# Negatively charged Ir(III) cyclometalated complexes containing a chelating bis-tetrazolato ligand: Synthesis, photophysics and study of reactivity with electrophiles.

Valentina Fiorini,[a]* Stefano Zacchini,[a] Paolo Raiteri,[b,c] Rita Mazzoni,[a] Valerio Zanotti,[a] Massimiliano Massi[b]* and Stefano Stagni[a]*

[a] *Department of Industrial Chemistry "Toso Montanari", University of Bologna, Viale Risorgimento 4, I-40136 Bologna, Italy*

[b] *Department of Chemistry, Curtin University, GPO Box U 1987, Perth, Australia, 6845*

[c] *Curtin Institute for Computation, Curtin University, GPO Box U 1987, Perth, Australia, 6845*

## Electronic Supplementary Information - ESI

## ESI-MS spettroscopy

**Figure S1:** ESI-MS spectrum of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** (negative ions region) [M]$^-$ = 713 *m/z*, $CH_3CN$.

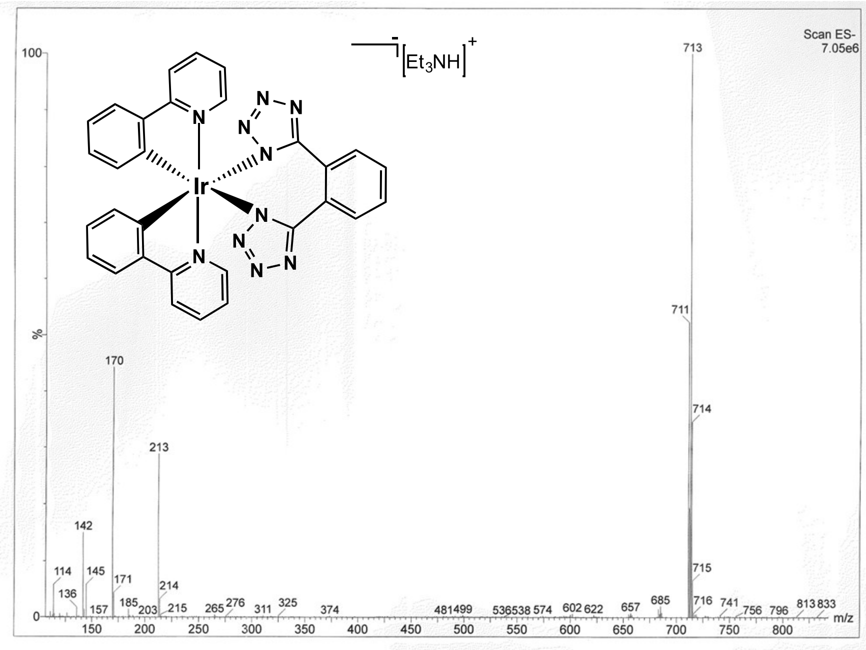



**Figure S2:** ESI-MS spectrum of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** (negative ions region) [M]$^-$ = 785 *m/z*, $CH_3CN$.

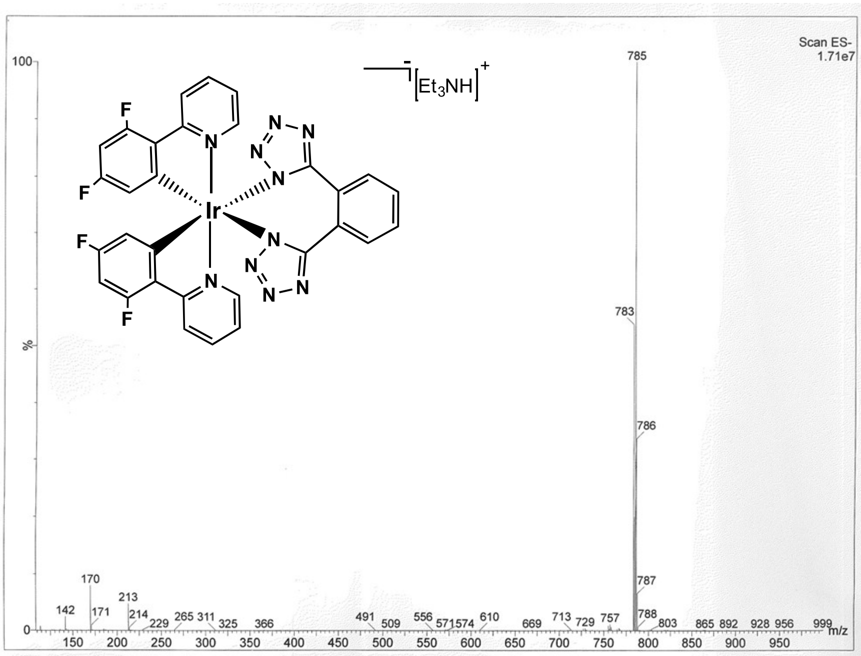


**Figure S3:** ESI-MS spectrum of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** (positive ions region) [M]$^-$ = 743 *m/z*, $CH_3CN$.

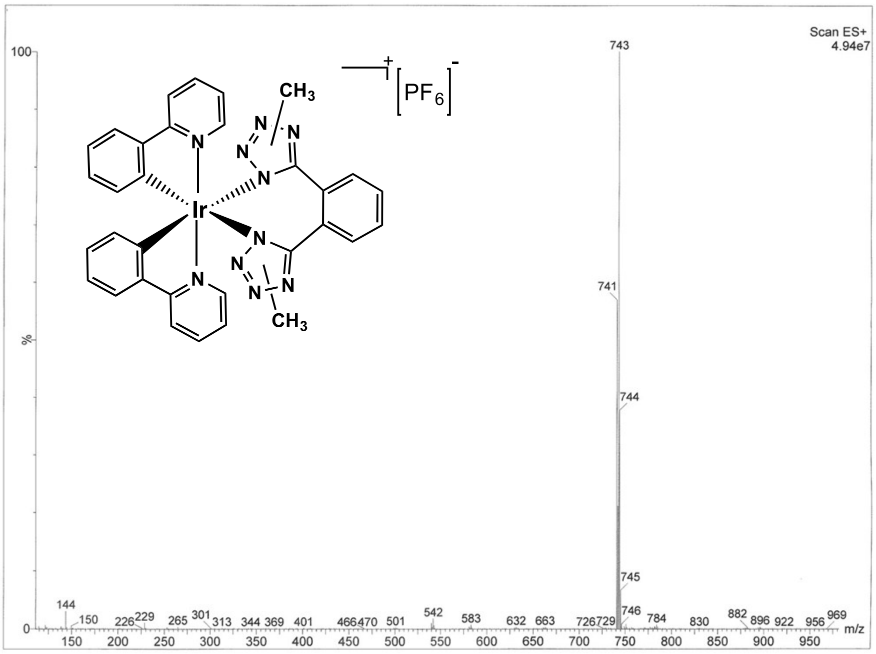



**Figure S4:** ESI-MS spectrum of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** (positive ions region) [M]$^-$ = 815 *m/z*, $CH_3CN$.

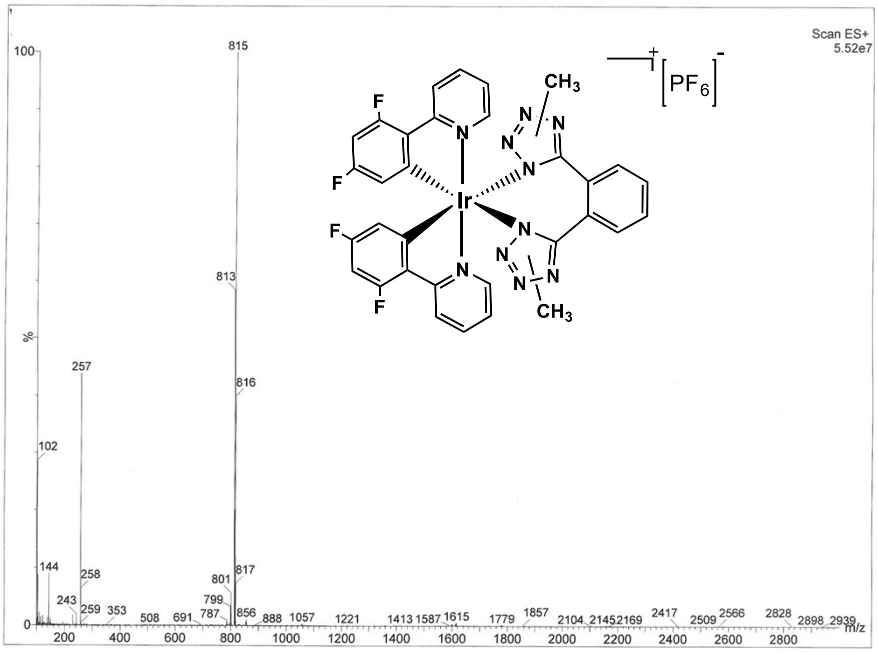
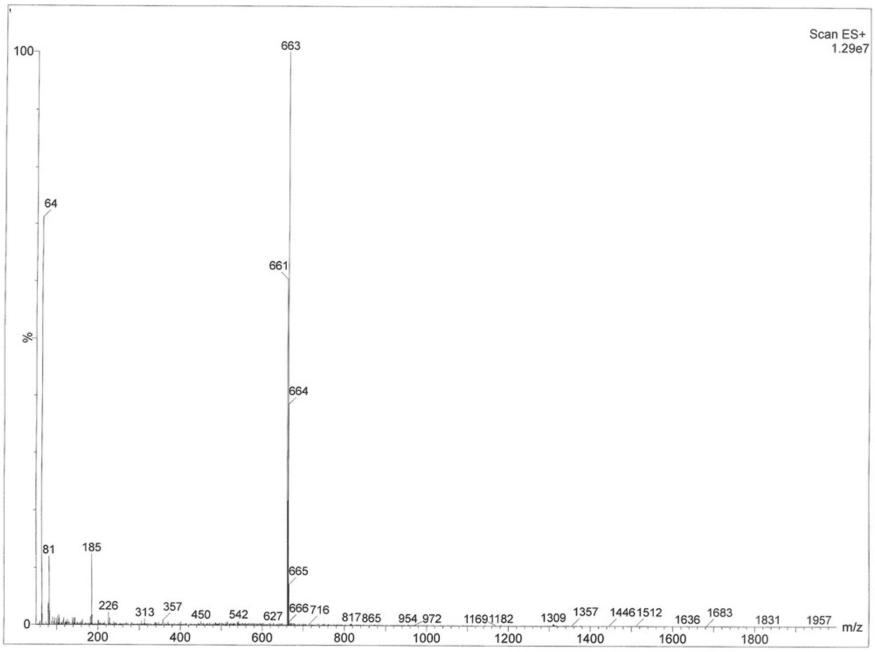


**Figure S5:** ESI-MS spectrum of **SS1** (positive and negative ions region), $CH_3CN$.



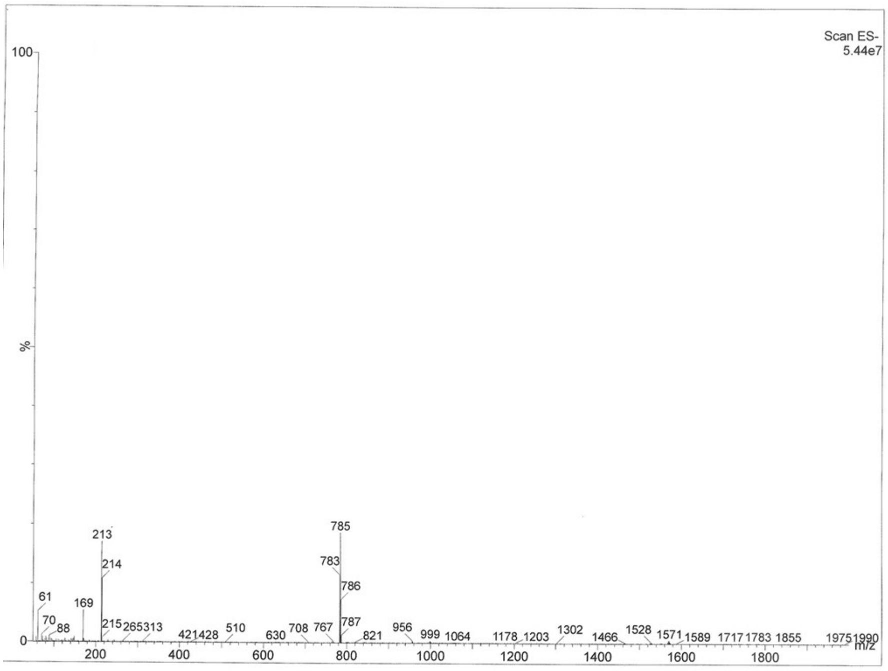
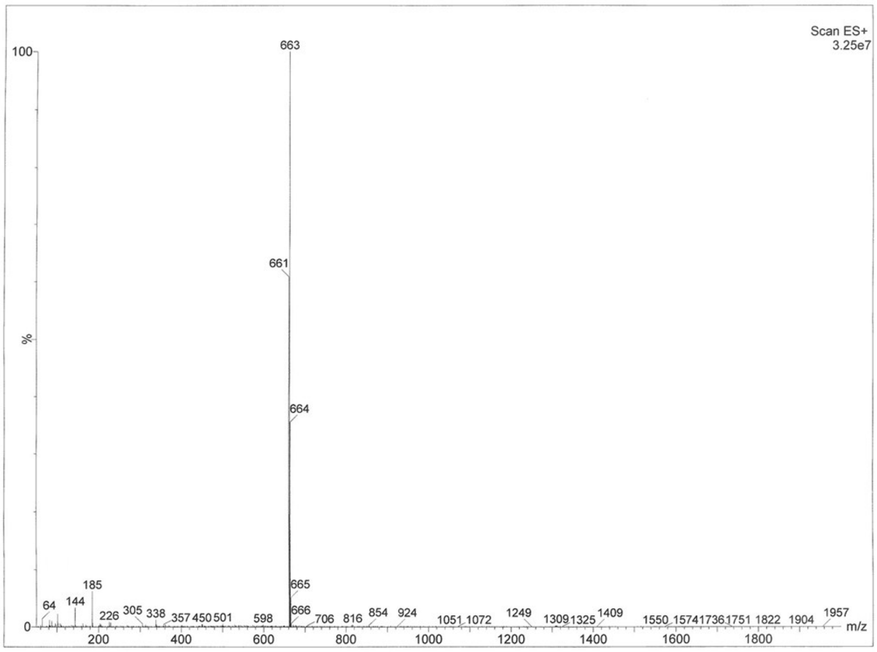
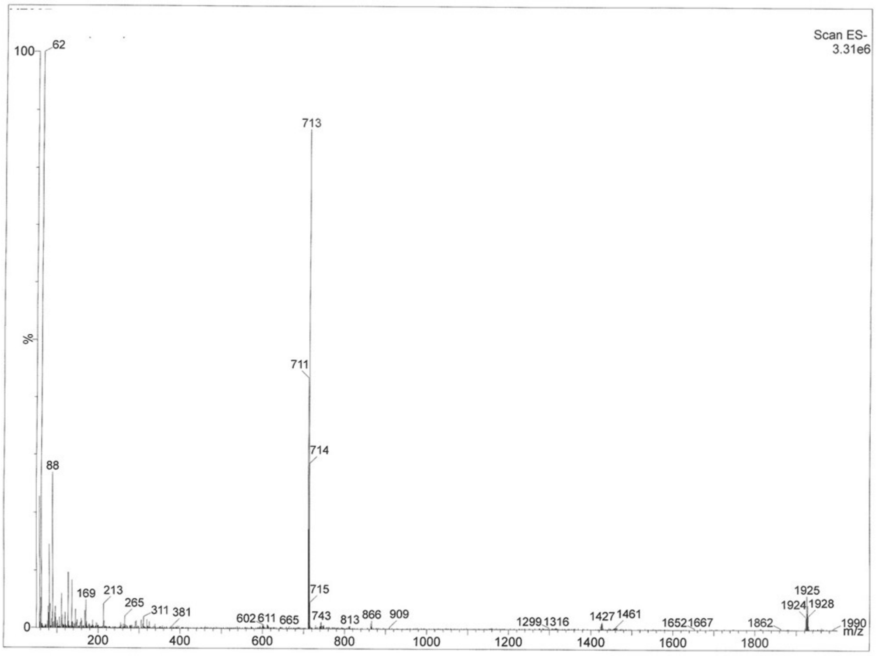



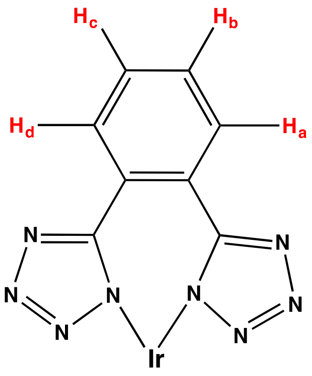
**Figure S6:** ESI-MS spectrum of **SS2** (positive and negative ions region), $CH_3CN$.



**NMR spectroscopy**

Hydrogen labeling adopted for 1,2 BTB and 1,2 $BTBMe_2$



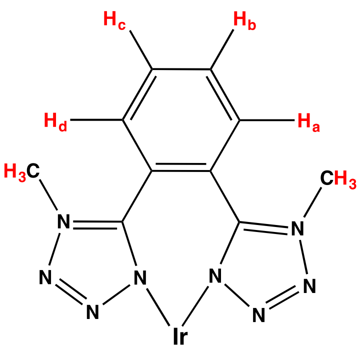



**Figure S7:** $^{1}$H Variable Temperature NMR of **$[Ir(ppy)_2(1,2\ BTB)]^-$** $CD_2Cl_2$, 600 MHz.

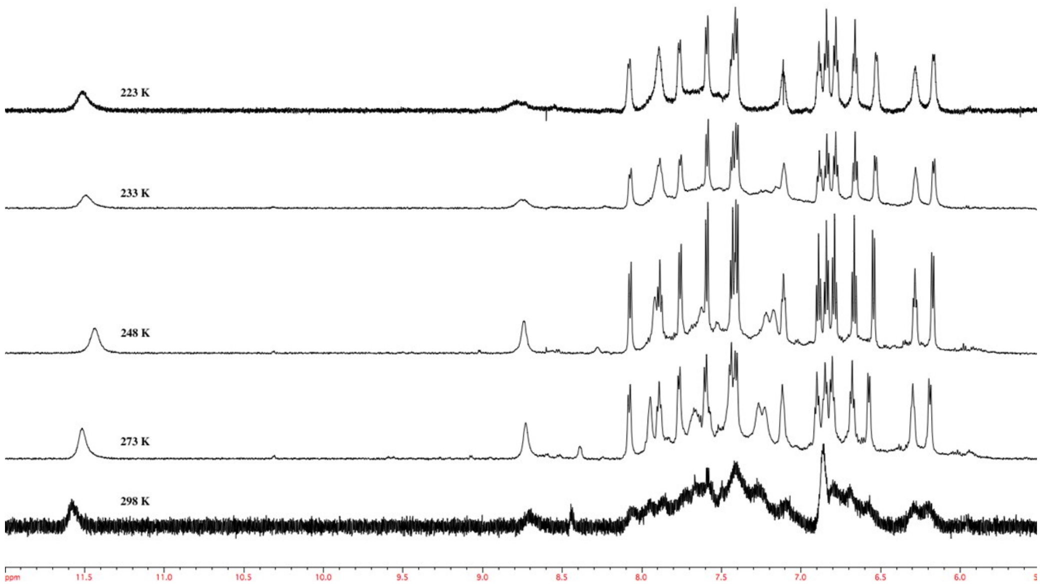
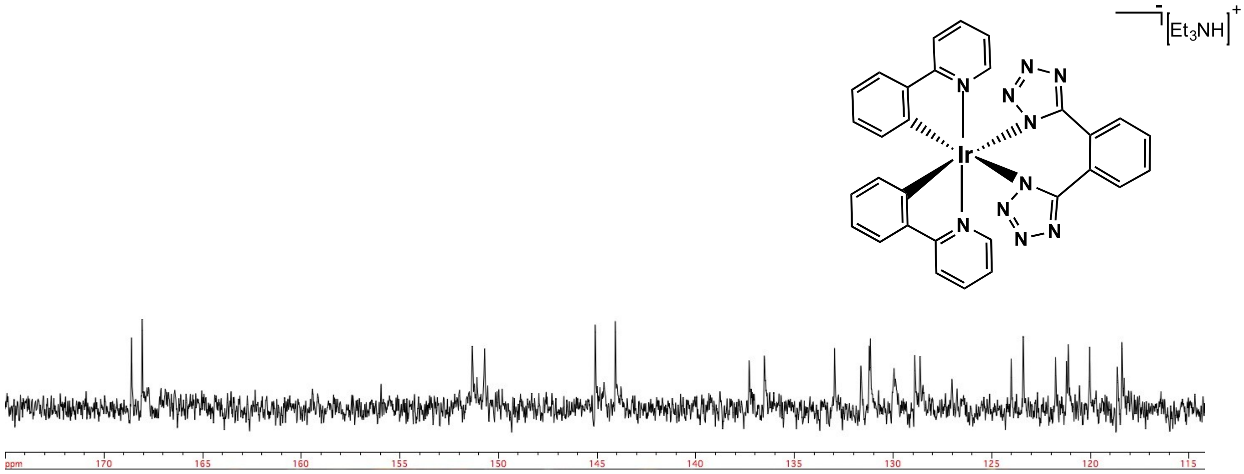



**Figure S8:** $^{13}$C NMR of **$[Ir(ppy)_2(1,2\ BTB)]^-$** $CD_2Cl_2$, 150.8 MHz, 248K.




**$[Ir(ppy)_2(1,2\ BTB)]^-$** Y = 76.5%, 0.058 g **$^{1}$H-NMR** (600 MHz), $CD_2Cl_2$, 248K, δ (ppm) = 11.45 (s, br, 1H), 8.73 (s, br, 1H, $H_d$), 8.02 (d, 1H, $J_{H-H}$ = 8.39 Hz, $H_c$), 7.84 (m, 2H, $H_b$ and ppy), 7.71 (d, 1H, $J_{H-H}$ = 7.79 Hz, $H_a$), 7.54 (m, 2H), 7.38 – 7.34 (m, 2H), 7.21 – 7.05 (m, 3H), 6.84 – 6.82 (m, 1H), 6.79 – 6.77 (m, 1H), 6.74 – 6.72 (m, 1H), 6.62 – 6.60 (m, 1H), 6.49 (d, 1H, $J_{H-H}$ = 7.79 Hz), 6.23 (m, 1H), 6.12 (d, 1H, $J_{H-H}$ = 7.79 Hz). **$^{13}$C-NMR** (150.8 MHz), $CD_2Cl_2$, 248K, δ (ppm) = 168.60, 168.06, 151.33, 150.70, 145.10, 144.08, 137.30, 136.53, 132.53, 131.63, 131.20, 131.15, 129.95, 128.90, 128.63. **ESI-MS** (*m/z*) $CH_3CN$, $[M]^-$ = 712; $[M]^+$= 102 ($Et_3NH$).

**Figure S9:** $^{1}$H Variable Temperature NMR of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $CD_2Cl_2$, 600 MHz.

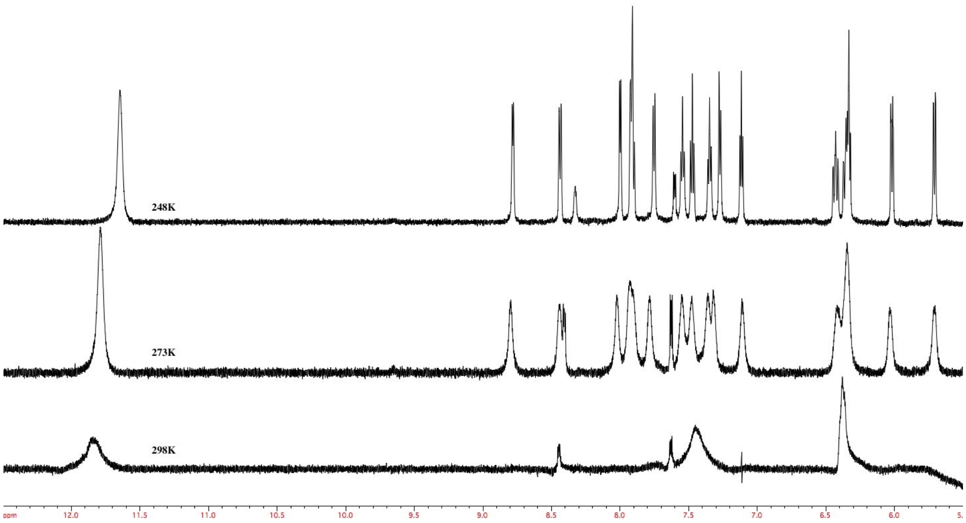
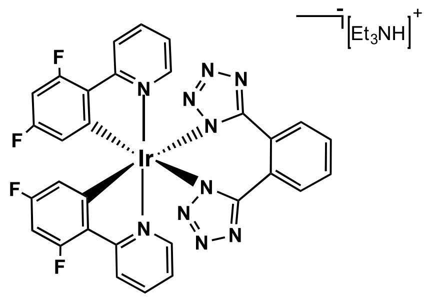
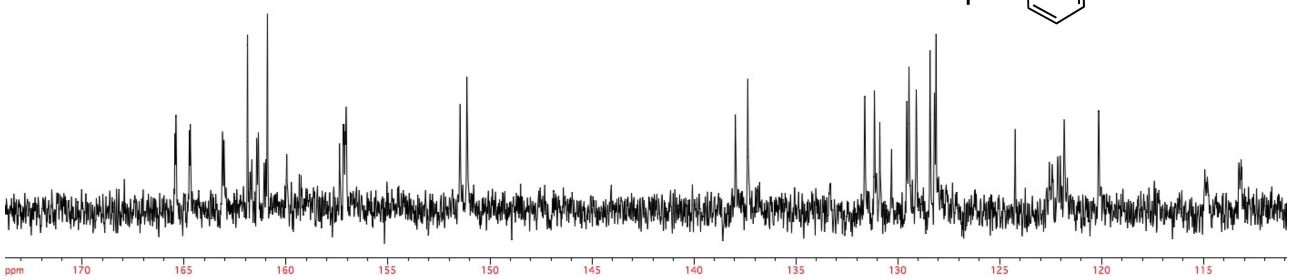



**Figure S10:** $^{13}$C NMR of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $CD_2Cl_2$, 600 MHz, 248K.




**[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** Y = 59%, 0.043 g **$^{1}$H-NMR** (600 MHz), $CD_2Cl_2$, 248K, δ (ppm) = 11.64 (s, br, 1H), 8.78 (d, 1H, $J_{H-H}$ = 5.99 Hz, $H_d$), 8.44 (d, 1H, $J_{H-H}$ = 8.99 Hz, $H_c$), 8.00 (d, 1H, $J_{H-H}$ = 4.79 Hz, $H_b$), 7.92 – 7.89 (m, 2H, $H_a$ and F$_2$ppy), 7.75 (m, 1H), 7.55 – 7.53 (m, 1H), 7.48 – 7.46 (m, 1H), 7.36 – 7.33 (m, 1H), 7.27 (m, 1H), 7.12 – 7.10 (m, 1H), 6.44 – 6.37 (m, 1H), 6.35 – 6.32 (m, 1H), 6.02 – 6.00 (m,1H), 5.71 – 5.69 (m, 1H). **$^{13}$C-NMR** (150.8 MHz), $CD_2Cl_2$, 248K, δ (ppm) = 165.42, 164.76, 163.13, 161.91, 161.46, 160.93, 157.74, 157.21, 151.48, 151.14, 137.98, 137.37, 131.63, 131.15, 130.74, 129.57, 129.54, 129.46, 129.20, 128.64, 128.43, 128.21, 128.14, 123.92, 122.51, 122.08, 121.85, 120.16, 114.63, 113.18. **ESI-MS** (*m/z*) [M]$^-$ = 784; [M]$^+$= 102 ($Et_3NH$).

**Figure S11:** $^{1}$H NMR of **$[Ir(ppy)_2(1,2\ BTBMe_2)]^+$** Acetone-*d$^6$*, 400 MHz, 298K.

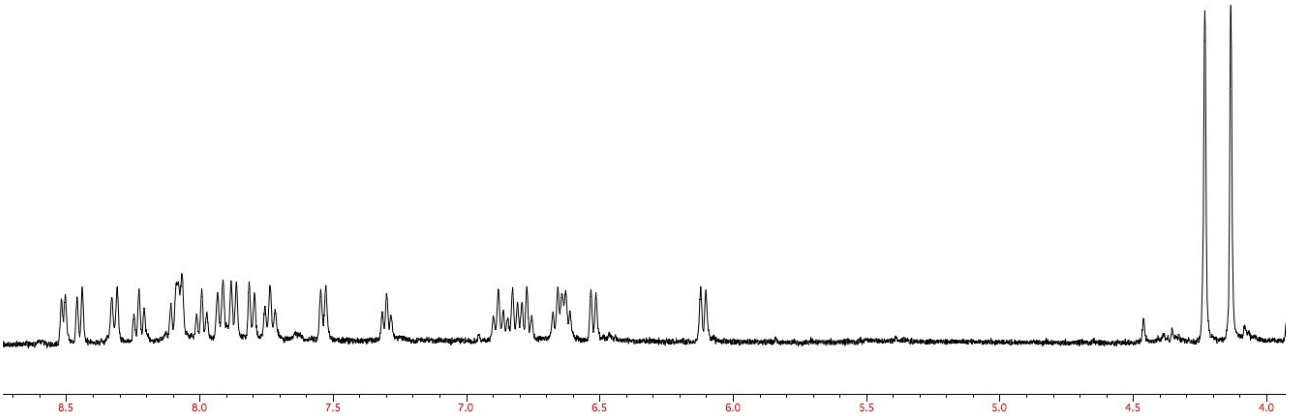
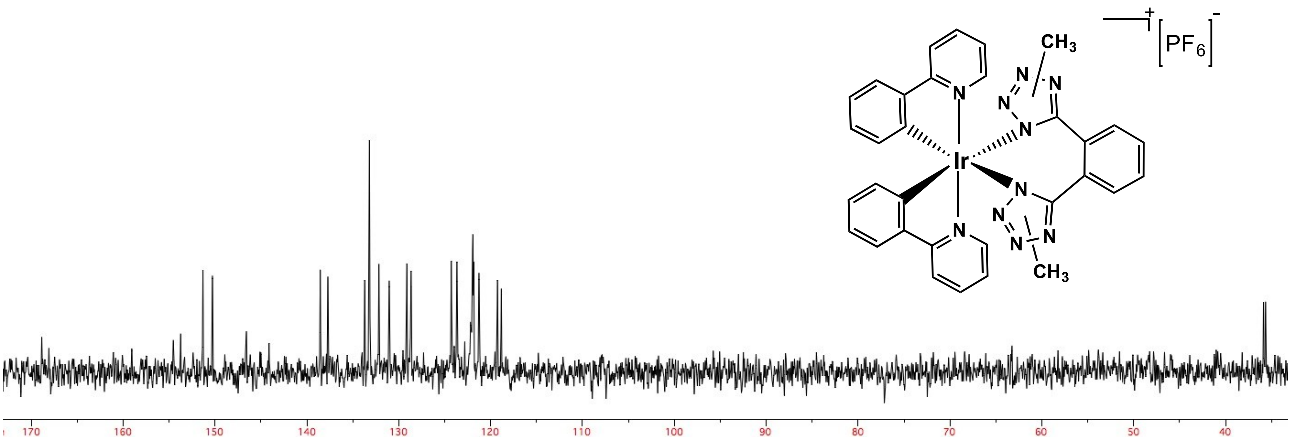



**Figure S12:** $^{13}$C NMR of **$[Ir(ppy)_2(1,2\ BTBMe_2)]^+$** Acetone-*d$^6$*, 298K.




**$[[Ir(ppy)_2(1,2\ BTBMe_2)]^+$** Y = 31.7%, 0.021 g **$^{1}$H-NMR** (400 MHz), Acetone-*d$^6$*, 298K, δ (ppm) = 8.51 (d, 1H, $J_{H-H}$ = 5.59 Hz), 8.44 (m, 1H, $H_d$), 8.32 (m, 1H), 8.25-8.19 (m, 1H, $H_c$), 8.09-8.05 (m, 2H), 8.00-7.96 (m, 1H, $H_b$), 7.92-7.85 (m, 2H), 7.80-7.78 (m, 1H, $H_a$), 7.74-7.70 (m, 1H), 7.53-7.51 (m, 1H), 7.30-7.29 (m, 1H), 6.87-6.76 (m, 3H), 6.66-6.61 (m, 2H), 6.52 (d, 1H, $J_{H-H}$ =7.59 Hz), 6.11 (d, 1H, $J_{H-H}$ = 7.59 Hz), 4.22 (s, 3H, $CH_3$), 4.12 (s, 3H, $CH_3$). **$^{13}$C-NMR** (100 MHz), Acetone-*d$^6$*, 298K, δ (ppm) = 168.86, 168.09, 154.54 (Ct), 153.74 (Ct), 151.32, 150.28, 146.58, 144.12, 138.54, 137.72, 133.71, 13.19, 132.16, 131.04, 129.12, 128.65, 124.28, 123.66, 122.82, 121.97, 121.92, 121.83, 121.27, 119.25, 118.84, 35.86, 35.63. **ESI-MS** (*m/z*) $[M]^+$ = 743; $[M]^-$= 145 ($PF_6$).

**Figure S13:** NOESY-NMR and $^{1}$H-NMR spectrum (overlaid) of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-$d^6$, 600 MHz, 298K.

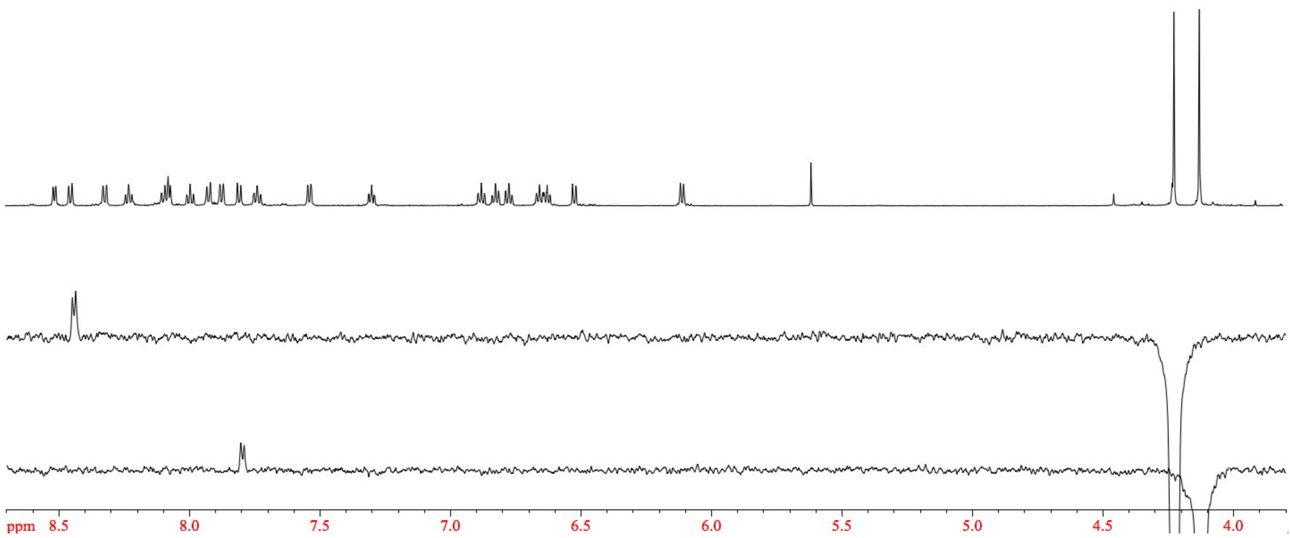



**Figure S14:** $^{1}$H-$^{1}$H COSY-NMR of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-$d^6$, 600 MHz, 298K.

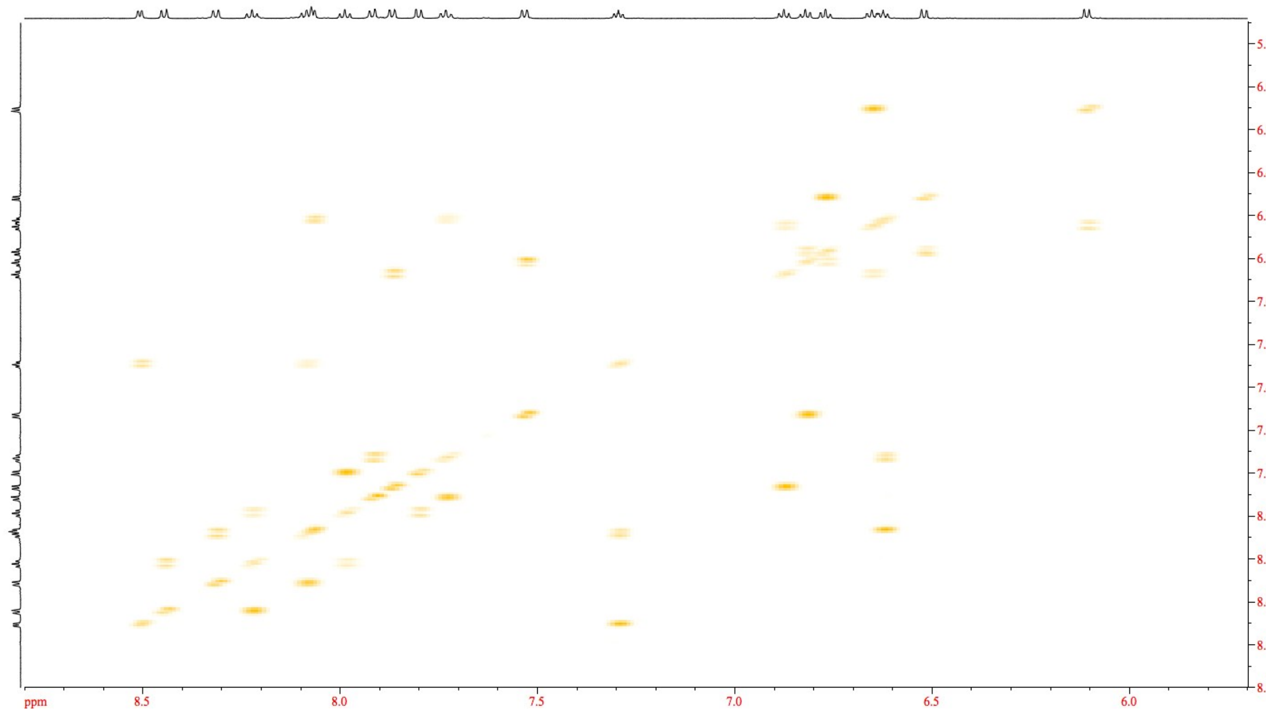


**Figure S15:** $^{1}$H NMR of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-*d*$^6$, 400 MHz, 298K.

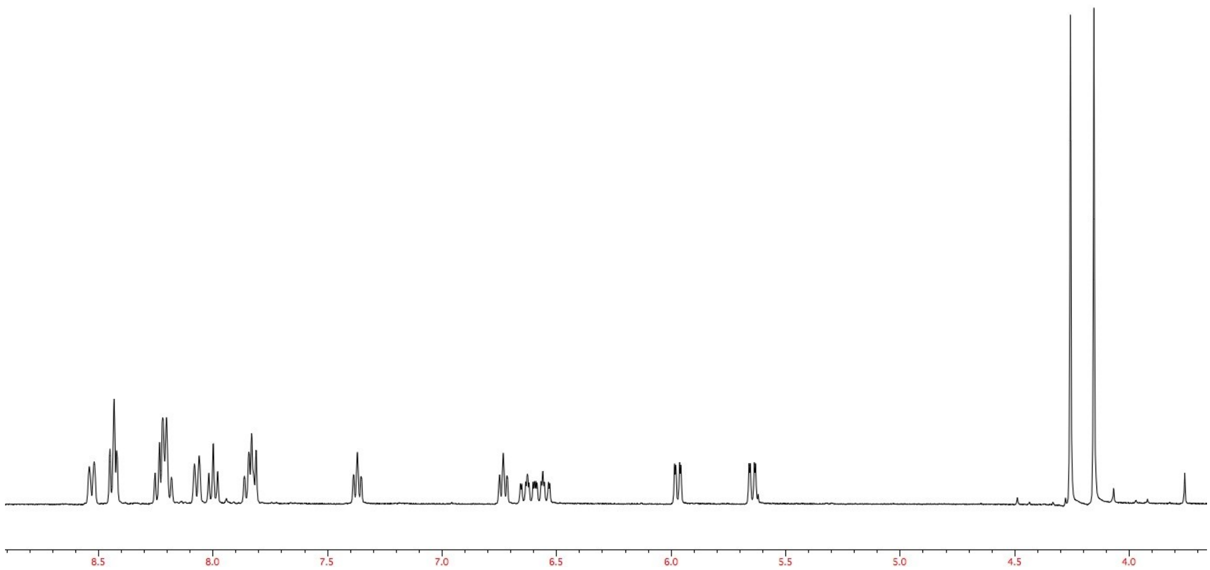
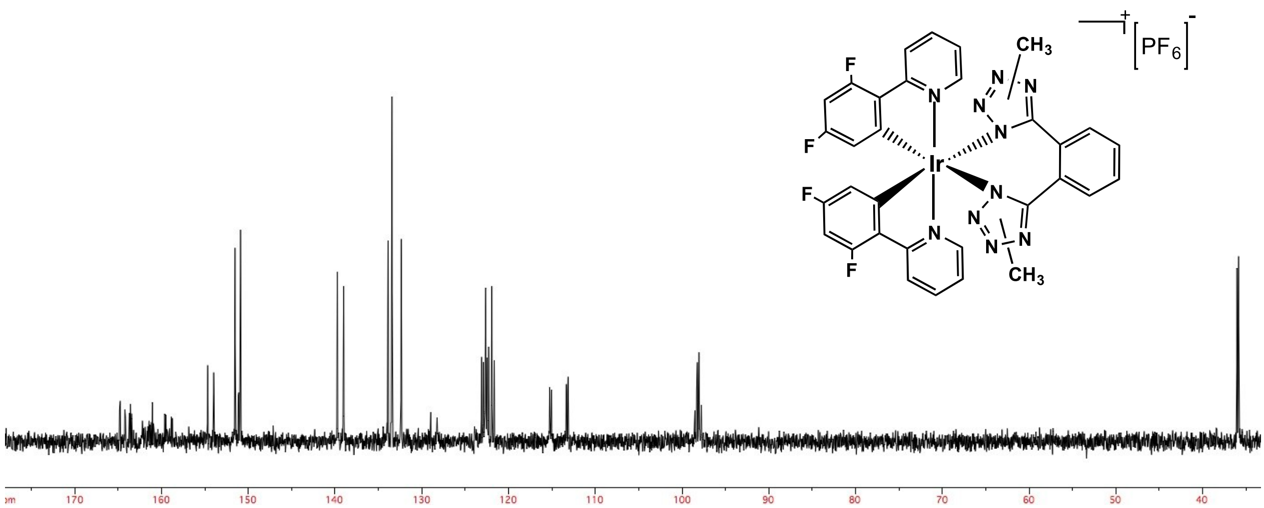



**Figure S16:** $^{13}$C NMR of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-*d*$^6$, 400 MHz, 298K.




**[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Y = 28.7%, 0.019 g **$^1$H-NMR** (400 MHz), Acetone-*d*$^6$, 298K, δ (ppm) = 8.52 (d, 1H, $J_{H\text{-}H}$ = 8.39 Hz), 8.43-8.41 (m, 2H, H$_d$ and F$_2$ppy), 8.24-8.17 (m, 3H, H$_c$ and F$_2$ppy), 8.07 (d, 1H, $J_{H\text{-}H}$ = 8.39 Hz), 8.00-7.96 (m, 1H, H$_b$), 7.85-7.80 (m, 2H, H$_a$ and F$_2$ppy), 7.37-7.34 (m, 1H), 6.73-6.70 (m, 1H), 6.64-6.51 (m, 2H), 5.97-5.94 (m, 1H), 5.64-5.62 (m, 1H), 4.24 (s, 3H, CH$_3$), 4.14 (s, 3H, CH$_3$). **$^{13}$C-NMR** (100 MHz), Acetone-*d*$^6$, 298K, δ (ppm) = 165.72, 165.10, 164.59, 161.93, 160.51, 159.94, 155.56 (Ct), 154.86 (Ct), 152.41, 152.03, 151.97, 151.86, 151.78, 140.61, 139.89, 134.76, 134.32, 133.25, 129.84, 129.11, 123.99, 123.78, 123.36, 122.82, 116.14, 114.23, 99.20, 99.12, 98.85, 98.66, 36.91, 36.72. **ESI-MS** (*m/z*) [M]$^+$ = 815; [M]$^-$= 145 (PF$_6$).

**Figure S17:** NOESY-NMR and $^1$H-NMR spectrum (overlaid) of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-$d^6$, 600 MHz, 298K.

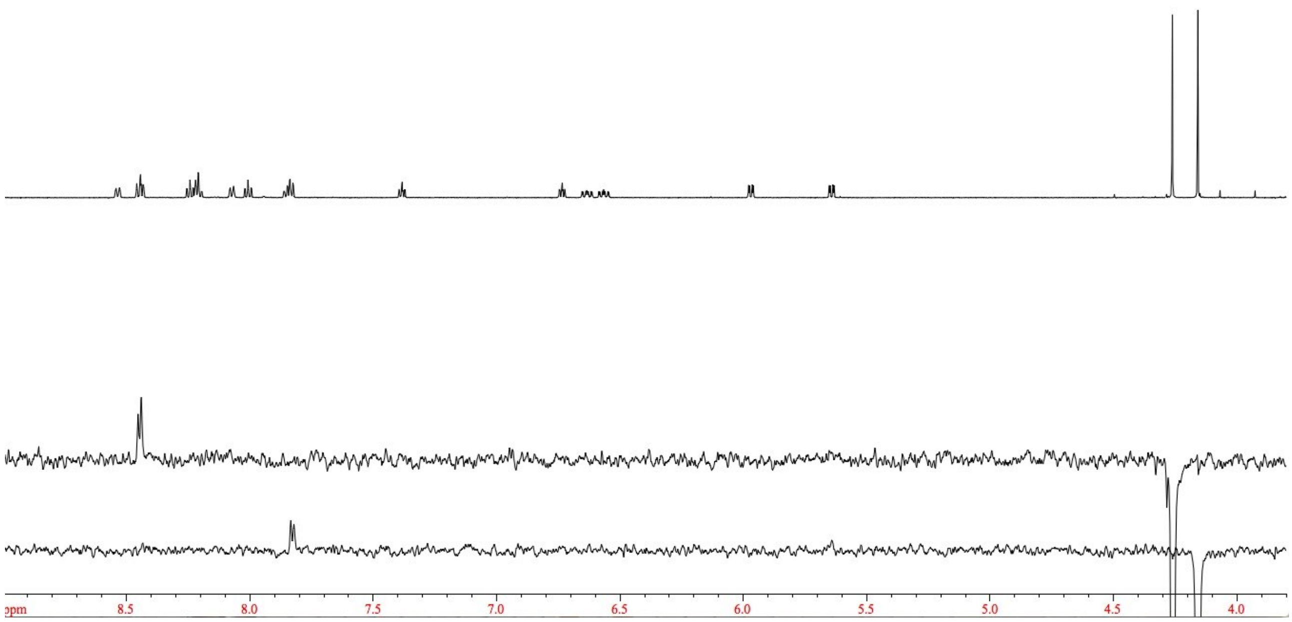



**Figure S18: $^1$**H-$^1$H COSY-NMR of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** Acetone-$d^6$, 600 MHz, 298K.

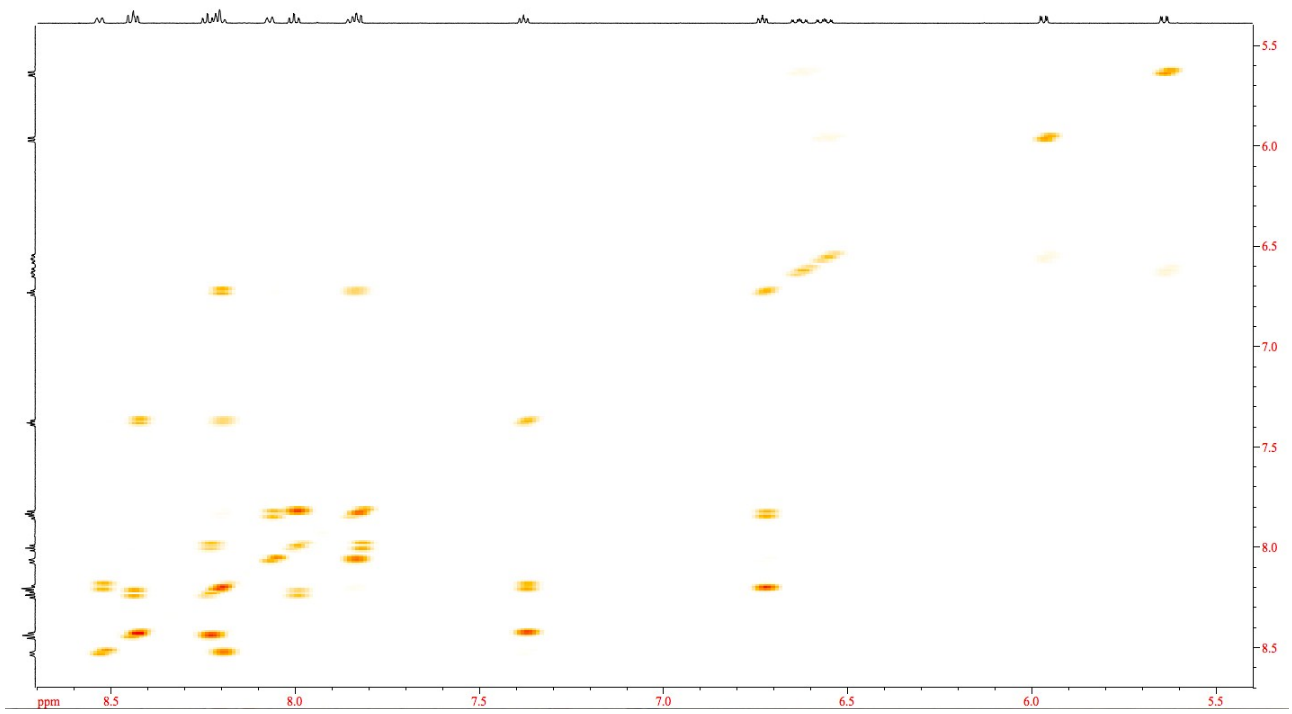
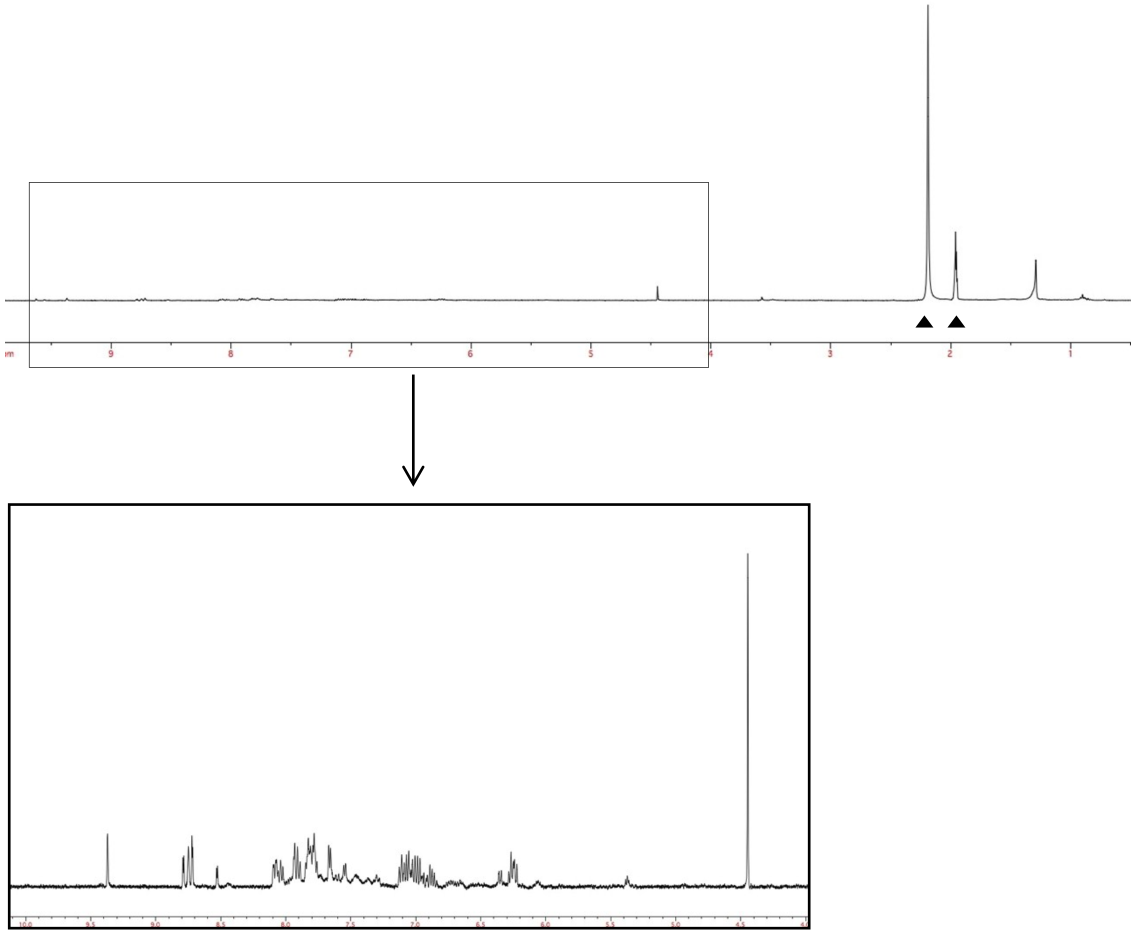
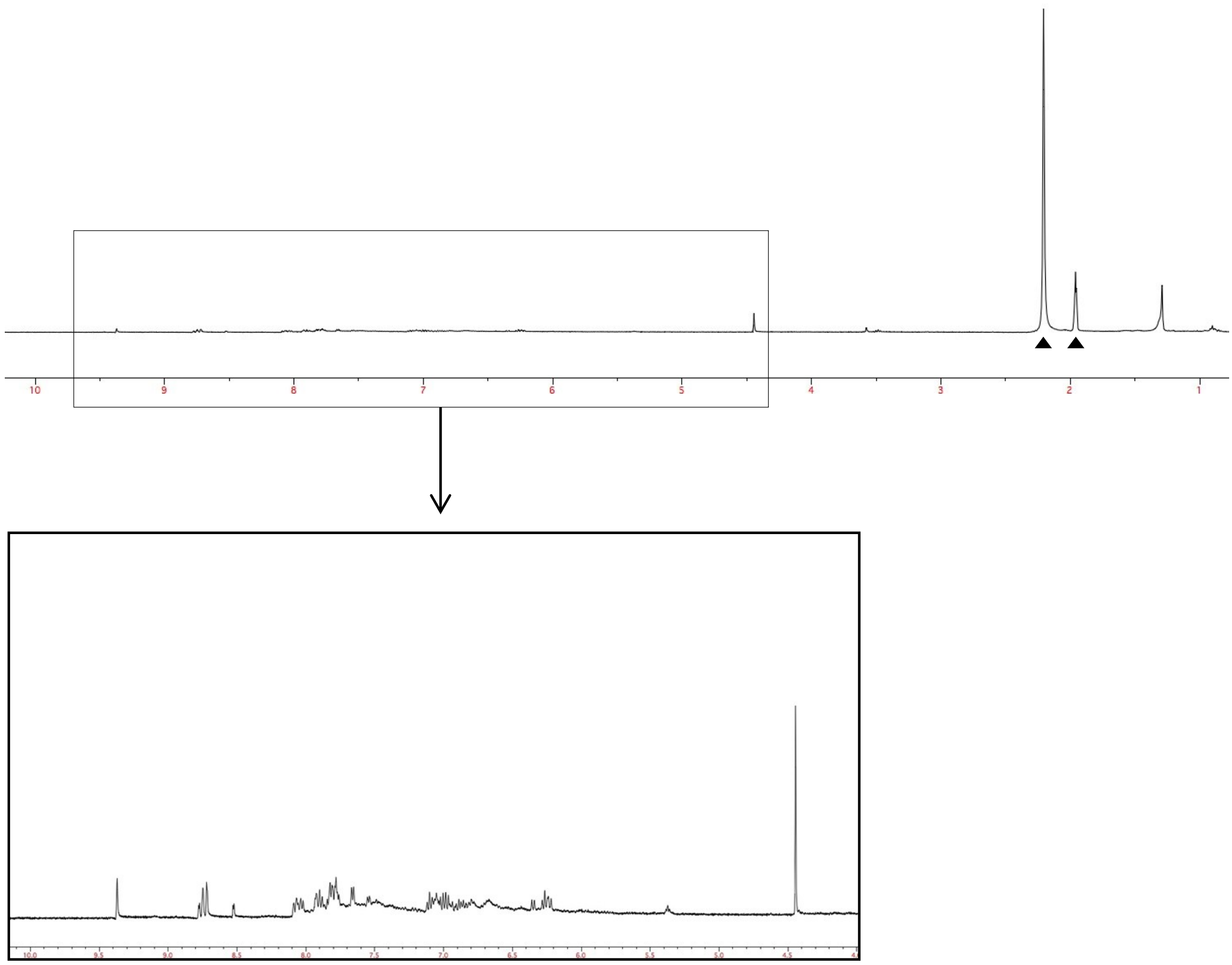


**Figure S19:** $^1$H NMR of **SS1** $CD_3CN$, 400 MHz, 298K.



▲= $^1$H signals of residual of non deuterated $CD_3CN$ and water.

**Figure S20:** $^{1}H$ NMR of **SS2** $CD_3CN$, 400 MHz, 298K.



▲= $^{1}H$ signals of residual of non deuterated $CD_3CN$ and water.

.

**Photophysical proprieties**

**Figure S21:** Absorption Profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, r.t.

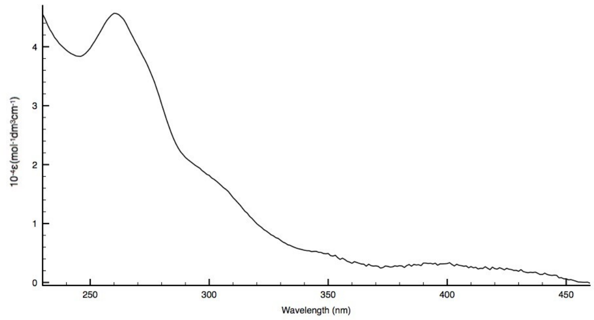



**Figure S22:** Excitation Profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, r.t.

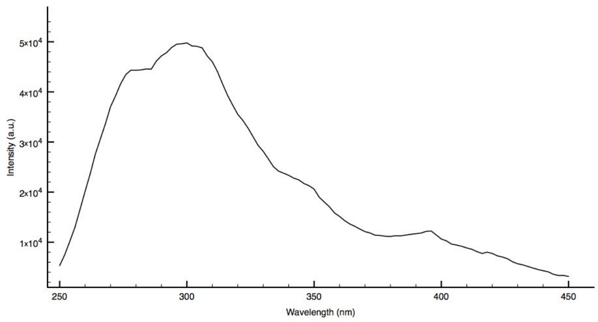



**Figure S23** Emission profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 298K.

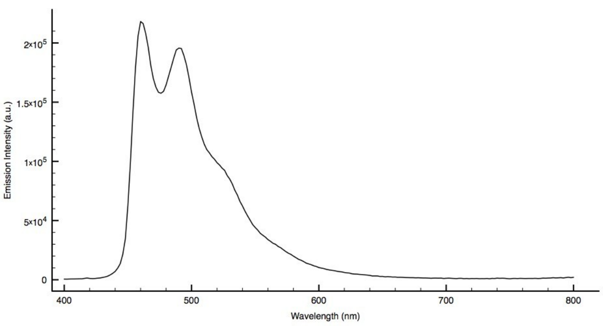



**Figure S24:** Emission profiles of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, oxygenated (black line) and deoxygenated solution (blue line).

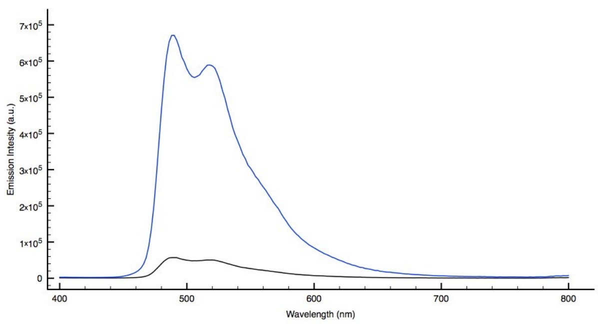


**Figure S25:** Emission profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 77 K.

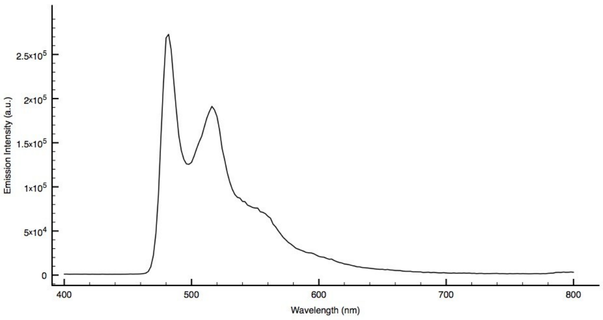



**Figure S26:** Normalized Emission profiles of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 298K (black line) and 77 K (blue line).

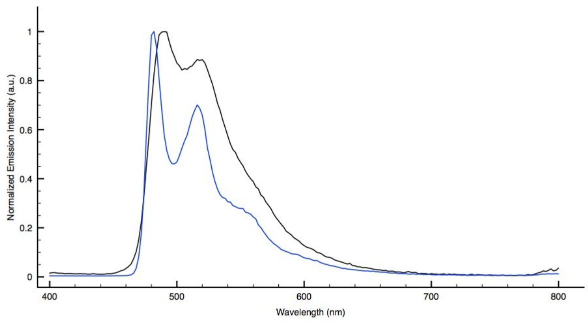



**Figure S27:** Emission Profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** neat solid matrix, r.t.

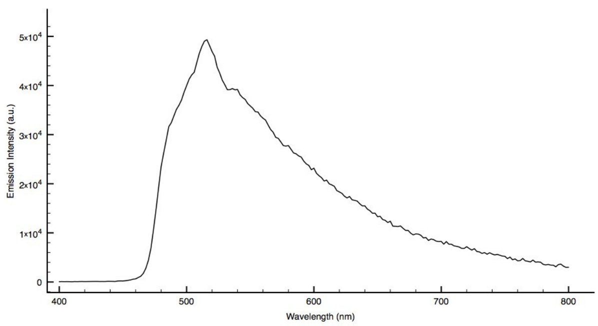



**Figure S28:** Excitation Profile of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** neat solid matrix, r.t.

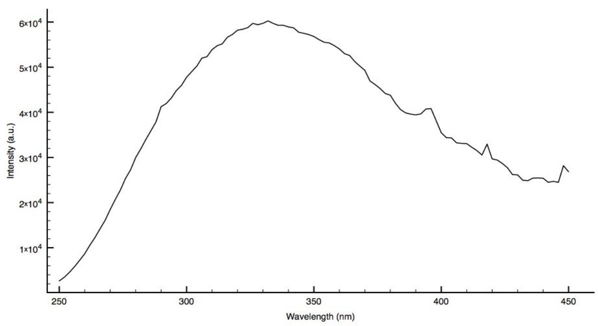


**Figure S29:** Absorption Profile of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, r.t.

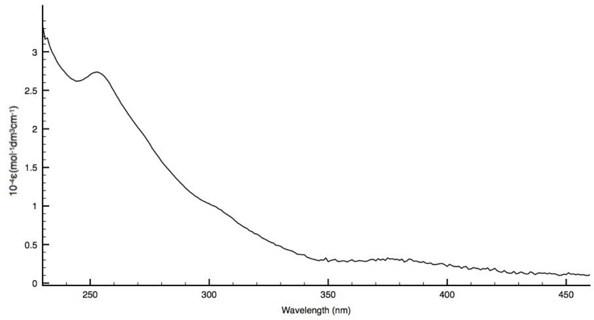



**Figure S30:** Excitation Profile of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, r.t.

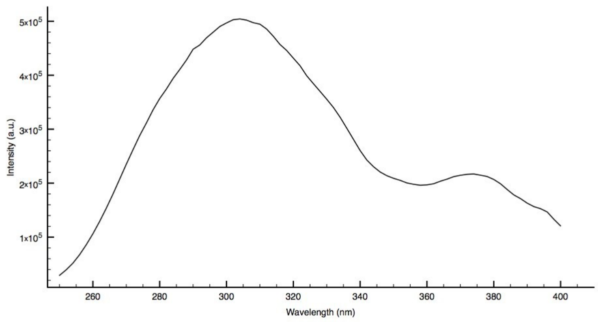



**Figure S31:** Emission profile of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 298K.



**Figure S32:** Emission profiles of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, oxygenated (black line) and deoxygenated solution (blue line).

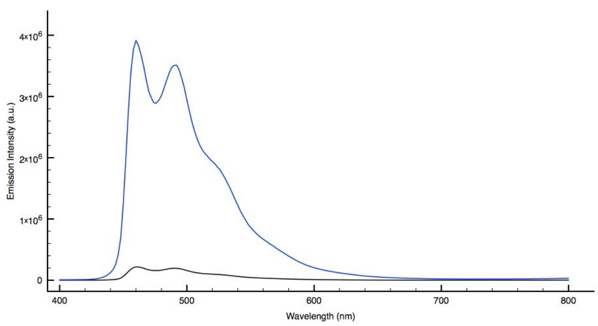


**Figure S33:** Emission profile of **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 77 K.

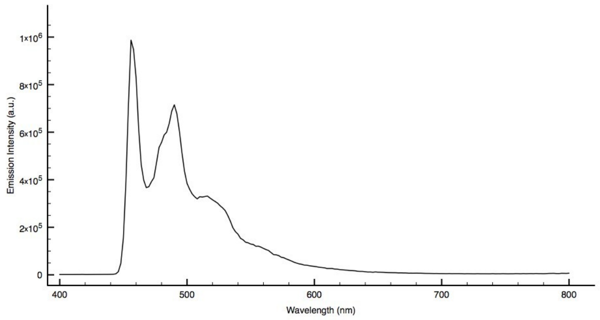



**Figure S34:** Normalized Emission profiles of **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** $10^{-5}$M, $CH_2Cl_2$, 298K (black line) and 77 K (blue line).

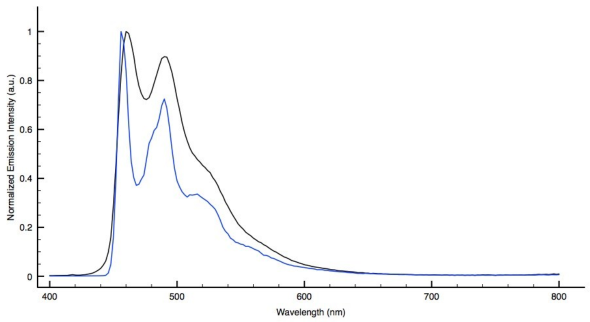



**Figure S35:** Emission Profile of **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** neat solid matrix, r.t.

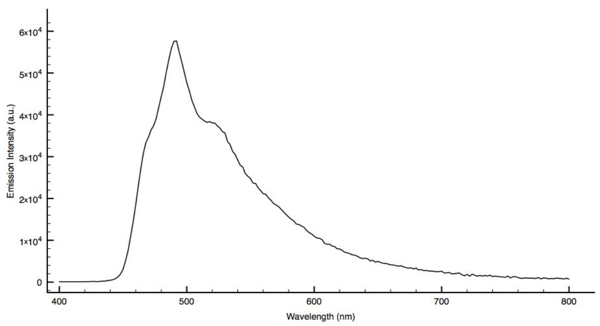



**Figure S36:** Excitation Profile of **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** neat solid matrix, r.t.

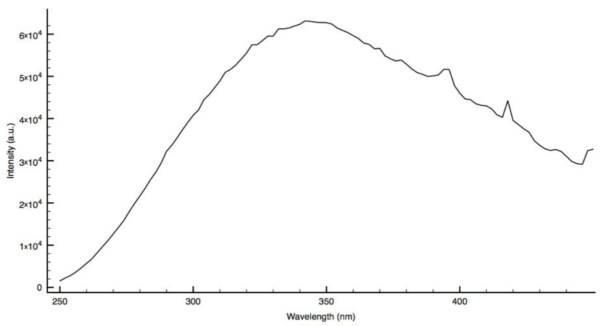


**Figure S37:** Absorption Profile of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** 10$^{-5}$M, $CH_2Cl_2$, r.t.

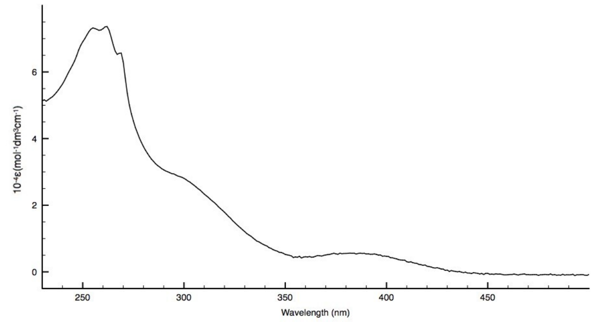



**Figure S38:** Absorption Profile of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** (red line) and **[Ir(ppy)$_2$(1,2 BTB)]$^-$** (blue line) 10$^{-5}$M, $CH_2Cl_2$, r.t.

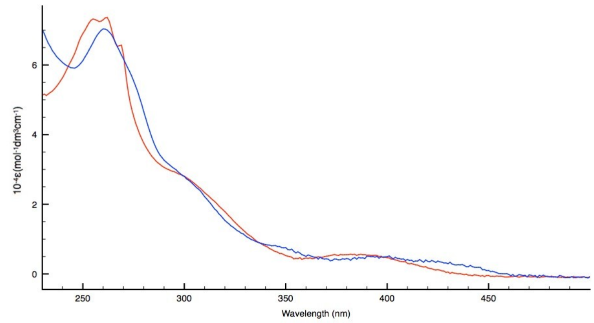



**Figure S39:** Excitation Profile of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** 10$^{-5}$M, $CH_2Cl_2$, r.t.

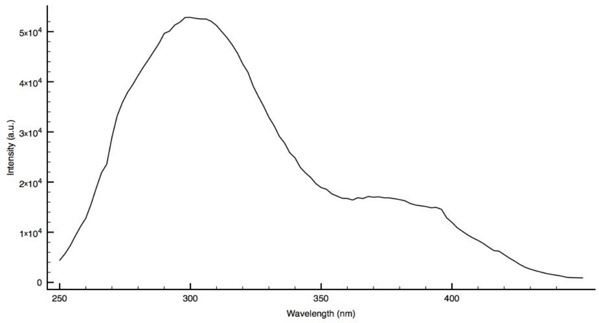



**Figure S40:** Emission profile of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** 10$^{-5}$M, $CH_2Cl_2$, 298K.

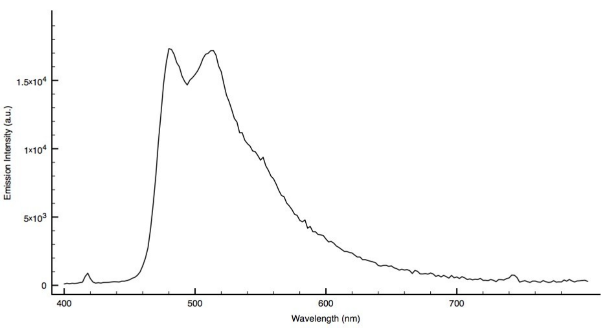


**Figure S41:** Emission profiles of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, oxygenated (black line) and deoxygenated solution (blue line).

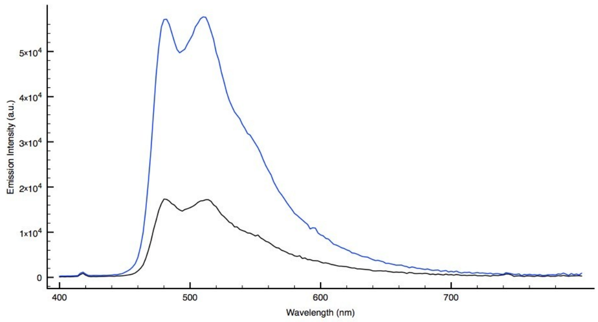



**Figure S42:** Emission profile of **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, 77 K.

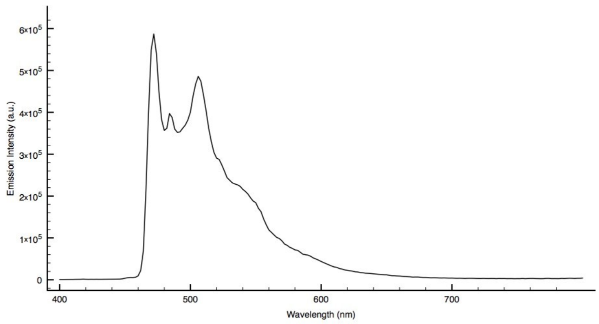



**Figure S43:** Absorption Profile of **[Ir(F$_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, r.t.

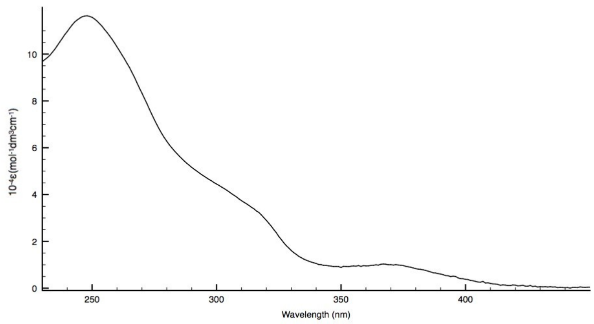


**Figure S44:** Absorption Profile of **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** (red line) and **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** (blue line) $10^{-5}$M, $CH_2Cl_2$, r.t.

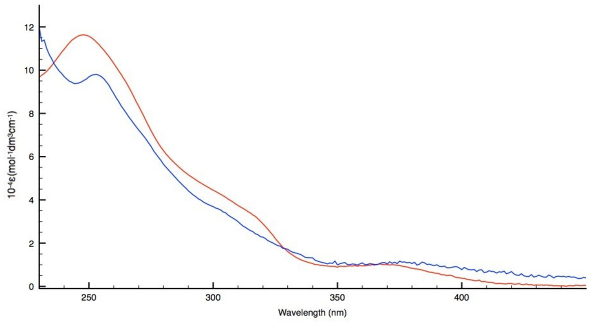



**Figure S45:** Excitation Profile of **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, r.t.

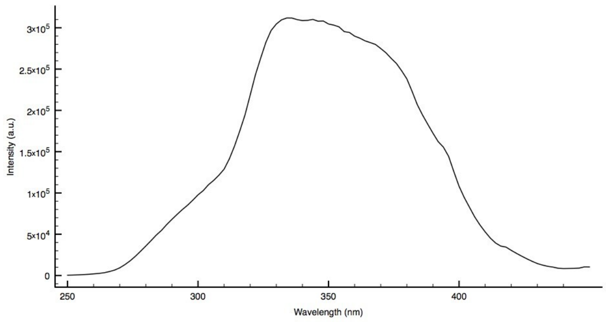



**Figure S46:** Emission profile of **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, 298K.

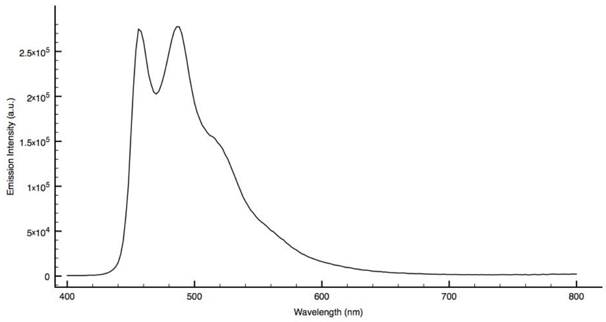


**Figure S47:** Emission profiles of **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, oxygenated (black line) and deoxygenated solution (blue line).

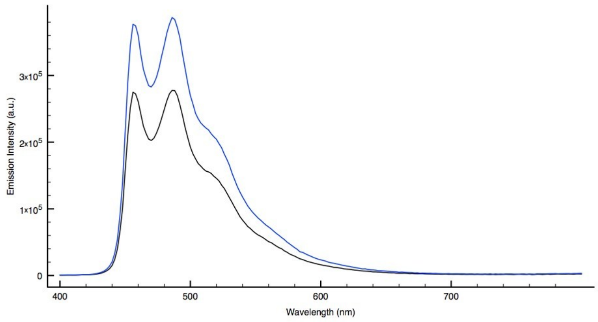
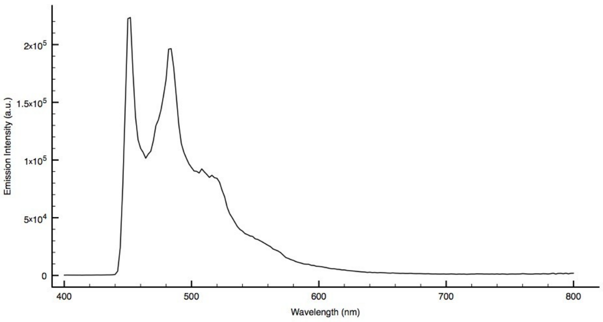



**Figure S48:** Emission profile of **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** $10^{-5}$M, $CH_2Cl_2$, 77K.



## Emission titration of Anionic Ir(III) tetrazolate complexes with $HOSO_2CF_3$

In the $HOSO_2CF_3$ emission titration a 10 mL stock solution of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** (1,23*10$^{-4}$M) in $CH_2Cl_2$ was prepared. 2 mL of the stock solution were then transferred to a quartz cuvette and the emission spectrum of the solution was measured after successive additions (10 µL aliquots for 12 additions) with $HOSO_2CF_3$ in $CH_2Cl_2$, 0,005 M. For the $HOSO_2CF_3$ emission titration of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$**, a 10 mL stock solution (1,13*10$^{-4}$M) in $CH_2Cl_2$ was prepared. 2 mL of the stock solution were then transferred to a quartz cuvette and the emission spectrum of the solution was measured after successive additions (10 µL aliquots for 12 additions) with $HOSO_2CF_3$ in $CH_2Cl_2$, 0,01 M.

**Figure S49:** Steady-state emission spectra showing the blue shift of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** (1,23*10$^{-4}$M), 10 µL aliquots for 12 additions with $HOSO_2CF_3$ in $CH_2Cl_2$, 0,005 M;

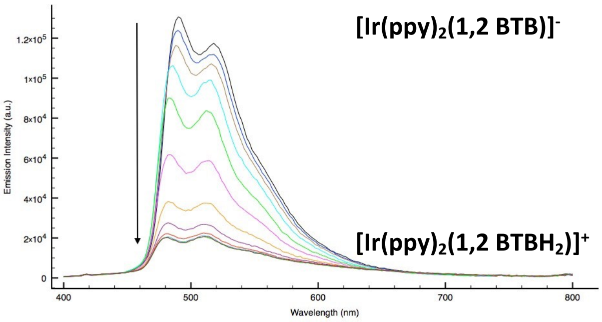



**Figure S50:** Steady-state emission spectra showing the back titration of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** + 110 µL of $HOSO_2CF_3$ 0,005 M, $CH_2Cl_2$ with $Et_3N$.

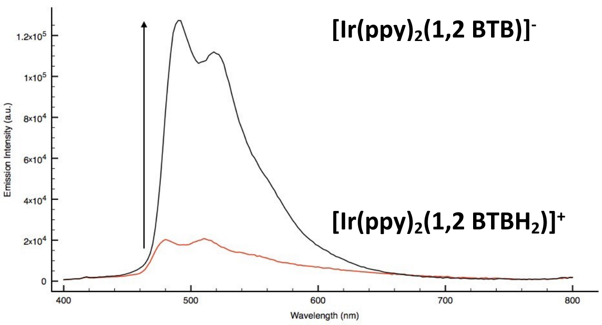


**Figure S51:** Decay time of **[Ir(ppy)$_2$(1,2 BTB)]$^-$** + 110 µL of $HOSO_2CF_3$ 0,005 M, $CH_2Cl_2$ (blue line) and **[Ir(ppy)$_2$(1,2 BTB)]$^-$ +** 110 µL of $HOSO_2CF_3$ 0,005 M, $CH_2Cl_2$ + $Et_3N$ (red line).

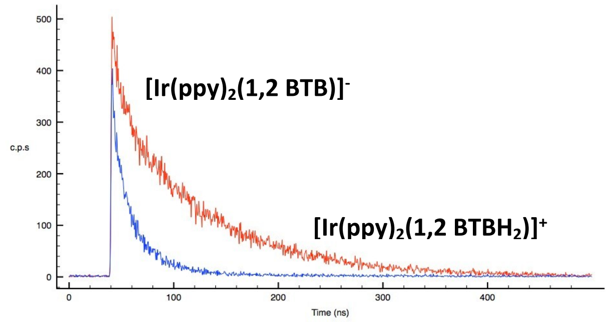



**Figure S52:** Steady-state emission spectra showing the blue shift of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** ($1{,}13*10^{-4}$M), 20 µL aliquots for 12 additions with $HOSO_2CF_3$ in $CH_2Cl_2$, 0,01 M;

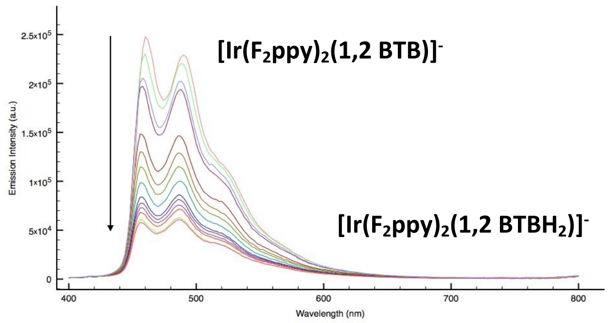



**Figure S53:** Steady-state emission spectra showing the back titration of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** + 260 µL of $HOSO_2CF_3$ 0,01 M, $CH_2Cl_2$ with $Et_3N$.

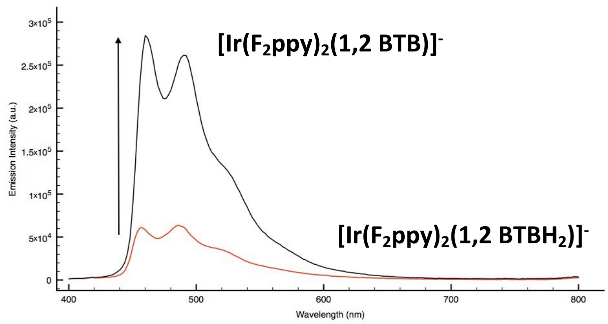



**Figure S54:** Decay time of **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$** + 260 µL of $HOSO_2CF_3$ 0,01 M, $CH_2Cl_2$ (red line) and **[Ir(F$_2$ppy)$_2$(1,2 BTB)]$^-$ +** 260 µL of $HOSO_2CF_3$ 0,01 M, $CH_2Cl_2$ + $Et_3N$ (blue line).

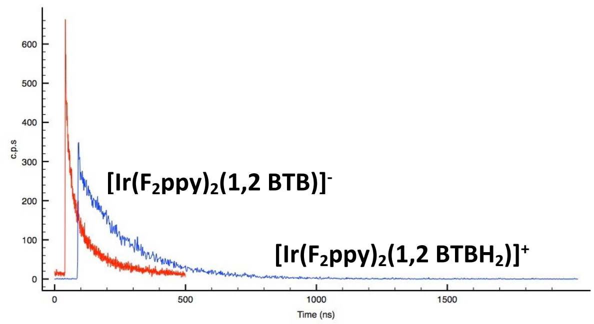


**Figure S55:** Left - Absorption profile **[IrTPYZ-Me]$^+$**, Right – Excitation profile **[IrTPYZ-Me]$^+$**, $\lambda_{emi}$ = 686 nm; $CH_2Cl_2$, r.t.

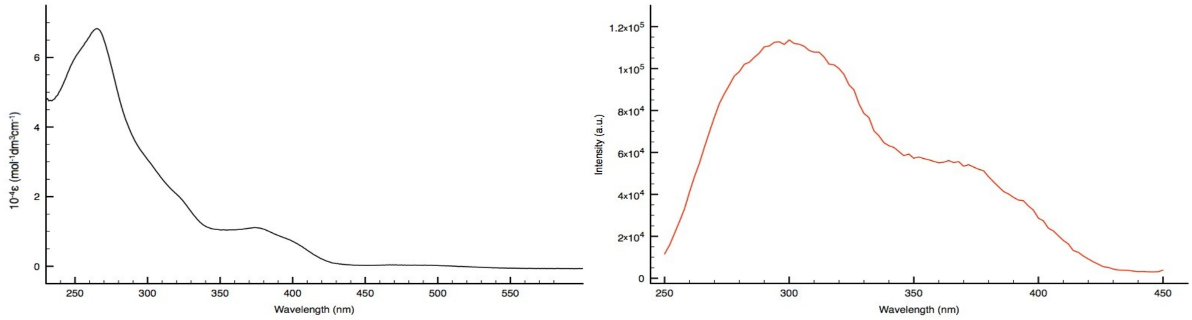



**Figure S56:** Emission spectra **[IrTPYZ-Me]$^+$**, 298K (black line), 77K (blue line), $CH_2Cl_2$.

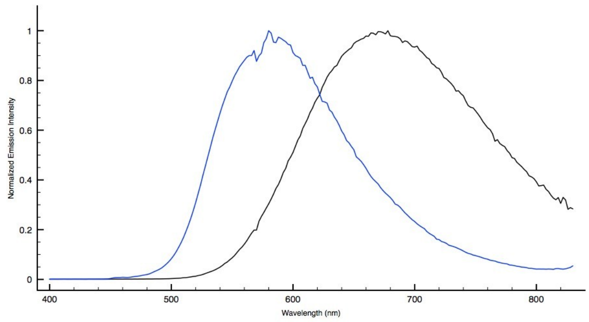



**Figure S57:** Emission spectra **[IrTPYZ-Me]$^+$** 298K oxygenated solution (black line), 298K deoxygenated solution (blue line), $CH_2Cl_2$.

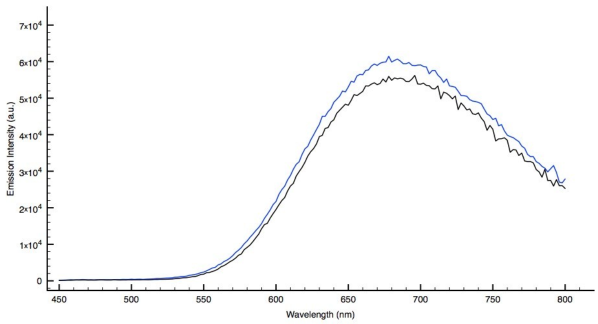


**Figure S58:** Absorption profile of **SS1** $10^{-5}$M, $CH_2Cl_2$, r.t.

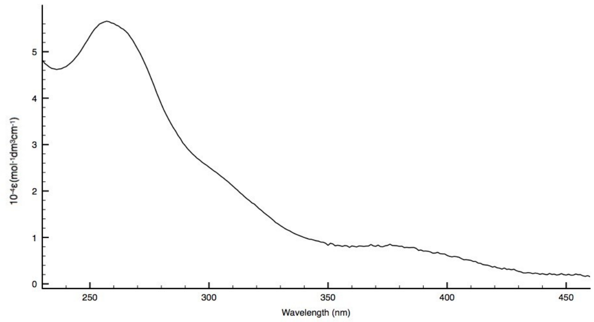



**Figure S59:** Emission profile of **SS1** $10^{-5}$M, $CH_2Cl_2$, 298K.

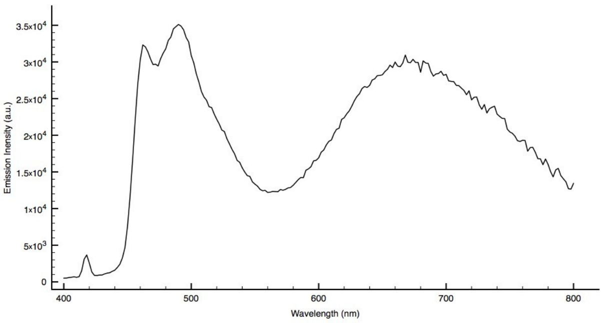



**Figure S60:** Excitation Profile of **SS1** $10^{-5}$M, $CH_2Cl_2$, r.t.

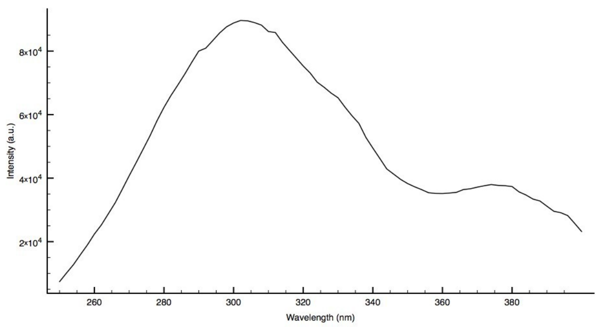



**Figure S61:** Emission profiles of **SS1** $10^{-5}$M, $CH_2Cl_2$, oxygenated (red line) and deoxygenated solution (blue line).

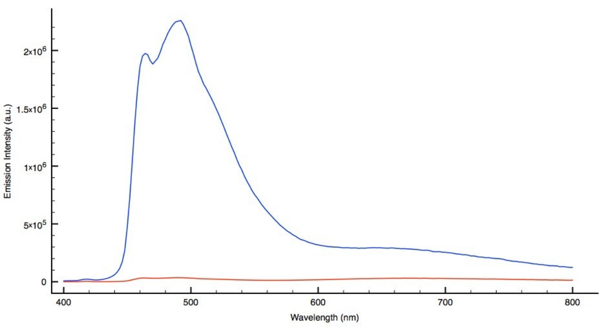


**Figure S62:** Emission profile of **SS1** $10^{-5}$M, $CH_2Cl_2$, 77 K.

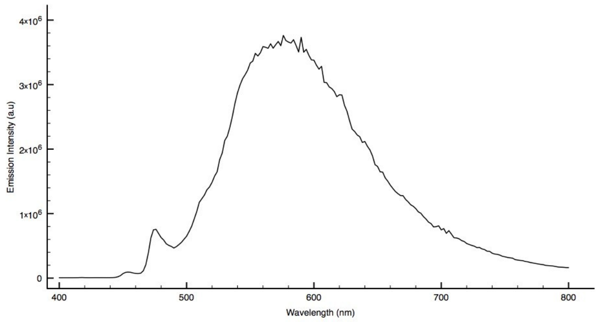



**Figure S63:** CIE of **SS1** (air equilibrated "Air" and deoxygenated solution "Ar") $10^{-5}$M, $CH_2Cl_2$

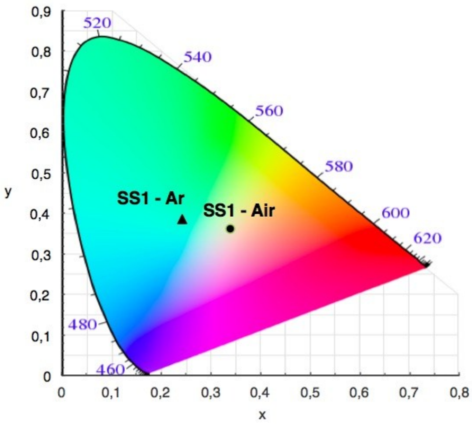



**Figure S64:** Absorption profile of **SS2** $10^{-5}$M, $CH_2Cl_2$, r.t.

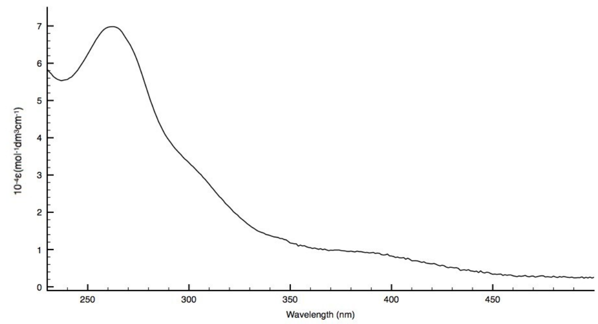



**Figure S65:** Emission profile of **SS2** $10^{-5}$M, $CH_2Cl_2$, 298K.

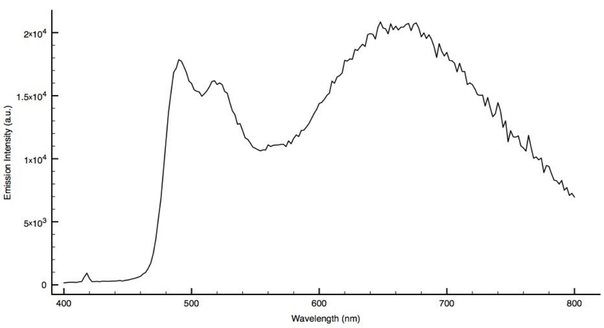


**Figure S66:** Excitation Profile of **SS2** $10^{-5}$M, $CH_2Cl_2$, r.t.

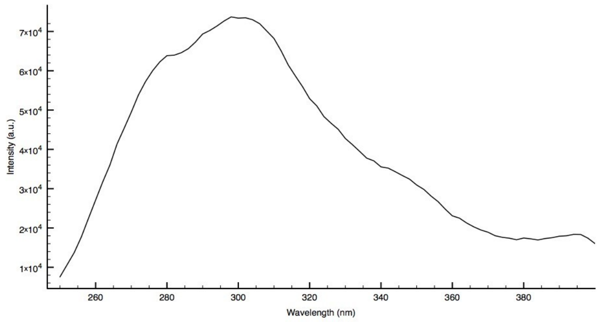



**Figure S67:** Emission profiles of **SS2** $10^{-5}$M, $CH_2Cl_2$, oxygenated (red line) and deoxygenated solution (blue line).

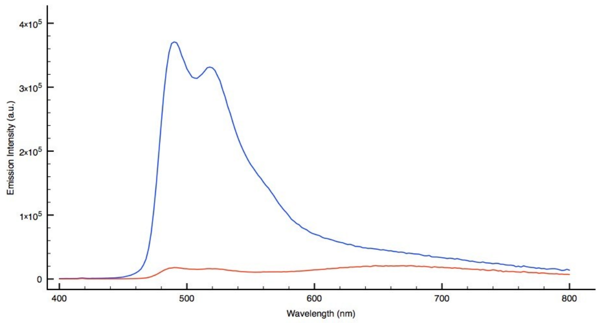



**Figure S68:** Emission profile of **SS2** $10^{-5}$M, $CH_2Cl_2$, 77 K.

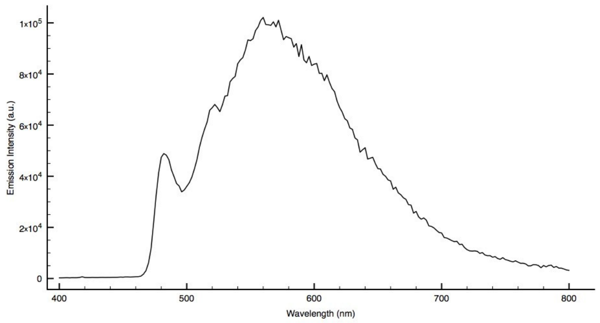



**Figure S69:** CIE of **SS2** (air equilibrated "Air" and deoxygenated solution "Ar") $10^{-5}$M, $CH_2Cl_2$

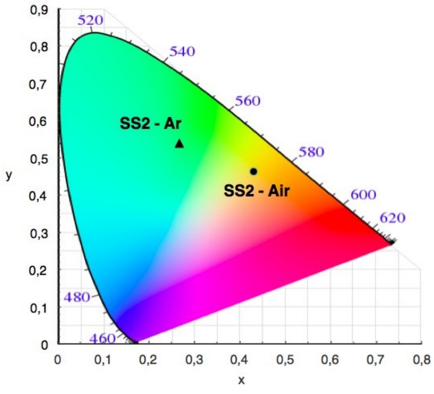


**Table S1:** Crystal data and collection details $[HNEt_3]^+[Ir(ppy)_2(1,2\ BTB)]^-$.

| | |
|---|---|
| **Formula** | $C_{36}H_{36}IrN_{11}$ |
| ***Fw*** | 814.96 |
| ***T*, K** | 100(2) |
| **$\lambda$, Å** | 0.71073 |
| **Crystal system** | Triclinic |
| **Space Group** | *P*1 |
| ***a*, Å** | 12.0892(5) |
| ***b*, Å** | 12.2178(5) |
| ***c*, Å** | 12.8423(6) |
| ***a*, °** | 72.808(3) |
| **$\beta$, °** | 73.021(2) |
| ***g*, °** | 63.995(2) |
| **Cell Volume, Å$^3$** | 1599.23(12) |
| ***Z*** | 2 |
| **$D_c$, g cm$^{-3}$** | 1.692 |
| **$\mu$, mm$^{-1}$** | 4.221 |
| **F(000)** | 812 |
| **Crystal size, mm** | 0.13×0.11×0.09 |
| **$\theta$ limits, °** | 1.91–25.03 |
| **Index ranges** | $-14 \leq h \leq 14$<br>$-14 \leq k \leq 10$<br>$-15 \leq l \leq 15$ |
| **Reflections collected** | 22006 |
| **Independent reflections** | 5648 [$R_{int}$ = 0.0638] |
| **Completeness to $\theta$ max** | 99.8% |
| **Data / restraints / parameters** | 5648 / 51 / 433 |
| **Goodness on fit on F$^2$** | 1.066 |
| **$R_1$ ($I$> 2$\sigma$($I$))** | 0.0444 |
| **$wR_2$ (all data)** | 0.1140 |
| **Largest diff. peak and hole, e Å$^{-3}$** | 3.463 / –1.933 |

**TD-DFT calculations**

**Figure S70**: Localization of the HOMO and LUMO orbitals for the anionic and cationic Ir(III) complexes.

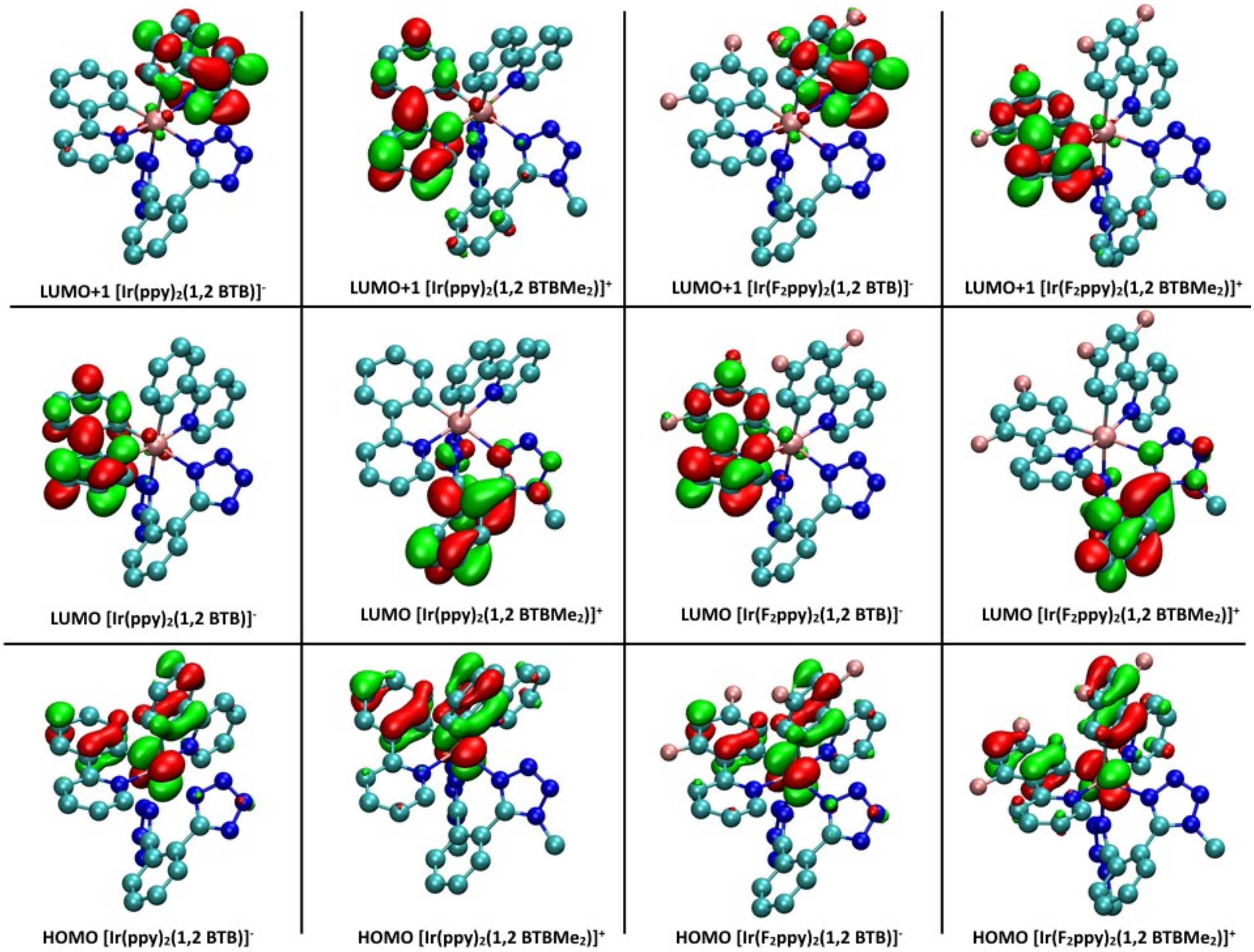


**Table S2:** List of all the computed electronic transitions for **[Ir(ppy)$_2$(1,2 BTB)]$^-$** with their character.

| Wavelength (nm) | Intensity(a.u.) | Levels | Character |
|---|---|---|---|
| 341.45 nm | 0.1842 | HOMO-1 -> LUMO | 6.2 % |
| | | HOMO -> LUMO | 84.9 % |
| | | HOMO -> LUMO+1 | 2.4 % |
| | | HOMO -> LUMO+1 | 2.4 % |
| 331.95 nm | 0.0615 | HOMO-2 -> LUMO+1 | 2.7 % |
| | | HOMO-1 -> LUMO | 2.2 % |
| | | HOMO-1 -> LUMO+1 | 3.6 % |
| | | HOMO -> LUMO | 2.1 % |
| | | HOMO -> LUMO+1 | 84.8 % |
| 286.38 nm | 0.0960 | HOMO-6 -> LUMO | 2.8 % |
| | | HOMO-4 -> LUMO | 2.2 % |
| | | HOMO-2 -> LUMO | 17.0 % |
| | | HOMO-1 -> LUMO | 45.0 % |
| | | HOMO-1 -> LUMO+1 | 2.1 % |
| | | HOMO -> LUMO | 2.5 % |
| | | HOMO -> LUMO+2 | 15.7 % |
| 281.09 nm | 0.1193 | HOMO-4 -> LUMO | 3.2 % |
| | | HOMO-2 -> LUMO | 3.9 % |
| | | HOMO-1 -> LUMO | 6.3 % |
| | | HOMO-1 -> LUMO+1 | 3.2 % |
| | | HOMO -> LUMO+2 | 62.7 % |
| | | HOMO -> LUMO+3 | 2.8 % |
| 276.76 nm | 0.0344 | HOMO-7 -> LUMO | 2.4 % |
| | | HOMO-5 -> LUMO | 2.2 % |
| | | HOMO-4 -> LUMO | 9.8 % |
| | | HOMO-3 -> LUMO | 67.4 % |
| | | HOMO-2 -> LUMO | 6.3 % |
| 273.61 nm | 0.0208 | HOMO-6 -> LUMO+1 | 7.3 % |
| | | HOMO-5 -> LUMO+1 | 3.6 % |
| | | HOMO-2 -> LUMO+1 | 28.8 % |
| | | HOMO-1 -> LUMO | 2.9 % |
| | | HOMO-1 -> LUMO+1 | 33.3 % |
| | | HOMO -> LUMO+3 | 3.7 % |
| | | HOMO -> LUMO+4 | 4.3 % |
| 271.31 nm | 0.0166 | HOMO-5 -> LUMO+1 | 2.5 % |
| | | HOMO-4 -> LUMO+1 | 2.5 % |
| | | HOMO-3 -> LUMO+1 | 14.4 % |
| | | HOMO-2 -> LUMO+1 | 8.2 % |
| | | HOMO-1 -> LUMO+2 | 7.4 % |
| | | HOMO -> LUMO+3 | 25.7 % |
| | | HOMO -> LUMO+4 | 23.2 % |
| 269.23 nm | 0.1108 | HOMO-3 -> LUMO+1 | 60.0 % |
| | | HOMO-2 -> LUMO+1 | 2.5 % |
| | | HOMO-1 -> LUMO+1 | 3.5 % |
| | | HOMO -> LUMO+3 | 5.7 % |
| | | HOMO -> LUMO+4 | 5.2 % |
| | | HOMO -> LUMO+8 | 2.0 % |
| 268.17 nm | 0.1902 | HOMO-6 -> LUMO | 10.5 % |
| | | HOMO-5 -> LUMO | 2.4 % |
| | | HOMO-4 -> LUMO | 11.4 % |

| | | | |
|---|---|---|---|
| | | HOMO-4 -> LUMO+1 | 5.3 % |
| | | HOMO-3 -> LUMO | 13.3 % |
| | | HOMO-2 -> LUMO | 29.5 % |
| | | HOMO-1 -> LUMO | 7.8 % |
| | | HOMO -> LUMO | 2.1 % |
| 266.45 nm | 0.5118 | HOMO-6 -> LUMO+1 | 2.5 % |
| | | HOMO-5 -> LUMO+1 | 3.5 % |
| | | HOMO-4 -> LUMO | 5.6 % |
| | | HOMO-4 -> LUMO+1 | 16.7 % |
| | | HOMO-3 -> LUMO+1 | 6.1 % |
| | | HOMO-2 -> LUMO+1 | 27.7 % |
| | | HOMO-1 -> LUMO+1 | 17.9 % |
| | | HOMO -> LUMO+1 | 2.2 % |
| | | HOMO -> LUMO+2 | 2.2 % |
| 254.39 nm | 0.0130 | HOMO-6 -> LUMO | 2.7 % |
| | | HOMO-3 -> LUMO+10 | 4.1 % |
| | | HOMO-3 -> LUMO+16 | 4.4 % |
| | | HOMO-2 -> LUMO+1 | 2.7 % |
| | | HOMO-1 -> LUMO | 2.1 % |
| | | HOMO -> LUMO+4 | 7.9 % |
| | | HOMO -> LUMO+8 | 4.2 % |
| | | HOMO -> LUMO+10 | 11.2 % |
| | | HOMO -> LUMO+13 | 4.0 % |
| | | HOMO -> LUMO+16 | 13.3 % |
| | | HOMO -> LUMO+19 | 2.7 % |
| 252.03 nm | 0.0271 | HOMO-6 -> LUMO | 7.3 % |
| | | HOMO-5 -> LUMO | 3.4 % |
| | | HOMO-4 -> LUMO | 4.4 % |
| | | HOMO-2 -> LUMO | 3.3 % |
| | | HOMO-2 -> LUMO+3 | 2.1 % |
| | | HOMO-2 -> LUMO+4 | 2.4 % |
| | | HOMO-1 -> LUMO | 3.4 % |
| | | HOMO-1 -> LUMO+2 | 2.0 % |
| | | HOMO -> LUMO+2 | 6.1 % |
| | | HOMO -> LUMO+3 | 33.1 % |
| | | HOMO -> LUMO+4 | 13.4 % |
| | | HOMO -> LUMO+7 | 2.0 % |
| 250.19 nm | 0.0144 | HOMO-6 -> LUMO | 7.8 % |
| | | HOMO-5 -> LUMO | 7.4 % |
| | | HOMO-4 -> LUMO | 6.5 % |
| | | HOMO-3 -> LUMO+10 | 2.3 % |
| | | HOMO-3 -> LUMO+16 | 2.4 % |
| | | HOMO-2 -> LUMO | 6.2 % |
| | | HOMO-1 -> LUMO | 4.9 % |
| | | HOMO -> LUMO+3 | 3.9 % |
| | | HOMO -> LUMO+4 | 23.7 % |
| | | HOMO -> LUMO+10 | 3.6 % |
| 247.50 nm | 0.0592 | HOMO-6 -> LUMO+10 | 2.7 % |
| | | HOMO-6 -> LUMO+16 | 2.3 % |
| | | HOMO-2 -> LUMO | 2.1 % |
| | | HOMO-2 -> LUMO+8 | 2.1 % |
| | | HOMO-2 -> LUMO+10 | 9.2 % |
| | | HOMO-2 -> LUMO+13 | 4.1 % |
| | | HOMO-2 -> LUMO+16 | 9.4 % |
| | | HOMO-2 -> LUMO+19 | 2.2 % |
| | | HOMO-1 -> LUMO+2 | 4.0 % |
| | | HOMO-1 -> LUMO+10 | 6.5 % |
| | | HOMO-1 -> LUMO+13 | 2.4 % |
| | | HOMO-1 -> LUMO+16 | 6.2 % |

| | | | |
|---|---|---|---|
| 245.26 nm | 0.2167 | HOMO-6 -> LUMO | 4.7 % |
| | | HOMO-4 -> LUMO | 7.3 % |
| | | HOMO-3 -> LUMO+2 | 4.4 % |
| | | HOMO-2 -> LUMO+2 | 14.2 % |
| | | HOMO-2 -> LUMO+10 | 2.1 % |
| | | HOMO-2 -> LUMO+16 | 2.4 % |
| | | HOMO-1 -> LUMO+2 | 25.6 % |
| | | HOMO-1 -> LUMO+4 | 2.9 % |
| 243.88 nm | 0.0124 | HOMO-6 -> LUMO+1 | 11.0 % |
| | | HOMO-5 -> LUMO+1 | 24.8 % |
| | | HOMO-4 -> LUMO+1 | 5.0 % |
| | | HOMO-2 -> LUMO+1 | 5.1 % |
| | | HOMO-2 -> LUMO+2 | 4.2 % |
| | | HOMO-1 -> LUMO+1 | 9.1 % |
| | | HOMO-1 -> LUMO+2 | 4.3 % |
| | | HOMO -> LUMO+1 | 2.1 % |
| | | HOMO -> LUMO+3 | 4.8 % |
| | | HOMO -> LUMO+8 | 4.3 % |
| 242.52 nm | 0.0254 | HOMO-7 -> LUMO+3 | 14.7 % |
| | | HOMO-7 -> LUMO+4 | 15.7 % |
| | | HOMO-6 -> LUMO+5 | 5.1 % |
| | | HOMO-5 -> LUMO+5 | 9.2 % |
| | | HOMO-4 -> LUMO+2 | 2.2 % |
| | | HOMO-4 -> LUMO+5 | 3.7 % |
| | | HOMO-3 -> LUMO+4 | 2.3 % |
| | | HOMO-2 -> LUMO+5 | 8.6 % |
| | | HOMO-1 -> LUMO+2 | 2.3 % |
| | | HOMO-1 -> LUMO+5 | 2.5 % |
| | | HOMO -> LUMO+5 | 7.4 % |
| 240.88 nm | 0.0234 | HOMO-3 -> LUMO+3 | 2.1 % |
| | | HOMO-3 -> LUMO+8 | 2.2 % |
| | | HOMO-3 -> LUMO+10 | 11.2 % |
| | | HOMO-3 -> LUMO+13 | 3.9 % |
| | | HOMO-3 -> LUMO+16 | 13.1 % |
| | | HOMO-3 -> LUMO+19 | 2.7 % |
| | | HOMO -> LUMO+10 | 9.1 % |
| | | HOMO -> LUMO+13 | 3.1 % |
| | | HOMO -> LUMO+16 | 7.6 % |
| 237.97 nm | 0.1896 | HOMO-3 -> LUMO+2 | 21.3 % |
| | | HOMO-3 -> LUMO+3 | 9.3 % |
| | | HOMO-3 -> LUMO+4 | 4.0 % |
| | | HOMO-1 -> LUMO+2 | 10.6 % |
| | | HOMO-1 -> LUMO+3 | 8.8 % |
| | | HOMO-1 -> LUMO+4 | 5.7 % |
| | | HOMO -> LUMO+4 | 2.2 % |
| | | HOMO -> LUMO+7 | 5.7 % |
| 232.52 nm | 0.1479 | HOMO-5 -> LUMO+3 | 3.9 % |
| | | HOMO-4 -> LUMO+2 | 10.7 % |
| | | HOMO-4 -> LUMO+3 | 2.2 % |
| | | HOMO-3 -> LUMO+2 | 8.1 % |
| | | HOMO-2 -> LUMO+2 | 7.3 % |
| | | HOMO-2 -> LUMO+3 | 6.5 % |
| | | HOMO-2 -> LUMO+4 | 10.6 % |
| | | HOMO-1 -> LUMO+4 | 18.0 % |
| | | HOMO -> LUMO+3 | 4.3 % |
| | | HOMO -> LUMO+4 | 5.1 % |
| 232.01 nm | 0.2294 | HOMO-5 -> LUMO+2 | 2.5 % |

| | | | |
|---|---|---|---|
| | | HOMO-5 -> LUMO+4 | 2.3 % |
| | | HOMO-4 -> LUMO+2 | 5.8 % |
| | | HOMO-4 -> LUMO+4 | 2.2 % |
| | | HOMO-3 -> LUMO+2 | 27.9 % |
| | | HOMO-2 -> LUMO+3 | 6.0 % |
| | | HOMO-2 -> LUMO+4 | 4.4 % |
| | | HOMO-1 -> LUMO+3 | 9.6 % |
| | | HOMO -> LUMO+7 | 8.0 % |
| | | HOMO -> LUMO+8 | 2.9 % |
| 230.49 nm | 0.1582 | HOMO-5 -> LUMO+1 | 3.2 % |
| | | HOMO-4 -> LUMO+3 | 2.2 % |
| | | HOMO-3 -> LUMO+2 | 9.0 % |
| | | HOMO-3 -> LUMO+3 | 4.1 % |
| | | HOMO-3 -> LUMO+4 | 6.2 % |
| | | HOMO-2 -> LUMO+2 | 9.3 % |
| | | HOMO-1 -> LUMO+3 | 4.5 % |
| | | HOMO -> LUMO+3 | 4.2 % |
| | | HOMO -> LUMO+7 | 10.1 % |
| | | HOMO -> LUMO+8 | 7.3 % |
| | | HOMO -> LUMO+17 | 3.5 % |
| | | HOMO -> LUMO+24 | 2.2 % |
| | | HOMO -> LUMO+26 | 2.3 % |
| 229.35 nm | 0.0577 | HOMO-6 -> LUMO+2 | 6.1 % |
| | | HOMO-4 -> LUMO+4 | 2.8 % |
| | | HOMO-3 -> LUMO+2 | 5.6 % |
| | | HOMO-2 -> LUMO+2 | 19.0 % |
| | | HOMO-2 -> LUMO+3 | 16.5 % |
| | | HOMO-2 -> LUMO+4 | 2.0 % |
| | | HOMO-1 -> LUMO+3 | 7.4 % |
| | | HOMO-1 -> LUMO+4 | 2.5 % |
| | | HOMO -> LUMO+7 | 4.8 % |
| | | HOMO -> LUMO+8 | 5.0 % |
| 226.83 nm | 0.5376 | HOMO-9 -> LUMO | 3.8 % |
| | | HOMO-8 -> LUMO | 2.2 % |
| | | HOMO-7 -> LUMO+3 | 2.4 % |
| | | HOMO-7 -> LUMO+4 | 4.2 % |
| | | HOMO-3 -> LUMO+3 | 8.3 % |
| | | HOMO -> LUMO+5 | 33.8 % |
| | | HOMO -> LUMO+7 | 5.8 % |
| | | HOMO -> LUMO+8 | 2.5 % |
| | | HOMO -> LUMO+10 | 2.4 % |
| 226.27 nm | 0.0708 | HOMO-6 -> LUMO+3 | 2.1 % |
| | | HOMO-6 -> LUMO+4 | 2.9 % |
| | | HOMO-4 -> LUMO+2 | 9.6 % |
| | | HOMO-3 -> LUMO+2 | 2.3 % |
| | | HOMO-2 -> LUMO+2 | 7.9 % |
| | | HOMO-2 -> LUMO+3 | 17.1 % |
| | | HOMO-2 -> LUMO+4 | 25.7 % |
| | | HOMO-1 -> LUMO+2 | 2.3 % |
| | | HOMO-1 -> LUMO+3 | 2.4 % |
| | | HOMO-1 -> LUMO+4 | 2.8 % |

**Table S3:** List of all the computed electronic transitions for **[Ir(ppy)$_2$(1,2 BTBMe$_2$)]$^+$** with their character.

| Wavelength(nm) | Intensity (a.u.) | Levels | Character |
|---|---|---|---|
| 329.58 nm | 0.2074 | HOMO-1 -> LUMO+1 | 9.6 % |
| | | HOMO -> LUMO | 2.1 % |
| | | HOMO -> LUMO+1 | 66.4 % |
| | | HOMO -> LUMO+2 | 13.7 % |
| | | HOMO -> LUMO+2 | 13.7 % |
| 320.67 nm | 0.0761 | HOMO-1 -> LUMO+2 | 9.4 % |
| | | HOMO -> LUMO+1 | 9.2 % |
| | | HOMO -> LUMO+2 | 61.7 % |
| | | HOMO -> LUMO+3 | 11.7 % |
| 304.64 nm | 0.0029 | HOMO -> LUMO | 91.5 % |
| 276.16 nm | 0.2848 | HOMO-3 -> LUMO+1 | 8.2 % |
| | | HOMO-2 -> LUMO+1 | 30.0 % |
| | | HOMO-2 -> LUMO+2 | 2.7 % |
| | | HOMO-1 -> LUMO+1 | 31.4 % |
| | | HOMO-1 -> LUMO+3 | 3.2 % |
| | | HOMO -> LUMO+1 | 6.9 % |
| 273.50 nm | 0.0702 | HOMO-4 -> LUMO+1 | 5.3 % |
| | | HOMO-2 -> LUMO+2 | 3.5 % |
| | | HOMO-1 -> LUMO+1 | 3.4 % |
| | | HOMO-1 -> LUMO+2 | 4.7 % |
| | | HOMO-1 -> LUMO+5 | 2.6 % |
| | | HOMO-1 -> LUMO+6 | 2.1 % |
| | | HOMO -> LUMO+3 | 2.9 % |
| | | HOMO -> LUMO+4 | 56.4 % |
| 268.90 nm | 0.2844 | HOMO-4 -> LUMO+1 | 6.2 % |
| | | HOMO-3 -> LUMO+2 | 4.6 % |
| | | HOMO-2 -> LUMO+2 | 19.1 % |
| | | HOMO-2 -> LUMO+3 | 4.0 % |
| | | HOMO-1 -> LUMO+2 | 28.6 % |
| | | HOMO-1 -> LUMO+4 | 5.6 % |
| | | HOMO -> LUMO+2 | 4.4 % |
| | | HOMO -> LUMO+4 | 6.2 % |
| 265.64 nm | 0.0606 | HOMO-4 -> LUMO+1 | 2.8 % |
| | | HOMO-1 -> LUMO+2 | 7.7 % |
| | | HOMO-1 -> LUMO+4 | 7.6 % |
| | | HOMO -> LUMO+1 | 2.5 % |
| | | HOMO -> LUMO+2 | 4.7 % |
| | | HOMO -> LUMO+3 | 11.2 % |
| | | HOMO -> LUMO+5 | 20.6 % |
| | | HOMO -> LUMO+6 | 12.0 % |
| | | HOMO -> LUMO+9 | 4.0 % |
| | | HOMO -> LUMO+11 | 2.5 % |
| 263.24 nm | 0.1081 | HOMO-5 -> LUMO+1 | 6.4 % |
| | | HOMO-4 -> LUMO | 15.5 % |
| | | HOMO-4 -> LUMO+1 | 19.0 % |
| | | HOMO-4 -> LUMO+2 | 3.8 % |
| | | HOMO-3 -> LUMO | 2.1 % |
| | | HOMO-2 -> LUMO | 2.8 % |
| | | HOMO-1 -> LUMO+1 | 3.0 % |
| | | HOMO-1 -> LUMO+2 | 2.6 % |
| | | HOMO -> LUMO+4 | 3.6 % |

| | | | |
|---|---|---|---|
| | | HOMO -> LUMO+5 | 3.0 % |
| 261.27 nm | 0.0557 | HOMO-5 -> LUMO+1 | 16.1 % |
| | | HOMO-5 -> LUMO+2 | 8.1 % |
| | | HOMO-4 -> LUMO+1 | 13.4 % |
| | | HOMO-2 -> LUMO+1 | 2.7 % |
| | | HOMO-1 -> LUMO | 3.2 % |
| | | HOMO-1 -> LUMO+1 | 3.2 % |
| | | HOMO -> LUMO+3 | 14.6 % |
| | | HOMO -> LUMO+5 | 8.0 % |
| | | HOMO -> LUMO+9 | 3.2 % |
| 260.48 nm | 0.0119 | HOMO-5 -> LUMO | 5.1 % |
| | | HOMO-5 -> LUMO+2 | 2.4 % |
| | | HOMO-4 -> LUMO | 26.9 % |
| | | HOMO-4 -> LUMO+2 | 2.5 % |
| | | HOMO-3 -> LUMO | 9.8 % |
| | | HOMO-3 -> LUMO+2 | 2.5 % |
| | | HOMO-2 -> LUMO | 5.9 % |
| | | HOMO-1 -> LUMO | 17.2 % |
| 259.35 nm | 0.1607 | HOMO-5 -> LUMO+1 | 33.3 % |
| | | HOMO-5 -> LUMO+3 | 2.4 % |
| | | HOMO-4 -> LUMO+1 | 10.6 % |
| | | HOMO-4 -> LUMO+2 | 3.5 % |
| | | HOMO-3 -> LUMO+1 | 12.1 % |
| | | HOMO-2 -> LUMO+1 | 6.2 % |
| | | HOMO-2 -> LUMO+2 | 3.5 % |
| | | HOMO -> LUMO+4 | 3.1 % |
| 256.38 nm | 0.1690 | HOMO-5 -> LUMO+2 | 19.7 % |
| | | HOMO-3 -> LUMO+2 | 5.0 % |
| | | HOMO-1 -> LUMO+2 | 2.7 % |
| | | HOMO -> LUMO+3 | 31.3 % |
| | | HOMO -> LUMO+5 | 2.5 % |
| 255.49 nm | 0.0121 | HOMO-5 -> LUMO+1 | 4.8 % |
| | | HOMO-5 -> LUMO+2 | 9.4 % |
| | | HOMO-4 -> LUMO+2 | 38.5 % |
| | | HOMO-4 -> LUMO+3 | 3.2 % |
| | | HOMO-2 -> LUMO+2 | 15.1 % |
| | | HOMO-2 -> LUMO+3 | 2.2 % |
| | | HOMO -> LUMO+3 | 3.6 % |
| | | HOMO -> LUMO+5 | 2.0 % |
| 251.75 nm | 0.0868 | HOMO-7 -> LUMO | 5.7 % |
| | | HOMO-5 -> LUMO | 54.7 % |
| | | HOMO-5 -> LUMO+1 | 2.5 % |
| | | HOMO-4 -> LUMO | 9.7 % |
| | | HOMO-3 -> LUMO | 4.3 % |
| | | HOMO-2 -> LUMO | 7.8 % |
| | | HOMO-1 -> LUMO | 3.1 % |
| 249.13 nm | 0.0056 | HOMO-5 -> LUMO+2 | 9.6 % |
| | | HOMO-4 -> LUMO+1 | 7.0 % |
| | | HOMO-4 -> LUMO+2 | 5.9 % |
| | | HOMO-3 -> LUMO+2 | 8.0 % |
| | | HOMO -> LUMO+3 | 5.7 % |
| | | HOMO -> LUMO+4 | 2.7 % |
| | | HOMO -> LUMO+5 | 10.9 % |
| | | HOMO -> LUMO+13 | 2.7 % |
| | | HOMO -> LUMO+14 | 7.3 % |
| | | HOMO -> LUMO+15 | 5.8 % |
| | | HOMO -> LUMO+16 | 3.6 % |

| | | | |
|---|---|---|---|
| 248.97 nm | 0.0657 | HOMO-4 -> LUMO+1 | 3.6 % |
| | | HOMO-3 -> LUMO+1 | 29.9 % |
| | | HOMO-3 -> LUMO+2 | 2.9 % |
| | | HOMO-2 -> LUMO+1 | 4.1 % |
| | | HOMO-1 -> LUMO | 2.2 % |
| | | HOMO-1 -> LUMO+1 | 10.3 % |
| | | HOMO -> LUMO+1 | 3.1 % |
| | | HOMO -> LUMO+4 | 5.9 % |
| | | HOMO -> LUMO+5 | 2.8 % |
| 245.20 nm | 0.0394 | HOMO-5 -> LUMO+14 | 2.5 % |
| | | HOMO-5 -> LUMO+16 | 2.3 % |
| | | HOMO-4 -> LUMO | 4.3 % |
| | | HOMO-3 -> LUMO | 2.0 % |
| | | HOMO-3 -> LUMO+1 | 2.5 % |
| | | HOMO-3 -> LUMO+2 | 10.1 % |
| | | HOMO-3 -> LUMO+3 | 3.8 % |
| | | HOMO-2 -> LUMO+4 | 2.7 % |
| | | HOMO-1 -> LUMO | 16.9 % |
| | | HOMO-1 -> LUMO+2 | 2.1 % |
| | | HOMO -> LUMO+5 | 6.8 % |
| | | HOMO -> LUMO+6 | 2.8 % |
| | | HOMO -> LUMO+10 | 2.7 % |
| 243.97 nm | 0.0147 | HOMO-5 -> LUMO | 3.4 % |
| | | HOMO-4 -> LUMO | 10.1 % |
| | | HOMO-3 -> LUMO | 3.7 % |
| | | HOMO-3 -> LUMO+2 | 4.7 % |
| | | HOMO-2 -> LUMO | 2.5 % |
| | | HOMO-1 -> LUMO | 37.0 % |
| | | HOMO-1 -> LUMO+1 | 2.4 % |
| | | HOMO -> LUMO+3 | 3.8 % |
| | | HOMO -> LUMO+5 | 4.2 % |
| 243.06 nm | 0.0271 | HOMO-4 -> LUMO+1 | 12.0 % |
| | | HOMO-4 -> LUMO+3 | 3.9 % |
| | | HOMO-4 -> LUMO+9 | 2.3 % |
| | | HOMO-4 -> LUMO+11 | 2.3 % |
| | | HOMO-4 -> LUMO+13 | 3.3 % |
| | | HOMO-4 -> LUMO+14 | 10.1 % |
| | | HOMO-4 -> LUMO+15 | 9.0 % |
| | | HOMO-4 -> LUMO+16 | 4.8 % |
| | | HOMO-2 -> LUMO+14 | 2.1 % |
| | | HOMO-1 -> LUMO | 3.2 % |
| | | HOMO -> LUMO+4 | 3.1 % |
| | | HOMO -> LUMO+6 | 2.2 % |
| 239.75 nm | 0.0701 | HOMO-5 -> LUMO+2 | 10.3 % |
| | | HOMO-5 -> LUMO+3 | 5.1 % |
| | | HOMO-5 -> LUMO+14 | 5.0 % |
| | | HOMO-5 -> LUMO+15 | 2.8 % |
| | | HOMO-5 -> LUMO+16 | 3.3 % |
| | | HOMO -> LUMO+5 | 9.8 % |
| | | HOMO -> LUMO+10 | 5.3 % |
| | | HOMO -> LUMO+14 | 3.4 % |
| | | HOMO -> LUMO+15 | 4.8 % |
| | | HOMO -> LUMO+19 | 3.9 % |
| 238.83 nm | 0.1026 | HOMO-10 -> LUMO | 2.5 % |
| | | HOMO-7 -> LUMO | 14.3 % |
| | | HOMO-6 -> LUMO+3 | 2.4 % |
| | | HOMO-5 -> LUMO+2 | 3.7 % |
| | | HOMO-3 -> LUMO+2 | 9.7 % |

| | | | |
|---|---|---|---|
| | | HOMO-2 -> LUMO+4 | 2.8 % |
| | | HOMO-1 -> LUMO+2 | 5.2 % |
| | | HOMO -> LUMO+2 | 2.6 % |
| | | HOMO -> LUMO+6 | 5.9 % |
| | | HOMO -> LUMO+10 | 4.2 % |
| | | HOMO -> LUMO+18 | 2.1 % |
| | | HOMO -> LUMO+19 | 5.5 % |
| 238.57 nm | 0.0683 | HOMO-10 -> LUMO | 4.1 % |
| | | HOMO-7 -> LUMO | 24.2 % |
| | | HOMO-6 -> LUMO | 2.7 % |
| | | HOMO-6 -> LUMO+3 | 5.1 % |
| | | HOMO-5 -> LUMO | 2.3 % |
| | | HOMO-5 -> LUMO+2 | 6.5 % |
| | | HOMO-3 -> LUMO+2 | 3.2 % |
| | | HOMO-2 -> LUMO | 2.5 % |
| | | HOMO-1 -> LUMO+2 | 2.7 % |
| | | HOMO -> LUMO+6 | 17.0 % |
| 237.88 nm | 0.1030 | HOMO-7 -> LUMO | 3.2 % |
| | | HOMO-2 -> LUMO+4 | 7.5 % |
| | | HOMO-1 -> LUMO+5 | 5.8 % |
| | | HOMO -> LUMO+5 | 9.3 % |
| | | HOMO -> LUMO+6 | 30.2 % |
| | | HOMO -> LUMO+11 | 4.8 % |
| | | HOMO -> LUMO+16 | 2.1 % |
| | | HOMO -> LUMO+19 | 2.4 % |
| 235.65 nm | 0.1065 | HOMO-4 -> LUMO+1 | 2.5 % |
| | | HOMO-4 -> LUMO+4 | 2.1 % |
| | | HOMO-3 -> LUMO+4 | 4.1 % |
| | | HOMO-2 -> LUMO+4 | 10.4 % |
| | | HOMO-2 -> LUMO+5 | 3.5 % |
| | | HOMO-2 -> LUMO+6 | 2.6 % |
| | | HOMO-1 -> LUMO+4 | 20.9 % |
| | | HOMO -> LUMO+4 | 4.5 % |
| | | HOMO -> LUMO+5 | 4.0 % |
| | | HOMO -> LUMO+7 | 7.0 % |
| | | HOMO -> LUMO+10 | 2.0 % |
| | | HOMO -> LUMO+12 | 2.2 % |
| | | HOMO -> LUMO+19 | 5.5 % |
| 232.36 nm | 0.0886 | HOMO-4 -> LUMO | 4.2 % |
| | | HOMO-2 -> LUMO | 15.6 % |
| | | HOMO-2 -> LUMO+4 | 3.5 % |
| | | HOMO-1 -> LUMO+5 | 4.5 % |
| | | HOMO -> LUMO+7 | 41.3 % |
| | | HOMO -> LUMO+10 | 5.4 % |
| | | HOMO -> LUMO+19 | 3.1 % |

**Table S4:** List of all the computed electronic transitions for **[Ir($F_2$ppy)$_2$(1,2 BTB)]$^-$** with their character.

| Wavelength (nm) | Intensity (a.u.) | Levels | Character |
|---|---|---|---|
| 322.42 nm | 0.1769 | HOMO-1 -> LUMO | 8.2 % |
| | | HOMO -> LUMO | 80.1 % |
| | | HOMO -> LUMO+1 | 3.6 % |
| | | HOMO -> LUMO+1 | 3.6 % |
| 314.42 nm | 0.0662 | HOMO-2 -> LUMO+1 | 5.1 % |
| | | HOMO-1 -> LUMO | 2.1 % |
| | | HOMO-1 -> LUMO+1 | 3.0 % |
| | | HOMO -> LUMO | 3.1 % |
| | | HOMO -> LUMO+1 | 81.1 % |
| 278.89 nm | 0.1608 | HOMO-5 -> LUMO | 5.2 % |
| | | HOMO-4 -> LUMO | 2.9 % |
| | | HOMO-3 -> LUMO | 3.2 % |
| | | HOMO-2 -> LUMO | 11.9 % |
| | | HOMO-1 -> LUMO | 55.6 % |
| | | HOMO-1 -> LUMO+1 | 3.0 % |
| | | HOMO -> LUMO | 5.1 % |
| 269.14 nm | 0.0719 | HOMO-7 -> LUMO | 6.3 % |
| | | HOMO-5 -> LUMO | 3.6 % |
| | | HOMO-4 -> LUMO | 47.1 % |
| | | HOMO-3 -> LUMO | 10.3 % |
| | | HOMO-2 -> LUMO | 14.3 % |
| | | HOMO-1 -> LUMO | 2.1 % |
| 267.79 nm | 0.1120 | HOMO-6 -> LUMO | 4.8 % |
| | | HOMO-5 -> LUMO+1 | 2.4 % |
| | | HOMO-3 -> LUMO | 17.5 % |
| | | HOMO-3 -> LUMO+1 | 4.2 % |
| | | HOMO-2 -> LUMO+1 | 6.2 % |
| | | HOMO-1 -> LUMO+1 | 13.2 % |
| | | HOMO -> LUMO+2 | 27.7 % |
| 265.84 nm | 0.0541 | HOMO-6 -> LUMO+1 | 5.8 % |
| | | HOMO-5 -> LUMO+1 | 17.3 % |
| | | HOMO-4 -> LUMO | 3.3 % |
| | | HOMO-2 -> LUMO+1 | 29.2 % |
| | | HOMO-1 -> LUMO | 2.2 % |
| | | HOMO-1 -> LUMO+1 | 24.0 % |
| 265.00 nm | 0.2341 | HOMO-6 -> LUMO | 5.3 % |
| | | HOMO-5 -> LUMO | 2.4 % |
| | | HOMO-4 -> LUMO+1 | 8.9 % |
| | | HOMO-3 -> LUMO | 23.7 % |
| | | HOMO-3 -> LUMO+1 | 5.5 % |
| | | HOMO-2 -> LUMO+1 | 17.5 % |
| | | HOMO-1 -> LUMO+1 | 9.3 % |
| | | HOMO-1 -> LUMO+2 | 2.0 % |
| | | HOMO -> LUMO+1 | 2.8 % |
| | | HOMO -> LUMO+4 | 2.3 % |
| 262.71 nm | 0.0840 | HOMO-7 -> LUMO+1 | 7.0 % |
| | | HOMO-4 -> LUMO+1 | 35.2 % |
| | | HOMO-3 -> LUMO+1 | 37.3 % |
| | | HOMO -> LUMO+4 | 2.4 % |
| 259.98 nm | 0.4551 | HOMO-5 -> LUMO | 10.2 % |

| | | | |
|---|---|---|---|
| | | HOMO-4 -> LUMO+1 | 2.4 % |
| | | HOMO-3 -> LUMO | 13.1 % |
| | | HOMO-2 -> LUMO | 5.2 % |
| | | HOMO-2 -> LUMO+1 | 6.3 % |
| | | HOMO-1 -> LUMO+1 | 4.5 % |
| | | HOMO -> LUMO+2 | 42.6 % |
| 255.15 nm | 0.0375 | HOMO-6 -> LUMO+1 | 2.1 % |
| | | HOMO-5 -> LUMO | 2.5 % |
| | | HOMO-2 -> LUMO | 2.3 % |
| | | HOMO-1 -> LUMO+1 | 3.0 % |
| | | HOMO-1 -> LUMO+2 | 5.5 % |
| | | HOMO -> LUMO+3 | 5.7 % |
| | | HOMO -> LUMO+4 | 42.6 % |
| | | HOMO -> LUMO+8 | 2.6 % |
| 250.86 nm | 0.0163 | HOMO-5 -> LUMO+1 | 2.6 % |
| | | HOMO-4 -> LUMO+10 | 6.0 % |
| | | HOMO-4 -> LUMO+13 | 3.9 % |
| | | HOMO-3 -> LUMO+10 | 2.4 % |
| | | HOMO-2 -> LUMO+1 | 3.5 % |
| | | HOMO -> LUMO+4 | 8.0 % |
| | | HOMO -> LUMO+9 | 3.0 % |
| | | HOMO -> LUMO+10 | 12.9 % |
| | | HOMO -> LUMO+11 | 4.1 % |
| | | HOMO -> LUMO+13 | 8.0 % |
| 246.54 nm | 0.0043 | HOMO-6 -> LUMO+10 | 2.4 % |
| | | HOMO-5 -> LUMO+10 | 8.3 % |
| | | HOMO-5 -> LUMO+11 | 2.1 % |
| | | HOMO-5 -> LUMO+13 | 4.8 % |
| | | HOMO-4 -> LUMO+10 | 2.0 % |
| | | HOMO-2 -> LUMO | 2.6 % |
| | | HOMO-2 -> LUMO+10 | 8.9 % |
| | | HOMO-2 -> LUMO+11 | 2.2 % |
| | | HOMO-2 -> LUMO+13 | 4.8 % |
| | | HOMO-1 -> LUMO+10 | 9.6 % |
| | | HOMO-1 -> LUMO+11 | 2.7 % |
| | | HOMO-1 -> LUMO+13 | 5.4 % |
| 244.15 nm | 0.0361 | HOMO-6 -> LUMO | 5.5 % |
| | | HOMO-5 -> LUMO+3 | 4.5 % |
| | | HOMO-3 -> LUMO+3 | 4.5 % |
| | | HOMO-2 -> LUMO+3 | 9.7 % |
| | | HOMO-1 -> LUMO+3 | 3.2 % |
| | | HOMO -> LUMO+2 | 4.7 % |
| | | HOMO -> LUMO+3 | 37.8 % |
| | | HOMO -> LUMO+4 | 2.4 % |
| | | HOMO -> LUMO+7 | 2.8 % |
| 242.92 nm | 0.0044 | HOMO-7 -> LUMO+3 | 12.5 % |
| | | HOMO-6 -> LUMO | 10.8 % |
| | | HOMO-5 -> LUMO | 5.3 % |
| | | HOMO-5 -> LUMO+5 | 3.8 % |
| | | HOMO-4 -> LUMO | 5.2 % |
| | | HOMO-4 -> LUMO+3 | 2.7 % |
| | | HOMO-2 -> LUMO+5 | 6.0 % |
| | | HOMO-1 -> LUMO | 3.3 % |
| | | HOMO -> LUMO+2 | 2.8 % |
| | | HOMO -> LUMO+4 | 4.1 % |
| | | HOMO -> LUMO+5 | 3.1 % |
| 241.85 nm | 0.0262 | HOMO-7 -> LUMO+3 | 10.5 % |
| | | HOMO-6 -> LUMO | 8.6 % |

| | | | |
|---|---|---|---|
| | | HOMO-5 -> LUMO+5 | 3.6 % |
| | | HOMO-4 -> LUMO | 4.8 % |
| | | HOMO-4 -> LUMO+3 | 3.7 % |
| | | HOMO-3 -> LUMO+5 | 2.8 % |
| | | HOMO-2 -> LUMO+2 | 5.2 % |
| | | HOMO-2 -> LUMO+3 | 4.8 % |
| | | HOMO-2 -> LUMO+5 | 2.7 % |
| | | HOMO-1 -> LUMO+2 | 10.9 % |
| | | HOMO -> LUMO+3 | 6.4 % |
| | | HOMO -> LUMO+4 | 2.9 % |
| 239.14 nm | 0.2631 | HOMO-6 -> LUMO+1 | 3.6 % |
| | | HOMO-3 -> LUMO+2 | 5.0 % |
| | | HOMO-3 -> LUMO+3 | 2.1 % |
| | | HOMO-3 -> LUMO+10 | 3.9 % |
| | | HOMO-3 -> LUMO+13 | 2.1 % |
| | | HOMO-2 -> LUMO+2 | 3.3 % |
| | | HOMO-1 -> LUMO+2 | 9.6 % |
| | | HOMO-1 -> LUMO+4 | 4.7 % |
| | | HOMO -> LUMO+4 | 3.9 % |
| | | HOMO -> LUMO+7 | 3.8 % |
| | | HOMO -> LUMO+8 | 6.1 % |
| | | HOMO -> LUMO+10 | 3.5 % |
| 237.26 nm | 0.0966 | HOMO-6 -> LUMO | 2.2 % |
| | | HOMO-3 -> LUMO+10 | 4.4 % |
| | | HOMO-3 -> LUMO+13 | 3.1 % |
| | | HOMO-2 -> LUMO+2 | 2.1 % |
| | | HOMO-1 -> LUMO+2 | 6.4 % |
| | | HOMO-1 -> LUMO+4 | 3.9 % |
| | | HOMO -> LUMO+4 | 4.6 % |
| | | HOMO -> LUMO+6 | 2.2 % |
| | | HOMO -> LUMO+7 | 2.9 % |
| | | HOMO -> LUMO+10 | 11.1 % |
| | | HOMO -> LUMO+11 | 4.4 % |
| | | HOMO -> LUMO+13 | 4.7 % |
| 235.39 nm | 0.0472 | HOMO-7 -> LUMO+1 | 3.8 % |
| | | HOMO-6 -> LUMO+1 | 13.8 % |
| | | HOMO-5 -> LUMO+1 | 5.7 % |
| | | HOMO-5 -> LUMO+2 | 2.2 % |
| | | HOMO-4 -> LUMO+1 | 2.6 % |
| | | HOMO-3 -> LUMO+4 | 3.3 % |
| | | HOMO-2 -> LUMO+2 | 2.3 % |
| | | HOMO-2 -> LUMO+4 | 2.2 % |
| | | HOMO-1 -> LUMO+1 | 2.0 % |
| | | HOMO-1 -> LUMO+2 | 20.4 % |
| | | HOMO -> LUMO+2 | 3.5 % |
| | | HOMO -> LUMO+3 | 2.3 % |
| | | HOMO -> LUMO+7 | 4.9 % |
| 229.78 nm | 0.2162 | HOMO-6 -> LUMO+1 | 8.3 % |
| | | HOMO-5 -> LUMO+1 | 4.5 % |
| | | HOMO-3 -> LUMO+2 | 2.2 % |
| | | HOMO-2 -> LUMO+1 | 2.1 % |
| | | HOMO-2 -> LUMO+4 | 3.9 % |
| | | HOMO-1 -> LUMO+1 | 4.3 % |
| | | HOMO-1 -> LUMO+2 | 3.9 % |
| | | HOMO-1 -> LUMO+3 | 2.7 % |
| | | HOMO -> LUMO+4 | 6.2 % |
| | | HOMO -> LUMO+7 | 19.4 % |
| | | HOMO -> LUMO+18 | 4.6 % |
| 227.06 nm | 0.3739 | HOMO-5 -> LUMO | 3.4 % |

| | | | |
|---|---|---|---|
| | | HOMO-5 -> LUMO+3 | 2.4 % |
| | | HOMO-4 -> LUMO+3 | 2.3 % |
| | | HOMO-3 -> LUMO+2 | 7.8 % |
| | | HOMO-3 -> LUMO+4 | 5.9 % |
| | | HOMO-2 -> LUMO | 4.3 % |
| | | HOMO-2 -> LUMO+3 | 12.0 % |
| | | HOMO-1 -> LUMO+3 | 2.0 % |
| | | HOMO-1 -> LUMO+4 | 10.5 % |
| | | HOMO -> LUMO+2 | 3.1 % |
| | | HOMO -> LUMO+3 | 6.2 % |
| | | HOMO -> LUMO+4 | 9.3 % |
| | | HOMO -> LUMO+7 | 6.9 % |
| | | HOMO -> LUMO+18 | 2.2 % |
| 226.46 nm | 0.1783 | HOMO-6 -> LUMO | 6.6 % |
| | | HOMO-5 -> LUMO | 8.6 % |
| | | HOMO-4 -> LUMO+2 | 4.3 % |
| | | HOMO-3 -> LUMO | 2.9 % |
| | | HOMO-3 -> LUMO+3 | 2.3 % |
| | | HOMO-3 -> LUMO+4 | 3.8 % |
| | | HOMO-2 -> LUMO | 3.6 % |
| | | HOMO-2 -> LUMO+2 | 7.3 % |
| | | HOMO-2 -> LUMO+4 | 3.0 % |
| | | HOMO-1 -> LUMO+3 | 5.6 % |
| | | HOMO -> LUMO+3 | 14.2 % |
| | | HOMO -> LUMO+7 | 4.4 % |
| | | HOMO -> LUMO+8 | 3.1 % |
| | | HOMO -> LUMO+18 | 3.3 % |
| 224.46 nm | 0.0265 | HOMO-7 -> LUMO | 2.8 % |
| | | HOMO-5 -> LUMO | 28.8 % |
| | | HOMO-3 -> LUMO+3 | 2.2 % |
| | | HOMO-2 -> LUMO | 29.1 % |
| | | HOMO-2 -> LUMO+3 | 3.4 % |
| | | HOMO-1 -> LUMO+3 | 2.8 % |
| | | HOMO -> LUMO+3 | 7.4 % |
| 223.06 nm | 0.0819 | HOMO-6 -> LUMO | 20.6 % |
| | | HOMO-4 -> LUMO | 18.4 % |
| | | HOMO-3 -> LUMO | 11.6 % |
| | | HOMO-3 -> LUMO+2 | 2.2 % |
| | | HOMO-2 -> LUMO | 10.8 % |
| | | HOMO-1 -> LUMO | 12.4 % |
| | | HOMO -> LUMO+5 | 2.1 % |
| | | HOMO -> LUMO+8 | 2.3 % |
| 222.57 nm | 0.0180 | HOMO-7 -> LUMO+2 | 4.0 % |
| | | HOMO-5 -> LUMO+2 | 4.0 % |
| | | HOMO-4 -> LUMO+2 | 46.2 % |
| | | HOMO-3 -> LUMO+2 | 8.8 % |
| | | HOMO-2 -> LUMO+2 | 5.4 % |
| | | HOMO-2 -> LUMO+4 | 3.9 % |
| | | HOMO-1 -> LUMO+3 | 2.0 % |
| | | HOMO-1 -> LUMO+4 | 7.5 % |
| 221.13 nm | 0.2752 | HOMO-13 -> LUMO | 2.0 % |
| | | HOMO-6 -> LUMO | 5.2 % |
| | | HOMO-6 -> LUMO+2 | 4.0 % |
| | | HOMO-5 -> LUMO | 4.9 % |
| | | HOMO-5 -> LUMO+2 | 3.9 % |
| | | HOMO-4 -> LUMO+4 | 2.4 % |
| | | HOMO-3 -> LUMO+2 | 17.5 % |
| | | HOMO-3 -> LUMO+4 | 2.8 % |
| | | HOMO-2 -> LUMO+2 | 14.9 % |

| | |
|---|---|
| HOMO-2 -> LUMO+3 | 3.3 % |
| HOMO-2 -> LUMO+4 | 2.6 % |
| HOMO -> LUMO+5 | 3.8 % |
| HOMO -> LUMO+8 | 3.4 % |

**Table S5:** List of all the computed electronic transitions for **[Ir($F_2$ppy)$_2$(1,2 BTBMe$_2$)]$^+$** with their character.

| Wavelength (nm) | Intensity (a.u.) | Levels | Character |
|---|---|---|---|
| 312.50 nm | 0.2176 | HOMO-1 -> LUMO+1 | 14.3 % |
| | | HOMO -> LUMO+1 | 62.7 % |
| | | HOMO -> LUMO+2 | 11.8 % |
| | | HOMO -> LUMO+2 | 11.8 % |
| 305.21 nm | 0.1027 | HOMO-1 -> LUMO+2 | 12.5 % |
| | | HOMO -> LUMO+1 | 9.0 % |
| | | HOMO -> LUMO+2 | 64.7 % |
| | | HOMO -> LUMO+3 | 4.8 % |
| 284.84 nm | 0.0033 | HOMO -> LUMO | 89.3 % |
| 272.90 nm | 0.3229 | HOMO-3 -> LUMO+1 | 3.9 % |
| | | HOMO-2 -> LUMO+1 | 42.4 % |
| | | HOMO-2 -> LUMO+2 | 3.2 % |
| | | HOMO-1 -> LUMO+1 | 25.4 % |
| | | HOMO -> LUMO+1 | 7.6 % |
| 267.24 nm | 0.2896 | HOMO-3 -> LUMO+2 | 3.5 % |
| | | HOMO-2 -> LUMO+1 | 3.1 % |
| | | HOMO-2 -> LUMO+2 | 27.8 % |
| | | HOMO-2 -> LUMO+3 | 2.3 % |
| | | HOMO-1 -> LUMO+2 | 37.9 % |
| | | HOMO -> LUMO+2 | 5.3 % |
| 260.82 nm | 0.0057 | HOMO-4 -> LUMO | 2.7 % |
| | | HOMO-4 -> LUMO+1 | 42.9 % |
| | | HOMO-4 -> LUMO+13 | 4.3 % |
| | | HOMO-1 -> LUMO+4 | 4.9 % |
| | | HOMO -> LUMO+4 | 19.3 % |
| 256.87 nm | 0.0327 | HOMO-5 -> LUMO+1 | 2.5 % |
| | | HOMO-5 -> LUMO+2 | 6.7 % |
| | | HOMO-5 -> LUMO+8 | 2.2 % |
| | | HOMO-5 -> LUMO+11 | 2.6 % |
| | | HOMO-5 -> LUMO+13 | 13.5 % |
| | | HOMO-5 -> LUMO+14 | 2.5 % |
| | | HOMO-4 -> LUMO+1 | 2.6 % |
| | | HOMO-4 -> LUMO+2 | 8.3 % |
| | | HOMO-3 -> LUMO+2 | 6.0 % |
| | | HOMO -> LUMO+3 | 2.6 % |
| | | HOMO -> LUMO+8 | 2.9 % |
| | | HOMO -> LUMO+9 | 2.4 % |
| | | HOMO -> LUMO+11 | 4.3 % |
| | | HOMO -> LUMO+13 | 8.2 % |
| 254.58 nm | 0.2963 | HOMO-5 -> LUMO+1 | 24.4 % |
| | | HOMO-4 -> LUMO | 3.5 % |
| | | HOMO-4 -> LUMO+1 | 4.9 % |
| | | HOMO-4 -> LUMO+13 | 3.6 % |
| | | HOMO-1 -> LUMO+1 | 5.4 % |
| | | HOMO -> LUMO+3 | 3.2 % |
| | | HOMO -> LUMO+4 | 20.2 % |
| | | HOMO -> LUMO+10 | 2.7 % |
| 253.04 nm | 0.0119 | HOMO-4 -> LUMO | 35.9 % |
| | | HOMO-4 -> LUMO+1 | 3.0 % |
| | | HOMO-4 -> LUMO+2 | 2.4 % |

| | | | |
|---|---|---|---|
| | | HOMO-3 -> LUMO | 2.6 % |
| | | HOMO-2 -> LUMO | 10.0 % |
| | | HOMO-1 -> LUMO | 21.2 % |
| | | HOMO -> LUMO+3 | 2.9 % |
| | | HOMO -> LUMO+5 | 2.8 % |
| 251.82 nm | 0.0384 | HOMO-5 -> LUMO+1 | 16.2 % |
| | | HOMO-5 -> LUMO+2 | 11.9 % |
| | | HOMO-4 -> LUMO | 6.1 % |
| | | HOMO-2 -> LUMO+1 | 2.9 % |
| | | HOMO-1 -> LUMO | 3.1 % |
| | | HOMO-1 -> LUMO+2 | 3.5 % |
| | | HOMO-1 -> LUMO+4 | 2.4 % |
| | | HOMO-1 -> LUMO+5 | 3.5 % |
| | | HOMO -> LUMO+3 | 2.1 % |
| | | HOMO -> LUMO+4 | 3.8 % |
| | | HOMO -> LUMO+5 | 11.5 % |
| | | HOMO -> LUMO+6 | 8.7 % |
| 251.64 nm | 0.1210 | HOMO-5 -> LUMO+1 | 18.8 % |
| | | HOMO-4 -> LUMO | 2.4 % |
| | | HOMO-4 -> LUMO+2 | 4.9 % |
| | | HOMO-4 -> LUMO+13 | 4.7 % |
| | | HOMO-3 -> LUMO+1 | 11.9 % |
| | | HOMO-2 -> LUMO+1 | 3.1 % |
| | | HOMO-1 -> LUMO+4 | 4.7 % |
| | | HOMO -> LUMO+4 | 9.7 % |
| | | HOMO -> LUMO+6 | 3.2 % |
| | | HOMO -> LUMO+13 | 4.2 % |
| 248.69 nm | 0.0289 | HOMO-5 -> LUMO+1 | 4.1 % |
| | | HOMO-5 -> LUMO+2 | 28.2 % |
| | | HOMO-4 -> LUMO+2 | 30.2 % |
| | | HOMO-2 -> LUMO+2 | 8.1 % |
| | | HOMO-1 -> LUMO+2 | 3.4 % |
| | | HOMO -> LUMO+13 | 2.8 % |
| 245.59 nm | 0.0111 | HOMO-7 -> LUMO | 17.3 % |
| | | HOMO-6 -> LUMO+3 | 5.8 % |
| | | HOMO-5 -> LUMO | 24.2 % |
| | | HOMO-5 -> LUMO+13 | 3.9 % |
| | | HOMO-3 -> LUMO | 2.7 % |
| | | HOMO-1 -> LUMO | 2.3 % |
| | | HOMO -> LUMO+3 | 14.7 % |
| | | HOMO -> LUMO+5 | 4.5 % |
| 244.79 nm | 0.1310 | HOMO-7 -> LUMO | 8.0 % |
| | | HOMO-5 -> LUMO | 15.8 % |
| | | HOMO-5 -> LUMO+1 | 3.0 % |
| | | HOMO-4 -> LUMO+2 | 4.5 % |
| | | HOMO-3 -> LUMO+2 | 2.5 % |
| | | HOMO-1 -> LUMO | 2.2 % |
| | | HOMO-1 -> LUMO+4 | 4.5 % |
| | | HOMO -> LUMO+3 | 12.1 % |
| | | HOMO -> LUMO+5 | 11.4 % |
| | | HOMO -> LUMO+6 | 3.2 % |
| | | HOMO -> LUMO+8 | 2.1 % |
| | | HOMO -> LUMO+9 | 2.5 % |
| | | HOMO -> LUMO+13 | 2.5 % |
| 242.97 nm | 0.0254 | HOMO-5 -> LUMO+13 | 2.2 % |
| | | HOMO-4 -> LUMO+1 | 2.8 % |
| | | HOMO-4 -> LUMO+8 | 2.2 % |
| | | HOMO-4 -> LUMO+13 | 13.7 % |

| | | | |
|---|---|---|---|
| | | HOMO-3 -> LUMO+1 | 22.0 % |
| | | HOMO-2 -> LUMO+4 | 4.6 % |
| | | HOMO-1 -> LUMO+1 | 2.5 % |
| | | HOMO -> LUMO+1 | 2.0 % |
| | | HOMO -> LUMO+10 | 2.5 % |
| 242.22 nm | 0.0366 | HOMO-5 -> LUMO | 3.4 % |
| | | HOMO-5 -> LUMO+13 | 6.8 % |
| | | HOMO-4 -> LUMO+2 | 10.7 % |
| | | HOMO-4 -> LUMO+13 | 2.4 % |
| | | HOMO-3 -> LUMO+2 | 18.5 % |
| | | HOMO -> LUMO+3 | 5.1 % |
| | | HOMO -> LUMO+10 | 2.6 % |
| | | HOMO -> LUMO+13 | 7.0 % |
| 239.71 nm | 0.0110 | HOMO-7 -> LUMO | 2.9 % |
| | | HOMO-5 -> LUMO+13 | 2.7 % |
| | | HOMO-4 -> LUMO | 14.8 % |
| | | HOMO-1 -> LUMO | 29.8 % |
| | | HOMO -> LUMO+3 | 7.6 % |
| | | HOMO -> LUMO+5 | 2.9 % |
| | | HOMO -> LUMO+13 | 4.1 % |
| 238.84 nm | 0.2881 | HOMO-5 -> LUMO+2 | 2.0 % |
| | | HOMO-4 -> LUMO+1 | 21.1 % |
| | | HOMO-4 -> LUMO+13 | 10.1 % |
| | | HOMO-3 -> LUMO+1 | 3.3 % |
| | | HOMO-2 -> LUMO+4 | 2.3 % |
| | | HOMO-1 -> LUMO | 2.2 % |
| | | HOMO-1 -> LUMO+4 | 3.1 % |
| | | HOMO -> LUMO+4 | 10.1 % |
| | | HOMO -> LUMO+10 | 3.3 % |
| 237.39 nm | 0.0518 | HOMO-5 -> LUMO | 7.5 % |
| | | HOMO-5 -> LUMO+13 | 2.3 % |
| | | HOMO-4 -> LUMO | 9.8 % |
| | | HOMO-3 -> LUMO | 3.3 % |
| | | HOMO-2 -> LUMO | 12.1 % |
| | | HOMO-1 -> LUMO | 15.2 % |
| | | HOMO-1 -> LUMO+1 | 2.1 % |
| | | HOMO -> LUMO+3 | 13.7 % |
| | | HOMO -> LUMO+4 | 2.6 % |
| | | HOMO -> LUMO+13 | 4.4 % |
| 235.95 nm | 0.0179 | HOMO-7 -> LUMO | 27.1 % |
| | | HOMO-6 -> LUMO | 4.2 % |
| | | HOMO-6 -> LUMO+3 | 5.1 % |
| | | HOMO-5 -> LUMO | 14.5 % |
| | | HOMO-3 -> LUMO | 3.0 % |
| | | HOMO-2 -> LUMO | 8.6 % |
| | | HOMO-1 -> LUMO | 2.1 % |
| | | HOMO -> LUMO+3 | 9.0 % |
| | | HOMO -> LUMO+13 | 2.5 % |
| 234.51 nm | 0.1023 | HOMO-5 -> LUMO+2 | 13.4 % |
| | | HOMO-5 -> LUMO+13 | 3.8 % |
| | | HOMO-3 -> LUMO+1 | 8.3 % |
| | | HOMO-1 -> LUMO+1 | 3.9 % |
| | | HOMO -> LUMO+1 | 2.5 % |
| | | HOMO -> LUMO+3 | 3.7 % |
| | | HOMO -> LUMO+5 | 7.6 % |
| | | HOMO -> LUMO+10 | 9.4 % |
| | | HOMO -> LUMO+13 | 3.4 % |
| | | HOMO -> LUMO+15 | 3.5 % |

| | | | |
|---|---|---|---|
| | | HOMO -> LUMO+19 | 7.5 % |
| 231.05 nm | 0.0402 | HOMO-5 -> LUMO+2 | 14.0 % |
| | | HOMO-5 -> LUMO+13 | 2.3 % |
| | | HOMO-3 -> LUMO+2 | 14.5 % |
| | | HOMO-2 -> LUMO+1 | 2.8 % |
| | | HOMO-2 -> LUMO+2 | 2.4 % |
| | | HOMO-1 -> LUMO+1 | 7.0 % |
| | | HOMO-1 -> LUMO+2 | 6.4 % |
| | | HOMO-1 -> LUMO+4 | 2.9 % |
| | | HOMO -> LUMO+2 | 6.5 % |
| | | HOMO -> LUMO+10 | 2.3 % |
| | | HOMO -> LUMO+15 | 3.4 % |
| | | HOMO -> LUMO+19 | 4.1 % |
| 229.91 nm | 0.0245 | HOMO-7 -> LUMO | 2.2 % |
| | | HOMO-5 -> LUMO | 13.5 % |
| | | HOMO-4 -> LUMO | 3.5 % |
| | | HOMO-2 -> LUMO | 51.6 % |
| | | HOMO-1 -> LUMO | 13.6 % |
| | | HOMO -> LUMO | 3.0 % |
| 228.31 nm | 0.1141 | HOMO-4 -> LUMO+4 | 3.6 % |
| | | HOMO-2 -> LUMO+1 | 6.9 % |
| | | HOMO-2 -> LUMO+4 | 16.4 % |
| | | HOMO-1 -> LUMO+1 | 10.6 % |
| | | HOMO-1 -> LUMO+2 | 2.3 % |
| | | HOMO-1 -> LUMO+4 | 8.6 % |
| | | HOMO -> LUMO+4 | 7.9 % |
| | | HOMO -> LUMO+5 | 5.5 % |
| | | HOMO -> LUMO+15 | 2.8 % |
| | | HOMO -> LUMO+19 | 3.9 % |
| 227.43 nm | 0.1530 | HOMO-2 -> LUMO+1 | 4.7 % |
| | | HOMO-2 -> LUMO+5 | 3.6 % |
| | | HOMO-1 -> LUMO+1 | 3.9 % |
| | | HOMO-1 -> LUMO+4 | 2.4 % |
| | | HOMO-1 -> LUMO+5 | 4.1 % |
| | | HOMO -> LUMO+5 | 32.1 % |
| | | HOMO -> LUMO+6 | 25.9 % |
| | | HOMO -> LUMO+9 | 3.9 % |
| | | HOMO -> LUMO+13 | 3.3 % |