Hybrid Charged Heterometallic Pt Ir Complexes: Tailoring Excited States by Taking the Best of Both Worlds

Ahmed M. Soliman, Daniel Fortin, Pierre D. Harvey* and Eli Zysman-Colman*.

Département de chimie, Université de Sherbrooke, 2500 Boul. Université, Sherbrooke, QC, J1K 2R1
Pierre.Harvey@usherbrooke.ca; Eli.Zysman-Colman@usherbrooke.ca

SUPPORTING INFORMATION

Table of Contents: Pages

Experimental section:

Synthesis S2-S10
Photophysical Characterization S10-S11
Computational Methodology S11

Molar Absorptivities of complexes S12
Absorption and emission spectra of individual complexes S13-S14
Comparison of calculated and experimental absorption spectra S15-S16
Visualisation of MOs of individual complexes S17-S18
Energy and composition of TD-DFT calculated transitions S19-S30
$^1$H, $^{13}$C and $^{31}$P NMR spectra of individual complexes S31-S55
References S56-S57
Experimental section

Synthesis:

General Procedures:

Commercial chemicals were used as supplied. All experiments were carried out with freshly distilled anhydrous solvents obtained from a Pure Solv™ solvent purification system from Innovative Technologies except where specifically mentioned. N,N,N-Triethylamine (Et₃N), N,N-diisopropylamine (i-Pr₂NH) were distilled over CaH₂ under a nitrogen atmosphere. PtCl₂(PBu₃)₂ was obtained following standard literature protocol¹ and heated to 165 °C to obtain the trans form. CuI,² [(ppy)₂Ir-μ-Cl]₃ dimer and 1-ethynyl-4-methylbenzene³ were purified or prepared following literature procedures. All reagents wherein the synthesis is not explicitly described in the SI were purchased and used without further purification. Flash column chromatography was performed using silica gel (Silia-P from Silicycle, 60 Å, 40-63 μm). Analytical thin layer chromatography (TLC) was performed with silica plates with aluminum backings (250 μm with indicator F-254). Compounds were visualized under UV light. ¹H and ¹³C NMR spectra were recorded on a Brucker Avance spectrometer at 400 MHz and 100 MHz, respectively or a Brucker Avance spectrometer at 300 MHz and 75MHz, respectively. ³¹P NMR spectra was recorded on a Brucker Avance spectrometer at 121 MHz. The following abbreviations have been used for multiplicity assignments: “s” for singlet, “d” for doublet, “t” for triplet and “m” for multiplet. Deuterated chloroform (CDCl₃) was used as the solvent of record. Melting points (Mp’s) were recorded using open end capillaries on a Meltemp melting point apparatus and are uncorrected. GC-MS samples were separated on a Shimadzu QP 2010 Plus equipped with a HP5-MS 30 m x 0.25 mm ID x 0.25 μm film thickness column. High resolution mass spectra were recorded on either a VG Micromass ZAB-2F or a Waters Synapt MS G1 (ES-Q-TOF) at the Université de Sherbrooke.

5-Bromo-2-iodopyridine (6):⁵

![5-Bromo-2-iodopyridine](image)
To a mixture of 2,5-dibromopyridine (4.00 g, 16.88 mmol, 1.00 equiv.) and KI (8.41 g, 50.63 mmol, 3.00 equiv.) was added HI (48 % wt., 20 mL). The reaction mixture was heated to reflux for 72 h. The reaction was followed by GC-MS and upon consumption of the starting material, was then cooled to 0 °C. An aqueous solution of KOH (40 %, 30 mL) followed by Et₂O (30 mL) was then added to the reaction mixture. The layers were separated and the aqueous phase was washed with Et₂O (2 x 30 mL). The combined organic phases were dried over MgSO₄, filtered and concentrated. The residue was purified by flash chromatography (10% EtOAc/Hexanes on silica gel) to yield 4.25 g of white solid (Yield: 90 %). Rf: 0.28 (10% EtOAc/Hexanes). Mp: 112.8-113.6°C. (Litt.: 112.5-113.5°C).

\[ \text{1H NMR (400 MHz, CDCl}_3 \text{) } \delta (ppm): \text{ 8.43 (d, } J = 2.5 \text{ Hz, 1H), 7.58 (dd, } J = 8.3 \text{ Hz, 1H), 7.42 (dd, } J = 8.4, 2.7 \text{ Hz, 1H).} \]

\[ \text{13C NMR (100 MHz, CDCl}_3 \text{) } \delta (ppm): 152.1, 140.5, 136.3, 121.4, 115.4. \]

\[ \text{LR-MS (EI, 70eV) (m/z): 283 (M}^+\text{), 75. HR-MS (EI, 70eV): Calculated (C}_5\text{H}_3\text{BrIN): 282.8494; Found: 282.8493. The 1H and 13C NMR spectrum each correspond to that found in the literature.} \]

5-bromo-2,2'-bipyridine (7):

To a solution of 2-bromopyridine (4.80 mL, 50.4 mmol, 1.05 equiv.) in THF (65 mL) at -78 °C was added n-BuLi 2.2 M in hexanes (24.0 mL, 52.8 mmol, 1.10 equiv.) over 40 min. The mixture was stirred for 30 min at -78 °C, then a solution of ZnCl₂ (7.19 g, 52.8 mmol, 1.10 equiv.) in THF (60 mL) was canulated in over 40 min. The mixture was stirred at room temperature for 2 h. The zincate solution was canulated into a mixture of 5-bromo-2-iodopyridine (6) (13.6 g, 48.0 mmol, 1.00 equiv.) and Pd(PPh₃)₄ (2.91 g, 2.52 mmol, 5 mol %) in THF (60 mL). The reaction mixture was heated to reflux for 16 h. The reaction was followed by GC-MS. Upon cooling to room temperature, a gray solid precipitate was observed. The reaction mixture was concentrated under reduced pressure, but not dried. The suspension was cooled to -20 °C. The gray solid was filtered and washed with cold THF (2 x 20 mL). It was added to an aqueous solution of EDTA:NaHCO₃ (sat.) (1:1,15 mL) then stirred for 2 h at room temperature. To the mixture was added DCM and then the phases were separated. The organic phase was further washed with an aqueous solution of EDTA:NaHCO₃ (sat.) (1:1, 2 x 15 mL). The organic phase was dried over MgSO₄ and concentrated under reduced pressure.
The residue was purified by flash chromatography (15% EtOAc/Hexanes on silica gel) to yield 7.00 g of white solid (Yield: 60%). **Rf:** 0.45 (10% EtOAc/Hexanes). **Mp:** 72-73.8°C. (Litt.: 74-75°C).\(^7\)

**1H NMR (300 MHz, CDCl\(_3\)) \(\delta\) (ppm):** 8.72 (d, \(J = 2.2\) Hz, 1H), 8.68 (d, \(J = 4.7\) Hz, 1H), 8.38 (d, \(J = 8.0\) Hz, 1H), 8.32 (d, \(J = 8.5\) Hz, 1H), 7.96 (dd, \(J = 8.5, 2.4\) Hz, 1H), 7.82 (td, \(J = 7.8, 1.8\) Hz, 1H), 7.33 (ddd, \(J = 7.3, 4.7, 1.1\) Hz, 1H).

**13C NMR (75 MHz, CDCl\(_3\)) \(\delta\) (ppm):** 155.1, 154.6, 150.1, 149.2, 139.4, 137.0, 123.9, 122.3, 121.1, 120.9. **LR-MS (EI, 70eV) \(m/z\):** 234 (M\(^+\)), 155, 128. **HR-MS (EI, 70eV):** Calculated (C\(_{10}\)H\(_7\)BrN\(_2\)) 233.9793; Found: 233.9797. The \(1H\) and \(13C\) NMR spectra each correspond to that found in the literature.\(^7\)

### 5-trimethylsilylethynyl-2,2'-bipyridine (8):

![](image)

To a solution of 5-bromo-2,2'-bipyridine (7) (2.00 g, 8.55 mmol, 1.00 equiv.) in THF (90 mL) and i-Pr\(_2\)NH (30 mL) was added TMSA (2.90 mL, 20.5 mmol, 2.40 equiv.), Pd(PPh\(_3\))\(_4\) (0.59 g, 0.51 mmol, 6 mol %) and CuI (0.25 mg, 1.37 mmol, 0.16 equiv.). The solution was degassed and stirred for 48 h at room temperature. The reaction was followed by GC-MS. The solvent was evaporated under reduced pressure. The residue was purified by flash chromatography (10% EtOAc/Hexanes on silica gel) to yield 2.03 g of gray solid (Yield: 94%). **Rf:** 0.38 (10% EtOAc/Hexanes). **Mp:** 53.2-54.7 °C. (Litt.: 55-56 °C).\(^8\) **1H NMR (300 MHz, CDCl\(_3\)) \(\delta\) (ppm):** 8.73 (d, \(J = 1.8\) Hz, 1H), 8.68 (d, \(J = 4.3\) Hz, 1H), 8.38 (dd, \(J = 11.7, 8.1\) Hz, 2H), 7.87 (dd, \(J = 8.3, 2.2\) Hz, 1H), 7.85 – 7.77 (m, 1H), 7.32 (ddd, \(J = 7.3, 4.7, 0.9\) Hz, 1H), 0.28 (s, 9H). **13C NMR (75 MHz, CDCl\(_3\)) \(\delta\) (ppm):** 155.4, 154.9, 152.0, 149.1, 139.8, 136.9, 123.9, 121.4, 120.0, 101.7, 99.1, -0.3. **LR-MS (EI, 70eV) \(m/z\):** 252 (M\(^+\)), 237, 221. **HR-MS (EI, 70eV):** Calculated (C\(_{15}\)H\(_{16}\)N\(_2\)Si): 252.1083; Found: 252.1088. The \(1H\) NMR spectrum corresponds to that found in the literature, but the \(13C\) NMR spectrum was found to be different.\(^9\)

### 5-Ethynyl-2,2'-bipyridine (5):

![](image)
To a solution of the protected 5-trimethylsilylethynyl-2,2'-bipyridine (8) (0.10 g, 0.40 mmol, 1.00 equiv.) in MeOH (5 mL) was added K$_2$CO$_3$ (0.13 g, 0.91 mmol, 2.30 equiv.). The reaction was stirred for 2 h at room temperature and followed by GC-MS. The reaction was poured into a solution of H$_2$O/Et$_2$O (1:1), the layers were separated and the organic phase was washed with H$_2$O (twice). The combined aqueous fractions were extracted with Et$_2$O (three times). The organic phase were combined and dried over MgSO$_4$, the organic phase was filtered and then concentrated under reduced pressure to yield 0.07 g of light brown solid (Yield: 99%). **Mp:** 87.6-88.5 °C. (Litt.: 87-89°C). **Rf:** 0.30 (10% EtOAc/Hexanes). *H NMR (300 MHz, CDCl$_3$) δ (ppm):* 8.78 (d, *J* = 1.4 Hz, 1H), 8.69 (d, *J* = 4.4 Hz, 1H), 8.40 (dd, *J* = 8.1, 4.3 Hz, 2H), 7.91 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.83 (td, *J* = 7.9, 1.6 Hz, 1H), 7.33 (dd, *J* = 7.4, 4.9, 0.5 Hz, 1H), 3.29 (s, 1H). C NMR (75 MHz, CDCl$_3$) δ (ppm): δ 155.4, 155.3, 152.2, 149.2, 140.0, 137.0, 124.0, 121.4, 120.2, 119.1, 81.32, 80.7. LR-MS (EI, 70eV) (*m/z*): 180 (M$^+$). HR-MS (EI, 70eV): Calculated (C$_{12}$H$_8$N$_2$): 180.0687; Found: 180.0682.

**Synthesis of 5’ and 2’:**

A) Procedure leading to (5’) as the major product:

**trans-(5-ethynyl-2,2’-bipyridine)-chloro-bis(tri-n-butylphosphine)platinum (5’):**

In A dry flask charged with excess trans-PtCl$_2$(PBu$_3$)$_2$ (0.99 g, 1.48 mmol, 8.90 equiv.), CuI (9.5 mg, 0.05 mmol, 0.30 equiv.) was added followed by DCM (50 mL) and i-Pr$_2$NH (50 mL). The
reaction mixture was purged with N₂ for 30 min, then 5-Ethynyl-2,2'-bipyridine (5) (30 mg, 0.17 mmol, 1.00 equiv.), dissolved in DCM (15 mL) and i-Pr₂NH (15 mL), was added dropwise over 2 h. The mixture was stirred at room temperature for 16 h. The solvent was removed under reduced pressure and the residue was redissolved in DCM (50 mL). The organic phase was washed with H₂O twice then dried over MgSO₄ and concentrated under reduced pressure. The residue was purified by flash chromatography (50% DCM/Hexanes on silica gel) to recuperate the excess trans-PtCl₂(PBu₃)₂, then (30% EtOAc/Hexanes) to yield 100 mg (Yield: 73%) of 5' and finally flushed with (20% MeOH/DCM) to yield 42 mg (Yield: 13%) of 2'. Rₚ: 0.75 (30% EtOAc/Hexanes).

**B) Procedure leading to (2') as the major product:**

**trans-bis(tri-n-butylphosphine)-bis(5-ethynyl-2,2'-bipyridine)platinum (2'):**

In A dry flask charged with excess trans-PtCl₂(PBu₃)₂ (0.40 g, 0.60 mmol, 4.00 equiv.), CuI (8.6 mg, 0.04 mmol, 0.3 equiv.) was added followed by DCM (30 mL) and i-Pr₂NH (30 mL). The reaction mixture was purged with N₂ for 30 min, then 5-Ethynyl-2,2'-bipyridine (5) (27 mg, 0.15 mmol, 1.00 equiv.), dissolved in DCM (10 mL) and i-Pr₂NH (10 mL), and added dropwise over 2 h. The mixture was stirred at room temperature for 16 h. The reaction was followed the same way as 5'. The residue was purified by flash chromatography (50% DCM/Hexanes on silica gel) to recuperate the excess trans-PtCl₂(PBu₃)₂, then (30% EtOAc/Hexanes) to yield 8 mg (Yield: 7%) of light yellow...
solid of 5' and finally flushed with (20% MeOH/DCM) to yield 80 mg (Yield: 28%) of 2'. **Rf**: 0.18 (20% MeOH/DCM). **Mp**: 138.7-140.8°C. **H NMR (400 MHz, CDCl3) δ (ppm)**: 8.58 (d, J = 4.1 Hz, 2H), 8.51 (s, 2H), 8.27 (d, J = 8.0 Hz, 2H), 8.18 (d, J = 8.2 Hz, 2H), 7.71 (t, d, J = 7.8, 0.9 Hz, 2H), 7.22 – 7.17 (m, 2H), 2.15 – 1.97 (m, 12H), 1.63 – 1.48 (m, 12H), 1.46 – 1.31 (m, 12H), 0.86 (t, J = 7.3 Hz, 18H). **C NMR (101 MHz, CDCl3) δ (ppm)**: 156.5, 151.9, 151.4, 149.4, 138.4, 137.0, 126.0, 123.4, 121.0, 120.4, 114.9, 106.5, 26.4, 24.7, 24.0, 13.8. **P NMR (162 MHz, CDCl3) δ (ppm)**: 4.31 (d, J = 2328.0 Hz). **LR-MS (EI, 70eV) (m/z)**: 957 (M+), 381, 173. **HR-MS (EI, 70eV):** Calculated (C48H68N4P2Pt): 956.4546; Found: 956.4539

*A dry flask charged with 5' (76 mg, 0.09, 1.00 equiv.), CuI (5.3 mg, 0.03 mmol, 0.30 equiv.), DCM (40 mL) and i-Pr2NH (6 mL) was purged with N2 for 30 min. Excess 1-ethyl-4-methylbenzene (50 mg, 0.43 mmol, 4.60 equiv.), dissolved in DCM (10 mL), was then added. The mixture was stirred at room temperature for 16 h. The solvent was removed under reduced pressure and the residue was redissolved in DCM (20 ml). The organic phase was washed with H2O twice then dried over MgSO4 and concentrated under reduced pressure. The residue was purified by flash chromatography (50% DCM/Hexane on silica gel) to yield 64 mg of yellow liquid (Yield: 78%). **Rf**: 0.84 (50% DCM/Hexanes). **H NMR (400 MHz, CDCl3) δ (ppm)**: 8.65 (d, J = 3.4 Hz, 1H), 8.57 (s, 1H), 8.36 – 8.31 (m, 1H), 8.23 (d, J = 8.4 Hz, 1H), 7.83 – 7.74 (m, 1H), 7.64 (td, J = 8.3, 1.8 Hz, 1H), 7.30 – 7.22 (m, 1H), 7.16 (d, J = 7.9 Hz, 2H), 7.01 (d, J = 7.9 Hz, 2H), 2.29 (s, 3H), 2.26 – 2.06 (m, 12H), 1.68 – 1.36 (m, 2H), 0.92 (t, J = 7.3 Hz, 18H). **C NMR (101 MHz, CDCl3) δ (ppm)**: 156.5, 151.7, 151.4, 149.4, 138.4, 137.0, 134.8, 130.8, 128.8, 126.2, 126.1, 123.3, 121.0, 120.4, 109.3, 106.1, 106.0, 105.9, 26.6, 24.7, 24.1, 21.5, 14.1. **P NMR (162 MHz, CDCl3) δ (ppm)**: 4.17 (d, J = 2349.4 Hz). **LR-MS (EI, 70eV) (m/z)**: 893 (M+); 381, 317. **HR-MS (EI, 70eV):** Calculated (C45H68N4P2Pt): 892.4484. **Found**: 892.4470.

**trans-(5-ethyl-2,2'-bipyridine)-4-tolylethynyl-bis(tri-n-butylphosphine)platinum (2):**

![reactant diagram]

[**[Ir(ppy)2(5-ethyl-2,2'-bipyridine)] Hexafluorophosphate (1):**]10
The dimeric complex $[(ppy)_2\text{Ir-μ-Cl}]_2$ (86 mg, 0.08 mmol, 0.45 equiv.) was dissolved in DCM (6 mL) and methanol (6 mL) and 5-ethynyl-2,2'-bipyridine (5) (32 mg, 0.18 mmol, 1.00 equiv.) was added. The mixture was heated to 60 °C over 18 h. The color of the solution turned from orange to red. The solution was cooled to RT and extracted with water (3 x 50 mL), then washed with ether (3 x 50 mL) to remove unreacted bipyridine (5). To the aqueous solution was slowly added a solution of NH$_4$PF$_6$ (10 mL, 10 % w/w in H$_2$O) under gentle stirring. The first drop caused the precipitation of an orange solid. The suspension was conserved for 2 h at 0 °C, filtered and the resulting solid was washed with cold water. The residue was purified by flash chromatography (10% MeOH/DCM on silica gel) to yield 110 mg of a red solid (Yield: 76%). **Rf**: 0.53 (10% MeOH/DCM). **Mp**: >350 °C.  

$^1$H NMR (300 MHz, CDCl$_3$) δ (ppm): 8.68 (d, $J = 6.5$ Hz, 2H), 8.17 (dd, $J = 13.1$, 4.8 Hz, 2H), 7.98 – 7.86 (m, 4H), 7.78 (t, $J = 7.6$ Hz, 2H), 7.69 (dd, $J = 7.7$, 4.0 Hz, 2H), 7.50 (t, $J = 6.9$ Hz, 2H), 7.42 (t, $J = 6.9$, 1H), 7.05 (t, $J = 6.9$ Hz, 4H), 6.98 – 6.86 (m, 2H), 6.27 (t, $J = 6.6$ Hz, 2H), 3.35 (s, 1H).  

$^{13}$C NMR (75 MHz, CDCl$_3$): δ (ppm): 168.0, 167.8, 155.4, 155.2, 152.8, 150.5, 149.8, 149.7, 148.9, 143.6, 143.5, 140.2, 138.5, 138.4, 131.9, 131.8, 131.2, 131.1, 128.5, 126.3, 125.2, 125.1, 125.0, 123.9, 123.7, 123.7, 123.1, 123.0, 120.0, 119.9, 85.6, 78.3. LR-MS (EI, 70eV) (m/z): 681 (M$^+$); 381, 317, 75. HR-MS (EI, 70eV): Calculated (C$_{34}$H$_{24}$IrN$_4$): 681.1630. Found: 681.1649. The $^1$H and $^{13}$C NMR spectra each correspond to that found in the literature.$^{10}$ The structure was resolved by single crystal X-ray diffractometry and has been deposited into the CCDB.

$trans$-$[\text{Ir}(ppy)_2(5\text{-Ethynyl-2,2'}\text{-bipyridine})]-4\text{-tolylethynyl-bis(tri-}n\text{-butylphosphine)platinum}$

Hexafluorophosphate (3):
The dimeric complex [(ppy)_2Ir-μ-Cl]_2 (15.20 mg, 0.01 mmol, 0.45 equiv.) was dissolved in DCM (5 mL) and methanol (5 mL), and 2 (28 mg, 0.03 mmol, 1.00 equiv.) was added and the mixture was heated to 60 °C over 18 h. The color of the solution turned from orange to red. The solution was cooled to RT and washed with water (3 x 50 mL) then extracted with ether (3x). The organic solution was evaporated to obtain the chloride complex as a red solid. This complex was dissolved in a minimum amount of methanol and a solution of NH_4PF_6 (3 mL, 10% w/w in H_2O) was slowly added under stirring. The resulting suspension was re-cooled to 0 °C for 2 h, filtered, washed with cold water and the solid was dried under vacuum. The residue was purified by flash chromatography (10% MeOH/DCM on silica gel) to yield 40 mg of red solid (Yield: 87%). Rf: 0.47 (10% MeOH/DCM). Mp: >350 °C. \(^{1}H\) NMR (300 MHz, CDCl\(_3\)) δ (ppm): 8.61 (d, J = 8.1 Hz, 1H), 8.45 (d, J = 8.5 Hz, 1H), 8.13 (t, J = 7.8 Hz, 1H), 7.99 – 7.82 (m, 3H), 7.77 (t, J = 8.1 Hz, 4H), 7.65 (dd, J = 16.7, 7.7 Hz, 3H), 7.52 (t, J = 4.8 Hz, 2H), 7.32 (dd, J = 12.5, 6.3 Hz, 2H), 7.14 (d, J = 7.8 Hz, 2H), 7.10 – 6.96 (m, 4H), 6.95 – 6.83 (m, 2H), 6.27 (d, J = 7.4 Hz, 2H), 2.29 (s, 3H), 2.11 – 1.81 (m, 12H), 1.72 – 1.26 (m, 24H), 0.87 (t, J = 7.0 Hz, 18H). \(^{13}C\) NMR (101 MHz, CDCl\(_3\)) δ (ppm): 169.0, 168.8, 153.2, 153.1, 151.9, 151.7, 151.6, 151.0, 149.9, 149.5, 144.6, 144.5, 141.3, 141.0, 140.5, 140.3, 139.1, 139.0, 136.1, 132.8, 132.8, 132.0, 131.7, 131.4, 131.2, 129.8, 128.2, 127.5, 127.3, 126.0, 125.9, 125.7, 124.5, 124.2, 123.7, 123.4, 120.7, 120.5, 27.4, 25.4, 25.0, 22.4, 14.8. \(^{31}P\) NMR (162 MHz, CDCl\(_3\)) δ (ppm): 5.28 (d, J = 2318.2 Hz). LR-MS (EI, 70eV) (m/z): 1394 (M\(^+\)); Calculated (C\(_{67}H_{84}IrN_4P_2Pt): 1394.5458. Found: 1394.5421.

trans-bis[Ir(ppy)(5-Ethynyl-2,2'-bipyridine)]-bis(tri-n-butylphosphine)platinum Hexafluorophosphate (4):
The dimeric complex \([\text{ppy})_2\text{Ir-μ-Cl}]_2\) (0.06 g, 0.05 mmol, 1.50 equiv.) was dissolved in DCM (6 mL) and methanol (6 mL) and Pt complex \(2'\) (35 mg, 0.04 mmol, 1 equiv.) was added as a solid. The mixture was heated to 60 °C over 18 h. The reaction was followed the same way as described for 1 to yield 33 mg of a red solid (Yield: 40%). Rf: 0.52 (10% MeOH/DCM). Mp: >350 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) (ppm): 8.46 (t, \(J = 9.1\) Hz, 4H), 8.00 (t, \(J = 8.1\) Hz, 4H), 7.95 – 7.88 (m, 4H), 7.87 – 7.71 (m, 8H), 7.64 (d, \(J = 7.5\) Hz, 4H), 7.60 – 7.52 (m, 2H), 7.46 (dd, \(J = 9.8, 5.6\) Hz, 4H), 7.29 (d, \(J = 6.4\) Hz, 4H), 6.99 (dt, \(J = 14.5, 6.8\) Hz, 2H), 6.91 – 6.80 (m, 4H), 6.77 (d, \(J = 7.6\) Hz, 2H), 6.23 (dd, \(J = 11.6, 7.6\) Hz, 4H), 1.91 – 1.66 (m, 12), 1.48 – 1.22 (m, 24), 0.86 (t, \(J = 6.7\) Hz, 18H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) (ppm): 167.9, 167.7, 155.8, 151.9, 151.0, 150.6, 150.3, 150.0, 148.7, 148.3, 143.5, 143.4, 140.3, 139.7, 138.1, 138.0, 131.6, 130.8, 130.6, 130.1, 130.0, 127.3, 126.3, 126.2, 124.8, 124.6, 123.4, 123.1, 122.6, 122.4, 119.7, 119.5, 110.1, 105.2, 26.2, 24.3, 23.8, 13.8. \(^{31}\)P NMR (162 MHz, CDCl\(_3\)) \(\delta\) (ppm): 4.38 (d, \(J = 2326.3\) Hz). LR-MS (EI, 70eV) (m/z): 979 (M\(^{2+}\)); 501, 360, 249. HR-MS (EI, 70eV): Calculated (C\(_{92}\)H\(_{100}\)Ir\(_2\)N\(_8\)P\(_2\)Pt): 979.3216 (M\(^{2+}\)); Found: 979.3270 (M\(^{2+}\)).

Photophysical characterization: All samples were prepared in 2-methyltetrahydrofuran (2-MeTHF), which was distilled over CaH\(_2\) under nitrogen or HPLC grade acetonitrile (ACN) for the external reference. Absorption spectra were recorded at room temperature and at 77 K in a 1.0 cm capped quartz cuvette and an NMR tube inserted into a liquid nitrogen filled quartz dewar, respectively, using a Shimadzu UV-1800 double beam spectrophotometer. Molar absorptivity determination was verified by linear least squares fit of values obtained from at least three independent solutions at varying concentrations with absorbances ranging from 0.01-2.6. Steady-state emission spectra were obtained by exciting at the lowest energy absorption maxima using a Horiba Jobin Yvon Fluorolog-3 spectrofluorometer equipped with double monochromators and a photomultiplier tube detector (Hamamatsu model R955). Emission quantum yields were determined...
using the optically dilute method. A stock solution with absorbance of ca. 0.5 was prepared and then four dilutions were prepared with dilution factors of 40, 20, 13.3 and 10 to obtain solutions with absorbances of ca. 0.013, 0.025, 0.038 and 0.05, respectively. The Beer-Lambert law was found to be linear at the concentrations of the solutions. The emission spectra were then measured after the solutions were rigorously degassed with solvent-saturated nitrogen gas (N$_2$) for 20 minutes prior to spectrum acquisition using septa-sealed quartz cells from Starna. For each sample, linearity between absorption and emission intensity was verified through linear regression analysis and additional measurements were acquired until the Pearson regression factor ($R^2$) for the linear fit of the data set surpassed 0.9. Individual relative quantum yield values were calculated for each solution and the values reported represent the slope value. The equation $\Phi_s = \Phi_r (A_r/A_s)(I_s/I_r)(n_s/n_r)^2$ was used to calculate the relative quantum yield of each of the sample, where $\Phi_r$ is the absolute quantum yield of the reference, $n$ is the refractive index of the solvent, $A$ is the absorbance at the excitation wavelength, and $I$ is the integrated area under the corrected emission curve. The subscripts s and r refer to the sample and reference, respectively. A solution of [Ru(bpy)$_3$](PF$_6$)$_2$ in ACN ($\Phi_r = 0.095\%$) was used as the external reference. The experimental uncertainty in the emission quantum yields is conservatively estimated to be 10%, though we have found that statistically we can reproduce PLQYs to 3% relative error. The emission lifetimes were measured on a TimeMaster model TM-3/2003 apparatus from PTI. The source was a nitrogen laser with high-resolution dye laser (fwhm ~1400 ps), and the excited state lifetimes were obtained from deconvolution or distribution lifetimes analysis.

**Computational Methodology.** Calculations were performed with Gaussian 09 at the Université de Sherbrooke with Mammouth super computer supported by Calcul Québec. The DFT and TDDFT were calculated with the B3LYP method. The 3-21G* basis set was used for C, H and N, and VDZ (valence double $\zeta$) with SBKJC effective core potentials for iridium and platinum. The predicted phosphorescence wavelengths were obtained by energy differences between the Triplet and Singlet optimized states. The calculated absorption spectra and related MO contributions were obtained from the TD-DFT/Singlets output file and gausssum 2.1. A THF quantum mechanical continuum solvation model was employed.
**Figure S1:** Absorptivities of 1 (blue), 2 (red), 3 (mauve), 4 (green):
**Figure S2:** Absorption (green) and emission spectra at 298 K (red) and 77 K (blue) for 1:

![Absorption and emission spectra for 1](image1)

**Figure S3:** Absorption (green) and emission spectra at 298 K (red) and 77 K (blue) for 2:

![Absorption and emission spectra for 2](image2)
Figure S4: Absorption (green) and emission spectra at 298 K (red) and 77 K (blue) for 3:

Figure S5: Absorption (green) and emission spectra at 298 K (red) and 77 K (blue) for 4:
**Figure S6:** Calculated and experimental absorption spectra for 1:

![Absorption spectra for 1](image1)

**Figure S7:** Calculated and experimental absorption spectra for 2:

![Absorption spectra for 2](image2)
**Figure S8:** Calculated and experimental absorption spectra for 3:

![Absorption spectra for 3](image1.png)

**Figure S9:** Calculated and experimental absorption spectra for 4:

![Absorption spectra for 4](image2.png)
Table S1: Visualization of MOs of 1:

<table>
<thead>
<tr>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMO</td>
<td><img src="image1" alt="Image" /></td>
<td>LUMO</td>
<td><img src="image2" alt="Image" /></td>
<td>HSOMO</td>
<td><img src="image3" alt="Image" /></td>
</tr>
<tr>
<td>-5.97</td>
<td></td>
<td>-3.04</td>
<td></td>
<td>-3.90</td>
<td></td>
</tr>
<tr>
<td>HOMO -1</td>
<td><img src="image4" alt="Image" /></td>
<td>LUMO+1</td>
<td><img src="image5" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-5.69</td>
<td></td>
<td>-2.06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HOMO -2</td>
<td><img src="image6" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-5.67</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table S2: Visualization of MOs of 2:

<table>
<thead>
<tr>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMO</td>
<td><img src="image7" alt="Image" /></td>
<td>LUMO</td>
<td><img src="image8" alt="Image" /></td>
<td>HSOMO</td>
<td><img src="image9" alt="Image" /></td>
</tr>
<tr>
<td>-5.27</td>
<td></td>
<td>-1.55</td>
<td></td>
<td>-3.18</td>
<td></td>
</tr>
<tr>
<td>HOMO -1</td>
<td><img src="image10" alt="Image" /></td>
<td>LUMO+1</td>
<td><img src="image11" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-5.79</td>
<td></td>
<td>-0.77</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HOMO -2</td>
<td><img src="image12" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-5.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Table S3:** Visualization of MOs of 3:

<table>
<thead>
<tr>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMO -5.53</td>
<td><img src="image1" alt="Image" /></td>
<td>LUMO -2.78</td>
<td><img src="image2" alt="Image" /></td>
<td>HSOMO -3.87</td>
<td><img src="image3" alt="Image" /></td>
</tr>
<tr>
<td>HOMO -1 -5.93</td>
<td><img src="image4" alt="Image" /></td>
<td>LUMO -1 -2.62</td>
<td><img src="image5" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HOMO -2 -6.25</td>
<td><img src="image6" alt="Image" /></td>
<td></td>
<td><img src="image7" alt="Image" /></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table S4:** Visualization of MOs of 4:

<table>
<thead>
<tr>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
<th>Orbital Energy (eV)</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMO -8.69</td>
<td><img src="image8" alt="Image" /></td>
<td>LUMO -5.81</td>
<td><img src="image9" alt="Image" /></td>
<td>HSOMO -6.82</td>
<td><img src="image10" alt="Image" /></td>
</tr>
<tr>
<td>HOMO -1 -6.81</td>
<td><img src="image11" alt="Image" /></td>
<td>LUMO+1 -5.03</td>
<td><img src="image12" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HOMO -2 -8.96</td>
<td><img src="image13" alt="Image" /></td>
<td></td>
<td><img src="image14" alt="Image" /></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table S5: Energy and composition of TD-DFT calculated transitions of 1:

<table>
<thead>
<tr>
<th>No.</th>
<th>Energy (cm⁻¹)</th>
<th>Wavelength (nm)</th>
<th>Oscillator Strength</th>
<th>Symmetry</th>
<th>Major contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18155.6556</td>
<td>550.7922552</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>HOMO→LUMO (98%)</td>
</tr>
<tr>
<td>2</td>
<td>23140.2584</td>
<td>432.1462629</td>
<td>0.0012</td>
<td>Singlet-A</td>
<td>H-2→LUMO (94%)</td>
</tr>
<tr>
<td>3</td>
<td>24080.6535</td>
<td>415.27109</td>
<td>0.0451</td>
<td>Singlet-A</td>
<td>H-1→LUMO (92%)</td>
</tr>
<tr>
<td>4</td>
<td>25446.968</td>
<td>382.9741256</td>
<td>0.0489</td>
<td>Singlet-A</td>
<td>HOMO→L-1 (96%)</td>
</tr>
<tr>
<td>5</td>
<td>25633.2833</td>
<td>390.1177957</td>
<td>0.0468</td>
<td>Singlet-A</td>
<td>H-3→LUMO (87%)</td>
</tr>
<tr>
<td>6</td>
<td>26384.9928</td>
<td>379.0032606</td>
<td>0.0333</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (12%), HOMO→L+3 (83%)</td>
</tr>
<tr>
<td>7</td>
<td>26810.0544</td>
<td>372.9943942</td>
<td>0.002</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (82%), HOMO→L+3 (12%)</td>
</tr>
<tr>
<td>8</td>
<td>27318.1872</td>
<td>366.0585003</td>
<td>0.0028</td>
<td>Singlet-A</td>
<td>H-4→LUMO (91%)</td>
</tr>
<tr>
<td>9</td>
<td>28289.2854</td>
<td>353.4907243</td>
<td>0.0085</td>
<td>Singlet-A</td>
<td>H-5→LUMO (96%)</td>
</tr>
<tr>
<td>10</td>
<td>28725.6344</td>
<td>348.1211135</td>
<td>0.0064</td>
<td>Singlet-A</td>
<td>HOMO→L+4 (98%)</td>
</tr>
<tr>
<td>11</td>
<td>30286.8703</td>
<td>326.979898</td>
<td>0.0122</td>
<td>Singlet-A</td>
<td>H-2→L+1 (73%)</td>
</tr>
<tr>
<td>12</td>
<td>30847.9375</td>
<td>324.1733427</td>
<td>0.4761</td>
<td>Singlet-A</td>
<td>H-6→LUMO (77%), H-2→L+2 (13%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-3→L+1 (61%), H-2→L+3 (14%), H-1→L+1 (51%)</td>
</tr>
<tr>
<td>13</td>
<td>30958.0352</td>
<td>322.7051969</td>
<td>0.013</td>
<td>Singlet-A</td>
<td>HOMO→L-5 (93%)</td>
</tr>
<tr>
<td>14</td>
<td>31387.2524</td>
<td>318.6003768</td>
<td>0.0214</td>
<td>Singlet-A</td>
<td>HOMO→L+5 (93%)</td>
</tr>
<tr>
<td>15</td>
<td>31646.9947</td>
<td>315.9857702</td>
<td>0.0083</td>
<td>Singlet-A</td>
<td>H-2→L+3 (23%), HOMO→L+6 (59%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-2→L+1 (13%), H-2→L+2 (11%), H-1→L+3 (47%)</td>
</tr>
<tr>
<td>16</td>
<td>31741.3622</td>
<td>315.04634</td>
<td>0.0311</td>
<td>Singlet-A</td>
<td>H-2→L+3 (32%), H-1→L+1 (18%), HOMO- →L+6 (22%)</td>
</tr>
<tr>
<td>17</td>
<td>31959.5187</td>
<td>312.796741</td>
<td>0.0405</td>
<td>Singlet-A</td>
<td>H-2→L+2 (61%), H-1→L+3 (16%)</td>
</tr>
<tr>
<td>18</td>
<td>32131.3304</td>
<td>311.201542</td>
<td>0.323</td>
<td>Singlet-A</td>
<td>H-1→L+2 (63%)</td>
</tr>
<tr>
<td>19</td>
<td>32482.5908</td>
<td>307.8572161</td>
<td>0.008</td>
<td>Singlet-A</td>
<td>H-7→LUMO (94%)</td>
</tr>
<tr>
<td>20</td>
<td>32914.9074</td>
<td>303.8137053</td>
<td>0.0012</td>
<td>Singlet-A</td>
<td>H-3→L+1 (58%), H-2→L+3 (10%)</td>
</tr>
<tr>
<td>21</td>
<td>33127.8388</td>
<td>301.8609224</td>
<td>0.0092</td>
<td>Singlet-A</td>
<td>H-3→L+3 (58%), H-1→L+3 (14%)</td>
</tr>
<tr>
<td>22</td>
<td>33502.8772</td>
<td>298.4889054</td>
<td>0.1298</td>
<td>Singlet-A</td>
<td>H-3→L+2 (31%), H-2→L+4 (49%)</td>
</tr>
<tr>
<td>23</td>
<td>33936.8185</td>
<td>294.6652168</td>
<td>0.0134</td>
<td>Singlet-A</td>
<td>H-3→L+4 (13%), H-1→L+4 (71%)</td>
</tr>
<tr>
<td>24</td>
<td>34150.2082</td>
<td>292.7729902</td>
<td>0.0587</td>
<td>Singlet-A</td>
<td>H-3→L+2 (40%), H-2→L+4 (48%)</td>
</tr>
<tr>
<td>25</td>
<td>34328.0006</td>
<td>291.3073862</td>
<td>0.0051</td>
<td>Singlet-A</td>
<td>H-3→L+2 (40%), H-2→L+4 (48%)</td>
</tr>
<tr>
<td>26</td>
<td>34745.7924</td>
<td>287.8045838</td>
<td>0.0239</td>
<td>Singlet-A</td>
<td>H-3→L+2 (40%), H-2→L+4 (48%)</td>
</tr>
<tr>
<td>27</td>
<td>34883.72</td>
<td>286.6636743</td>
<td>0.1516</td>
<td>H-2→L+1 (67%)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-5→L+1 (36%), H-4→L+3 (25%), H-1→L+5 (14%)</td>
</tr>
<tr>
<td>28</td>
<td>35287.8056</td>
<td>283.3840064</td>
<td>0.0396</td>
<td>Singlet-A</td>
<td>H-5→L+1 (43%), H-4→L+3 (40%)</td>
</tr>
<tr>
<td>29</td>
<td>35527.3548</td>
<td>281.4732488</td>
<td>0.0008</td>
<td>Singlet-A</td>
<td>H-5→L+1 (43%), H-4→L+3 (40%)</td>
</tr>
<tr>
<td>30</td>
<td>35705.6046</td>
<td>280.0668706</td>
<td>0.0458</td>
<td>Singlet-A</td>
<td>H-4→L+2 (48%), H-3→L+4 (16%)</td>
</tr>
<tr>
<td>31</td>
<td>35815.2568</td>
<td>279.2103066</td>
<td>0.004</td>
<td>Singlet-A</td>
<td>H-4→L+2 (48%), HOMO→L+7 (64%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-3→L+4 (49%), H-1→L+4 (14%), HOMO- →L+7 (21%)</td>
</tr>
<tr>
<td>32</td>
<td>35893.5312</td>
<td>278.6017182</td>
<td>0.0123</td>
<td>Singlet-A</td>
<td>H-5→L+3 (50%), H-2→L+5 (12%)</td>
</tr>
<tr>
<td>33</td>
<td>35941.2057</td>
<td>278.2215981</td>
<td>0.0099</td>
<td>Singlet-A</td>
<td>H-5→L+3 (50%), H-2→L+5 (12%)</td>
</tr>
<tr>
<td>34</td>
<td>36066.1369</td>
<td>277.2683975</td>
<td>0.0056</td>
<td>Singlet-A</td>
<td>H-9→LUMO (51%)</td>
</tr>
<tr>
<td>35</td>
<td>36697.6734</td>
<td>272.4968387</td>
<td>0.0045</td>
<td>Singlet-A</td>
<td>H-5→L+2 (73%)</td>
</tr>
<tr>
<td>36</td>
<td>36784.78192</td>
<td>271.8515505</td>
<td>0.0064</td>
<td>Singlet-A</td>
<td>H-2→L+5 (57%), H-1→L+6 (23%)</td>
</tr>
<tr>
<td>Number</td>
<td>Value1</td>
<td>Value2</td>
<td>Value3</td>
<td>Value4</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>38692.24784</td>
<td>271.0670033</td>
<td>0.0035</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+6 (57%), H-1-&gt;L+5 (28%)</td>
</tr>
<tr>
<td>38</td>
<td>37956.92064</td>
<td>269.5641532</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-10-&gt;LUMO (92%)</td>
</tr>
<tr>
<td>39</td>
<td>37766.36544</td>
<td>264.7858719</td>
<td>0.0154</td>
<td>Singlet-A</td>
<td>H-11-&gt;LUMO (-16%), H-6-&gt;L+2 (48%), H-4-&gt;L+4 (12%)</td>
</tr>
<tr>
<td>40</td>
<td>37687.18541</td>
<td>264.0808881</td>
<td>0.0014</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+4 (74%)</td>
</tr>
<tr>
<td>41</td>
<td>37931.71024</td>
<td>263.6316669</td>
<td>0.3458</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+1 (19%), H-5-&gt;L+3 (-11%), H-1-&gt;L+6 (32%)</td>
</tr>
<tr>
<td>42</td>
<td>38111.57312</td>
<td>262.3874897</td>
<td>0.1284</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+3 (10%), H-2-&gt;L+6 (-18%), H-1-&gt;L+5 (39%)</td>
</tr>
<tr>
<td>43</td>
<td>38322.08528</td>
<td>260.946134</td>
<td>0.126</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+1 (64%)</td>
</tr>
<tr>
<td>44</td>
<td>38519.69248</td>
<td>259.6074723</td>
<td>0.0734</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+5 (65%)</td>
</tr>
<tr>
<td>45</td>
<td>38725.36528</td>
<td>258.2286811</td>
<td>0.0181</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+4 (80%)</td>
</tr>
<tr>
<td>46</td>
<td>38822.95904</td>
<td>257.5795418</td>
<td>0.0073</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+6 (76%), H-1-&gt;L+6 (-13%)</td>
</tr>
<tr>
<td>47</td>
<td>39102.0288</td>
<td>255.7412059</td>
<td>0.0102</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+3 (86%)</td>
</tr>
<tr>
<td>48</td>
<td>39573.05984</td>
<td>252.6971642</td>
<td>0.0855</td>
<td>Singlet-A</td>
<td>H-11-&gt;LUMO (-23%), HOMO-&gt;L+11 (32%)</td>
</tr>
<tr>
<td>49</td>
<td>39616.62408</td>
<td>252.2542324</td>
<td>0.0555</td>
<td>Singlet-A</td>
<td>H-11-&gt;LUMO (38%), H-6-&gt;L+2 (10%), HOMO-&gt;L+11 (20%)</td>
</tr>
<tr>
<td>50</td>
<td>39988.11596</td>
<td>250.1176986</td>
<td>0.0221</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+4 (67%)</td>
</tr>
<tr>
<td>51</td>
<td>40122.3272</td>
<td>249.2377066</td>
<td>0.0664</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+5 (19%), HOMO-&gt;L+8 (50%), HOMO-&gt;L+14 (12%)</td>
</tr>
<tr>
<td>52</td>
<td>40438.49087</td>
<td>247.2594729</td>
<td>0.0079</td>
<td>Singlet-A</td>
<td>H-12-&gt;LUMO (95%)</td>
</tr>
<tr>
<td>53</td>
<td>40561.9024</td>
<td>246.5367601</td>
<td>0.1197</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+5 (72%), HOMO-&gt;L+8 (-10%)</td>
</tr>
<tr>
<td>54</td>
<td>40803.06384</td>
<td>245.0796352</td>
<td>0.035</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+6 (91%)</td>
</tr>
<tr>
<td>55</td>
<td>40955.98989</td>
<td>244.1049332</td>
<td>0.0015</td>
<td>Singlet-A</td>
<td>H-13-&gt;LUMO (88%)</td>
</tr>
<tr>
<td>56</td>
<td>41116.81568</td>
<td>243.2094955</td>
<td>0.0103</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+5 (-18%), H-1-&gt;L+7 (58%)</td>
</tr>
<tr>
<td>57</td>
<td>41149.07808</td>
<td>243.0188031</td>
<td>0.011</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+5 (65%), H-1-&gt;L+7 (12%)</td>
</tr>
<tr>
<td>58</td>
<td>41193.43888</td>
<td>242.7571058</td>
<td>0.0156</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+1 (21%), H-7-&gt;L+1 (32%), H-2-&gt;L+7 (38%)</td>
</tr>
<tr>
<td>59</td>
<td>41289.25552</td>
<td>242.3111315</td>
<td>0.0023</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+1 (21%), H-7-&gt;L+1 (32%), H-2-&gt;L+7 (15%)</td>
</tr>
<tr>
<td>60</td>
<td>41427.34128</td>
<td>241.3864779</td>
<td>0.0015</td>
<td>Singlet-A</td>
<td>H-7-&gt;L+2 (67%)</td>
</tr>
<tr>
<td>61</td>
<td>41667.66298</td>
<td>241.1517255</td>
<td>0.0312</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+6 (7%)</td>
</tr>
<tr>
<td>62</td>
<td>41659.63056</td>
<td>240.5045348</td>
<td>0.0004</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+1 (-19%), H-8-&gt;L+3 (17%), H-7-&gt;L+3 (23%)</td>
</tr>
<tr>
<td>63</td>
<td>41798.35888</td>
<td>239.2438428</td>
<td>0.0329</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+11 (38%)</td>
</tr>
<tr>
<td>64</td>
<td>41846.75248</td>
<td>238.9671697</td>
<td>0.0124</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+11 (21%), H-1-&gt;L+11 (12%)</td>
</tr>
<tr>
<td>65</td>
<td>42712.99929</td>
<td>234.1207709</td>
<td>0.0014</td>
<td>Singlet-A</td>
<td>H-15-&gt;LUMO (-34%), H-3-&gt;L+7 (35%)</td>
</tr>
<tr>
<td>66</td>
<td>42771.8786</td>
<td>233.7984851</td>
<td>0.0016</td>
<td>Singlet-A</td>
<td>H-15-&gt;LUMO (56%), H-3-&gt;L+7 (21%)</td>
</tr>
<tr>
<td>67</td>
<td>42775.48992</td>
<td>233.7896678</td>
<td>0.0206</td>
<td>Singlet-A</td>
<td>H-14-&gt;LUMO (52%), H-3-&gt;L+7 (20%)</td>
</tr>
<tr>
<td>68</td>
<td>43027.55632</td>
<td>232.4092013</td>
<td>0.0093</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+2 (57%), H-7-&gt;L+4 (12%)</td>
</tr>
<tr>
<td>69</td>
<td>43037.43264</td>
<td>230.913</td>
<td>0.0037</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+3 (-19%), H-8-&gt;L+3 (18%), HOMO-&gt;L+9 (20%)</td>
</tr>
<tr>
<td>70</td>
<td>43380.02304</td>
<td>230.5208855</td>
<td>0.0033</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+1 (82%)</td>
</tr>
<tr>
<td>71</td>
<td>43495.36112</td>
<td>229.9053752</td>
<td>0.0107</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+1 (82%)</td>
</tr>
<tr>
<td>72</td>
<td>43600.21392</td>
<td>229.3566728</td>
<td>0.0329</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+3 (22%), H-8-&gt;L+3 (-15%), HOMO-&gt;L+9 (18%), HOMO-&gt;L+11 (10%)</td>
</tr>
<tr>
<td>73</td>
<td>43916.38544</td>
<td>227.705443</td>
<td>0.0179</td>
<td>Singlet-A</td>
<td>H-16-&gt;LUMO (55%)</td>
</tr>
<tr>
<td>74</td>
<td>43995.42382</td>
<td>227.2963438</td>
<td>0.0051</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+6 (84%)</td>
</tr>
<tr>
<td>75</td>
<td>44185.77848</td>
<td>226.3171726</td>
<td>0.0165</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (76%)</td>
</tr>
<tr>
<td>76</td>
<td>44212.39298</td>
<td>226.1809264</td>
<td>0.0227</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+1 (69%)</td>
</tr>
<tr>
<td>77</td>
<td>44369.67216</td>
<td>225.3791726</td>
<td>0.0047</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+2 (10%), H-8-&gt;L+4 (28%), H-7-&gt;L+4 (38%)</td>
</tr>
<tr>
<td>78</td>
<td>44432.58384</td>
<td>225.0600603</td>
<td>0.0613</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+4 (10%), HOMO-&gt;L+8 (10%), HOMO-&gt;L+10 (23%), HOMO-&gt;L+13 (17%), HOMO-&gt;L+14 (-19%)</td>
</tr>
<tr>
<td>79</td>
<td>44576.15152</td>
<td>224.3952031</td>
<td>0.0073</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+7 (85%)</td>
</tr>
<tr>
<td>80</td>
<td>44675.74528</td>
<td>223.8451228</td>
<td>0.0045</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+2 (79%)</td>
</tr>
<tr>
<td>81</td>
<td>44918.13295</td>
<td>222.62336</td>
<td>0.0008</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+3 (61%)</td>
</tr>
<tr>
<td>82</td>
<td>45135.09764</td>
<td>221.5570705</td>
<td>0.0096</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+8 (52%)</td>
</tr>
<tr>
<td>83</td>
<td>45211.7208</td>
<td>221.1815835</td>
<td>0.001</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+1 (11%), H-9-&gt;L+1 (25%), H-8-&gt;L+1 (20%), H-7-&gt;L+1 (24%)</td>
</tr>
<tr>
<td>84</td>
<td>45377.06556</td>
<td>220.3756428</td>
<td>0.0024</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+7 (12%), HOMO-&gt;L+10 (40%), HOMO-&gt;L+13 (13%)</td>
</tr>
<tr>
<td>85</td>
<td>45405.29521</td>
<td>220.22424</td>
<td>0.0044</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+7 (71%)</td>
</tr>
<tr>
<td>86</td>
<td>45707.75521</td>
<td>218.781254</td>
<td>0.0043</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+2 (47%)</td>
</tr>
<tr>
<td>87</td>
<td>45778.89312</td>
<td>218.47847</td>
<td>0.0028</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+2 (11%), H-1-&gt;L+8 (33%), HOMO-&gt;L+12 (-12%)</td>
</tr>
<tr>
<td>88</td>
<td>45981.17904</td>
<td>217.4802867</td>
<td>0.0012</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+2 (-11%), H-9-&gt;L+4 (-28%), H-8-&gt;L+4 (30%)</td>
</tr>
<tr>
<td>89</td>
<td>46031.99232</td>
<td>217.240217</td>
<td>0.001</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+3 (-14%), H-9-&gt;L+3 (-24%), H-8-&gt;L+3 (-18%), H-7-&gt;L+3 (24%)</td>
</tr>
<tr>
<td>90</td>
<td>46315.90144</td>
<td>215.91911</td>
<td>0.0007</td>
<td>Singlet-A</td>
<td>H-18-&gt;LUMO (36%), H-11-&gt;L+2 (33%), H-6-&gt;L+7 (15%)</td>
</tr>
<tr>
<td>91</td>
<td>46496.57088</td>
<td>215.0695236</td>
<td>0.0014</td>
<td>Singlet-A</td>
<td>H-19-&gt;LUMO (25%), H-3-&gt;L+8 (19%), HOMO-&gt;L+12 (32%)</td>
</tr>
<tr>
<td>92</td>
<td>46583.67936</td>
<td>214.6674573</td>
<td>0.0016</td>
<td>Singlet-A</td>
<td>H-19-&gt;LUMO (58%), H-6-&gt;L+7 (13%)</td>
</tr>
<tr>
<td>93</td>
<td>46689.33872</td>
<td>214.1816585</td>
<td>0.0017</td>
<td>Singlet-A</td>
<td>H-20-&gt;LUMO (-22%), H-15-&gt;LUMO (-12%), H-6-&gt;L+7 (30%)</td>
</tr>
<tr>
<td>94</td>
<td>47035.35296</td>
<td>212.2611</td>
<td>0.0028</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+9 (19%), HOMO-&gt;L+13 (17%), HOMO-&gt;L+14 (25%)</td>
</tr>
<tr>
<td>95</td>
<td>47045.83824</td>
<td>212.5580529</td>
<td>0.0095</td>
<td>Singlet-A</td>
<td>H-11-&gt;L+1 (61%)</td>
</tr>
<tr>
<td>96</td>
<td>47131.33385</td>
<td>212.1730755</td>
<td>0.0016</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+9 (46%), H-2-&gt;L+10 (-11%)</td>
</tr>
<tr>
<td>97</td>
<td>47156.01568</td>
<td>212.0170605</td>
<td>0.0333</td>
<td>Singlet-A</td>
<td>H-20-&gt;LUMO (24%), H-11-&gt;L+1 (-18%), H-11-&gt;L+2 (18%), H-11-&gt;L+4 (13%)</td>
</tr>
<tr>
<td>98</td>
<td>47195.85841</td>
<td>211.8829986</td>
<td>0.0006</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+4 (-22%), H-8-&gt;L+4 (25%), H-7-&gt;L+5 (-16%)</td>
</tr>
<tr>
<td>99</td>
<td>47260.38332</td>
<td>211.15951</td>
<td>0.0018</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+4 (11%), H-8-&gt;L+5 (19%), H-7-&gt;L+5 (38%)</td>
</tr>
<tr>
<td>100</td>
<td>47489.44624</td>
<td>210.5731019</td>
<td>0.0085</td>
<td>Singlet-A</td>
<td>H-12-&gt;L+1 (30%), H-8-&gt;L+6 (16%), H-7-&gt;L+6 (26%)</td>
</tr>
</tbody>
</table>
Table S6: Energy and composition of TD-DFT calculated transitions of 2:

<table>
<thead>
<tr>
<th>No.</th>
<th>Energy (cm⁻¹)</th>
<th>Wavelength (nm)</th>
<th>Oscillator Strength</th>
<th>Symmetry</th>
<th>Major contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>28194.11136</td>
<td>354.6839931</td>
<td>1.4361</td>
<td>Singlet-A</td>
<td>HOMO→LUMO (85%)</td>
</tr>
<tr>
<td>2</td>
<td>28408.85632</td>
<td>352.0053848</td>
<td>0.0759</td>
<td>Singlet-A</td>
<td>HOMO→L+1 (84%)</td>
</tr>
<tr>
<td>3</td>
<td>28867.58836</td>
<td>346.4092555</td>
<td>0.2333</td>
<td>Singlet-A</td>
<td>H-2→LUMO (23%), H-1→LUMO (62%)</td>
</tr>
<tr>
<td>4</td>
<td>30972.22192</td>
<td>323.2352286</td>
<td>0.6913</td>
<td>Singlet-A</td>
<td>H-1→L+1 (62%)</td>
</tr>
<tr>
<td>5</td>
<td>31097.72736</td>
<td>321.5669069</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-2→LUMO (49%), H-1→LUMO (27%)</td>
</tr>
<tr>
<td>6</td>
<td>32207.55392</td>
<td>310.4861681</td>
<td>0.0009</td>
<td>Singlet-A</td>
<td>H-6→LUMO (16%), H-5→LUMO (55%), H-2→LUMO (-12%)</td>
</tr>
<tr>
<td>7</td>
<td>33058.47472</td>
<td>302.4942949</td>
<td>0.0073</td>
<td>Singlet-A</td>
<td>H-3→LUMO (95%)</td>
</tr>
<tr>
<td>8</td>
<td>34725.57376</td>
<td>291.7529571</td>
<td>0.012</td>
<td>Singlet-A</td>
<td>H-8→L+1 (20%), H-6→L+1 (27%), H-5→L+1 (-10%), H-2→L+1 (84%)</td>
</tr>
<tr>
<td>9</td>
<td>34350.58384</td>
<td>291.1158671</td>
<td>0.0069</td>
<td>Singlet-A</td>
<td>H-9→LUMO (-10%), H-7→LUMO (35%), HOMO→L+4 (19%)</td>
</tr>
<tr>
<td>10</td>
<td>35020.8352</td>
<td>285.5440336</td>
<td>0.004</td>
<td>Singlet-A</td>
<td>H-8→L+1 (-11%), H-7→LUMO (-12%), H-5→L+1 (23%), HOMO→L+2 (-18%)</td>
</tr>
<tr>
<td>11</td>
<td>35136.17328</td>
<td>284.6069753</td>
<td>0.0555</td>
<td>Singlet-A</td>
<td>H-2→L+1 (24%), HOMO→L+2 (42%)</td>
</tr>
<tr>
<td>12</td>
<td>35361.20352</td>
<td>282.7958046</td>
<td>0.0031</td>
<td>Singlet-A</td>
<td>H-3→L+1 (92%)</td>
</tr>
<tr>
<td>13</td>
<td>35470.08912</td>
<td>281.9270818</td>
<td>0.0007</td>
<td>Singlet-A</td>
<td>HOMO→L+3 (55%), HOMO→L+4 (15%)</td>
</tr>
<tr>
<td>14</td>
<td>36012.09744</td>
<td>277.8644674</td>
<td>0.0034</td>
<td>Singlet-A</td>
<td>HOMO→L+4 (55%)</td>
</tr>
<tr>
<td>15</td>
<td>36150.82576</td>
<td>276.6185842</td>
<td>0.0318</td>
<td>Singlet-A</td>
<td>H-1→L+2 (-28%), H-1→L+3 (-13%), H-1→L+4 (32%)</td>
</tr>
<tr>
<td>16</td>
<td>36273.42288</td>
<td>275.6839362</td>
<td>0.0346</td>
<td>Singlet-A</td>
<td>H-1→L+3 (60%)</td>
</tr>
<tr>
<td>17</td>
<td>36455.70544</td>
<td>274.3058561</td>
<td>0.015</td>
<td>Singlet-A</td>
<td>H-4→LUMO (51%), HOMO→L+4 (11%)</td>
</tr>
<tr>
<td>18</td>
<td>36915.44464</td>
<td>270.8893282</td>
<td>0.0284</td>
<td>Singlet-A</td>
<td>H-2→L+2 (24%), H-2→L+5 (12%), H-1→L+4 (25%)</td>
</tr>
<tr>
<td>19</td>
<td>37228.38992</td>
<td>268.6122076</td>
<td>0.004</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (11%), HOMO→L+5 (75%)</td>
</tr>
<tr>
<td>20</td>
<td>37504.23344</td>
<td>266.6365656</td>
<td>0.0085</td>
<td>Singlet-A</td>
<td>HOMO→L+7 (91%)</td>
</tr>
<tr>
<td>21</td>
<td>37579.24532</td>
<td>266.1043455</td>
<td>0.0005</td>
<td>Singlet-A</td>
<td>H-8→L+1 (31%), H-6→L+1 (10%), H-5→L+1 (14%), H-4→L+1 (20%)</td>
</tr>
<tr>
<td>22</td>
<td>37987.30288</td>
<td>263.2454385</td>
<td>0.0004</td>
<td>Singlet-A</td>
<td>H-1→L+3 (-12%), H-1→L+6 (89%)</td>
</tr>
<tr>
<td>23</td>
<td>38318.85904</td>
<td>260.9681042</td>
<td>0.0139</td>
<td>Singlet-A</td>
<td>H-4→L+6 (10%), HOMO→L+3 (-12%), HOMO→L+6 (36%)</td>
</tr>
<tr>
<td>24</td>
<td>38435.81024</td>
<td>260.1740392</td>
<td>0.0024</td>
<td>Singlet-A</td>
<td>H-6→L+3 (15%), H-5→L+3 (13%), H-4→L+3 (29%), HOMO→L+1 (22%)</td>
</tr>
<tr>
<td>25</td>
<td>38679.39136</td>
<td>258.5356099</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-6→L+2 (-11%), H-5→L+2 (30%), H-5→L+5 (-12%)</td>
</tr>
<tr>
<td>26</td>
<td>38758.43424</td>
<td>258.0083586</td>
<td>0.003</td>
<td>Singlet-A</td>
<td>H-6→LUMO (59%), H-5→LUMO (21%)</td>
</tr>
<tr>
<td>27</td>
<td>39033.4712</td>
<td>256.1903846</td>
<td>0.0705</td>
<td>Singlet-A</td>
<td>H-1→L+2 (53%), H-1→L+4 (15%)</td>
</tr>
<tr>
<td>28</td>
<td>39289.15072</td>
<td>254.5231907</td>
<td>0.0047</td>
<td>Singlet-A</td>
<td>H-1→L+7 (85%)</td>
</tr>
<tr>
<td>29</td>
<td>39544.02368</td>
<td>252.8827132</td>
<td>0.0051</td>
<td>Singlet-A</td>
<td>H-6→L+1 (25%), H-5→L+1 (50%)</td>
</tr>
<tr>
<td>30</td>
<td>39794.86384</td>
<td>251.28871</td>
<td>0.0168</td>
<td>Singlet-A</td>
<td>H-6→L+3 (-16%), H-4→L+6 (22%), HOMO→L+6 (25%)</td>
</tr>
<tr>
<td>31</td>
<td>39966.65112</td>
<td>250.2085418</td>
<td>0.0045</td>
<td>Singlet-A</td>
<td>H-9→LUMO (32%), H-8→LUMO (20%), H-7→LUMO (22%)</td>
</tr>
<tr>
<td>32</td>
<td>40058.60886</td>
<td>249.6342299</td>
<td>0.0025</td>
<td>Singlet-A</td>
<td>H-2→L+2 (-17%), H-2→L+4 (44%), H-1→L+5 (15%)</td>
</tr>
<tr>
<td>33</td>
<td>40230.40624</td>
<td>248.5682083</td>
<td>0.0468</td>
<td>Singlet-A</td>
<td>H-10→LUMO (90%)</td>
</tr>
<tr>
<td>34</td>
<td>40578.84016</td>
<td>246.4338547</td>
<td>0.0164</td>
<td>Singlet-A</td>
<td>H-2→L+4 (-17%), H-1→L+5 (60%)</td>
</tr>
<tr>
<td>35</td>
<td>40621.58784</td>
<td>246.1745228</td>
<td>0.0234</td>
<td>Singlet-A</td>
<td>H-3→L+1 (23%), H-7→L+1 (38%), H-3→L+7 (14%)</td>
</tr>
<tr>
<td>37</td>
<td>40972.44144</td>
<td>244.0664908</td>
<td>0.0485</td>
<td>Singlet-A</td>
<td>H-9→LUMO (20%), H-8→LUMO (53%)</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
<td>-------------</td>
<td>--------</td>
<td>-----------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>38</td>
<td>41123.28616</td>
<td>243.1713346</td>
<td>0.0406</td>
<td>Singlet-A</td>
<td>H-3→L+7 (76%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-3→L+2 (17%), H-3→L+4 (22%), H-2→L+2 (14%)</td>
</tr>
<tr>
<td>39</td>
<td>41881.43456</td>
<td>238.7692806</td>
<td>0.026</td>
<td>Singlet-A</td>
<td>H-3→L+2 (19%), H-3→L+4 (32%), H-2→L+2 (10%)</td>
</tr>
<tr>
<td>40</td>
<td>41902.45012</td>
<td>238.8457856</td>
<td>0.0289</td>
<td>Singlet-A</td>
<td>H-9→L+1 (137%), H-7→L+1 (37%)</td>
</tr>
<tr>
<td>41</td>
<td>42060.49088</td>
<td>237.7523185</td>
<td>0.0357</td>
<td>Singlet-A</td>
<td>H-10→L+1 (94%)</td>
</tr>
<tr>
<td>42</td>
<td>42284.71456</td>
<td>236.4902777</td>
<td>0.0013</td>
<td>Singlet-A</td>
<td>H-9→L+1 (10%), H-2→L+3 (71%)</td>
</tr>
<tr>
<td>43</td>
<td>42438.93152</td>
<td>235.5217063</td>
<td>0.0265</td>
<td>Singlet-A</td>
<td>H-11→LUMO (27%), H-2→L+5 (28%)</td>
</tr>
<tr>
<td>44</td>
<td>42577.33184</td>
<td>234.9773171</td>
<td>0.0338</td>
<td>Singlet-A</td>
<td>H-11→LUMO (22%), H-2→L+5 (26%)</td>
</tr>
<tr>
<td>45</td>
<td>42742.03408</td>
<td>233.9617245</td>
<td>0.0136</td>
<td>Singlet-A</td>
<td>HOMO→L+6 (89%)</td>
</tr>
<tr>
<td>46</td>
<td>43157.41248</td>
<td>231.7099063</td>
<td>0.0029</td>
<td>Singlet-A</td>
<td>H-3→L+3 (22%), HOMO→L+8 (11%)</td>
</tr>
<tr>
<td>47</td>
<td>43496.16768</td>
<td>229.905312</td>
<td>0.01</td>
<td>Singlet-A</td>
<td>H-3→L+3 (30%), H-3→L+6 (11%)</td>
</tr>
<tr>
<td>48</td>
<td>43524.39728</td>
<td>229.7561971</td>
<td>0.0015</td>
<td>Singlet-A</td>
<td>H-4→L+3 (11%), H-3→L+3 (32%), H-2→L+6 (18%)</td>
</tr>
<tr>
<td>49</td>
<td>43542.1416</td>
<td>229.6656%</td>
<td>0.0012</td>
<td>Singlet-A</td>
<td>H-3→L+2 (45%), H-3→L+4 (34%), H-3→L+5 (12%)</td>
</tr>
<tr>
<td>50</td>
<td>43674.41744</td>
<td>228.9669923</td>
<td>0.0055</td>
<td>Singlet-A</td>
<td>H-12→L+1 (11%), H-11→L+1 (28%), H-4→L+2 (11%)</td>
</tr>
<tr>
<td>51</td>
<td>43761.52592</td>
<td>228.5112274</td>
<td>0.0101</td>
<td>Singlet-A</td>
<td>H-12→LUMO (43%), H-11→LUMO (11%), H-9→LUMO (12%)</td>
</tr>
<tr>
<td>52</td>
<td>43877.67056</td>
<td>227.8191%</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-14→LUMO (17%), H-7→L+2 (11%), H-4→L+5 (16%)</td>
</tr>
<tr>
<td>53</td>
<td>44227.71756</td>
<td>226.1025561</td>
<td>0.0042</td>
<td>Singlet-A</td>
<td>H-4→L+6 (10%), H-2→L+6 (35%)</td>
</tr>
<tr>
<td>54</td>
<td>44295.98</td>
<td>225.9377433</td>
<td>0.0004</td>
<td>Singlet-A</td>
<td>H-11→L+1 (10%), H-4→L+4 (15%), H-1→L+8 (13%)</td>
</tr>
<tr>
<td>55</td>
<td>44369.67216</td>
<td>225.3791726</td>
<td>0.0032</td>
<td>Singlet-A</td>
<td>H-4→L+4 (22%), H-1→L+8 (10%), HOMO→L+9 (13%)</td>
</tr>
<tr>
<td>56</td>
<td>44651.1616</td>
<td>223.9583393</td>
<td>0.0788</td>
<td>Singlet-A</td>
<td>H-7→L+6 (16%), H-5→L+6 (17%), H-5→L+5 (-14%)</td>
</tr>
<tr>
<td>57</td>
<td>44713.26672</td>
<td>223.8426929</td>
<td>0.0042</td>
<td>Singlet-A</td>
<td>H-5→L+4 (14%), HOMO→L+9 (35%)</td>
</tr>
<tr>
<td>58</td>
<td>44805.38192</td>
<td>222.6655417</td>
<td>0.0018</td>
<td>Singlet-A</td>
<td>H-8→L+6 (30%), H-6→L+6 (29%)</td>
</tr>
<tr>
<td>59</td>
<td>44910.13952</td>
<td>222.6232443</td>
<td>0.0102</td>
<td>Singlet-A</td>
<td>H-12→L+1 (33%), H-11→L+1 (10%)</td>
</tr>
<tr>
<td>60</td>
<td>44951.20192</td>
<td>222.4627626</td>
<td>0.0129</td>
<td>Singlet-A</td>
<td>H-2→L+7 (77%)</td>
</tr>
<tr>
<td>61</td>
<td>45077.02528</td>
<td>221.8425004</td>
<td>0.2722</td>
<td>Singlet-A</td>
<td>H-6→L+4 (-10%), H-5→L+4 (13%), H-4→L+4 (15%)</td>
</tr>
<tr>
<td>62</td>
<td>45281.08486</td>
<td>220.8427649</td>
<td>0.071</td>
<td>Singlet-A</td>
<td>H-3→L+2 (-13%), H-3→L+5 (82%)</td>
</tr>
<tr>
<td>63</td>
<td>45503.69552</td>
<td>219.7623706</td>
<td>0.0018</td>
<td>Singlet-A</td>
<td>H-3→L+3 (-14%), H-3→L+6 (83%)</td>
</tr>
<tr>
<td>64</td>
<td>45605.32208</td>
<td>219.2726528</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-13→L+1 (19%), H-8→L+3 (13%), H-5→L+3 (-11%), H-4→L+3 (10%)</td>
</tr>
<tr>
<td>65</td>
<td>45781.95872</td>
<td>218.4266528</td>
<td>0.0124</td>
<td>Singlet-A</td>
<td>H-16→LUMO (15%), H-6→L+2 (10%), H-4→L+2 (15%)</td>
</tr>
<tr>
<td>66</td>
<td>45936.81824</td>
<td>217.6903056</td>
<td>0.0099</td>
<td>Singlet-A</td>
<td>H-13→L+1 (13%), H-12→L+1 (-10%)</td>
</tr>
<tr>
<td>67</td>
<td>46004.59928</td>
<td>217.3697125</td>
<td>0.0171</td>
<td>Singlet-A</td>
<td>H-5→L+2 (16%), H-4→L+2 (10%), H-1→L+9 (17%)</td>
</tr>
<tr>
<td>68</td>
<td>46255.73072</td>
<td>216.2361757</td>
<td>0.0095</td>
<td>Singlet-A</td>
<td>H-1→L+9 (12%)</td>
</tr>
<tr>
<td>69</td>
<td>46332.03264</td>
<td>215.3833%</td>
<td>0.0068</td>
<td>Singlet-A</td>
<td>H-13→L+1 (13%), H-12→L+1 (11%), H-9→L+3 (-11%), H-7→L+3 (10%)</td>
</tr>
<tr>
<td>70</td>
<td>46575.61376</td>
<td>214.7046517</td>
<td>0.0065</td>
<td>Singlet-A</td>
<td>H-7→L+4 (57%)</td>
</tr>
<tr>
<td>71</td>
<td>46960.34288</td>
<td>212.5456343</td>
<td>0.0053</td>
<td>Singlet-A</td>
<td>H-6→L+4 (19%), H-5→L+4 (12%)</td>
</tr>
<tr>
<td>72</td>
<td>47161.98288</td>
<td>212.60519</td>
<td>0.0147</td>
<td>Singlet-A</td>
<td>H-6→L+3 (22%), H-5→L+3 (42%)</td>
</tr>
<tr>
<td>73</td>
<td>47214.40928</td>
<td>211.7997483</td>
<td>0.0032</td>
<td>Singlet-A</td>
<td>H-5→L+8 (10%), H-4→L+8 (38%)</td>
</tr>
<tr>
<td>74</td>
<td>47378.14096</td>
<td>211.0067800</td>
<td>0.0029</td>
<td>Singlet-A</td>
<td>H-10→L+2 (-16%), H-10→L+4 (42%)</td>
</tr>
<tr>
<td>75</td>
<td>47481.38064</td>
<td>210.6088716</td>
<td>0.0859</td>
<td>Singlet-A</td>
<td>H-14→LUMO (-12%), H-5→L+6 (12%), H-4→L+5 (42%)</td>
</tr>
<tr>
<td>76</td>
<td>47515.25616</td>
<td>210.4587202</td>
<td>0.0084</td>
<td>Singlet-A</td>
<td>H-4→L+5 (42%)</td>
</tr>
<tr>
<td></td>
<td>47739.47984</td>
<td>209.4702337</td>
<td>0.0059</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+7 (25%), H-9-&gt;L+4 (-13%)</td>
</tr>
<tr>
<td>----</td>
<td>-------------</td>
<td>-------------</td>
<td>--------</td>
<td>-----------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td>78</td>
<td>47929.02144</td>
<td>208.5418552</td>
<td>0.0322</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+7 (11%), H-9-&gt;L+2 (-14%), H-7-&gt;L+7 (20%)</td>
</tr>
<tr>
<td>79</td>
<td>47990.32</td>
<td>208.3753557</td>
<td>0.0423</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+7 (-12%), H-4-&gt;L+7 (40%)</td>
</tr>
<tr>
<td></td>
<td>48136.30736</td>
<td>207.7433968</td>
<td>0.0021</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+6 (16%), H-5-&gt;L+6 (27%), H-4-&gt;L+6 (-13%)</td>
</tr>
<tr>
<td>80</td>
<td>48144.37296</td>
<td>207.7711</td>
<td>0.0094</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+7 (19%), H-9-&gt;L+4 (10%)</td>
</tr>
<tr>
<td>81</td>
<td>48447.63952</td>
<td>206.408405</td>
<td>0.0003</td>
<td>Singlet-A</td>
<td>H-13-&gt;LUMO (91%)</td>
</tr>
<tr>
<td>82</td>
<td>48700.89936</td>
<td>205.335017</td>
<td>0.0097</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+2 (-14%), H-2-&gt;L+9 (27%)</td>
</tr>
<tr>
<td>83</td>
<td>48754.13232</td>
<td>205.1108188</td>
<td>0.0136</td>
<td>Singlet-A</td>
<td>H-16-&gt;LUMO (-14%), H-8-&gt;L+2 (27%)</td>
</tr>
<tr>
<td>84</td>
<td>48863.58248</td>
<td>204.66525</td>
<td>0.0141</td>
<td>Singlet-A</td>
<td>H-7-&gt;L+3 (30%), H-2-&gt;L+8 (11%)</td>
</tr>
<tr>
<td>85</td>
<td>48954.95576</td>
<td>204.2693697</td>
<td>0.0026</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (15%), H-15-&gt;LUMO (16%), H-2-&gt;L+8 (12%)</td>
</tr>
<tr>
<td>86</td>
<td>49078.39944</td>
<td>203.3755</td>
<td>0.0054</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (11%), H-15-&gt;LUMO (21%), H-2-&gt;L+9 (-15%)</td>
</tr>
<tr>
<td>87</td>
<td>49096.11376</td>
<td>203.6821091</td>
<td>0.0178</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+5 (21%), H-2-&gt;L+8 (-12%)</td>
</tr>
<tr>
<td>88</td>
<td>49158.21888</td>
<td>203.4245428</td>
<td>0.0185</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+6 (24%), H-5-&gt;L+6 (-20%)</td>
</tr>
<tr>
<td>89</td>
<td>49214.67808</td>
<td>203.9095</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-9-&gt;L+2 (-10%), H-9-&gt;L+4 (-13%), H-8-&gt;L+4 (13%), H-7-&gt;L+3 (14%)</td>
</tr>
<tr>
<td>90</td>
<td>49425.9968</td>
<td>202.1221773</td>
<td>0.0237</td>
<td>Singlet-A</td>
<td>H-14-&gt;L+1 (96%)</td>
</tr>
<tr>
<td>91</td>
<td>49546.9808</td>
<td>201.822645</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (13%), H-8-&gt;L+4 (20%)</td>
</tr>
<tr>
<td>92</td>
<td>49647.8001</td>
<td>201.4167907</td>
<td>0.0117</td>
<td>Singlet-A</td>
<td>H-19-&gt;L+1 (13%), H-16-&gt;L+1 (31%), H-2-&gt;L+8 (15%)</td>
</tr>
<tr>
<td>93</td>
<td>49787.35588</td>
<td>200.8085</td>
<td>0.0034</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (34%), H-15-&gt;LUMO (-33%)</td>
</tr>
<tr>
<td>94</td>
<td>49825.244</td>
<td>200.7014577</td>
<td>0.0016</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+3 (78%)</td>
</tr>
<tr>
<td>95</td>
<td>49934.93616</td>
<td>200.2605945</td>
<td>0.0011</td>
<td>Singlet-A</td>
<td>H-13-&gt;LUMO (-11%), H-18-&gt;LUMO (52%)</td>
</tr>
<tr>
<td>96</td>
<td>49966.23472</td>
<td>200.0150623</td>
<td>0.0052</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+8 (16%), H-6-&gt;L+8 (-10%), H-4-&gt;L+8 (11%), H-3-&gt;L+8 (-14%), H-2-&gt;L+8 (-13%)</td>
</tr>
<tr>
<td>97</td>
<td>50025.77048</td>
<td>199.9898967</td>
<td>0.0029</td>
<td>Singlet-A</td>
<td>H-19-&gt;LUMO (43%), H-18-&gt;LUMO (28%)</td>
</tr>
<tr>
<td>98</td>
<td>50138.99584</td>
<td>199.19455</td>
<td>0.0016</td>
<td>Singlet-A</td>
<td>H-10-&gt;L+3 (65%), H-10-&gt;L+6 (10%)</td>
</tr>
</tbody>
</table>
Table S7: Energy and composition of TD-DFT calculated transitions of 3:

<table>
<thead>
<tr>
<th>No.</th>
<th>Energy (cm(^{-1}))</th>
<th>Wavelength (nm)</th>
<th>Oscillator Strength</th>
<th>Symmetry</th>
<th>Major contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>19829.2776</td>
<td>504.3048063</td>
<td>0.2067</td>
<td>Singlet-A</td>
<td>H-1-&gt;LUMO (-45%), HOMO-&gt;LUMO (53%)</td>
</tr>
<tr>
<td>2</td>
<td>19920.41888</td>
<td>501.9974761</td>
<td>0.195</td>
<td>Singlet-A</td>
<td>H-1-&gt;LUMO (53%), HOMO-&gt;LUMO (44%)</td>
</tr>
<tr>
<td>3</td>
<td>24293.5872</td>
<td>411.6312637</td>
<td>0.2634</td>
<td>Singlet-A</td>
<td>H-4-&gt;LUMO (-10%), H-2-&gt;LUMO (74%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>H-6-&gt;LUMO (36%), H-5-&gt;LUMO (-27%), H-4-&gt;LUMO (12%)</td>
</tr>
<tr>
<td>4</td>
<td>24823.49712</td>
<td>402.8441259</td>
<td>0.0797</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+1 (97%)</td>
</tr>
<tr>
<td>5</td>
<td>25314.69216</td>
<td>395.0275175</td>
<td>0.0431</td>
<td>Singlet-A</td>
<td>H-4-&gt;LUMO (13%), H-3-&gt;LUMO (64%)</td>
</tr>
<tr>
<td>6</td>
<td>25860.73328</td>
<td>388.6863777</td>
<td>0.0488</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+1 (89%)</td>
</tr>
<tr>
<td>7</td>
<td>26235.78368</td>
<td>381.1589057</td>
<td>0.0059</td>
<td>Singlet-A</td>
<td>H-5-&gt;LUMO (57%), H-4-&gt;LUMO (-15%), H-2-&gt;LUMO (-10%)</td>
</tr>
<tr>
<td>8</td>
<td>26274.49855</td>
<td>380.5971778</td>
<td>0.0034</td>
<td>Singlet-A</td>
<td>H-5-&gt;LUMO (-92%)</td>
</tr>
<tr>
<td>9</td>
<td>26725.3566</td>
<td>374.1763593</td>
<td>0.0134</td>
<td>Singlet-A</td>
<td>H-6-&gt;LUMO (51%), H-4-&gt;LUMO (23%)</td>
</tr>
<tr>
<td>10</td>
<td>27031.6944</td>
<td>370.2100228</td>
<td>0.0079</td>
<td>Singlet-A</td>
<td>H-9-&gt;LUMO (54%)</td>
</tr>
<tr>
<td>11</td>
<td>27160.10144</td>
<td>368.1871374</td>
<td>0.0066</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+2 (89%)</td>
</tr>
<tr>
<td>12</td>
<td>27319.80032</td>
<td>365.0384662</td>
<td>0.0291</td>
<td>Singlet-A</td>
<td>H-8-&gt;LUMO (74%)</td>
</tr>
<tr>
<td>13</td>
<td>27798.70352</td>
<td>359.7160655</td>
<td>0.1843</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+3 (86%)</td>
</tr>
<tr>
<td>14</td>
<td>28096.5176</td>
<td>355.9159944</td>
<td>0.0107</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+3 (68%)</td>
</tr>
<tr>
<td>15</td>
<td>28408.65532</td>
<td>352.0053848</td>
<td>0.2549</td>
<td>Singlet-A</td>
<td>H-7-&gt;LUMO (54%), H-4-&gt;LUMO (-16%), H-1-&gt;L+3 (-11%)</td>
</tr>
<tr>
<td>16</td>
<td>29320.87568</td>
<td>341.055934</td>
<td>0.0204</td>
<td>Singlet-A</td>
<td>H-9-&gt;LUMO (54%)</td>
</tr>
<tr>
<td>17</td>
<td>29830.6216</td>
<td>335.2260015</td>
<td>0.0047</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+4 (80%)</td>
</tr>
<tr>
<td>18</td>
<td>30009.6792</td>
<td>333.2285356</td>
<td>0.0131</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+4 (59%)</td>
</tr>
<tr>
<td>19</td>
<td>30249.22624</td>
<td>330.5869684</td>
<td>0.0111</td>
<td>Singlet-A</td>
<td>H-10-&gt;LUMO (91%)</td>
</tr>
<tr>
<td>20</td>
<td>30313.75104</td>
<td>329.832925</td>
<td>0.0307</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+1 (27%), H-6-&gt;L+1 (-11%), H-4-&gt;L+1 (-21%), H-2-&gt;L+1 (15%)</td>
</tr>
<tr>
<td>21</td>
<td>30778.3296</td>
<td>324.903922</td>
<td>0.0052</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+1 (15%), H-6-&gt;L+2 (-10%), H-3-&gt;L+1 (41%)</td>
</tr>
<tr>
<td>22</td>
<td>31276.78368</td>
<td>319.72597</td>
<td>0.0045</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+1 (63%)</td>
</tr>
<tr>
<td>23</td>
<td>31368.73152</td>
<td>318.7887911</td>
<td>0.0142</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+5 (64%)</td>
</tr>
<tr>
<td>24</td>
<td>31418.7824</td>
<td>318.2814002</td>
<td>0.1645</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+5 (68%), HOMO-&gt;L+7 (-15%)</td>
</tr>
<tr>
<td>25</td>
<td>31454.22688</td>
<td>317.9222951</td>
<td>0.0037</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+6 (63%)</td>
</tr>
<tr>
<td>26</td>
<td>31674.41776</td>
<td>315.7121964</td>
<td>0.0908</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+2 (51%)</td>
</tr>
<tr>
<td>27</td>
<td>31901.86768</td>
<td>313.4612713</td>
<td>0.0167</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+1 (22%), H-2-&gt;L+2 (-22%), H-1-&gt;L+6 (27%)</td>
</tr>
<tr>
<td>28</td>
<td>31968.0056</td>
<td>313.812758</td>
<td>0.0926</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+6 (75%), HOMO-&gt;L+7 (-19%)</td>
</tr>
<tr>
<td>29</td>
<td>32106.73922</td>
<td>311.4611416</td>
<td>0.0851</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+2 (-13%), H-2-&gt;L+3 (38%)</td>
</tr>
<tr>
<td>30</td>
<td>32257.56064</td>
<td>310.0048423</td>
<td>0.1228</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+2 (10%), HOMO-&gt;L+5 (20%), HOMO-&gt;L+6 (11%), HOMO-&gt;L+7 (45%)</td>
</tr>
<tr>
<td>31</td>
<td>32273.69184</td>
<td>309.8490941</td>
<td>0.0029</td>
<td>Singlet-A</td>
<td>H-2-&gt;L+2 (28%), H-2-&gt;L+3 (28%)</td>
</tr>
<tr>
<td>32</td>
<td>32898.92648</td>
<td>304.0073968</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-11-&gt;LUMO (99%)</td>
</tr>
<tr>
<td>33</td>
<td>33012.5008</td>
<td>302.9155549</td>
<td>0.0054</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+1 (38%), H-7-&gt;L+1 (12%)</td>
</tr>
<tr>
<td>34</td>
<td>33187.52432</td>
<td>301.3180456</td>
<td>0.0167</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+2 (41%), H-7-&gt;L+2 (12%), H-3-&gt;L+2 (-15%)</td>
</tr>
<tr>
<td>35</td>
<td>33438.36448</td>
<td>299.0576888</td>
<td>0.0973</td>
<td>Singlet-A</td>
<td>H-12-&gt;LUMO (47%), H-2-&gt;L+3 (32%)</td>
</tr>
<tr>
<td>S</td>
<td>Comp</td>
<td>H5-&gt;L5 (13%)</td>
<td>H4-&gt;L5 (30%)</td>
<td>H4-&gt;L6 (-12%)</td>
<td>H5-&gt;L6 (11%)</td>
</tr>
<tr>
<td>-----</td>
<td>------------</td>
<td>--------------</td>
<td>--------------</td>
<td>---------------</td>
<td>--------------</td>
</tr>
<tr>
<td>77</td>
<td>3866.26016</td>
<td>258.643476</td>
<td>0.0428</td>
<td></td>
<td></td>
</tr>
<tr>
<td>78</td>
<td>38734.23744</td>
<td>258.695332</td>
<td>0.0062</td>
<td></td>
<td></td>
</tr>
<tr>
<td>79</td>
<td>38868.93295</td>
<td>257.2748764</td>
<td>0.0428</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>38910.87408</td>
<td>256.9795678</td>
<td>0.0043</td>
<td></td>
<td></td>
</tr>
<tr>
<td>81</td>
<td>39252.04996</td>
<td>254.7656</td>
<td>0.0001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>82</td>
<td>39408.5216</td>
<td>253.752224</td>
<td>0.006</td>
<td></td>
<td></td>
</tr>
<tr>
<td>83</td>
<td>39485.1448</td>
<td>253.7598032</td>
<td>0.0066</td>
<td></td>
<td></td>
</tr>
<tr>
<td>84</td>
<td>39666.6208</td>
<td>252.1011318</td>
<td>0.0142</td>
<td></td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>39755.3424</td>
<td>251.57145</td>
<td>0.0116</td>
<td></td>
<td></td>
</tr>
<tr>
<td>86</td>
<td>39795.6704</td>
<td>251.283517</td>
<td>0.0364</td>
<td></td>
<td></td>
</tr>
<tr>
<td>87</td>
<td>39886.81168</td>
<td>250.75171</td>
<td>0.0022</td>
<td></td>
<td></td>
</tr>
<tr>
<td>88</td>
<td>39990.05335</td>
<td>250.0621945</td>
<td>0.1015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>89</td>
<td>40072.32045</td>
<td>249.5468128</td>
<td>0.01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>40125.23215</td>
<td>249.2316</td>
<td>0.0007</td>
<td></td>
<td></td>
</tr>
<tr>
<td>91</td>
<td>40199.75896</td>
<td>248.7577228</td>
<td>0.0005</td>
<td></td>
<td></td>
</tr>
<tr>
<td>92</td>
<td>40265.92768</td>
<td>248.3246202</td>
<td>0.1275</td>
<td></td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>40344.93775</td>
<td>247.862571</td>
<td>0.0172</td>
<td></td>
<td></td>
</tr>
<tr>
<td>94</td>
<td>40729.66688</td>
<td>245.55252</td>
<td>0.015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>95</td>
<td>40738.70304</td>
<td>245.346374</td>
<td>0.0066</td>
<td></td>
<td></td>
</tr>
<tr>
<td>96</td>
<td>40793.38512</td>
<td>245.1377833</td>
<td>0.0077</td>
<td></td>
<td></td>
</tr>
<tr>
<td>97</td>
<td>40805.48352</td>
<td>245.0561025</td>
<td>0.0088</td>
<td></td>
<td></td>
</tr>
<tr>
<td>98</td>
<td>40942.59872</td>
<td>244.2443888</td>
<td>0.0033</td>
<td></td>
<td></td>
</tr>
<tr>
<td>99</td>
<td>40964.37584</td>
<td>244.1111</td>
<td>0.0196</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>41013.576</td>
<td>243.8217094</td>
<td>0.0065</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## Table S8: Energy and composition of TD-DFT calculated transitions of 4:

<table>
<thead>
<tr>
<th>No.</th>
<th>Energy (cm⁻¹)</th>
<th>Wavelength (nm)</th>
<th>Oscillator Strength</th>
<th>Symmetry</th>
<th>Major contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>17574.9424</td>
<td>568.991075</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>HOMO→LUMO (62%), HOMO→L+1 (-36%)</td>
</tr>
<tr>
<td>2</td>
<td>17612.0446</td>
<td>567.7932618</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-1→LUMO (64%), H-1→L+1 (34%)</td>
</tr>
<tr>
<td>3</td>
<td>21617.42112</td>
<td>402.588688</td>
<td>0.0175</td>
<td>Singlet-A</td>
<td>HOMO→LUMO (37%), HOMO→L+1 (61%)</td>
</tr>
<tr>
<td>4</td>
<td>21713.40176</td>
<td>460.5450639</td>
<td>0.001</td>
<td>Singlet-A</td>
<td>H-1→LUMO (35%), H-1→L+1 (63%)</td>
</tr>
<tr>
<td>5</td>
<td>22068.8332</td>
<td>453.7875721</td>
<td>0.9277</td>
<td>Singlet-A</td>
<td>H-2→LUMO (87%)</td>
</tr>
<tr>
<td>6</td>
<td>22926.468</td>
<td>436.1770858</td>
<td>0.0953</td>
<td>Singlet-A</td>
<td>H-5→LUMO (48%), H-5→L+1 (-18%)</td>
</tr>
<tr>
<td>7</td>
<td>23187.62944</td>
<td>431.6367381</td>
<td>0.0748</td>
<td>Singlet-A</td>
<td>H-3→LUMO (61%), H-3→L+1 (27%)</td>
</tr>
<tr>
<td>8</td>
<td>23549.93888</td>
<td>424.6295522</td>
<td>0.0112</td>
<td>Singlet-A</td>
<td>H-4→LUMO (63%), H-4→L+1 (26%)</td>
</tr>
<tr>
<td>9</td>
<td>23674.95568</td>
<td>422.3872743</td>
<td>0.0163</td>
<td>Singlet-A</td>
<td>H-2→L+1 (63%)</td>
</tr>
<tr>
<td>10</td>
<td>24168.5704</td>
<td>413.7605094</td>
<td>0.0596</td>
<td>Singlet-A</td>
<td>H-9→LUMO (10%), H-8→LUMO (12%), H-7→LUMO (44%)</td>
</tr>
<tr>
<td>11</td>
<td>24692.8344</td>
<td>404.9757852</td>
<td>0.1381</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (49%), HOMO→L+3 (22%), HOMO→L+4 (15%)</td>
</tr>
<tr>
<td>12</td>
<td>24745.2608</td>
<td>404.1177857</td>
<td>0.0352</td>
<td>Singlet-A</td>
<td>H-1→L+2 (-14%), H-1→L+3 (66%), H-1→L+4 (-14%)</td>
</tr>
<tr>
<td>13</td>
<td>24806.59936</td>
<td>403.1191853</td>
<td>0.0343</td>
<td>Singlet-A</td>
<td>H-9→LUMO (52%), H-8→L+1 (-21%)</td>
</tr>
<tr>
<td>14</td>
<td>25323.56432</td>
<td>394.8891188</td>
<td>0.021</td>
<td>Singlet-A</td>
<td>H-9→L+1 (-13%), H-8→LUMO (41%), H-7→LUMO (13%), H-7→L+1 (-11%)</td>
</tr>
<tr>
<td>15</td>
<td>25382.12192</td>
<td>393.8229358</td>
<td>0.0852</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (-15%), HOMO→L+4 (16%), HOMO→L+5 (37%)</td>
</tr>
<tr>
<td>16</td>
<td>25813.9528</td>
<td>387.3873977</td>
<td>0.0066</td>
<td>Singlet-A</td>
<td>H-1→L+6 (72%)</td>
</tr>
<tr>
<td>17</td>
<td>25843.7952</td>
<td>386.9400682</td>
<td>0.0044</td>
<td>Singlet-A</td>
<td>H-1→L+4 (33%), H-1→L+5 (-19%), H-1→L+6 (-23%)</td>
</tr>
<tr>
<td>18</td>
<td>25878.4776</td>
<td>386.4214949</td>
<td>0.0055</td>
<td>Singlet-A</td>
<td>HOMO→L+7 (77%)</td>
</tr>
<tr>
<td>19</td>
<td>25990.58944</td>
<td>384.7546445</td>
<td>0.0026</td>
<td>Singlet-A</td>
<td>H-10→LUMO (18%), H-9→L+1 (-12%), H-7→L+1 (20%), HOMO→L+7 (11%)</td>
</tr>
<tr>
<td>20</td>
<td>26066.40608</td>
<td>383.6355487</td>
<td>0.0114</td>
<td>Singlet-A</td>
<td>H-12→L+1 (-11%), H-11→LUMO (60%), H-10→L+1 (-14%), H-6→LUMO (-10%)</td>
</tr>
<tr>
<td>21</td>
<td>26457.5788</td>
<td>377.9634077</td>
<td>0.0219</td>
<td>Singlet-A</td>
<td>H-12→LUMO (17%), H-11→L+1 (-13%), H-10→LUMO (13%), H-3→LUMO (11%), H-3→L+1 (29%)</td>
</tr>
<tr>
<td>22</td>
<td>26506.78784</td>
<td>377.2618569</td>
<td>0.0047</td>
<td>Singlet-A</td>
<td>H-12→LUMO (-15%), H-3→LUMO (-18%), H-3→L+1 (38%)</td>
</tr>
<tr>
<td>23</td>
<td>26570.56068</td>
<td>376.3571522</td>
<td>0.0005</td>
<td>Singlet-A</td>
<td>H-4→LUMO (-29%), H-4→L+1 (69%)</td>
</tr>
<tr>
<td>24</td>
<td>26736.65744</td>
<td>374.0183313</td>
<td>0.0005</td>
<td>Singlet-A</td>
<td>H-13→LUMO (98%)</td>
</tr>
<tr>
<td>25</td>
<td>27203.65568</td>
<td>367.5976537</td>
<td>0.002</td>
<td>Singlet-A</td>
<td>H-12→LUMO (-18%), H-10→LUMO (15%), H-5→LUMO (19%), H-5→L+1 (25%)</td>
</tr>
<tr>
<td>26</td>
<td>27280.72888</td>
<td>366.5651756</td>
<td>0.0029</td>
<td>Singlet-A</td>
<td>HOMO→L+8 (56%), HOMO→L+9 (-39%)</td>
</tr>
<tr>
<td>27</td>
<td>27468.20736</td>
<td>364.0572488</td>
<td>0.0025</td>
<td>Singlet-A</td>
<td>H-1→L+8 (35%), H-1→L+9 (60%)</td>
</tr>
<tr>
<td>28</td>
<td>27544.83056</td>
<td>363.0445277</td>
<td>0.0033</td>
<td>Singlet-A</td>
<td>H-14→LUMO (18%), H-5→LUMO (15%), H-6→L+1 (-12%), H-5→L+1 (11%)</td>
</tr>
<tr>
<td>29</td>
<td>27860.32592</td>
<td>361.9211742</td>
<td>0.0095</td>
<td>Singlet-A</td>
<td>H-15→LUMO (-15%), H-14→LUMO (23%), H-14→L+1 (-11%), H-6→L+1 (17%)</td>
</tr>
<tr>
<td>30</td>
<td>27656.13584</td>
<td>361.5834135</td>
<td>0.003</td>
<td>Singlet-A</td>
<td>H-15→LUMO (20%), H-15→L+1 (10%), H-14→LUMO (17%), H-5→L+1 (-14%)</td>
</tr>
<tr>
<td>31</td>
<td>27743.24432</td>
<td>360.4481107</td>
<td>0.0149</td>
<td>Singlet-A</td>
<td>H-15→LUMO (15%), H-6→L+1 (32%)</td>
</tr>
<tr>
<td>32</td>
<td>27804.54288</td>
<td>359.6534582</td>
<td>0.002</td>
<td>Singlet-A</td>
<td>H-13→L+1 (89%)</td>
</tr>
<tr>
<td>33</td>
<td>28353.31024</td>
<td>352.686825</td>
<td>0.0122</td>
<td>Singlet-A</td>
<td>H-12→L+1 (-15%), H-10→L+1 (49%), H-8→LUMO (11%), H-9→L+1 (36%), H-8→LUMO (14%), H-8→L+1 (14%), H-7→L+1 (13%)</td>
</tr>
<tr>
<td>34</td>
<td>28389.29888</td>
<td>352.2454021</td>
<td>0.101</td>
<td>Singlet-A</td>
<td>H-9→LUMO (11%), H-9→L+1 (15%), H-8→LUMO (14%), H-8→L+1 (43%)</td>
</tr>
<tr>
<td>37</td>
<td>29404.75792</td>
<td>340.0810177</td>
<td>0.0007</td>
<td>Singlet-A</td>
<td>HOMO→L+2 (-23%), HOMO→L+3 (72%)</td>
</tr>
<tr>
<td>38</td>
<td>29433.79408</td>
<td>339.745531</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-1→L+2 (71%), H-1→L+3 (22%)</td>
</tr>
<tr>
<td>39</td>
<td>29631.40128</td>
<td>337.479821</td>
<td>0.0003</td>
<td>Singlet-A</td>
<td>HOMO→L+4 (66%), HOMO→L+5 (-34%)</td>
</tr>
<tr>
<td>40</td>
<td>29693.5064</td>
<td>336.7798898</td>
<td>0.0006</td>
<td>Singlet-A</td>
<td>H-12→L+1 (13%), H-11→LUMO (24%), H-11→L+1 (44%)</td>
</tr>
<tr>
<td>41</td>
<td>29797.52824</td>
<td>335.5980312</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-1→L+4 (31%), H-1→L+5 (69%)</td>
</tr>
<tr>
<td>42</td>
<td>29809.65104</td>
<td>335.461827</td>
<td>0.0006</td>
<td>Singlet-A</td>
<td>H-12→LUMO (-17%), H-12→L+1 (40%), H-11→L+1 (-17%)</td>
</tr>
<tr>
<td>43</td>
<td>29988.70736</td>
<td>333.458544</td>
<td>0.0072</td>
<td>Singlet-A</td>
<td>H-5→L+2 (-10%), H-2→L+2 (44%)</td>
</tr>
<tr>
<td>44</td>
<td>30062.10432</td>
<td>332.6447109</td>
<td>0.0028</td>
<td>Singlet-A</td>
<td>H-6→L+3 (-13%), H-2→L+3 (33%)</td>
</tr>
<tr>
<td>45</td>
<td>30149.2128</td>
<td>331.6836186</td>
<td>0.0081</td>
<td>Singlet-A</td>
<td>H-2→L+4 (42%)</td>
</tr>
<tr>
<td>46</td>
<td>30234.70816</td>
<td>330.7457094</td>
<td>0.0142</td>
<td>Singlet-A</td>
<td>HOMO→L+10 (75%)</td>
</tr>
<tr>
<td>47</td>
<td>30325.04288</td>
<td>329.760457</td>
<td>0.0065</td>
<td>Singlet-A</td>
<td>H-1→L+11 (72%)</td>
</tr>
<tr>
<td>48</td>
<td>30354.8856</td>
<td>329.4362605</td>
<td>0.0097</td>
<td>Singlet-A</td>
<td>H-1→L+11 (72%)</td>
</tr>
<tr>
<td>49</td>
<td>30525.87632</td>
<td>327.590923</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>HOMO→L+6 (60%)</td>
</tr>
<tr>
<td>50</td>
<td>30542.81408</td>
<td>327.471</td>
<td>0.0068</td>
<td>Singlet-A</td>
<td>H-14→LUMO (27%), H-14→L+1 (69%)</td>
</tr>
<tr>
<td>51</td>
<td>30608.952</td>
<td>326.7018093</td>
<td>0.0167</td>
<td>Singlet-A</td>
<td>H-3→L+2 (27%), H-3→L+3 (10%)</td>
</tr>
<tr>
<td>52</td>
<td>30640.40784</td>
<td>326.364413</td>
<td>0.0096</td>
<td>Singlet-A</td>
<td>H-15→LUMO (-25%), H-15→L+1 (69%)</td>
</tr>
<tr>
<td>53</td>
<td>30712.19168</td>
<td>325.2650</td>
<td>0.0021</td>
<td>Singlet-A</td>
<td>H-4→L+2 (-11%), H-4→L+3 (47%)</td>
</tr>
<tr>
<td>54</td>
<td>30751.71312</td>
<td>325.1851386</td>
<td>0</td>
<td>Singlet-A</td>
<td>H-1→L+7 (69%)</td>
</tr>
<tr>
<td>55</td>
<td>30939.0416</td>
<td>323.2099495</td>
<td>0.0015</td>
<td>Singlet-A</td>
<td>H-1→L+12 (70%)</td>
</tr>
<tr>
<td>56</td>
<td>30972.71056</td>
<td>322.8648646</td>
<td>0.0087</td>
<td>Singlet-A</td>
<td>H-5→L+2 (15%), H-2→L+2 (24%), H-2→L+3 (11%), H-2→L+4 (15%)</td>
</tr>
<tr>
<td>57</td>
<td>30988.0352</td>
<td>322.7051969</td>
<td>0.0183</td>
<td>Singlet-A</td>
<td>H-6→L+3 (23%), H-2→L+3 (25%), H-1→L+12 (-17%)</td>
</tr>
<tr>
<td>58</td>
<td>30999.32704</td>
<td>322.587848</td>
<td>0.0083</td>
<td>Singlet-A</td>
<td>HOMO→L+13 (86%)</td>
</tr>
<tr>
<td>59</td>
<td>31175.96808</td>
<td>320.7599323</td>
<td>0.0017</td>
<td>Singlet-A</td>
<td>H-3→L+7 (15%), HOMO→L+5 (15%), HOMO→L+9 (23%)</td>
</tr>
<tr>
<td>60</td>
<td>31334.04944</td>
<td>319.1416424</td>
<td>0.0224</td>
<td>Singlet-A</td>
<td>H-3→L+7 (-12%), HOMO→L+5 (24%), HOMO→L+9 (33%)</td>
</tr>
<tr>
<td>61</td>
<td>31349.37408</td>
<td>318.9856351</td>
<td>0.0086</td>
<td>Singlet-A</td>
<td>H-1→L+8 (50%), H-1→L+9 (-41%)</td>
</tr>
<tr>
<td>62</td>
<td>31388.89552</td>
<td>318.5840035</td>
<td>0.0002</td>
<td>Singlet-A</td>
<td>H-6→L+6 (-19%), H-4→L+6 (20%)</td>
</tr>
<tr>
<td>63</td>
<td>31412.15792</td>
<td>318.25689</td>
<td>0.012</td>
<td>Singlet-A</td>
<td>H-5→L+7 (24%), H-3→L+2 (-10%), H-3→L+5 (17%)</td>
</tr>
<tr>
<td>64</td>
<td>31449.38752</td>
<td>317.9712162</td>
<td>0.0081</td>
<td>Singlet-A</td>
<td>H-4→L+4 (22%), H-4→L+5 (-15%), H-4→L+6 (-14%)</td>
</tr>
<tr>
<td>65</td>
<td>31508.2664</td>
<td>317.3770297</td>
<td>0.0254</td>
<td>Singlet-A</td>
<td>H-5→L+5 (19%)</td>
</tr>
<tr>
<td>66</td>
<td>31638.12256</td>
<td>316.0743809</td>
<td>0.0022</td>
<td>Singlet-A</td>
<td>H-3→L+5 (-10%), H-3→L+7 (15%), H-2→L+7 (-10%)</td>
</tr>
<tr>
<td>67</td>
<td>31709.09984</td>
<td>315.3668837</td>
<td>0.0083</td>
<td>Singlet-A</td>
<td>H-4→L+4 (22%), H-4→L+6 (-11%), H-4→L+6 (11%), H-2→L+6 (-14%)</td>
</tr>
<tr>
<td>68</td>
<td>31733.29684</td>
<td>315.1264148</td>
<td>0.0181</td>
<td>Singlet-A</td>
<td>H-4→L+6 (11%), H-3→L+7 (15%), H-2→L+6 (-14%)</td>
</tr>
<tr>
<td>69</td>
<td>31806.6936</td>
<td>314.3992307</td>
<td>0.0057</td>
<td>Singlet-A</td>
<td>H-16→L+1 (63%), H-2→L+6 (-14%)</td>
</tr>
<tr>
<td>70</td>
<td>32112.37984</td>
<td>311.1411</td>
<td>0.1433</td>
<td>Singlet-A</td>
<td>H-6→L+6 (14%), H-2→L+6 (23%)</td>
</tr>
<tr>
<td>71</td>
<td>32187.88982</td>
<td>310.6806742</td>
<td>0.0601</td>
<td>Singlet-A</td>
<td>H-2→L+7 (52%)</td>
</tr>
<tr>
<td>72</td>
<td>32222.072</td>
<td>310.3462744</td>
<td>0.031</td>
<td>Singlet-A</td>
<td>H-2→L+7 (-11%), H-2→L+8 (50%)</td>
</tr>
<tr>
<td>73</td>
<td>32271.27126</td>
<td>309.8731265</td>
<td>0.0704</td>
<td>Singlet-A</td>
<td>H-2→L+6 (-13%), H-2→L+9 (49%)</td>
</tr>
<tr>
<td>74</td>
<td>32277.72464</td>
<td>309.8111813</td>
<td>0.01</td>
<td>Singlet-A</td>
<td>H-7→L+2 (13%), H-2→L+8 (-10%)</td>
</tr>
<tr>
<td>75</td>
<td>32604.8144</td>
<td>306.7072448</td>
<td>0.0214</td>
<td>Singlet-A</td>
<td>H-8→L+3 (19%), H-8→L+6 (10%)</td>
</tr>
<tr>
<td>76</td>
<td>32710.84736</td>
<td>305.7098867</td>
<td>0.0298</td>
<td>Singlet-A</td>
<td>H-8→L+3 (19%), H-8→L+6 (10%)</td>
</tr>
<tr>
<td>Number</td>
<td>33002.01552</td>
<td>303.0117962</td>
<td>0.0324</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+8 (36%), H-3-&gt;L+9 (-25%)</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>-------------</td>
<td>--------</td>
<td>-----------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td></td>
<td>33025.40576</td>
<td>302.7971881</td>
<td>0.0397</td>
<td>Singlet-A</td>
<td>H-8-&gt;L+6 (23%)</td>
</tr>
<tr>
<td></td>
<td>33092.35024</td>
<td>302.1846417</td>
<td>0.0747</td>
<td>Singlet-A</td>
<td>H-5-&gt;L+8 (21%), H-5-&gt;L+9 (-17%)</td>
</tr>
<tr>
<td></td>
<td>33131.06512</td>
<td>301.8315277</td>
<td>0.0481</td>
<td>Singlet-A</td>
<td></td>
</tr>
<tr>
<td></td>
<td>33184.29808</td>
<td>301.3473413</td>
<td>0.0105</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+9 (20%), H-4-&gt;L+9 (28%)</td>
</tr>
<tr>
<td></td>
<td>33237.53104</td>
<td>300.86666</td>
<td>0.0122</td>
<td>Singlet-A</td>
<td>H-6-&gt;L+9 (16%), H-4-&gt;L+9 (12%)</td>
</tr>
<tr>
<td></td>
<td>33354.48224</td>
<td>299.8097805</td>
<td>0.0075</td>
<td>Singlet-A</td>
<td>H-7-&gt;L+4 (12%)</td>
</tr>
<tr>
<td></td>
<td>33526.27952</td>
<td>298.2734781</td>
<td>0.0103</td>
<td>Singlet-A</td>
<td>H-7-&gt;L+5 (19%)</td>
</tr>
<tr>
<td></td>
<td>33589.99776</td>
<td>297.7076709</td>
<td>0.0034</td>
<td>Singlet-A</td>
<td>H-17-&gt;LUMO (95%)</td>
</tr>
<tr>
<td></td>
<td>33631.93888</td>
<td>297.94445</td>
<td>0.0283</td>
<td>Singlet-A</td>
<td>H-11-&gt;L+2 (11%)</td>
</tr>
<tr>
<td></td>
<td>33675.49312</td>
<td>296.3518505</td>
<td>0.009</td>
<td>Singlet-A</td>
<td>H-12-&gt;L+3 (20%), H-11-&gt;L+3 (-11%), H-10-&gt;L+3 (13%)</td>
</tr>
<tr>
<td></td>
<td>33802.12304</td>
<td>255.84</td>
<td>0.0255</td>
<td>Singlet-A</td>
<td></td>
</tr>
<tr>
<td></td>
<td>33829.54608</td>
<td>255.595914</td>
<td>0.0064</td>
<td>Singlet-A</td>
<td>H-19-&gt;L+1 (18%), H-18-&gt;LUMO (42%)</td>
</tr>
<tr>
<td></td>
<td>33872.29376</td>
<td>255.2265374</td>
<td>0.0168</td>
<td>Singlet-A</td>
<td>H-18-&gt;LUMO (-10%), H-9-&gt;L+5 (13%)</td>
</tr>
<tr>
<td></td>
<td>33983.59904</td>
<td>294.26</td>
<td>0.0088</td>
<td>Singlet-A</td>
<td>H-19-&gt;LUMO (51%), H-18-&gt;L+1 (26%)</td>
</tr>
<tr>
<td></td>
<td>34208.62928</td>
<td>292.3239022</td>
<td>0.0007</td>
<td>Singlet-A</td>
<td>H-1-&gt;L+10 (62%), H-1-&gt;L+14 (25%)</td>
</tr>
<tr>
<td></td>
<td>34233.63264</td>
<td>292.1103964</td>
<td>0.0004</td>
<td>Singlet-A</td>
<td>HOMO-&gt;L+11 (74%), HOMO-&gt;L+14 (15%)</td>
</tr>
<tr>
<td></td>
<td>34271.54096</td>
<td>291.7872882</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+2 (-22%), H-3-&gt;L+3 (72%)</td>
</tr>
<tr>
<td></td>
<td>34338.97744</td>
<td>290.721</td>
<td>0.0025</td>
<td>Singlet-A</td>
<td>H-4-&gt;L+2 (56%), H-4-&gt;L+3 (18%)</td>
</tr>
<tr>
<td></td>
<td>34414.30288</td>
<td>290.5768647</td>
<td>0.0166</td>
<td>Singlet-A</td>
<td>H-11-&gt;L+5 (14%), H-4-&gt;L+2 (12%)</td>
</tr>
<tr>
<td></td>
<td>34478.02032</td>
<td>290.0388546</td>
<td>0.0154</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+4 (13%)</td>
</tr>
<tr>
<td></td>
<td>34498.18432</td>
<td>289.8703279</td>
<td>0.0094</td>
<td>Singlet-A</td>
<td>H-3-&gt;L+4 (29%), H-3-&gt;L+5 (-16%)</td>
</tr>
<tr>
<td></td>
<td>34553.83696</td>
<td>289.4034608</td>
<td>0.0077</td>
<td>Singlet-A</td>
<td>H-11-&gt;L+7 (10%)</td>
</tr>
<tr>
<td></td>
<td>34558.67632</td>
<td>289.9362</td>
<td>0.0215</td>
<td>Singlet-A</td>
<td>H-16-&gt;L+3 (15%)</td>
</tr>
</tbody>
</table>
**Figure S9**: $^1$H NMR data for 5-Bromo-2-iodopyridine (6):
Figure S10: $^{13}$C NMR data for 5-Bromo-2-iodopyridine (6):
Figure S11: $^1$H NMR data for 5-bromo-2,2'-bipyridine (7):
**Figure S12:** $^{13}$C NMR data for 5-bromo-2,2'-bipyridine (7):
Figure S13: $^1$H NMR data for 5-trimethylsilyl-2,2'-bipyridine (8):
Figure S14: $^{13}$C NMR data for 5-trimethylsilylethynyl-2,2'-bipyridine (8):
Figure S15: $^1$H NMR data for 5-Ethynyl-2,2'-bipyridine (5):
Figure S16: $^{13}$C NMR data for 5-Ethynyl-2,2'-bipyridine (5):
**Figure S17:** $^1$H NMR data for *trans-(5-ethynyl-2,2'-bipyridine)-chloro-bis(tri-*n*-butylphosphine)platinum (5'):
Figure S18: $^{13}$C NMR data for trans-(5-ethynyl-2,2'-bipyridine)-chloro-bis(tri-n-butylphosphine)platinum (5'):
**Figure S19**: $^{31}$P NMR data for trans-(5-ethynyl-2,2'-bipyridine)-chloro-bis(tri-n-butylphosphine)platinum (5'): 

![NMR spectrum and structure diagram](image)
Figure S20: $^{1}$H NMR data for trans-(5-ethynyl-2,2'-bipyridine)-4-tolylethynyl-bis(tri-$n$-butylphosphine)platinum (2):
Figure S21: $^{13}$C NMR data for *trans*- (5-ethynyl-2,2'-bipyridine)-4-tolylethynyl-bis(tri-*n*-butylphosphine)platinum (2):
Figure S22: $^{31}$P NMR data for trans-(5-ethynyl-2,2'-bipyridine)-4-tolylethynyl-bis(tri-$n$-butylphosphine)platinum (2):
Figure S23: $^1$H NMR data for trans-bis(tri-$n$-butylphosphine)-bis(5-ethynyl-2,2'-bipyridine)platinum (2'):
Figure S24: $^{13}$C NMR data for *trans*-bis(tri-*n*-butylphosphine)-bis(5-ethynyl-2,2'-bipyridine)platinum (2'): 
Figure S25: $^{31}$P NMR data for trans-bis(tri-$n$-butylphosphine)-bis(5-ethynyl-2,2'-bipyridine)platinum (2'): 

![NMR Spectrogram](image-url)
Figure S26: $^1$H NMR data for [Ir(ppy)$_2$(5-ethynyl-2,2'-bipyridine)] Hexafluorophosphate (1):
Figure S27: $^{13}$C NMR data for $[\text{Ir} \text{(ppy)}_2(5\text{-ethynyl-2,2'}\text{-bipyridine})] \text{ Hexafluorophosphate (1)}$: 

![NMR spectrum of Ir complex with 5-ethynyl-2,2'-bipyridine]
Figure S28: $^1$H NMR data for trans-[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-4-tolylethynyl-bis(tri-$n$-butylphosphine)platinum Hexafluorophosphate (3):
Figure S29: $^{13}$C NMR data for $trans$-[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-4-tolylethynyl-bis(tri-$n$-butylphosphine)platinum Hexafluorophosphate (3):
Figure S30: $^{31}$P NMR data for $trans$-[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-4-tolylethynyl-bis(tri-$n$-butylphosphine)platinum Hexafluorophosphate (3):
Figure S31: $^1$H NMR data for \textit{trans}-bis[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-bis(tri-\textit{n}-butylphosphine)platinum Hexafluorophosphate (4):
Figure S32: $^{13}$C NMR data for trans-bis[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-bis(tri-n-butyolphosphine)platinum Hexafluorophosphate (4):
**Figure S33:** $^{31}$P NMR data for *trans*-bis[Ir(ppy)$_2$(5-Ethynyl-2,2'-bipyridine)]-bis(tri-\textit{n}-butylphosphine)platinum Hexafluorophosphate (4):
References:


(21). N. M. O’Boyle, *GaussSum 2.0*, Dublin City University; Dubin Ireland, 2006.