.981323	0.039297	H	-3.635404	-2.983433	0.036108
H	-5.357237	4.232117	-2.597494	H	-5.360818	4.235422	-2.585313
H	-2.972017	3.172165	0.834941	H	-2.975690	3.167866	0.844887
H	-1.372873	2.802747	4.843208	H	-1.361186	2.772280	4.859328
H	1.059690	3.681719	3.485470	H	1.049540	3.681610	3.504335
H	1.471887	2.770132	2.008943	H	1.435247	2.828960	1.985471
H	1.684656	2.022372	3.606380	H	1.695377	2.026013	3.549719
H	-3.945662	0.425117	4.441487	H	-3.903706	0.372723	4.474061
H	-4.622584	1.403982	3.120689	H	-4.614377	1.339574	3.161848
H	-4.088741	2.186028	4.634665	H	-4.076984	2.130671	4.669846
H	-2.492007	-4.128788	4.232202	H	-2.491391	-4.131844	4.234366
H	1.059991	-3.423935	2.792548	H	1.066468	-3.398725	2.792046

H	0.291959	-4.828602	2.017275	H	0.301704	-4.826087	2.056137
H	0.203193	-4.632849	3.782582	H	0.224854	-4.589165	3.816683
H	-4.952404	-1.318855	2.681453	H	-4.964461	-1.341781	2.669489
H	-4.682187	-1.979021	4.316256	H	-4.705997	-2.016157	4.300194
H	-5.227623	-3.049747	3.012874	H	-5.229547	-3.077974	2.980744
H	5.947472	0.201050	3.420094	H	6.008753	0.230413	3.418959
H	4.994267	-3.859664	2.283301	H	5.058005	-3.830920	2.259509
H	5.201943	4.622455	2.068563	H	5.181095	4.636172	2.039105
H	2.866526	3.072149	-1.208811	H	2.839139	3.053830	-1.235996
H	6.136833	-2.242893	3.858740	H	6.222585	-2.205526	3.849521
H	3.723748	-2.912271	0.334361	H	3.765655	-2.927324	0.334636
H	2.648444	-4.552807	-3.753631	H	2.638904	-4.568378	-3.729837
H	-0.113954	-4.930250	-3.411604	H	-0.142857	-4.897672	-3.408345
H	-0.169247	-5.100083	-1.642963	H	-0.172503	-5.104228	-1.643089
H	-0.959696	-3.710484	-2.424498	H	-0.967559	-3.694568	-2.383472
H	4.861025	-2.487950	-3.969773	H	4.876189	-2.558595	-3.947220
H	5.037404	-1.563849	-2.454682	H	5.044715	-1.583657	-2.463056
H	5.345769	-3.319803	-2.480668	H	5.342352	-3.339993	-2.424902
H	1.264275	2.133156	-5.146752	H	1.233313	2.071005	-5.174678
H	-1.742389	1.660335	-3.751854	H	-1.756426	1.656082	-3.771399
H	-1.481729	2.536997	-2.228479	H	-1.495964	2.518468	-2.239737
H	-1.077476	3.307610	-3.785485	H	-1.085675	3.301044	-3.789301
H	4.539385	0.836199	-3.343567	H	4.523032	0.821584	-3.389090
H	3.768372	-0.212419	-4.555534	H	3.735144	-0.288490	-4.532465
H	4.006872	1.513830	-4.907985	H	3.955273	1.419970	-4.973475

Table S18 Optimized Geometries of $[Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4]$ (**2c$_1$**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	-2.643784	0.153896	0.651458	Pt	-2.620659	0.253528	0.680351
Pt	2.643461	0.171778	-0.645994	Pt	2.615320	0.076289	-0.668146
Ag	0.506207	-1.567955	1.478396	Ag	0.434567	-1.616444	1.442321
Ag	-0.501720	-1.527941	-1.515741	Ag	-0.630922	-1.459389	-1.551131
N	-3.389484	0.580542	-1.234147	N	-3.340981	0.741650	-1.200788
N	3.377277	0.561092	1.252898	N	3.410478	0.366314	1.224454
N	-2.017680	-0.105730	2.575280	N	-1.996578	-0.061822	2.604176
N	-0.850538	-0.732038	2.892769	N	-0.857777	-0.748087	2.899381
N	-2.856255	-1.966405	0.411040	N	-2.938445	-1.844221	0.433261
N	-1.990112	-2.611168	-0.427726	N	-2.135301	-2.507807	-0.450491
N	2.024096	-0.047538	-2.577022	N	1.951110	-0.052481	-2.591882
N	0.844959	-0.642490	-2.910475	N	0.740808	-0.582079	-2.925244
N	2.865910	-1.952737	-0.453001	N	2.732765	-2.060472	-0.545169
N	2.002490	-2.619653	0.370899	N	1.862884	-2.708263	0.287150
C	-2.385262	2.150082	0.676315	C	-2.248172	2.209472	0.706208
C	2.382732	2.167682	-0.631773	C	2.463624	2.082549	-0.587257
C	-3.898715	-0.277610	-2.124184	C	-3.941354	-0.100042	-2.122550
C	-4.417156	0.149714	-3.358090	C	-4.429637	0.385188	-3.331635
C	-4.402612	1.499619	-3.678845	C	-4.328919	1.738120	-3.659790
C	-3.800884	3.848795	-2.968716	C	-3.537366	4.009266	-2.889173
C	-3.268090	4.675390	-2.016999	C	-2.909355	4.840188	-1.886801
C	-2.196887	4.981320	0.243154	C	-1.827240	5.022672	0.364421
C	-1.729238	4.391605	1.410008	C	-1.411241	4.382403	1.527509
C	-1.817434	2.997344	1.629752	C	-1.606919	3.003307	1.711783
C	-2.838304	2.773207	-0.523844	C	-2.643405	2.875190	-0.472491
C	-3.380047	1.919408	-1.529151	C	-3.246001	2.057683	-1.482464
C	-3.874078	2.427272	-2.756669	C	-3.714165	2.635171	-2.713846
C	-2.765268	4.170302	-0.765136	C	-2.464450	4.280054	-0.690040
C	3.878090	-0.314477	2.130562	C	3.883448	-0.562164	2.062295
C	4.389023	0.088776	3.375718	C	4.447030	-0.226324	3.304860
C	4.376009	1.432607	3.721038	C	4.519717	1.104902	3.688887
C	3.783619	3.795772	3.050941	C	4.051869	3.517215	3.100964
C	3.257231	4.640943	2.112059	C	3.554433	4.419249	2.199955
C	2.196421	4.990542	-0.146632	C	2.460555	4.896915	-0.019460
C	1.732554	4.423333	-1.326062	C	1.932944	4.392517	-1.201078
C	1.819652	3.033290	-1.571441	C	1.928822	3.007394	-1.486479

C	2.831714	2.767573	0.581653	C	2.976592	2.619452	0.630935
C	3.367650	1.894251	1.573177	C	3.485427	1.687564	1.582975
C	3.855350	2.378338	2.812802	C	4.032155	2.105578	2.821926
C	2.759439	4.160028	0.848741	C	2.995865	4.005582	0.938119
C	-0.742971	-0.766239	4.239500	C	-0.737485	-0.807863	4.243844
C	-1.866982	-0.150485	4.799988	C	-1.824485	-0.146110	4.826328
C	-2.654098	0.255852	3.714014	C	-2.602481	0.313416	3.755269
C	0.435961	-1.389424	4.922285	C	0.417212	-1.497759	4.903273
C	-3.975731	0.959259	3.727498	C	-3.889170	1.078220	3.789795
C	-2.264737	-3.935295	-0.399751	C	-2.467370	-3.818056	-0.435738
C	-3.330942	-4.150400	0.482210	C	-3.508863	-4.003679	0.482875
C	-3.672699	-2.880859	0.973582	C	-3.774009	-2.732009	1.011950
C	-1.513797	-4.914779	-1.249104	C	-1.795538	-4.811885	-1.332878
C	-4.731614	-2.509528	1.965224	C	-4.777405	-2.334666	2.049988
C	0.733274	-0.631907	-4.257533	C	0.608209	-0.519858	-4.268915
C	1.865356	-0.014987	-4.801405	C	1.759327	0.063172	-4.810965
C	2.662166	0.341714	-3.705760	C	2.588667	0.345505	-3.718330
C	-0.442390	-1.239469	-4.959331	C	-0.604381	-1.050686	-4.969841
C	3.989870	1.033517	-3.699345	C	3.947945	0.973274	-3.712226
C	2.283457	-3.941500	0.314799	C	2.079763	-4.039746	0.189471
C	3.351334	-4.132503	-0.570489	C	3.111931	-4.256287	-0.731352
C	3.687322	-2.850991	-1.034220	C	3.494326	-2.979931	-1.173090
C	1.535488	-4.941523	1.142449	C	1.311565	-5.026259	1.014771
C	4.744745	-2.454376	-2.017596	C	4.539587	-2.608279	-2.178995
H	-3.883188	-1.329430	-1.840767	H	-4.004999	-1.147648	-1.839737
H	-4.822665	-0.592174	-4.047060	H	-4.898326	-0.318570	-4.022559
H	-4.797256	1.849827	-4.635973	H	-4.708812	2.123292	-4.607282
H	-4.178038	4.255465	-3.909944	H	-3.882073	4.471701	-3.817149
H	-3.217528	5.752128	-2.200265	H	-2.790215	5.909017	-2.074884
H	-2.122482	6.061152	0.094194	H	-1.666955	6.096040	0.236168
H	-1.277538	5.020033	2.182414	H	-0.916484	4.962145	2.310558
H	-1.427298	2.587299	2.563457	H	-1.257915	2.529996	2.630653
H	3.861234	-1.361063	1.828523	H	3.801676	-1.596150	1.729226
H	4.787976	-0.666813	4.053529	H	4.819613	-1.023374	3.949369
H	4.765502	1.764257	4.686858	H	4.952101	1.384742	4.652832
H	4.156618	4.184106	4.001521	H	4.472555	3.855009	4.050950
H	3.207767	5.714211	2.314942	H	3.576800	5.487365	2.432860
H	2.122999	6.067539	0.022066	H	2.460953	5.971524	0.178696
H	1.284744	5.066706	-2.088376	H	1.507938	5.083183	-1.934619

H	1.432391	2.641434	-2.514054	H	1.495000	2.666963	-2.428611
H	-2.091938	-0.017589	5.855251	H	-2.031991	-0.019770	5.885957
H	1.373019	-0.860589	4.678835	H	1.374757	-1.004624	4.664842
H	0.564811	-2.443926	4.625356	H	0.497425	-2.549058	4.579531
H	0.305755	-1.359978	6.014106	H	0.295574	-1.488929	5.996356
H	-4.303752	1.118662	4.765265	H	-4.202423	1.238815	4.831777
H	-4.751874	0.375644	3.208027	H	-4.695552	0.539906	3.267481
H	-3.920285	1.938137	3.226828	H	-3.793382	2.062295	3.303975
H	-3.801387	-5.098370	0.732326	H	-4.014713	-4.934096	0.729456
H	-0.477876	-4.580416	-1.416313	H	-0.750938	-4.524328	-1.529936
H	-1.986608	-5.043340	-2.238732	H	-2.308840	-4.891619	-2.307238
H	-1.481625	-5.904973	-0.769745	H	-1.796243	-5.813957	-0.877867
H	-5.333557	-1.658524	1.608936	H	-5.353075	-1.450178	1.734279
H	-4.290741	-2.218426	2.932533	H	-4.288782	-2.087183	3.006555
H	-5.406782	-3.359855	2.141025	H	-5.484664	-3.156930	2.232352
H	2.088833	0.151191	-5.852269	H	1.973681	0.254791	-5.859378
H	-1.376300	-1.058357	-4.403368	H	-1.513361	-0.895488	-4.367337
H	-0.330184	-2.331796	-5.074815	H	-0.517007	-2.132709	-5.171913
H	-0.555862	-0.810052	-5.966181	H	-0.745937	-0.544075	-5.936494
H	4.755549	0.437462	-3.178815	H	4.683363	0.340930	-3.191227
H	3.937702	2.007205	-3.188048	H	3.944008	1.948754	-3.201321
H	4.329085	1.202082	-4.732036	H	4.294731	1.125427	-4.744932
H	3.826935	-5.072536	-0.840042	H	3.535088	-5.209895	-1.038032
H	1.517704	-5.924595	0.648019	H	1.250307	-5.999566	0.504916
H	0.494855	-4.619851	1.305192	H	0.285961	-4.671854	1.202645
H	2.000693	-5.079977	2.134382	H	1.789569	-5.197121	1.995527
H	5.335894	-1.601370	-1.648533	H	5.158274	-1.769575	-1.822994
H	4.303211	-2.155604	-2.982304	H	4.085488	-2.299032	-3.134666
H	5.430011	-3.294567	-2.202848	H	5.200569	-3.464540	-2.378682

Table S19 Optimized Geometries of $[Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4]$ (**2c$_2$**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	-2.642356	0.102794	0.641651	Pt	-2.601322	0.245369	0.750632
Pt	2.643273	0.115022	-0.642860	Pt	2.577490	0.017546	-0.711283
Ag	0.585554	-1.535437	1.517338	Ag	0.471994	-1.706867	1.368613
Ag	-0.573777	-1.533238	-1.520482	Ag	-0.790915	-1.371654	-1.600758
N	-2.358809	2.153649	0.639946	N	-2.134873	2.260072	0.853224
N	2.352243	2.165496	-0.633602	N	2.547340	2.072498	-0.448197
N	-1.946923	-0.133027	2.655243	N	-1.858009	-0.183431	2.716769
N	-0.743894	-0.697280	2.957144	N	-0.715847	-0.895240	2.930832
N	-2.878662	-1.912107	0.458395	N	-3.019800	-1.727439	0.451542
N	-2.023948	-2.597431	-0.355277	N	-2.273797	-2.418501	-0.459128
N	1.950398	-0.117691	-2.659097	N	1.757641	0.072784	-2.679967
N	0.750057	-0.687310	-2.960516	N	0.553996	-0.484243	-2.996463
N	2.887646	-1.899310	-0.467343	N	2.618719	-2.025844	-0.785467
N	2.041661	-2.590376	0.350672	N	1.780801	-2.735242	0.025409
C	-3.395325	0.501561	-1.182951	C	-3.381957	0.816826	-1.015403
C	3.388660	0.509567	1.185868	C	3.500308	0.115552	1.049253
C	-3.972854	-0.327514	-2.147636	C	-4.065899	0.099591	-1.999587
C	-4.489555	0.202320	-3.353552	C	-4.571511	0.742292	-3.154492
C	-4.445549	1.561732	-3.636072	C	-4.410841	2.105871	-3.364481
C	-3.786764	3.874606	-2.881828	C	-3.516539	4.302914	-2.512399
C	-3.230575	4.694568	-1.937430	C	-2.855789	5.013141	-1.547039
C	-2.120924	4.925686	0.322244	C	-1.650976	5.012861	0.674769
C	-1.651536	4.291748	1.463110	C	-1.202221	4.274871	1.759543
C	-1.785658	2.898761	1.590049	C	-1.460256	2.895174	1.816460
C	-2.807624	2.761056	-0.504693	C	-2.565784	2.970618	-0.237712
C	-3.373476	1.895324	-1.487269	C	-3.242411	2.218133	-1.243177
C	-3.878622	2.449390	-2.692891	C	-3.733687	2.883468	-2.396760
C	-2.714623	4.160618	-0.704315	C	-2.350230	4.364759	-0.365533
C	3.968024	-0.321099	2.148099	C	4.035028	-0.940228	1.859298
C	4.477743	0.205495	3.358381	C	4.725022	-0.655731	3.050823
C	4.425042	1.563159	3.647745	C	4.910683	0.653480	3.485163
C	3.757132	3.876259	2.902470	C	4.535821	3.098299	3.081158
C	3.201288	4.698125	1.959538	C	3.980738	4.136976	2.246723
C	2.102639	4.935276	-0.304815	C	2.706210	4.827964	0.176259
C	1.643135	4.304983	-1.451671	C	2.036697	4.378551	-0.963219
C	1.783172	2.913135	-1.584216	C	1.957097	3.022351	-1.262335

C	2.792675	2.769418	0.516184	C	3.170557	2.474167	0.680026
C	3.358275	1.901659	1.497039	C	3.707581	1.435222	1.505534
C	3.856501	2.452422	2.707098	C	4.399699	1.758837	2.717686
C	2.693331	4.167691	0.721593	C	3.298280	3.855386	1.059864
C	-0.588089	-0.687930	4.300551	C	-0.522282	-1.012405	4.263970
C	-1.718282	-0.101907	4.881562	C	-1.565439	-0.359124	4.929010
C	-2.555143	0.233932	3.807784	C	-2.389865	0.151292	3.915187
C	0.624676	-1.267740	4.961927	C	0.641534	-1.765764	4.831999
C	-3.893032	0.910103	3.834393	C	-3.645869	0.959745	4.042943
C	-2.335346	-3.909768	-0.286256	C	-2.703377	-3.698792	-0.474110
C	-3.413055	-4.070312	0.594120	C	-3.748183	-3.832872	0.449630
C	-3.728565	-2.781091	1.046039	C	-3.918434	-2.561916	1.016450
C	-1.605816	-4.930853	-1.103809	C	-2.113440	-4.711829	-1.406257
C	-4.787542	-2.352212	2.011567	C	-4.887146	-2.120851	2.067488
C	0.588535	-0.666519	-4.303467	C	0.342639	-0.324978	-4.321348
C	1.711064	-0.066278	-4.883978	C	1.442804	0.339160	-4.877924
C	2.551119	0.264338	-3.810565	C	2.316241	0.573490	-3.808332
C	-0.624454	-1.245882	-4.964794	C	-0.907377	-0.810680	-4.989128
C	3.893209	0.932317	-3.832994	C	3.651643	1.253737	-3.820900
C	2.358432	-3.901048	0.276293	C	1.974166	-4.051057	-0.212851
C	3.430777	-4.054676	-0.611930	C	2.958116	-4.188290	-1.200552
C	3.737293	-2.763032	-1.063127	C	3.340963	-2.882822	-1.539133
C	1.638682	-4.927168	1.096232	C	1.232365	-5.104113	0.551379
C	4.785855	-2.327238	-2.036994	C	4.347342	-2.426571	-2.547840
H	-4.030755	-1.404146	-1.976920	H	-4.216475	-0.975538	-1.886335
H	-4.935966	-0.480156	-4.082285	H	-5.103664	0.145856	-3.900966
H	-4.847924	1.950355	-4.574631	H	-4.806027	2.582684	-4.264665
H	-4.175757	4.301558	-3.810177	H	-3.893745	4.815499	-3.401389
H	-3.171899	5.772850	-2.103857	H	-2.700757	6.088960	-1.657744
H	-2.031817	6.009195	0.209302	H	-1.461018	6.087342	0.614602
H	-1.178204	4.852052	2.270012	H	-0.645305	4.742372	2.571933
H	-1.428496	2.364289	2.470350	H	-1.119693	2.281297	2.649849
H	4.032748	-1.396455	1.972082	H	3.909242	-1.976197	1.543436
H	4.925732	-0.478176	4.085021	H	5.126400	-1.479345	3.646898
H	4.822224	1.949259	4.589548	H	5.450297	0.856230	4.413770
H	4.140437	4.300598	3.834374	H	5.060823	3.370833	3.998795
H	3.137373	5.775391	2.130564	H	4.098670	5.179232	2.553043
H	2.008795	6.017908	-0.187393	H	2.780047	5.891275	0.410283
H	1.173320	4.867351	-2.259192	H	1.560114	5.088240	-1.642355

H	1.435929	2.382010	-2.470414	H	1.428734	2.640674	-2.132979
H	-1.911943	0.052113	5.940502	H	-1.712898	-0.273187	6.002946
H	0.738438	-0.867873	5.980748	H	0.722102	-1.590939	5.915051
H	1.539837	-1.029383	4.396953	H	1.590006	-1.454564	4.364539
H	0.558229	-2.366949	5.041653	H	0.536301	-2.853272	4.674811
H	-4.482556	0.573428	4.701393	H	-4.171486	0.711968	4.977742
H	-4.463046	0.693374	2.919285	H	-4.326050	0.773302	3.199063
H	-3.797285	2.007641	3.912940	H	-3.437610	2.044129	4.062291
H	-3.912286	-4.996451	0.867896	H	-4.318761	-4.729434	0.678915
H	-0.571247	-4.609994	-1.301684	H	-1.092988	-4.423830	-1.702575
H	-2.096388	-5.095399	-2.079154	H	-2.713556	-4.813497	-2.327368
H	-1.572828	-5.900311	-0.583720	H	-2.067581	-5.704930	-0.933210
H	-5.344370	-1.481420	1.631710	H	-5.398599	-1.190886	1.773716
H	-4.353318	-2.069695	2.984216	H	-4.379834	-1.931571	3.027154
H	-5.500623	-3.172003	2.182170	H	-5.648739	-2.897158	2.231360
H	1.896721	0.100848	-5.942400	H	1.594370	0.607533	-5.920630
H	-1.538350	-1.016732	-4.393999	H	-1.790115	-0.231837	-4.669063
H	-0.553301	-2.344043	-5.054194	H	-1.104435	-1.869663	-4.752752
H	-0.744188	-0.837823	-5.979661	H	-0.820026	-0.717963	-6.081755
H	4.306631	1.003493	-2.816276	H	4.362825	0.758014	-3.143458
H	3.832020	1.951259	-4.252216	H	3.578581	2.306877	-3.499524
H	4.608810	0.369760	-4.455178	H	4.074374	1.244438	-4.836658
H	3.932149	-4.977960	-0.891369	H	3.352787	-5.111333	-1.617791
H	1.610419	-5.896745	0.576132	H	1.040059	-5.985631	-0.079017
H	0.602649	-4.613278	1.297725	H	0.265143	-4.721060	0.911338
H	2.133665	-5.088451	2.069900	H	1.805219	-5.446081	1.431116
H	5.345962	-1.457555	-1.659460	H	5.014497	-1.657752	-2.127568
H	4.340180	-2.040447	-3.003206	H	3.858331	-1.991046	-3.434164
H	5.497794	-3.145426	-2.219745	H	4.963285	-3.275091	-2.879589

Table S20 Optimized Geometries of $[Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4]$ (**2c$_3$**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	2.609978	0.135533	-0.714640	Pt	2.627405	0.205281	-0.650660
Pt	-2.620561	0.158546	0.693658	Pt	-2.627063	0.070546	0.614785
Ag	-0.665376	-1.376162	-1.574171	Ag	-0.524218	-1.440036	-1.575070
Ag	0.512033	-1.717749	1.362294	Ag	0.566345	-1.634930	1.461021
N	3.457876	0.341640	1.166332	N	3.336812	0.527283	1.272852
N	-2.248857	2.193142	0.790236	N	-2.352231	2.120500	0.706118
N	1.889025	0.094876	-2.620568	N	2.013018	0.062497	-2.596623
N	0.676058	-0.435214	-2.942210	N	0.826187	-0.507696	-2.945726
N	2.761676	-2.000926	-0.710708	N	2.864143	-1.915400	-0.565021
N	1.919433	-2.711362	0.098385	N	2.030158	-2.618790	0.257109
N	-1.878241	-0.236866	2.670124	N	-1.957362	-0.257248	2.627007
N	-0.725993	-0.926788	2.898985	N	-0.767819	-0.854468	2.919792
N	-2.942347	-1.831333	0.400361	N	-2.853515	-1.934937	0.337789
N	-2.141657	-2.492106	-0.485735	N	-1.988596	-2.578855	-0.498887
C	2.432989	2.132126	-0.525966	C	2.343814	2.171739	-0.541617
C	-3.412434	0.685951	-1.080663	C	-3.361549	0.545635	-1.198892
C	3.971721	-0.620417	1.939342	C	3.875667	-0.404593	2.141942
C	4.564228	-0.340097	3.182393	C	4.360727	-0.029447	3.391489
C	4.623836	0.969832	3.635202	C	4.318648	1.300437	3.811492
C	4.100324	3.401285	3.187888	C	3.660202	3.657690	3.187148
C	3.566639	4.340809	2.347972	C	3.097235	4.586361	2.231845
C	2.411117	4.915014	0.182665	C	2.072389	4.976552	-0.021373
C	1.860752	4.463404	-1.010154	C	1.640745	4.437094	-1.229606
C	1.864202	3.094034	-1.363991	C	1.760297	3.063623	-1.501115
C	2.970582	2.614642	0.704544	C	2.752168	2.736361	0.684511
C	3.520298	1.643250	1.592610	C	3.297843	1.822844	1.644599
C	4.094986	2.005668	2.836124	C	3.769803	2.291100	2.920675
C	2.980384	3.983776	1.081192	C	2.645488	4.131872	0.993400
C	-4.056882	-0.066807	-2.064792	C	-3.923756	-0.243569	-2.204898
C	-4.584048	0.546832	-3.225911	C	-4.429741	0.336262	-3.392449
C	-4.483490	1.915152	-3.442210	C	-4.389446	1.706777	-3.614292
C	-3.691955	4.154427	-2.597339	C	-3.750280	3.987686	-2.752600
C	-3.069327	4.898064	-1.631848	C	-3.207363	4.767493	-1.767566
C	-1.883676	4.962758	0.599368	C	-2.118914	4.904075	0.509691
C	-1.413661	4.251327	1.692786	C	-1.656861	4.222876	1.625701
C	-1.612496	2.862273	1.756087	C	-1.788421	2.825630	1.691414

C	-2.699981	2.877808	-0.308694	C	-2.791712	2.775507	-0.415519
C	-3.334629	2.090769	-1.314874	C	-3.343490	1.951466	-1.440929
C	-3.847538	2.727438	-2.475001	C	-3.837730	2.555226	-2.626702
C	-2.545001	4.279112	-0.442836	C	-2.701781	4.182286	-0.553656
C	0.499141	-0.304563	-4.275370	C	0.698968	-0.429139	-4.288216
C	1.625081	0.320506	-4.823295	C	1.829924	0.208287	-4.814299
C	2.485932	0.558629	-3.744313	C	2.641445	0.504480	-3.712500
C	-0.737260	-0.800387	-4.960847	C	-0.489481	-0.994165	-5.003380
C	3.838553	1.200886	-3.750631	C	3.972380	1.189813	-3.684777
C	2.150100	-4.030805	-0.088771	C	2.301031	-3.935937	0.122597
C	3.162814	-4.175210	-1.044850	C	3.334258	-4.085949	-0.811330
C	3.518882	-2.868758	-1.413438	C	3.659025	-2.785515	-1.223692
C	1.413784	-5.078305	0.689129	C	1.581222	-4.973486	0.928194
C	4.533730	-2.419184	-2.418491	C	4.683053	-2.345721	-2.223473
C	-0.552793	-1.045310	4.235485	C	-0.638318	-0.924043	4.264506
C	-1.617932	-0.415510	4.886480	C	-1.771573	-0.356001	4.855813
C	-2.436682	0.081403	3.860615	C	-2.582619	0.052401	3.786705
C	0.619284	-1.772320	4.820810	C	0.554024	-1.557442	4.913796
C	-3.720484	0.848484	3.965442	C	-3.912682	0.743118	3.827246
C	-2.512105	-3.790906	-0.502978	C	-2.301489	-3.892964	-0.501013
C	-3.573526	-3.967106	0.394667	C	-3.390715	-4.096463	0.356196
C	-3.816119	-2.701924	0.948591	C	-3.711410	-2.831556	0.869242
C	-1.853247	-4.781171	-1.413088	C	-1.563295	-4.873549	-1.359435
C	-4.825860	-2.297592	1.975832	C	-4.783000	-2.450759	1.841131
H	3.900118	-1.636208	1.552192	H	3.894986	-1.431442	1.786074
H	4.968983	-1.162792	3.772977	H	4.779870	-0.801669	4.039736
H	5.078021	1.206225	4.600725	H	4.696953	1.599234	4.790345
H	4.541733	3.696560	4.142639	H	4.011206	4.038035	4.149348
H	3.581567	5.395923	2.634755	H	3.036972	5.646304	2.487008
H	2.406464	5.978706	0.433365	H	1.976838	6.048189	0.171704
H	1.413057	5.185013	-1.699283	H	1.197806	5.094190	-1.982326
H	1.413012	2.794439	-2.312000	H	1.399039	2.670035	-2.452193
H	-4.159467	-1.147003	-1.946204	H	-3.978297	-1.326849	-2.081913
H	-5.084139	-0.076583	-3.972507	H	-4.864698	-0.315569	-4.155377
H	-4.893836	2.368911	-4.347511	H	-4.783118	2.134429	-4.539490
H	-4.084686	4.645080	-3.491954	H	-4.130672	4.453082	-3.665878
H	-2.959828	5.978855	-1.748227	H	-3.149826	5.852025	-1.886751
H	-1.739589	6.044025	0.533879	H	-2.029864	5.991322	0.443341
H	-0.884328	4.747205	2.506735	H	-1.187387	4.748546	2.457613

H	-1.255228	2.268316	2.597014	H	-1.435007	2.255486	2.550343
H	1.802642	0.567949	-5.866888	H	2.042678	0.423856	-5.858413
H	-0.781714	-0.420398	-5.992286	H	-0.639284	-0.485641	-5.967725
H	-1.648310	-0.470082	-4.436118	H	-1.407188	-0.872631	-4.406653
H	-0.761920	-1.902844	-5.009169	H	-0.364316	-2.071156	-5.211554
H	4.143224	1.420298	-4.784582	H	4.323384	1.369231	-4.711571
H	4.600632	0.546588	-3.299350	H	4.730018	0.585573	-3.162586
H	3.845788	2.143445	-3.181296	H	3.923206	2.160970	-3.166161
H	3.589952	-5.101788	-1.420967	H	3.797807	-5.012515	-1.141242
H	0.418823	-4.717395	0.992784	H	0.543417	-4.666036	1.131312
H	1.959029	-5.364483	1.605808	H	2.073758	-5.145979	1.901260
H	1.278662	-5.991175	0.089146	H	1.556786	-5.935986	0.395363
H	5.106205	-1.555088	-2.047223	H	5.259790	-1.484067	-1.852525
H	4.055548	-2.114659	-3.364154	H	4.214208	-2.046065	-3.175090
H	5.239580	-3.232689	-2.642520	H	5.386445	-3.164375	-2.435185
H	-1.782808	-0.336849	5.958488	H	-1.983949	-0.259246	5.917895
H	1.573801	-1.379880	4.432460	H	1.490124	-1.246866	4.422367
H	0.586098	-2.850154	4.586204	H	0.503861	-2.659375	4.867576
H	0.629444	-1.667476	5.915758	H	0.613966	-1.271508	5.974489
H	-4.199574	0.936987	2.979344	H	-4.461210	0.598365	2.885204
H	-3.555959	1.867504	4.356785	H	-3.805337	1.830870	3.985209
H	-4.425520	0.349176	4.649637	H	-4.528432	0.354766	4.653494
H	-4.108038	-4.887718	0.615537	H	-3.893803	-5.034760	0.576404
H	-1.800539	-5.775126	-0.942790	H	-1.520726	-5.862765	-0.878566
H	-0.829339	-4.463413	-1.663316	H	-0.531757	-4.536281	-1.545180
H	-2.409455	-4.893890	-2.360121	H	-2.054175	-5.004508	-2.339708
H	-5.376289	-1.396009	1.664262	H	-5.351569	-1.576671	1.486734
H	-4.345804	-2.074441	2.942437	H	-4.359037	-2.193440	2.825196
H	-5.551657	-3.108530	2.134622	H	-5.484060	-3.286720	1.979681

Table S21 Optimized Geometries of $[PtAu_2(dfppy)(\mu\text{-}Me_2pz)_3]$ (**3b**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	1.363254	0.676057	-0.426908	Pt	1.374788	0.655468	-0.435464
Au	-1.014718	-1.873284	-0.429940	Au	-1.045853	-1.869840	-0.408909
Au	-2.131847	0.943161	0.168383	Au	-2.115206	0.970509	0.168256
N	1.600656	1.923758	1.194782	N	1.616100	1.912223	1.136937
N	1.291596	-0.715654	-1.945392	N	1.265709	-0.754145	-1.952211
N	0.387130	-1.740481	-1.920855	N	0.351143	-1.770022	-1.908116
N	0.088734	2.109906	-1.458718	N	0.113271	2.095037	-1.480417
N	-1.222280	2.273109	-1.096524	N	-1.193462	2.276969	-1.113067
N	-2.445786	-1.809083	1.051518	N	-2.470332	-1.769813	1.076705
N	-2.937482	-0.561380	1.326300	N	-2.938405	-0.511289	1.343173
C	2.398092	1.434839	2.199253	C	2.446883	1.401071	2.194573
C	2.627864	2.216698	3.344730	C	2.674894	2.219050	3.353906
C	2.051739	3.477859	3.455764	C	2.120872	3.466816	3.458175
C	1.244542	3.956032	2.421894	C	1.303065	3.945451	2.385878
C	1.044653	3.145725	1.310474	C	1.088424	3.137710	1.272537
C	2.555380	-0.484455	0.682292	C	2.547033	-0.504816	0.648124
C	2.933335	0.099559	1.931789	C	2.942326	0.117741	1.941515
C	3.766888	-0.632583	2.792216	C	3.795106	-0.657614	2.809865
C	4.241467	-1.898918	2.483640	C	4.234624	-1.906632	2.483963
C	3.853404	-2.438861	1.260248	C	3.832215	-2.462787	1.238164
C	3.029520	-1.765138	0.364461	C	3.013883	-1.787135	0.343772
C	0.636648	-2.572644	-2.957719	C	0.575570	-2.610384	-2.943607
C	1.739232	-2.080475	-3.657591	C	1.672971	-2.134501	-3.663060
C	2.130834	-0.912670	-2.985442	C	2.086517	-0.966870	-3.004484
C	-0.195071	-3.788815	-3.217468	C	-0.275769	-3.816563	-3.185721
C	3.288251	-0.013203	-3.283310	C	3.247959	-0.081921	-3.329145
C	-1.743695	3.335044	-1.754100	C	-1.703671	3.341649	-1.774607
C	-0.739104	3.886047	-2.551589	C	-0.695474	3.875143	-2.579567
C	0.395987	3.088146	-2.337346	C	0.430316	3.064724	-2.365315
C	-3.172828	3.748846	-1.594140	C	-3.126585	3.774682	-1.610900
C	1.756531	3.240130	-2.942143	C	1.791174	3.198980	-2.973361
C	-3.844759	-0.658589	2.318754	C	-3.843261	-0.584116	2.339865
C	-3.939893	-2.007503	2.691171	C	-3.961424	-1.928119	2.723421
C	-3.039604	-2.700062	1.871524	C	-3.077082	-2.643382	1.906040
C	-4.560207	0.539827	2.855794	C	-4.533618	0.631263	2.871575
C	-2.698893	-4.156024	1.837074	C	-2.762939	-4.105536	1.882303

F	4.148584	-0.114842	3.989354	F	4.182497	-0.135850	4.000978
F	4.300473	-3.671195	0.940525	F	4.278811	-3.699973	0.946313
H	3.258952	1.823436	4.135770	H	3.301477	1.820456	4.147331
H	2.233256	4.082804	4.346678	H	2.297894	4.083908	4.339731
H	0.771302	4.937203	2.464847	H	0.839150	4.931386	2.419658
H	0.421188	3.463660	0.477885	H	0.462725	3.480338	0.450283
H	4.886202	-2.440882	3.173626	H	4.877663	-2.466691	3.162575
H	2.765453	-2.257875	-0.569977	H	2.740957	-2.280920	-0.587676
H	2.204725	-2.514570	-4.538406	H	2.120114	-2.578720	-4.548349
H	-1.225454	-3.518791	-3.501930	H	-1.295594	-3.533735	-3.495089
H	-0.258211	-4.429710	-2.323395	H	-0.367120	-4.431151	-2.275944
H	0.240594	-4.380313	-4.035331	H	0.160877	-4.438289	-3.980359
H	3.531561	0.609531	-2.411271	H	3.514945	0.543622	-2.466324
H	3.077924	0.654253	-4.135183	H	3.028212	0.582817	-4.180692
H	4.176427	-0.609193	-3.545160	H	4.124310	-0.689027	-3.604989
H	-0.818782	4.752361	-3.203314	H	-0.766632	4.738979	-3.235496
H	-3.472875	3.751706	-0.534272	H	-3.422024	3.785168	-0.549828
H	-3.852662	3.061247	-2.124777	H	-3.817374	3.094228	-2.136560
H	-3.328336	4.758157	-2.002085	H	-3.270304	4.784551	-2.021720
H	1.858360	2.639795	-3.861193	H	1.878922	2.608890	-3.900490
H	2.542887	2.916685	-2.244926	H	2.573403	2.853268	-2.282414
H	1.938715	4.291137	-3.212536	H	1.991640	4.249861	-3.231050
H	-4.583007	-2.431517	3.457832	H	-4.609004	-2.334208	3.495997
H	-5.649944	0.379064	2.869932	H	-5.624822	0.484839	2.906812
H	-4.347876	1.423002	2.235182	H	-4.320548	1.503028	2.235327
H	-4.245602	0.764596	3.888639	H	-4.197900	0.866420	3.895430
H	-2.586987	-4.511662	0.801112	H	-2.649597	-4.468983	0.849243
H	-3.485556	-4.748538	2.325985	H	-3.564120	-4.680810	2.368290
H	-1.748815	-4.358130	2.359999	H	-1.820978	-4.322371	2.414071

Table S22 Optimized Geometries of $[PtAu_2(bzq)(\mu\text{-}Me_2pz)_3]$ (**3c**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	1.468914	0.016785	-0.616427	Pt	-1.468983	0.007849	-0.597902
Au	-1.714766	-1.489175	-0.063440	Au	1.679026	1.500480	-0.045289
Au	-1.563033	1.606321	0.048373	Au	1.561174	-1.601155	-0.030534
N	2.211128	-1.450150	0.645466	N	-2.203200	1.388068	0.761541
N	0.614885	-1.494670	-1.937537	N	-0.690307	1.590214	-1.864986
N	-0.542117	-2.148943	-1.607484	N	0.483097	2.216890	-1.545338
N	0.845081	1.631482	-1.725809	N	-0.839589	-1.543852	-1.808580
N	-0.318750	2.285071	-1.432813	N	0.312251	-2.226148	-1.531076
N	-2.856126	-0.621190	1.417094	N	2.839987	0.591949	1.396106
N	-2.788845	0.745140	1.463328	N	2.788615	-0.776034	1.402206
C	2.091074	-2.776583	0.528042	C	-2.109581	2.768896	0.707338
C	2.652181	-3.661115	1.464332	C	-2.650250	3.568409	1.708382
C	3.353204	-3.159135	2.550220	C	-3.305751	3.006824	2.804304
C	4.197762	-1.119910	3.778205	C	-4.044255	0.860764	3.906410
C	4.289226	0.243680	3.844128	C	-4.117522	-0.586258	3.907570
C	3.760103	2.506017	2.870545	C	-3.577542	-2.753221	2.778244
C	3.148654	3.235821	1.860059	C	-2.989431	-3.404030	1.699125
C	2.454164	2.608212	0.799571	C	-2.353160	-2.687795	0.670246
C	2.991404	0.485357	1.772654	C	-2.896495	-0.616381	1.799671
C	2.902201	-0.936644	1.713519	C	-2.831618	0.816627	1.807866
C	3.494757	-1.763497	2.699894	C	-3.417165	1.573389	2.882898
C	3.691984	1.094430	2.847061	C	-3.551334	-1.317579	2.865863
C	2.357670	1.217569	0.726174	C	-2.291839	-1.256815	0.700633
C	-0.752777	-3.162558	-2.480163	C	0.659654	3.284401	-2.358673
C	0.304658	-3.176402	-3.390914	C	-0.437083	3.359790	-3.218430
C	1.142184	-2.113459	-3.015001	C	-1.264755	2.279149	-2.873536
C	-1.958066	-4.046081	-2.400898	C	1.869810	4.160302	-2.272573
C	2.426823	-1.681803	-3.650216	C	-2.587278	1.902741	-3.464423
C	-0.427709	3.369967	-2.233374	C	0.423903	-3.269321	-2.384767
C	0.703360	3.426185	-3.049411	C	-0.694592	-3.270624	-3.220506
C	1.486969	2.317217	-2.696045	C	-1.471002	-2.171280	-2.824413
C	-1.609524	4.285545	-2.174767	C	1.598064	-4.196131	-2.358830
C	2.824389	1.914633	-3.231107	C	-2.788919	-1.721237	-3.369334
C	-3.569048	1.185349	2.470583	C	3.576301	-1.237164	2.394349
C	-4.157237	0.071806	3.086117	C	4.153151	-0.135545	3.040957
C	-3.679311	-1.049957	2.394906	C	3.660285	1.000687	2.384666

C	-3.694896	2.639633	2.796814	C	3.718669	-2.698810	2.677919
C	-3.947023	-2.503716	2.623184	C	3.912072	2.449895	2.655855
H	1.530900	-3.138754	-0.332342	H	-1.588904	3.181016	-0.152030
H	2.523667	-4.734246	1.319188	H	-2.549274	4.651700	1.618323
H	3.795307	-3.832343	3.288976	H	-3.731496	3.629363	3.592742
H	4.658859	-1.745393	4.546092	H	-4.496234	1.412185	4.734176
H	4.827904	0.712766	4.671798	H	-4.620956	-1.095962	4.731248
H	4.290604	3.010661	3.681534	H	-4.066476	-3.324872	3.571014
H	3.201660	4.327829	1.882273	H	-3.019331	-4.495453	1.650207
H	1.988545	3.233459	0.035919	H	-1.897078	-3.233077	-0.156063
H	0.449321	-3.865303	-4.219296	H	-0.615390	4.102583	-3.991747
H	-2.863866	-3.525101	-2.754120	H	2.763743	3.654172	-2.674173
H	-2.149998	-4.369441	-1.365517	H	2.090249	4.435722	-1.228986
H	-1.819185	-4.941127	-3.024577	H	1.716299	5.083456	-2.849940
H	2.248834	-0.984189	-4.485966	H	-2.465473	1.326045	-4.396847
H	2.965327	-2.550992	-4.058201	H	-3.167584	2.805023	-3.712090
H	3.077412	-1.175191	-2.923592	H	-3.174180	1.294021	-2.762662
H	0.934658	4.176250	-3.801055	H	-0.920647	-3.977391	-4.014527
H	-1.822192	4.599809	-1.140524	H	1.817419	-4.536767	-1.334532
H	-2.518536	3.796313	-2.562671	H	2.507517	-3.704705	-2.742970
H	-1.424515	5.185399	-2.778876	H	1.401011	-5.079218	-2.983539
H	3.384311	1.334546	-2.483572	H	-3.392623	-1.234725	-2.589583
H	3.411768	2.807274	-3.495120	H	-3.350401	-2.581811	-3.763081
H	2.732812	1.298678	-4.140687	H	-2.663243	-1.001983	-4.194734
H	-4.846758	0.077688	3.926133	H	4.844944	-0.157933	3.878797
H	-3.722024	3.248641	1.880096	H	3.722161	-3.282778	1.744722
H	-2.841843	2.990604	3.402055	H	2.885716	-3.070599	3.298704
H	-4.614424	2.829524	3.369302	H	4.655303	-2.898970	3.218366
H	-3.167648	-2.961822	3.256017	H	3.097849	2.893928	3.253507
H	-3.965999	-3.054214	1.670164	H	3.982136	3.020770	1.717166
H	-4.913951	-2.645625	3.127758	H	4.849815	2.581650	3.214919

Table S23 Optimized Geometries of $[Pt_2Ag_2(bpy)_2(\mu\text{-}Me_2pz)_4]^{2+}$ (**4d**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	3.070529	0.117071	0.493694	Pt	2.911709	0.196083	0.320076
Pt	-3.062489	0.344762	-0.363106	Pt	-2.870752	0.360383	-0.327961
Ag	-0.357445	-1.441884	1.154438	Ag	-0.373327	-1.344887	1.430927
Ag	0.383217	-0.633440	-1.728489	Ag	0.259277	-1.246415	-1.594301
N	3.932773	0.818413	-1.245156	N	3.605291	0.661263	-1.565285
N	3.326313	2.106402	0.981974	N	2.953732	2.252600	0.439780
N	2.389364	-0.449859	2.329325	N	2.395829	-0.101530	2.266787
N	1.088999	-0.790561	2.581654	N	1.164224	-0.542212	2.662908
N	2.839138	-1.777994	-0.192382	N	2.867275	-1.811631	0.012396
N	1.901946	-2.025514	-1.163432	N	1.856882	-2.361488	-0.734414
N	-3.350120	2.292672	0.253259	N	-2.697791	2.399829	-0.320258
N	-3.965499	0.025348	1.464573	N	-3.380852	0.759229	1.613899
N	-2.806138	-1.628558	-0.763734	N	-3.074966	-1.621243	-0.088092
N	-1.879992	-2.341100	-0.044946	N	-2.087948	-2.332429	0.541633
N	-2.360930	0.829387	-2.214656	N	-2.447996	0.204436	-2.284586
N	-1.063890	0.658925	-2.612416	N	-1.300977	-0.349696	-2.771447
C	4.311421	2.129310	-1.208339	C	3.826783	1.991196	-1.781557
C	5.002401	2.703728	-2.278358	C	4.399781	2.432560	-2.977671
C	5.310855	1.928506	-3.396381	C	4.753371	1.505026	-3.957368
C	4.917182	0.590732	-3.419812	C	4.523499	0.148988	-3.720141
C	4.231077	0.069605	-2.325045	C	3.948994	-0.235057	-2.511166
C	3.943154	2.857033	0.023115	C	3.432287	2.883222	-0.673026
C	4.185129	4.218009	0.228758	C	3.521818	4.276905	-0.718906
C	3.788029	4.816974	1.423957	C	3.111614	5.031325	0.380297
C	3.144041	4.040638	2.387437	C	2.608049	4.373195	1.502557
C	2.928083	2.689323	2.129405	C	2.541957	2.982168	1.494706
C	0.968039	-0.998247	3.913882	C	1.152262	-0.579675	4.016408
C	2.205262	-0.778692	4.528076	C	2.393621	-0.150783	4.496149
C	3.087080	-0.442308	3.496938	C	3.162278	0.137465	3.364590
C	-0.322797	-1.430113	4.537489	C	-0.038917	-1.052789	4.789769
C	4.554190	-0.152512	3.588860	C	4.582439	0.611704	3.304050
C	2.035741	-3.316692	-1.549420	C	2.061262	-3.700395	-0.788824
C	3.073396	-3.901854	-0.814257	C	3.215839	-4.009802	-0.063238
C	3.560473	-2.901160	0.035329	C	3.699158	-2.792818	0.433303
C	1.185065	-3.913794	-2.627802	C	1.162413	-4.609082	-1.568539
C	4.662622	-2.980523	1.043249	C	4.896144	-2.540365	1.293162

C	-4.002701	2.425826	1.444768	C	-3.068546	3.007097	0.882919
C	-4.271199	3.691407	1.973285	C	-3.046531	4.424053	0.977769
C	-3.861945	4.830100	1.279878	C	-2.642022	5.195330	-0.086500
C	-3.178422	4.677495	0.073482	C	-2.225511	4.553029	-1.285314
C	-2.938412	3.392471	-0.406636	C	-2.271702	3.179413	-1.353443
C	-4.376508	1.158463	2.105155	C	-3.444743	2.119584	1.926817
C	-5.101435	1.082002	3.297199	C	-3.861189	2.512372	3.226662
C	-5.411495	-0.166377	3.837267	C	-4.199145	1.572255	4.171454
C	-4.984723	-1.315168	3.171427	C	-4.127428	0.193670	3.830541
C	-4.264994	-1.180302	1.986295	C	-3.720966	-0.157843	2.563744
C	-2.009974	-3.646699	-0.380260	C	-2.489439	-3.614010	0.617686
C	-3.034200	-3.769632	-1.326737	C	-3.778675	-3.731911	0.022787
C	-3.517878	-2.474270	-1.546740	C	-4.121465	-2.463376	-0.404047
C	-1.170192	-4.714389	0.250460	C	-1.664938	-4.675351	1.256576
C	-4.614550	-2.025222	-2.459746	C	-5.354773	-1.991761	-1.098900
C	-0.947811	1.157789	-3.865543	C	-1.378252	-0.339920	-4.118236
C	-2.186453	1.660275	-4.277385	C	-2.607924	0.251122	-4.510655
C	-3.062142	1.431422	-3.212460	C	-3.259703	0.588632	-3.341270
C	0.337551	1.093249	-4.630635	C	-0.314427	-0.908468	-4.991092
C	-4.517764	1.773153	-3.114318	C	-4.584731	1.253236	-3.156885
H	5.309156	3.747883	-2.238947	H	4.582428	3.493595	-3.141677
H	5.856622	2.365709	-4.234079	H	5.210359	1.839522	-4.890150
H	5.140581	-0.054892	-4.269657	H	4.793692	-0.611903	-4.453023
H	3.901490	-0.967394	-2.293695	H	3.755529	-1.279126	-2.269327
H	4.681666	4.810458	-0.538223	H	3.909731	4.774510	-1.606547
H	3.979378	5.877422	1.596223	H	3.183352	6.119918	0.356015
H	2.813391	4.466246	3.335299	H	2.270602	4.921823	2.382271
H	2.436226	2.036698	2.849520	H	2.161546	2.417704	2.345050
H	2.442773	-0.868525	5.584829	H	2.706175	-0.069757	5.533867
H	-0.381931	-2.528658	4.619394	H	-0.029090	-2.149367	4.911593
H	-1.185791	-1.088729	3.943733	H	-0.980893	-0.773027	4.291728
H	-0.420396	-1.020528	5.553807	H	-0.044499	-0.612361	5.797182
H	4.929175	0.368287	2.696550	H	4.886103	0.868730	2.279556
H	5.131817	-1.086109	3.690564	H	5.270269	-0.167721	3.669862
H	4.775768	0.461459	4.474807	H	4.730416	1.494897	3.945198
H	3.437763	-4.923028	-0.888209	H	3.659770	-4.991051	0.082027
H	1.241301	-5.010970	-2.598184	H	1.094885	-5.596148	-1.088113
H	1.521239	-3.593691	-3.628619	H	1.541701	-4.771722	-2.591648
H	0.128495	-3.621822	-2.520768	H	0.145025	-4.194537	-1.649601

H	5.365973	-2.139024	0.947253	H	5.406754	-1.606958	1.013296
H	5.226605	-3.913897	0.911579	H	5.612545	-3.368268	1.199665
H	4.263605	-2.968514	2.070051	H	4.611140	-2.461974	2.354943
H	-4.796742	3.791193	2.921801	H	-3.360694	4.896943	1.907821
H	-4.073343	5.822518	1.681444	H	-2.637600	6.283479	-0.010000
H	-2.835119	5.538719	-0.500424	H	-1.877310	5.123271	-2.146307
H	-2.412239	3.215973	-1.344006	H	-1.959597	2.650612	-2.252339
H	-5.433474	1.989526	3.799296	H	-3.917088	3.573660	3.466824
H	-5.984071	-0.237067	4.763504	H	-4.526322	1.880313	5.165361
H	-5.207926	-2.311935	3.553015	H	-4.406928	-0.583977	4.540975
H	-3.909486	-2.043914	1.427251	H	-3.667101	-1.201598	2.263097
H	-3.391911	-4.682942	-1.794650	H	-4.371782	-4.637707	-0.071930
H	-1.532312	-4.964245	1.262227	H	-2.138598	-5.019308	2.192442
H	-0.117279	-4.404311	0.339486	H	-0.653866	-4.313030	1.491017
H	-1.205885	-5.635654	-0.347708	H	-1.586720	-5.556441	0.600215
H	-4.222826	-1.408701	-3.283969	H	-5.141506	-1.719746	-2.145223
H	-5.371374	-1.429272	-1.925668	H	-5.785090	-1.109314	-0.600931
H	-5.118218	-2.897146	-2.898527	H	-6.110817	-2.788138	-1.105726
H	-2.429210	2.115652	-5.233862	H	-2.967849	0.394880	-5.525935
H	0.400601	0.171153	-5.233007	H	-0.671272	-1.827633	-5.486898
H	1.206014	1.113853	-3.952985	H	0.589896	-1.157139	-4.416389
H	0.421138	1.943722	-5.323138	H	-0.046559	-0.199441	-5.790663
H	-5.009700	1.620239	-4.086147	H	-5.155018	1.213792	-4.094873
H	-4.674235	2.830130	-2.838699	H	-4.468294	2.313156	-2.878300
H	-5.030635	1.151097	-2.367381	H	-5.175905	0.772671	-2.365020

Table S24 Optimized Geometries of $[Pt_2Au_2(bpy)_2(\mu\text{-}Me_2pz)_4]^{2+}$ (**5d**) by the B3LYP method.

	Singlet				Triplet		
	x	*y*	*z*		*x*	*y*	*z*
Pt	-0.977051	-0.421839	3.100382	Pt	-3.216796	0.086124	-0.569249
Pt	0.977051	0.421839	-3.100382	Pt	3.218179	-0.087637	0.567599
Au	0.606444	-1.527338	-0.013500	Au	0.001917	-1.557348	-0.242250
Au	-0.606444	1.527338	0.013500	Au	-0.006134	1.562195	0.239500
N	-0.422839	1.231530	4.190471	N	-4.125652	1.181444	0.887996
N	0.577179	-1.209928	4.193426	N	-4.115379	-1.413750	0.476124
N	-1.452052	-2.157381	2.135588	N	-2.378913	-1.110456	-2.024519
N	-1.059967	-2.392742	0.844658	N	-1.052738	-1.436925	-1.994236
N	-2.529213	0.487043	2.138284	N	-2.391889	1.679673	-1.585355
N	-2.403901	0.972722	0.864317	N	-1.064501	1.982358	-1.463784
N	0.422839	-1.231530	-4.190471	N	4.130367	-1.191492	-0.881084
N	-0.577179	1.209928	-4.193426	N	4.125897	1.405811	-0.479529
N	1.452052	2.157381	-2.135588	N	2.379338	1.115098	2.017688
N	1.059967	2.392742	-0.844658	N	1.052169	1.438732	1.988852
N	2.529213	-0.487043	-2.138284	N	2.384453	-1.674277	1.587048
N	2.403901	-0.972722	-0.864317	N	1.056438	-1.972237	1.463593
C	0.588261	1.019604	5.082431	C	-4.875299	0.439875	1.780358
C	1.029612	2.050116	5.916255	C	-5.577434	1.090454	2.813405
C	0.430299	3.307395	5.834904	C	-5.518486	2.469135	2.936067
C	-0.596994	3.509475	4.913053	C	-4.745862	3.206846	2.017615
C	-0.996037	2.447007	4.105567	C	-4.070953	2.527225	1.017276
C	1.148716	-0.347317	5.083504	C	-4.869949	-0.990467	1.553079
C	2.186723	-0.769928	5.917635	C	-5.566726	-1.934271	2.332248
C	2.642373	-2.086196	5.839002	C	-5.497947	-3.282622	2.021488
C	2.051398	-2.953719	4.920282	C	-4.721862	-3.693741	0.919993
C	1.020897	-2.478699	4.112428	C	-4.052772	-2.732638	0.180577
C	-1.667701	-3.525995	0.416758	C	-0.702544	-1.985742	-3.199365
C	-2.473483	-4.016950	1.444700	C	-1.826367	-2.000376	-4.009974
C	-2.314845	-3.131864	2.516908	C	-2.872251	-1.439990	-3.240668
C	-1.426473	-4.098726	-0.943809	C	0.677832	-2.486230	-3.473733
C	-2.931711	-3.205804	3.878210	C	-4.298297	-1.250027	-3.629243
C	-3.629082	1.362927	0.436311	C	-0.724092	2.881817	-2.438616
C	-4.556619	1.113122	1.448684	C	-1.854335	3.146316	-3.196284
C	-3.831638	0.559807	2.509691	C	-2.895026	2.372283	-2.632730
C	-3.848480	1.982434	-0.907532	C	0.654669	3.444892	-2.552683
C	-4.339959	0.112792	3.844000	C	-4.323678	2.309330	-3.052382

C	-0.588261	-1.019604	-5.082431	C	4.885318	-0.455480	-1.773430
C	-1.029612	-2.050116	-5.916255	C	5.589483	-1.111771	-2.801375
C	-0.430299	-3.307395	-5.834904	C	5.527902	-2.490939	-2.918580
C	0.596994	-3.509475	-4.913053	C	4.750486	-3.222935	-1.999793
C	0.996037	-2.447007	-4.105567	C	4.073396	-2.537482	-1.004843
C	-1.148716	0.347317	-5.083504	C	4.882806	0.976198	-1.552091
C	-2.186723	0.769928	-5.917635	C	5.584299	1.914957	-2.333049
C	-2.642373	2.086196	-5.839002	C	5.519650	3.264572	-2.026644
C	-2.051398	2.953719	-4.920282	C	4.742477	3.681981	-0.928508
C	-1.020897	2.478699	-4.112428	C	4.067628	2.725644	-0.188016
C	1.667701	3.525995	-0.416758	C	0.702241	1.986203	3.194400
C	2.473483	4.016950	-1.444700	C	1.827456	2.005567	4.003089
C	2.314845	3.131864	-2.516908	C	2.873759	1.447714	3.232639
C	1.426473	4.098726	0.943809	C	-0.680278	2.479815	3.471102
C	2.931711	3.205804	-3.878210	C	4.301079	1.262299	3.619322
C	3.629082	-1.362927	-0.436311	C	0.707959	-2.862286	2.443963
C	4.556619	-1.113122	-1.448684	C	1.835156	-3.129792	3.204465
C	3.831638	-0.559807	-2.509691	C	2.880981	-2.363174	2.640158
C	3.848480	-1.982434	0.907532	C	-0.675148	-3.415132	2.558858
C	4.339959	-0.112792	-3.844000	C	4.307938	-2.301822	3.065799
H	1.833895	1.874985	6.629309	H	-6.173156	0.505438	3.513280
H	0.763908	4.117053	6.485984	H	-6.067953	2.974042	3.731901
H	-1.093714	4.475178	4.815179	H	-4.676363	4.293081	2.073632
H	-1.793070	2.544671	3.369601	H	-3.463486	3.049651	0.279635
H	2.637442	-0.079332	6.628965	H	-6.165840	-1.599456	3.178345
H	3.449040	-2.426998	6.490061	H	-6.042694	-4.013229	2.621184
H	2.374882	-3.990632	4.825231	H	-4.645012	-4.743231	0.636191
H	0.520193	-3.110016	3.379315	H	-3.443046	-2.996797	-0.682401
H	-3.096757	-4.906679	1.421133	H	-1.898658	-2.373772	-5.027830
H	-0.451056	-4.610262	-0.998167	H	0.874188	-3.431083	-2.940678
H	-1.437288	-3.311020	-1.713060	H	1.438261	-1.757141	-3.153647
H	-2.205194	-4.834427	-1.188862	H	0.805589	-2.673848	-4.548441
H	-2.567077	-2.401675	4.531558	H	-4.888536	-0.825963	-2.806815
H	-2.699877	-4.172152	4.353838	H	-4.743277	-2.215635	-3.921640
H	-4.028975	-3.132832	3.821929	H	-4.382873	-0.587821	-4.506458
H	-5.624991	1.309323	1.422582	H	-1.934997	3.821534	-4.043813
H	-4.912529	1.933249	-1.178255	H	0.760553	3.998225	-3.495545
H	-3.266654	1.461119	-1.683401	H	1.414286	2.648069	-2.529008
H	-3.548505	3.043659	-0.916879	H	0.872753	4.140223	-1.725771

H	-3.526246	0.011257	4.575936	H	-4.928067	1.728443	-2.343628
H	-4.853228	-0.859066	3.772446	H	-4.422064	1.854755	-4.052044
H	-5.071640	0.836366	4.233982	H	-4.741762	3.326166	-3.127111
H	-1.833895	-1.874985	-6.629309	H	6.188230	-0.530920	-3.502097
H	-0.763908	-4.117053	-6.485984	H	6.077970	-3.000314	-3.711144
H	1.093714	-4.475178	-4.815179	H	4.677655	-4.309126	-2.052160
H	1.793070	-2.544671	-3.369601	H	3.460528	-3.055294	-0.268397
H	-2.637442	0.079332	-6.628965	H	6.184215	1.575420	-3.176645
H	-3.449040	2.426998	-6.490061	H	6.068297	3.991360	-2.627444
H	-2.374882	3.990632	-4.825231	H	4.668854	4.732622	-0.648184
H	-0.520193	3.110016	-3.379315	H	3.457565	2.994553	0.673328
H	3.096757	4.906679	-1.421133	H	1.900180	2.380148	5.020470
H	0.451056	4.610262	0.998167	H	-0.883402	3.422427	2.936924
H	1.437288	3.311020	1.713060	H	-1.437057	1.745655	3.153876
H	2.205194	4.834427	1.188862	H	-0.806909	2.668546	4.545789
H	2.567077	2.401675	-4.531558	H	4.890770	0.836282	2.797386
H	2.699877	4.172152	-4.353838	H	4.744934	2.229385	3.908372
H	4.028975	3.132832	-3.821929	H	4.388268	0.602711	4.498265
H	5.624991	-1.309323	-1.422582	H	1.909806	-3.799713	4.056703
H	4.912529	-1.933249	1.178255	H	-0.791078	-3.950189	3.511091
H	3.266654	-1.461119	1.683401	H	-1.428931	-2.613684	2.515068
H	3.548505	-3.043659	0.916879	H	-0.892452	-4.124625	1.743663
H	3.526246	-0.011257	-4.575936	H	4.918683	-1.731683	2.353506
H	4.853228	0.859066	-3.772446	H	4.404181	-1.835749	4.060378
H	5.071640	-0.836366	-4.233982	H	4.720780	-3.319447	3.154926

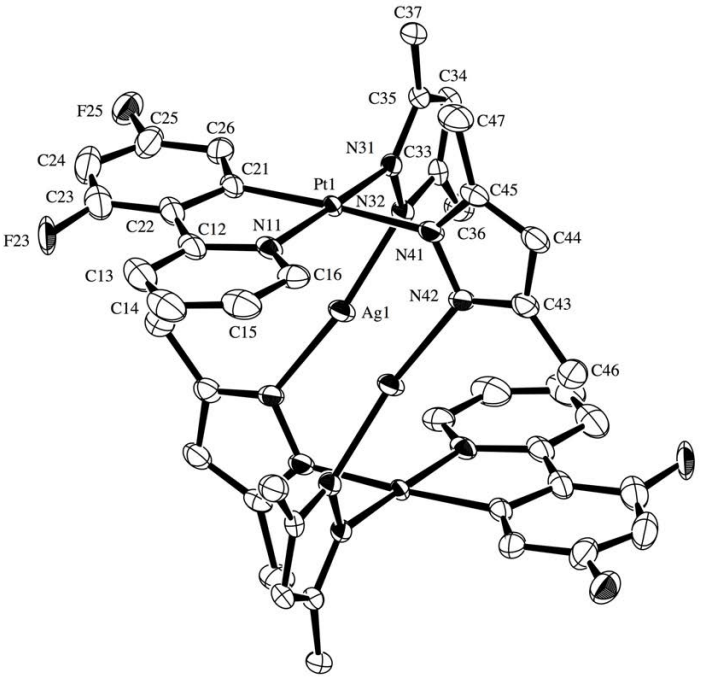


Fig. S1 Molecular structure of $[Pt_2Ag_2(dfppy)_2(\mu\text{-}Me_2pz)_4]$ (**2b**) with the atom numbering scheme (50% probability ellipsoids).

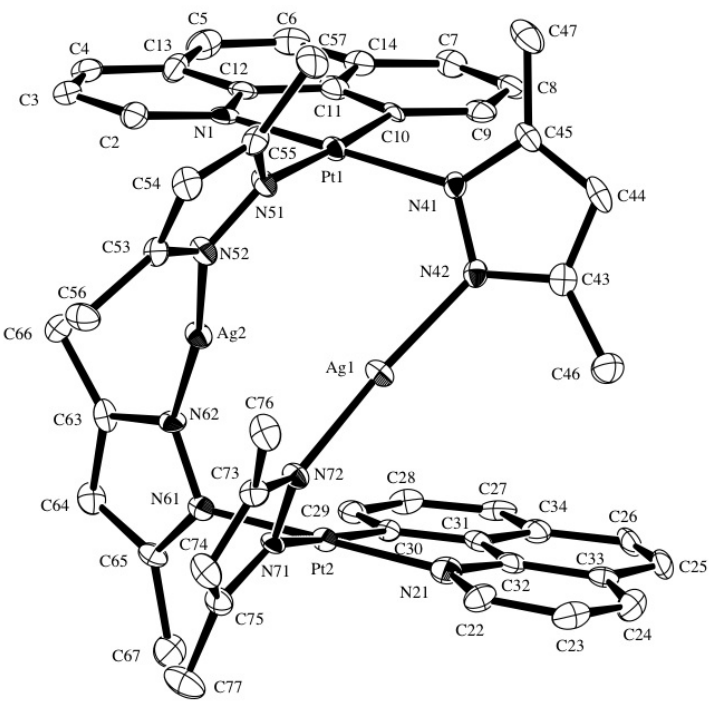


Fig. S2 Molecular structure of $[Pt_2Ag_2(bzq)_2(\mu\text{-}Me_2pz)_4]$ (**2c**) with the atom numbering scheme (50% probability ellipsoids).

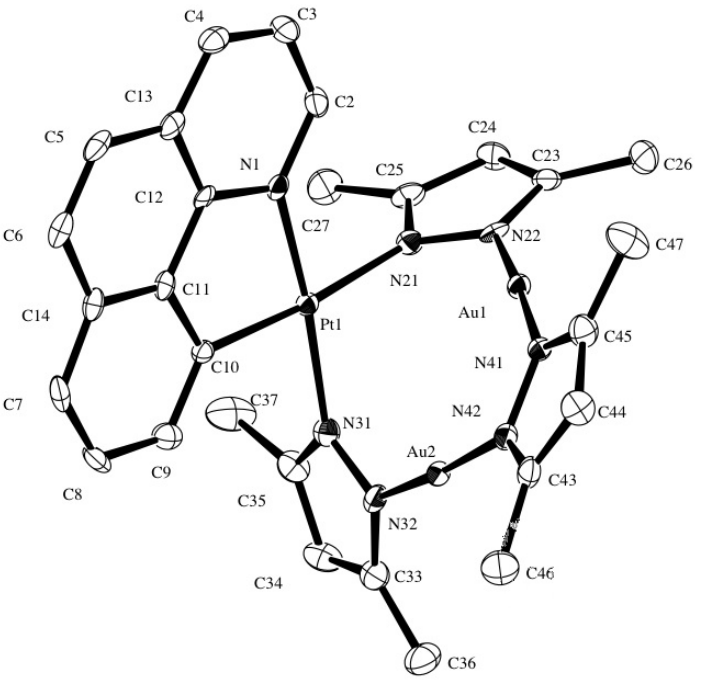


Fig. S3 Molecular structure of $[PtAu_2(bzq)(Me_2pz)_3]$ (**3c**) with the atom numbering scheme (50% probability ellipsoids).

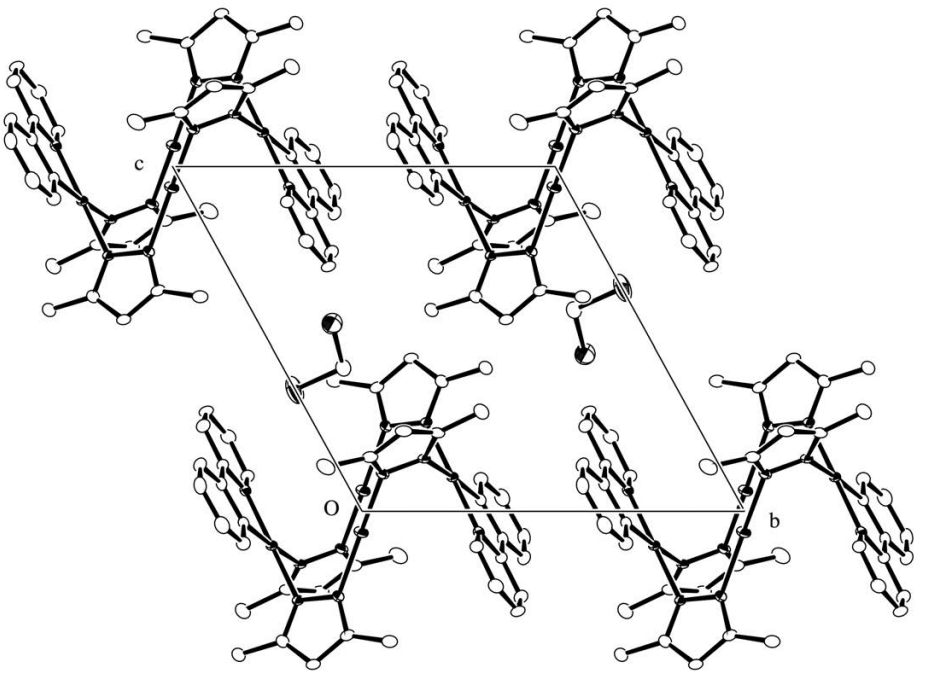


Fig. S4 Crystal structure of **2a**·$2CH_2Cl_2$ viewed along the a-axis.

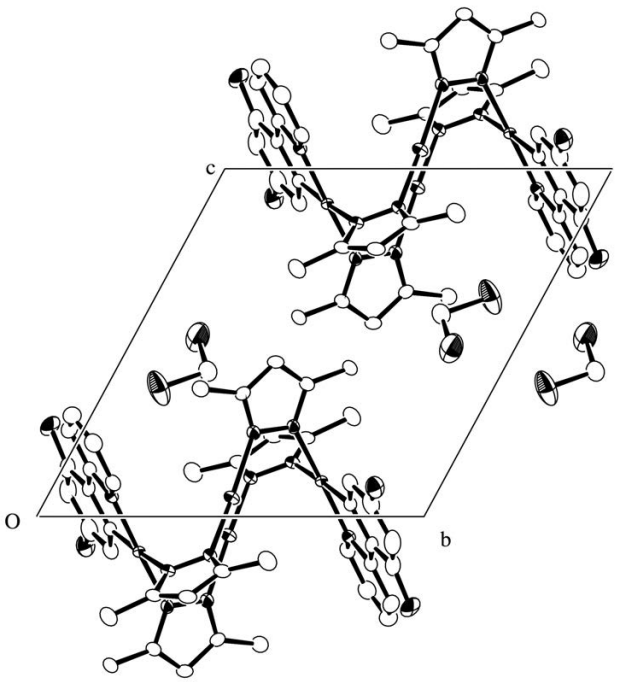


Fig. S5 Crystal structure of **2b**•$2CH_2Cl_2$ viewed along the a-axis.

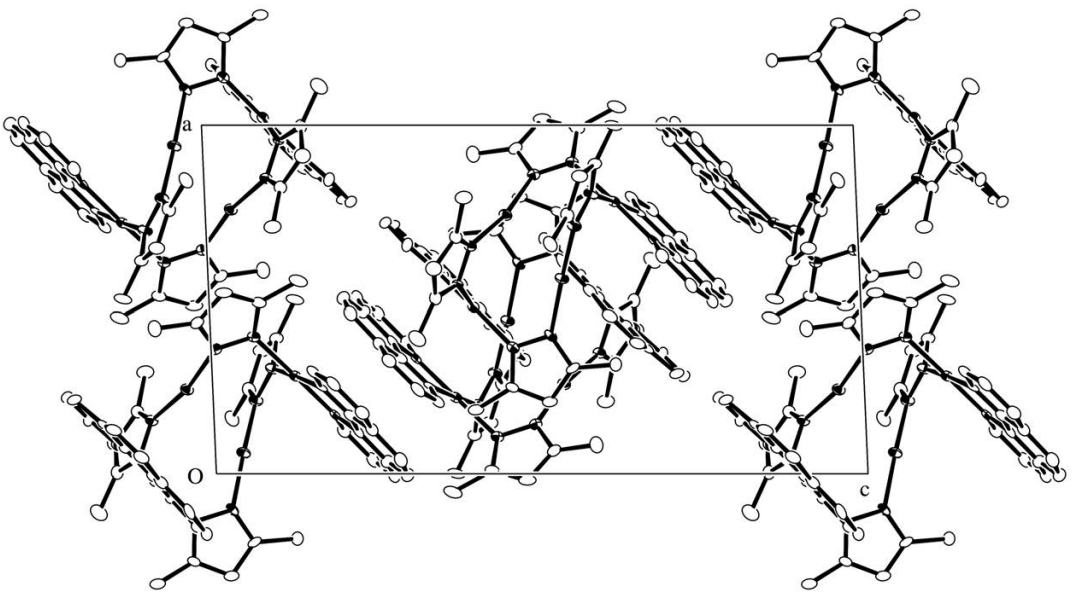


Fig. S6 Crystal structure of **2c** viewed along the b-axis.

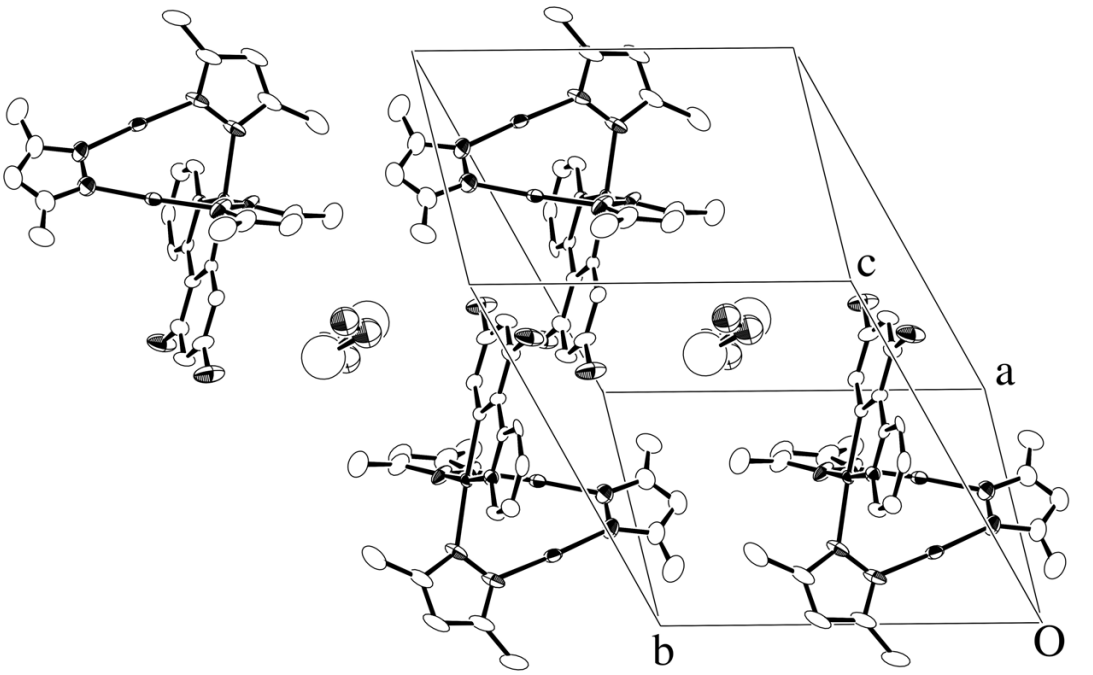


Fig. S7 Crystal structure of **3b**•0.5CH_2Cl_2.

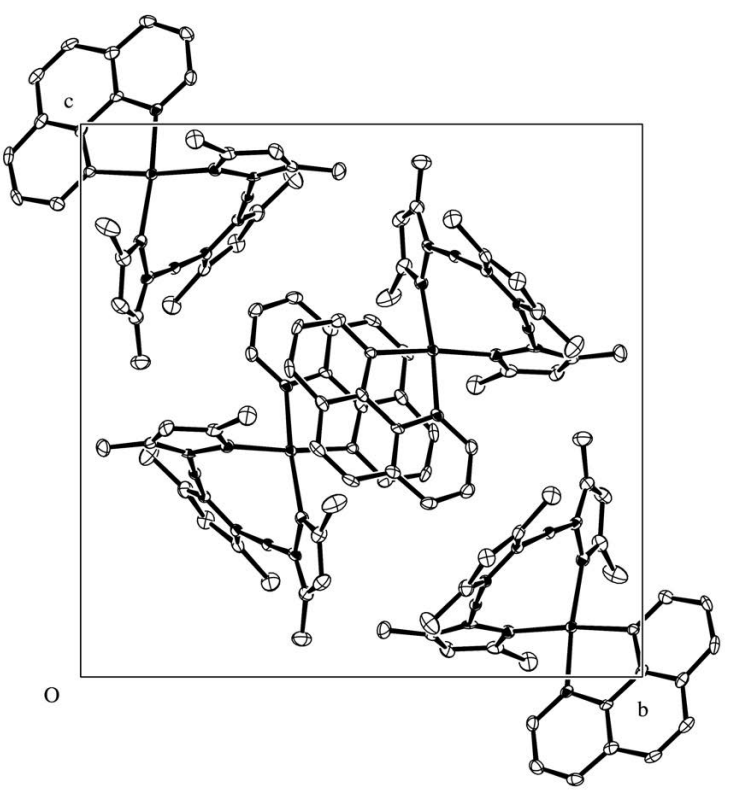


Fig. S8 Crystal structure of **3c** viewed along the a-axis.

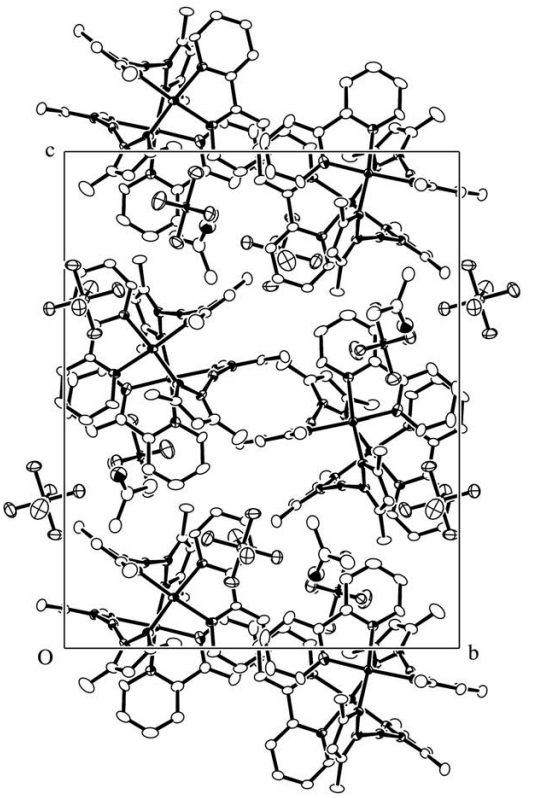


Fig. S9 Crystal structure of **4d**•$(CH_3)_2CO$ viewed along the a-axis.

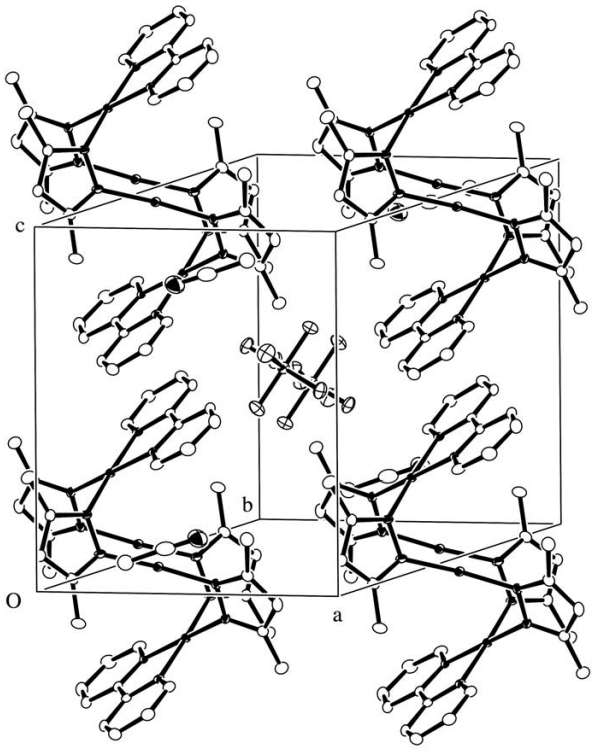


Fig. S10 Crystal structure of **5d**•$2CH_3CN$.

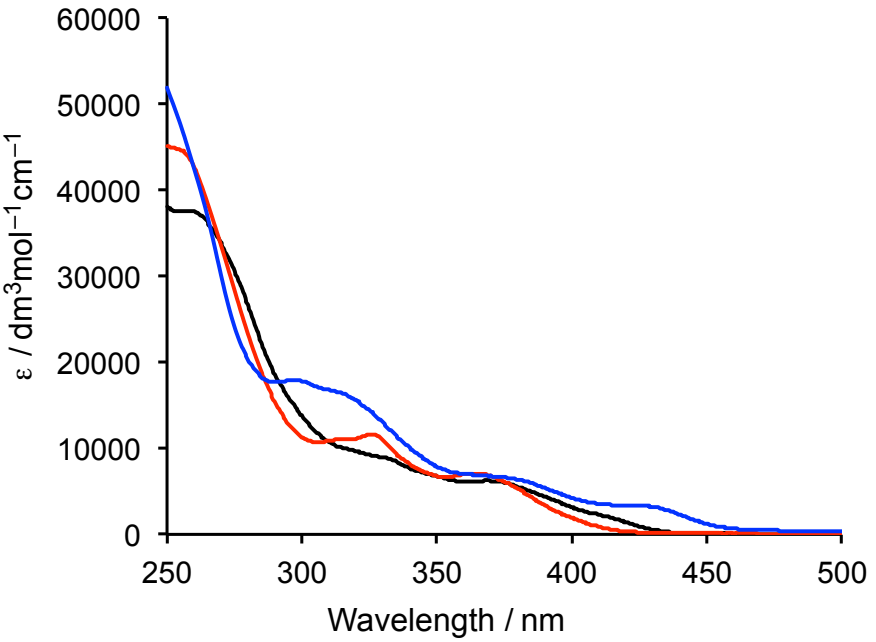


Fig. S11 Electronic absorption spectra of **2a** (———), **2b** (———) and **2c** (———) in CH_2Cl_2 at 298 K.

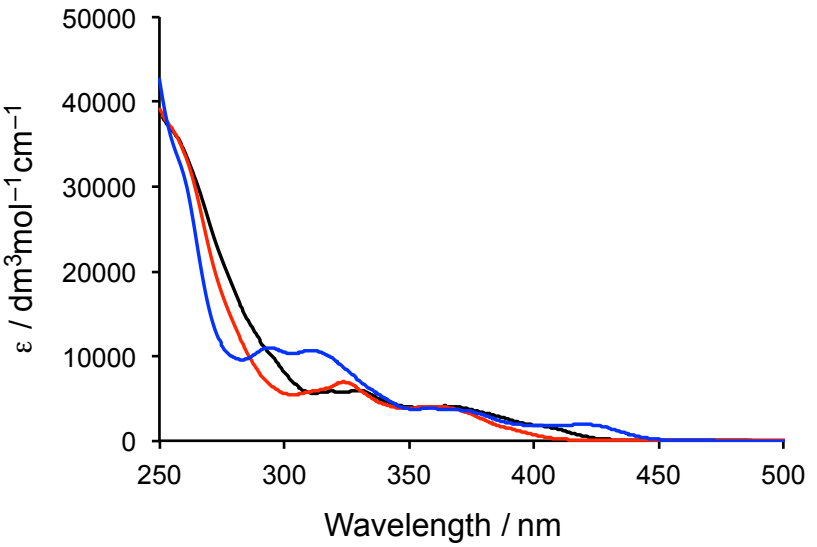


Fig. S12 Electronic absorption spectra of **3a** (———), **3b** (———) and **3c** (———) in CH_2Cl_2 at 298 K.

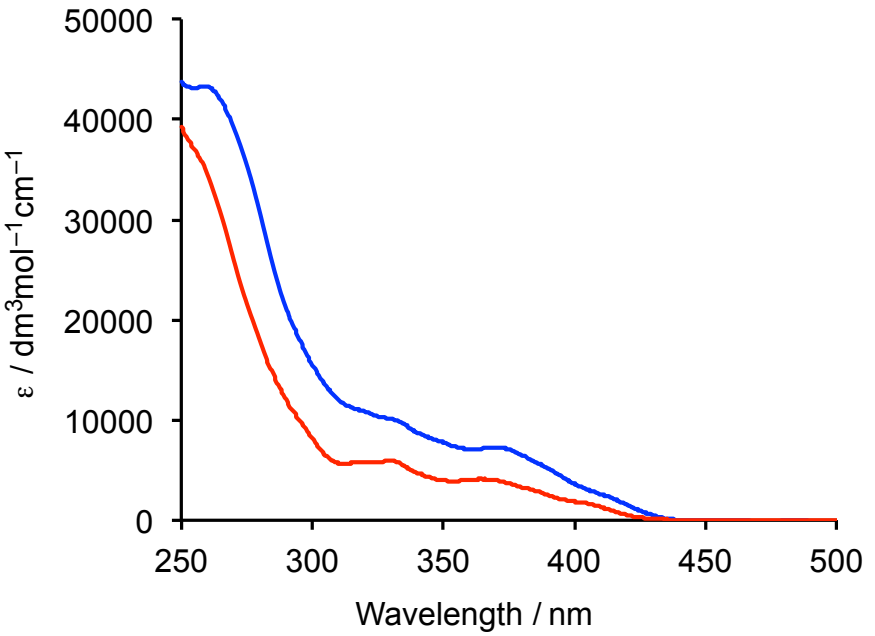


Fig. S13 Electronic absorption spectra of **2a** ( ) and **3a** ( ) in CH_2Cl_2 at 298 K.

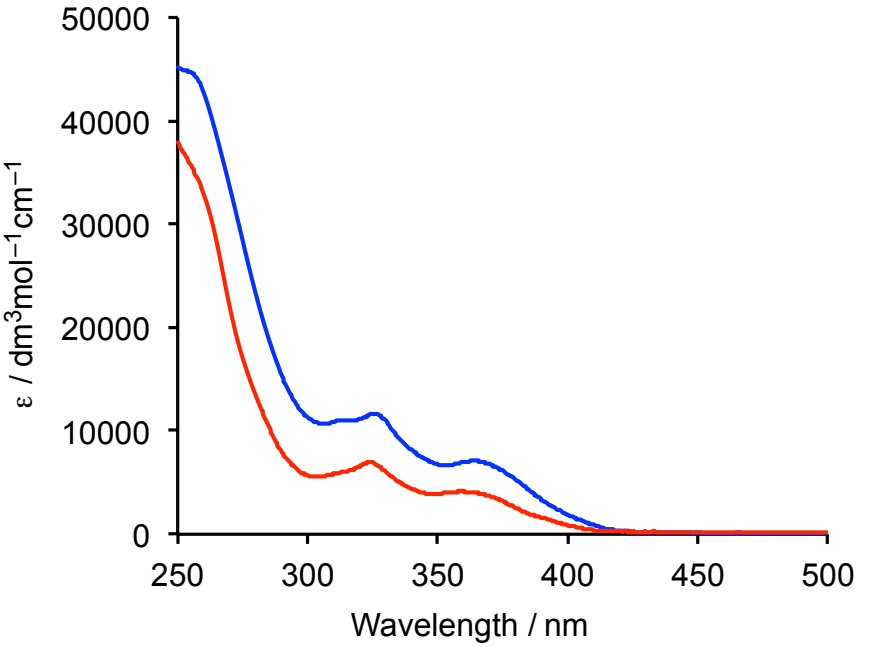


Fig. S14 Electronic absorption spectra of **2b** ( ) and **3b** ( ) in CH_2Cl_2 at 298 K.

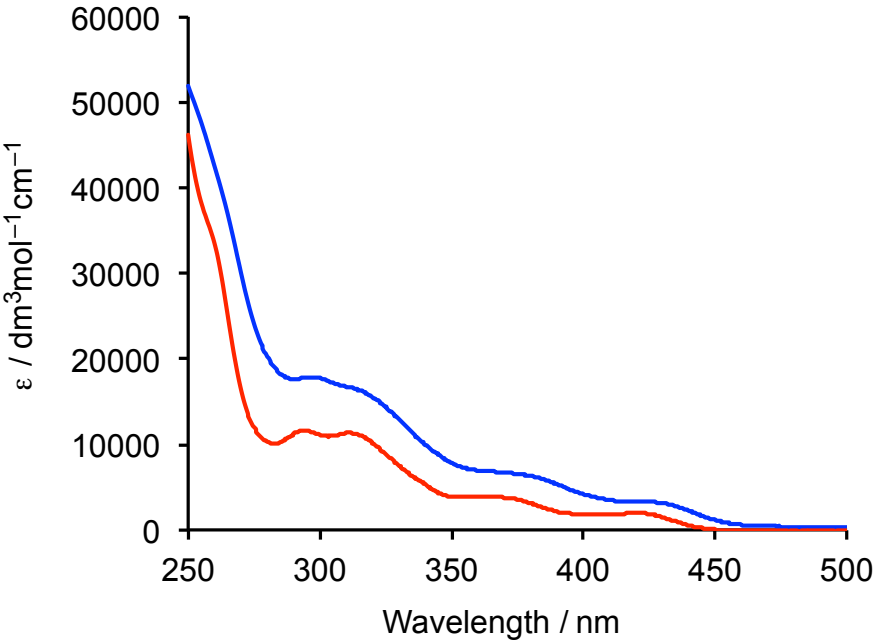


Fig. S15 Electronic absorption spectra of **2c** ( ) and **3c** ( ) in CH_2Cl_2 at 298 K.

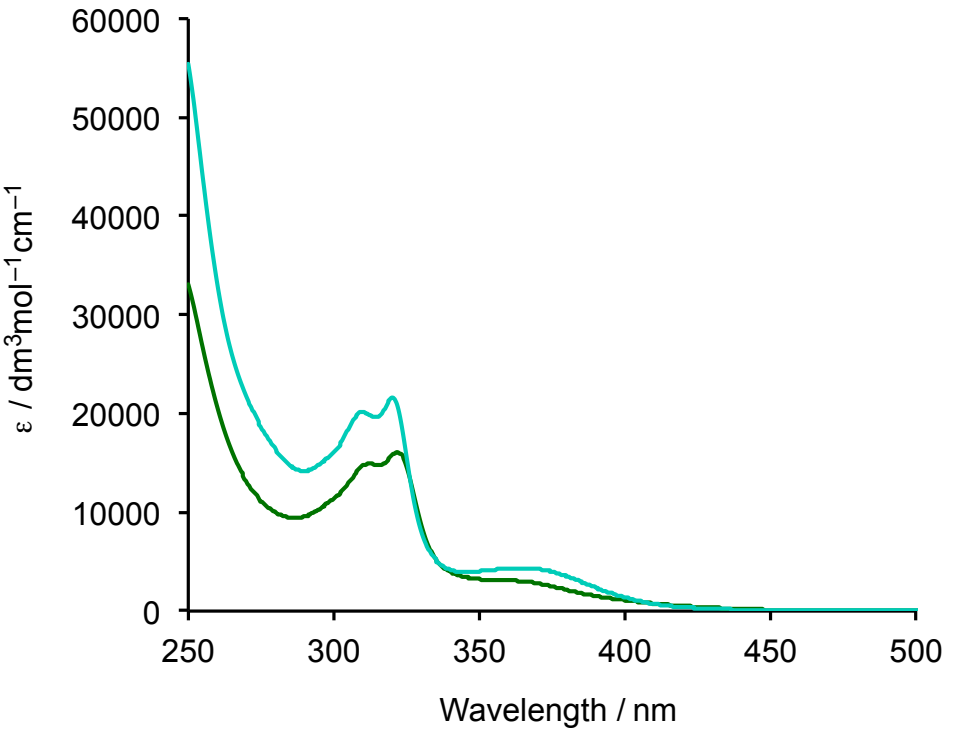


Fig. S16 Electronic absorption spectra of **4d** ( ) and **5d** ( ) in CH_3CN at 298 K.

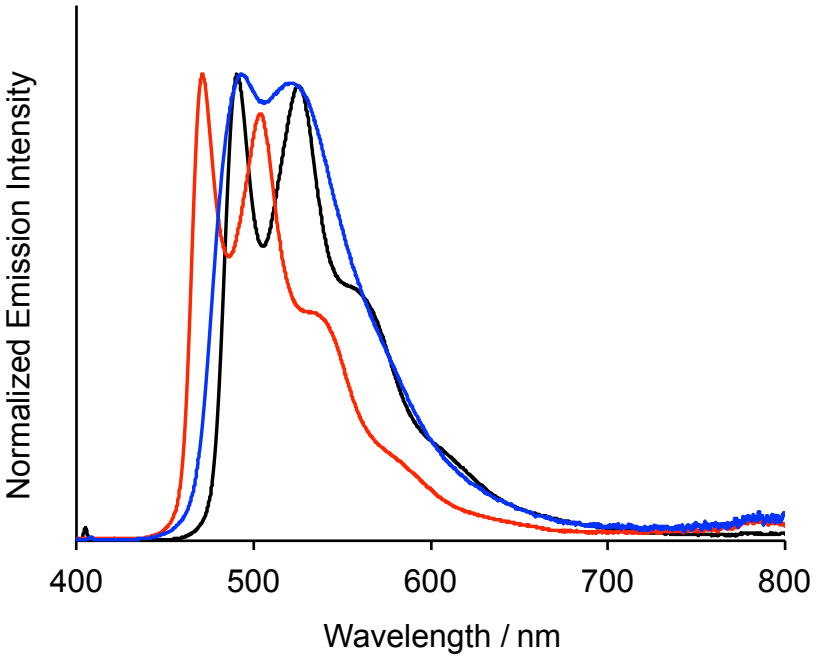


Fig. S17 Normalized emission spectra of **2a** (——), **2b** (——) and **2c** (——) in CH_2Cl_2 at 295 K (λ_{ex} = 350 nm).

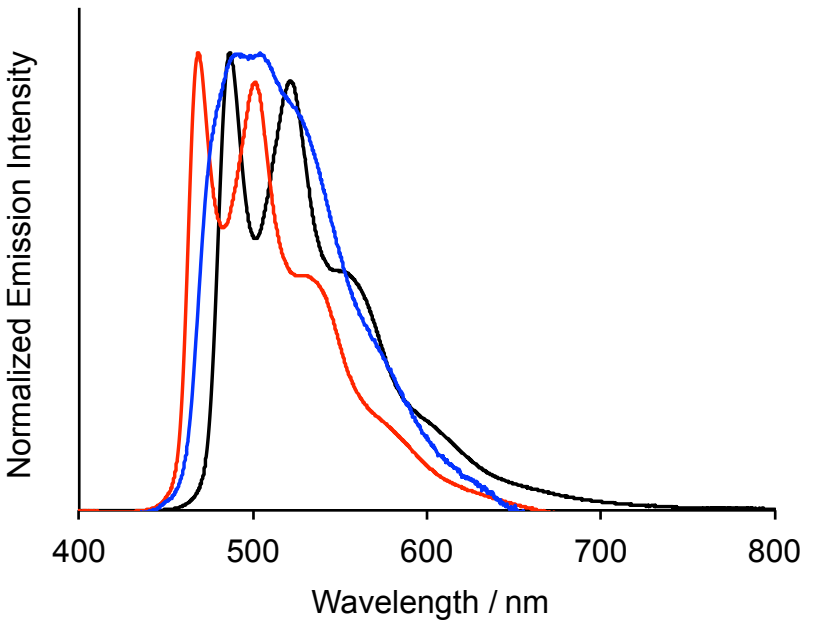


Fig. S18 Normalized emission spectra of **3a** (——), **3b** (——) and **3c** (——) in CH_2Cl_2 at 295 K (λ_{ex} = 350 nm).

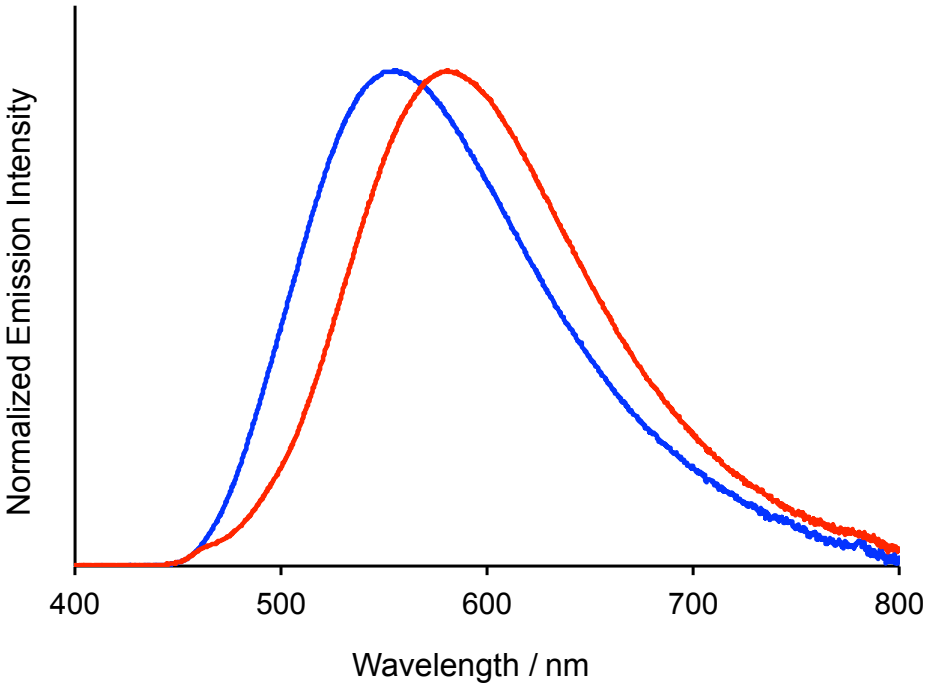


Fig. S19 Normalized emission spectra of **4d** (———) and **5d** (———) in CH_2Cl_2 at 295 K (λ_{ex} = 350 nm).

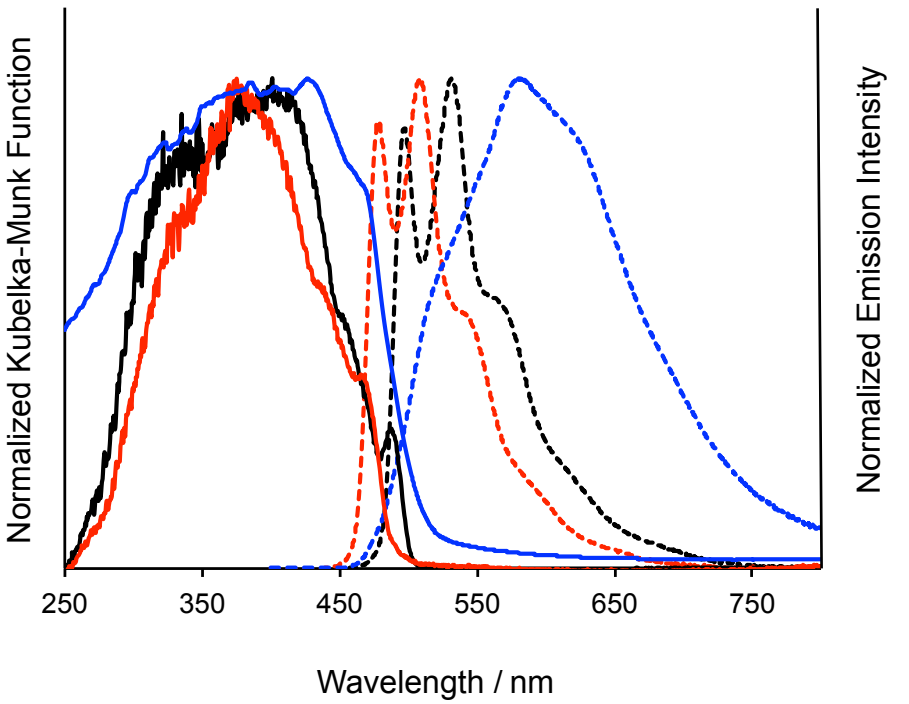


Fig. S20 UV-Vis diffuse reflectance spectra (solid line) and normalized solid state emission spectra (broken line) of **2a** (——— , - - -), **2b** (——— , - - -) and **2c** (——— , - - -) at 295 K (λ_{ex} = 350 nm).

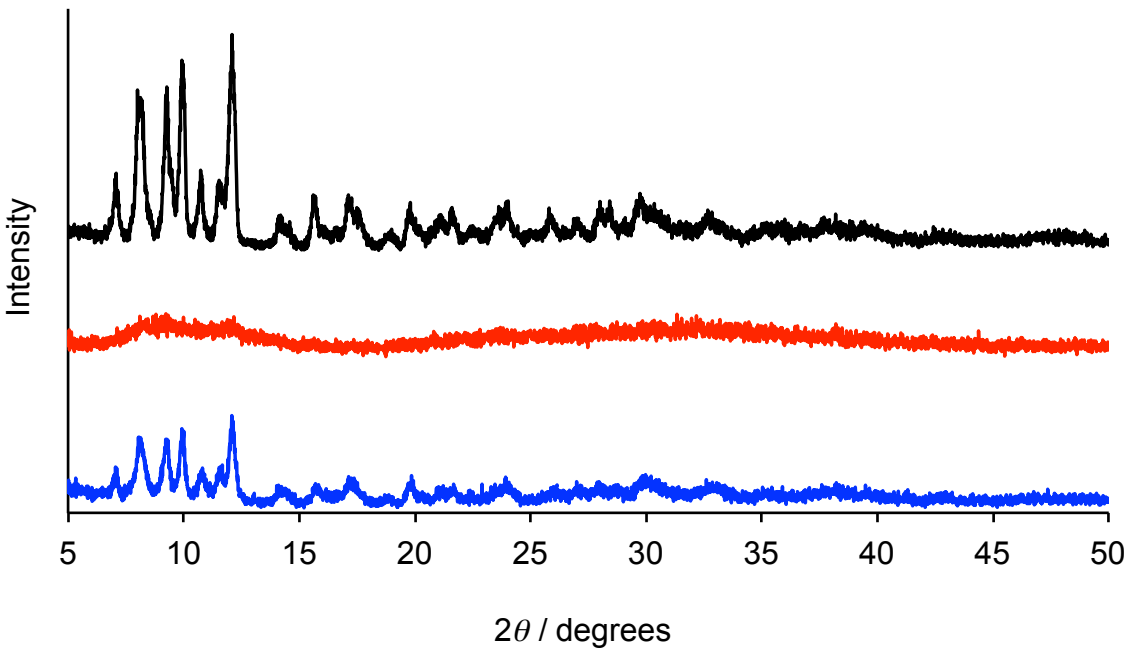
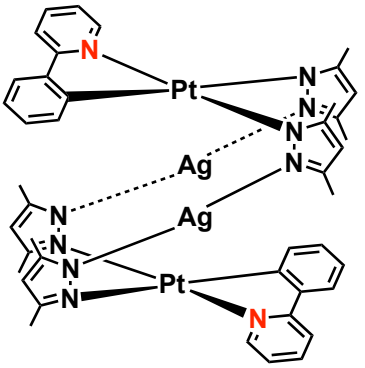
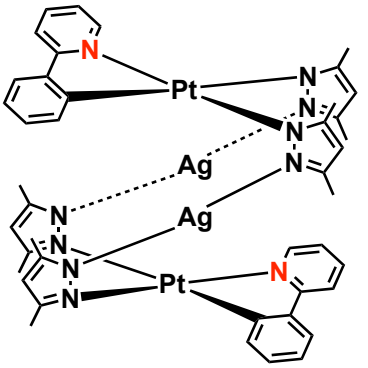


Fig. S21 Powder X-ray diffraction patterns of **5d**: unground sample (——), completely ground sample (——) and ground sample with a drop of CH_2Cl_2 added (——).

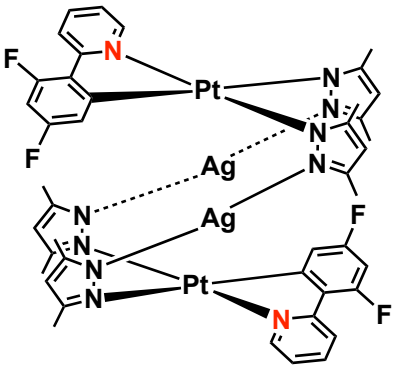


C_i isomer ($2a_1$)

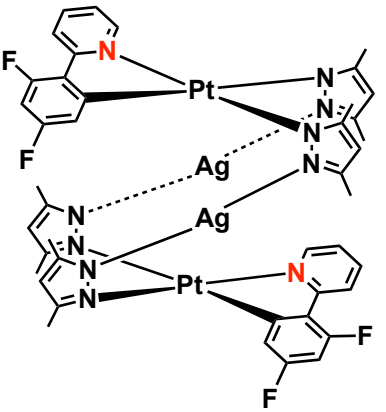


C_2 isomer ($2a_2$)

$[Pt_2Ag_2(ppy)_2(Me_2pz)_4]$ (2a)

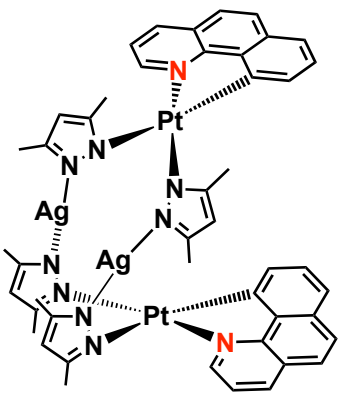


C_i isomer ($2b_1$)

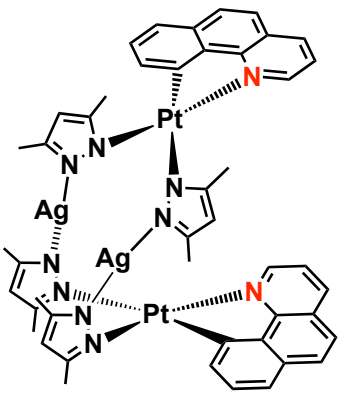


C_2 isomer ($2b_2$)

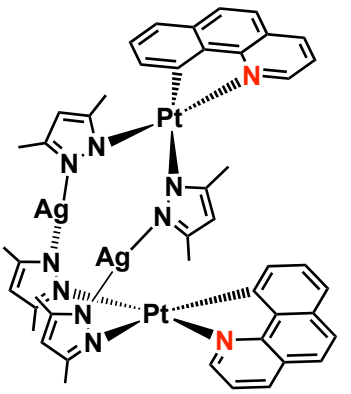
$[Pt_2Ag_2(dfppy)_2(Me_2pz)_4]$ (2b)



($2c_1$)



($2c_2$)



($2c_3$)

$[Pt_2Ag_2(bzq)_2(Me_2pz)_4]$ (2c)

Fig. S22 Notation of geometrical isomers of **2a**, **2b** and **2c** used in the computational methods.

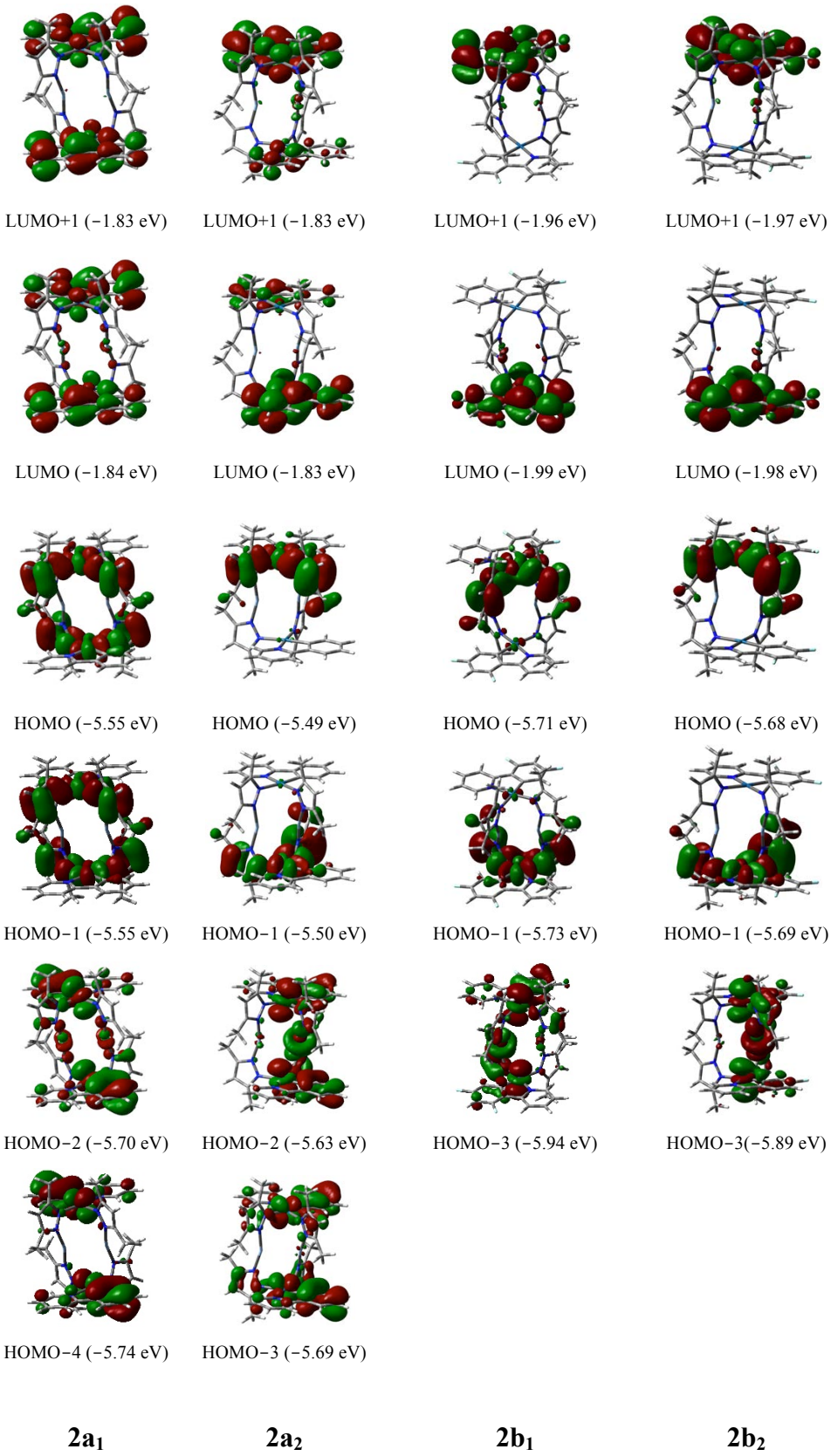


Fig. S23 Molecular orbitals of the singlet states for **2a$_1$**, **2a$_2$**, **2b$_1$** and **2b$_2$** by the B3LYP method.

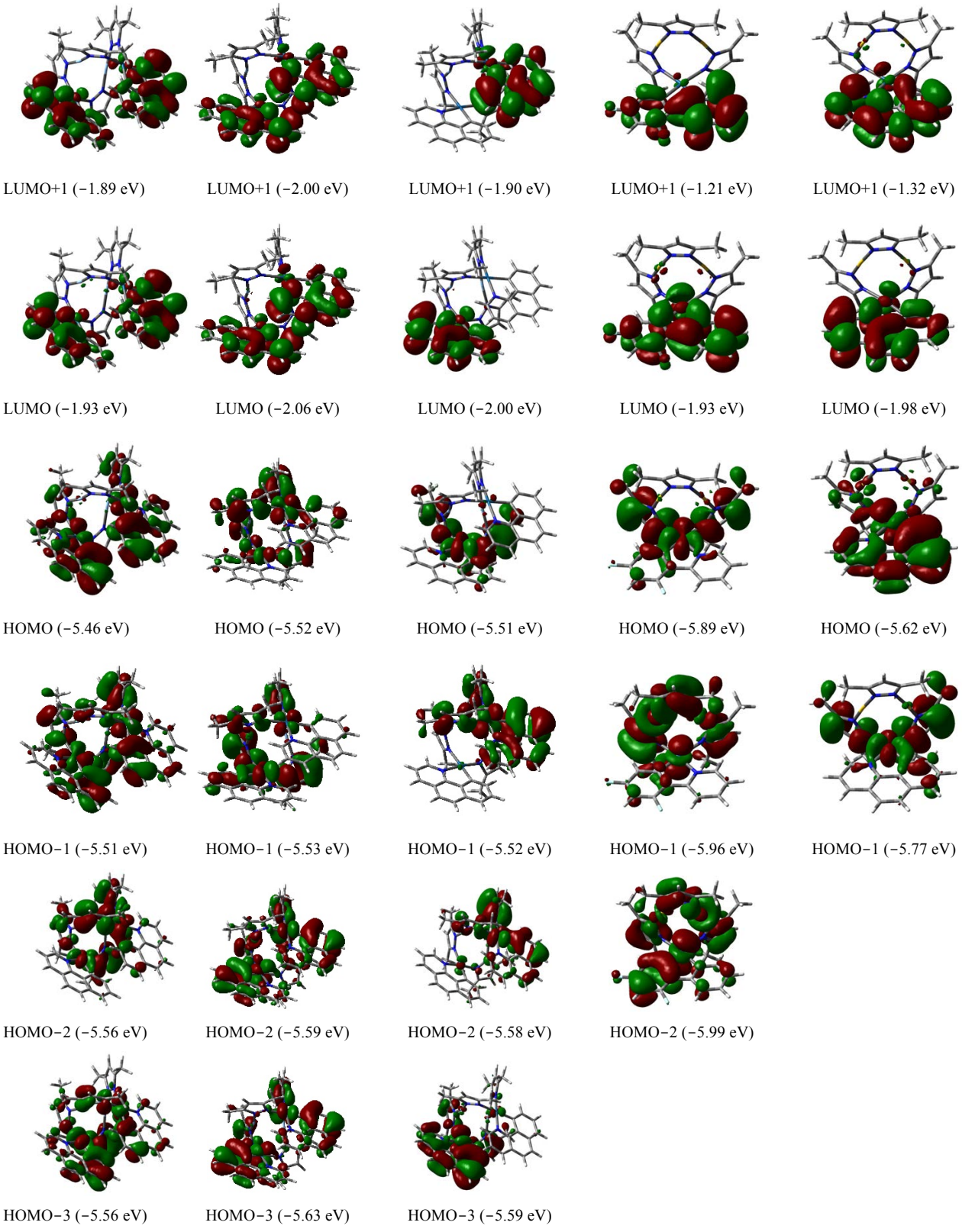


Fig. S24 Molecular orbitals of the singlet states for **2c$_1$**, **2c$_2$**, **2c$_3$**, **3b** and **3c** by the B3LYP method.

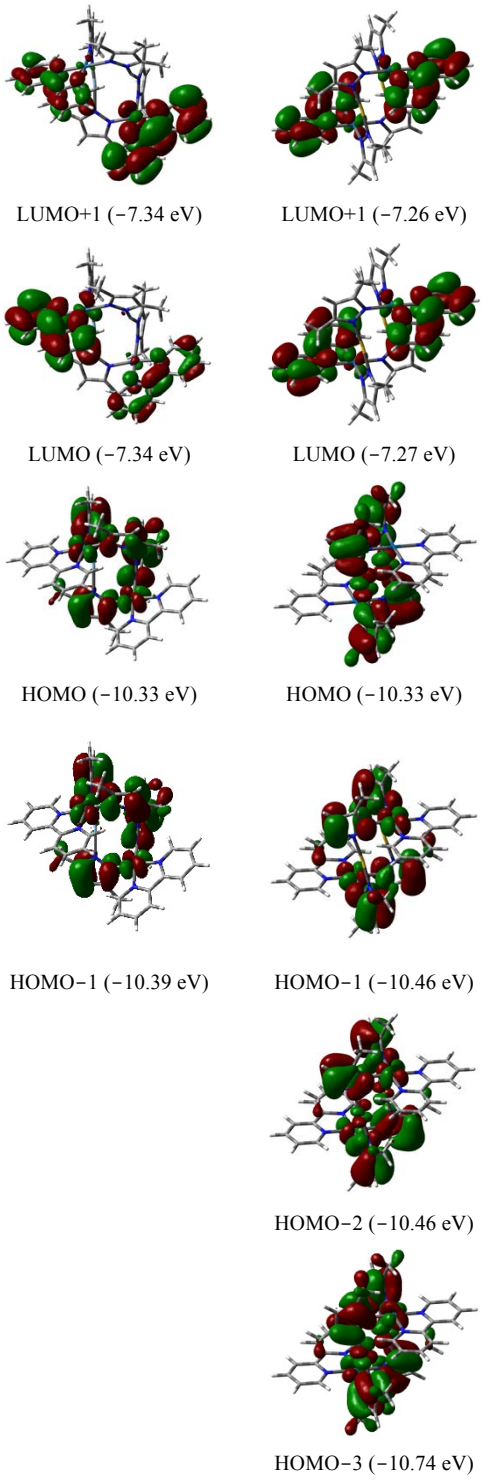


Fig. S25 Molecular orbitals of the singlet states for **4d** and **5d** by the B3LYP method.

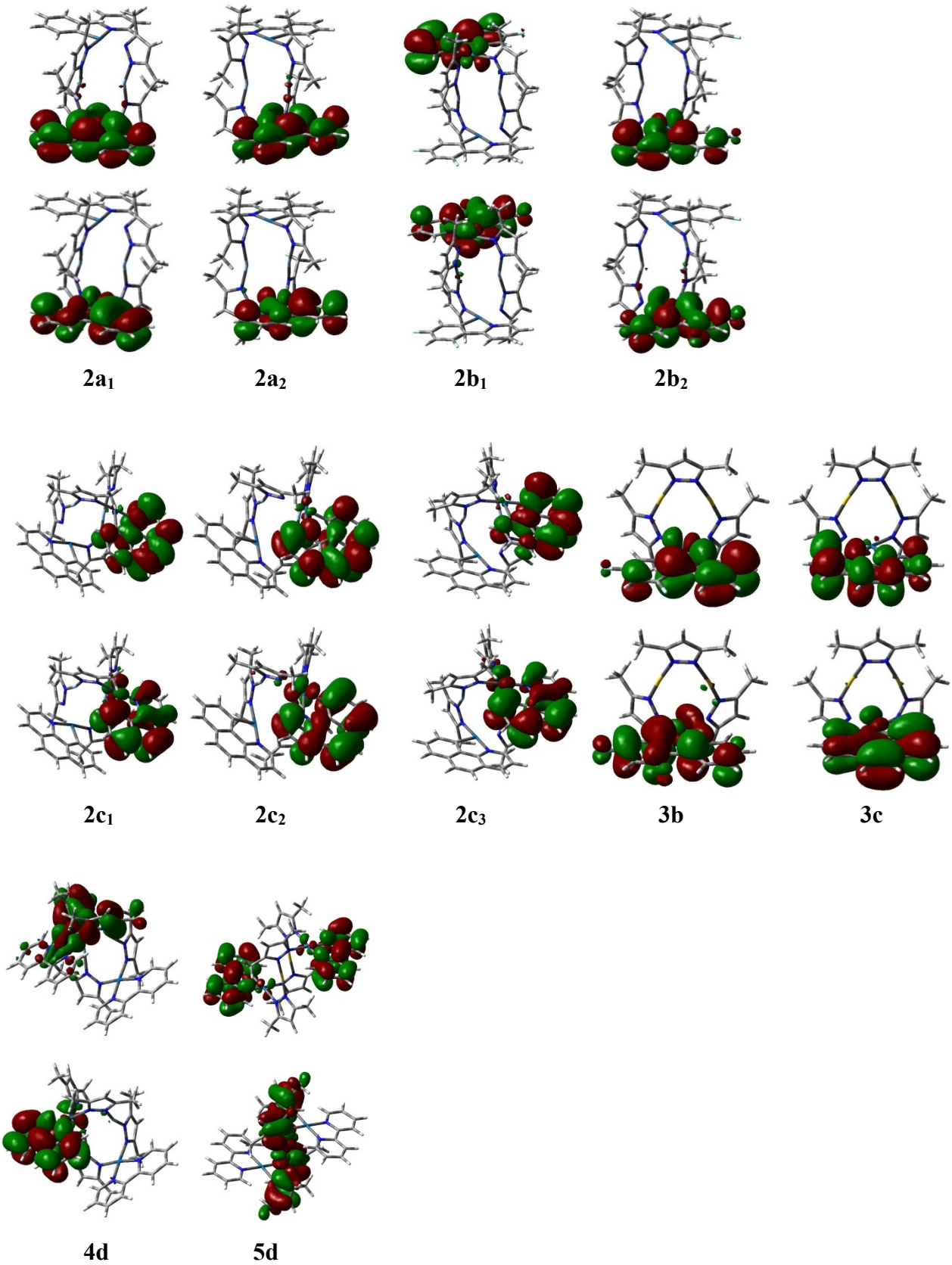


Fig. S26 Singly occupied molecular orbitals of the triplet states for **2a**$_1$, **2a**$_2$, **2b**$_1$, **2b**$_2$, **2c**$_1$, **2c**$_2$, **2c**$_3$, **3b**, **3c, 4d** and **5d** by the B3LYP method.