# Supplementary Information

## Photoluminescence and electroluminescence of an iridium(III) complex with 2',6'-bis(trifluoromethyl)-2,4'-bipyridine and 2-(5-phenyl-1,3,4-thiadiazol-2-yl)phenol ligands

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**Table S1.** Parameters associated with the single crystal diffraction data collection for **Ir(BTBP)$_2$TDZ**.

| | **Ir(BTBP)$_2$TDZ** |
|---|---|
| Formula | $C_{38}H_{19}F_{12}IrN_6OS$ |
| Formula weight | 1027.85 |
| T (K) | 296(2) |
| Wavelength (Å) | 0.71073 |
| Crystal system | Monoclinic |
| Space group | $P2_1/n$ |
| *a* (Å) | 10.5833(4) |
| *b* (Å) | 24.6297(8) |
| *c* (Å) | 15.5661(5) |
| *α* (deg) | 90.00 |
| *β* (deg) | 102.3490(10) |
| *γ* (deg) | 90.00 |
| *V* (Å$^3$) | 3963.6(2) |
| *Z* | 4 |
| $\rho_{calcd}$ (g/cm$^3$) | 1.722 |
| *μ* (Mo Kα) (mm$^{-1}$) | 3.517 |
| *F* (000) | 1992 |
| Range of transm factors (deg) | 1.574-25.009 |
| Reflns collected | 22135 |
| Unique($R_{int}$) | 6990(0.0304) |
| $R_1{}^a$, $wR_2{}^b$ [I > 2s(I)] | 0.0286, 0.0686 |
| $R_1{}^a$, $wR_2{}^b$ (all data) | 0.0358, 0.0707 |
| GOF on $F^2$ | 1.057 |
| CCDC number | 1524694 |

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

GOF = $[(\Sigma w|F_o| - |F_c|)^2/(N_{obs} - N_{param})]^{1/2}$ .

**Table S2.** The table of selected bond lengths and angles of **Ir(BTBP)$_2$TDZ**.

| Selected Bond | Bond Length (Å) | Selected Angle | Bond Angle (°) |
|---|---|---|---|
| Ir(1)-C(1) | 2.022(4) | C(22)-Ir(1)-C(1) | 99.02 (16) |
| Ir(1)-C(22) | 2.020(4) | C(22)-Ir(1)-N(3) | 80.46 (17) |
| Ir(1)-N(3) | 2.032(3) | C(1)-Ir(1)-N(3) | 101.88 (15) |
| Ir(1)-N(2) | 2.049(3) | C(22)-Ir(1)-N(2) | 105.59 (16) |
| Ir(1)-N(1) | 2.125(3) | C(1)-Ir(1)-N(2) | 80.94 (14) |
| Ir(1)-O(1) | 2.110(3) | N(3)-Ir(1)-N(2) | 172.96 (13) |
| | | C(22)-Ir(1)-N(1) | 90.94 (15) |
| | | C(1)-Ir(1)-N(1) | 168.81 (14) |
| | | N(3)-Ir(1)-N(1) | 84.70 (13) |
| | | N(2)-Ir(1)-N(1) | 91.53 (12) |
| | | C(22)-Ir(1)-O(1) | 171.25 (14) |
| | | C(1)-Ir(1)-O(1) | 85.61 (14) |
| | | N(3)-Ir(1)-O(1) | 91.35 (13) |
| | | N(2)-Ir(1)-O(1) | 82.40 (12) |
| | | N(1)-Ir(1)-O(1) | 85.20 (12) |

**Table S3.** Electrochemical data of **Ir(BTBP)$_2$TDZ**.

| Complex | $E_{ox}$ (V) [a] | $E_{red}$ (V) | HOMO (eV) [b] | LUMO (eV) | $E_g$ (eV) |
|---|---|---|---|---|---|
| **Ir(BTBP)$_2$TDZ** | 0.93 | -1.42 | -5.58 | -3.04 | 2.54 |

[a] Oxidation potential measured in solution at 0.05 mV/s.

[b] The HOMO energy levels were calculated from the equation: HOMO (eV) = $E_{ox}$ - $E^{+}_{Fc}{}^{+}/Fc$ + 4.8.

**Table S4.** Percentage distributions of HOMO and LUMO in **Ir(BTBP)$_2$TDZ**.

| Complex | Orbital | Energy/eV (Calculated) | $E_{gap}$/eV (Calculated) | Composition (%) | | |
|---|---|---|---|---|---|---|
| | | | | Ir | BTBP | TDZ |
| **Ir(BTBP)$_2$TDZ** | HOMO | -5.493 | 3.301 | 14.73 | 5.31 | 79.96 |
| | LUMO | -2.192 | | 1.39 | 41.77 | 56.84 |