# Supporting Information

# Phenothiazine and phenothiazine sulfone derivatives: AIE, HTMs for doping free fluorescent and multiple-resonance TADF OLEDs

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## Contents

## General methods

Chemicals were used as received unless otherwise indicated. All oxygen or moisture sensitive reactions were performed under a nitrogen/argon atmosphere. $^{1}$H NMR (500 MHz) and $^{13}$C NMR (126 MHz) spectra were recorded on a Bruker 500 MHz FT-NMR spectrometer at room temperature. $^{1}$H NMR chemical shifts are reported in parts per million (ppm) relative to the solvent residual peak ($CDCl_3$, 7.26 ppm). Multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) and the coupling constants, *J*, are given in hertz. $^{13}$C NMR chemical shifts are reported relative to the solvent residual peak ($CDCl_3$, 77.0 ppm). UV-visible absorption spectra were recorded on a PerkinElmer Lambda 35 instrument. Emission spectra were taken in a Fluoromax-4C, S/n.1579D-1417- FM Fluorescence software Ver 3.8.0.60. The relative quantum yields in solution were calculated using Quinine sulphate in 0.5 M $H_2SO_4$ as standard for **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$** and **$PTZO_2$-$(TPE)_2$**. All the measurements were carried out at 25 °C. HRMS was recorded with a Bruker-Daltonics micrOTOF-Q II mass spectrometer.

## Optical characterization

Ultraviolet-visible (UV-Vis) absorbance spectra of the films of the compounds were recorded Perkin Elmer Lambda 35 spectrometer. Toluene solutions (1 mg/ml) were drop casted on the quartz substrates for photophysical measurements (Figure S$$). The photoluminescence spectra of the solid state of the materials and doped in ZEONEX were measured in air and vacuum at room temperature by Edinburgh Instruments' FLS980 Fluorescence Spectrometer with a excitation wavelength of 340 nm. Photoluminescence quantum yields (PLQY) of the compounds in solid state (spin coated on quartz) and in toluene were obtained using the integrated sphere. PL decay curves were measured by utilizing the PicoQuant LDH-D-C-375 laser (wavelength 374 nm) as the excitation source. Since the PL decay was fitted with two $\tau$

components the average lifetime was calculated using the intensity average lifetime Equation (1): [52]

$$<\tau>_f = \frac{\int_0^x t \sum a_i exp(-t/\tau_i) dt}{\int_0^x \sum a_i exp(-t/\tau_i) dt} = \frac{\sum a_i \tau_i^2}{\sum a_i \tau_i} \quad (1)$$

**Thermal characterization**

Thermal properties of the synthesized compounds were analysed using differential scanning calorimetry (DSC) technique performed with Perkin Elmer DSC 8500 equipment at heating and cooling rates of 10°C/min under nitrogen atmosphere. An empty aluminum pan was used as a reference. Thermogravimetric analysis (TGA) was performed using Perkin Elmer TGA 4000 apparatus at a heating rate of 20°C/min under nitrogen atmosphere. Melting points were measured by MEL-TEMP (Electrothermal) melting point apparatus.

**Ionization potential**

Ionization potential ($IP^{PE}$) of the solid samples were estimated by electron photoemission spectrometry in air. The samples were vacuum-deposited ($2\times10^{-6}$ mbar) onto fluorine doped tin oxide (FTO) coated glass substrates, exploiting setup consisting of ASBN-D130-CM deep UV deuterium light source, CM110 1/8m monochromator and 6517B Keithley electrometer**.** Photoelectron emission spectra was recorded exciting the samples from low energy to high energy with the step of 1 nm and recording electron photoemission current at different excitation energies.

For charge mobilities, time of flight technique (TOF) was used. The samples were vacuum-deposited ($2\times10^{-6}$ mbar) onto indium doped tin oxide (ITO) coated glass substrates. The TOF

setup contains a laser (EKSPLA NL300) used for excitation at 355 nm wavelength. For electron and hole transport in deposited layers at different electric fields, a variety of positive external voltages (U) were applied. TDS 3032C oscilloscope (Tektronix) was used to record the photocurrent transients of holes or electrons.

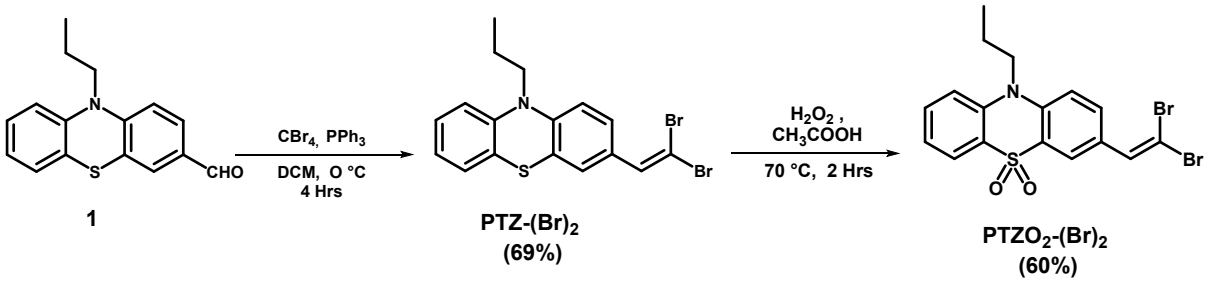
**Electrochemical properties**

Electrochemical properties of the compounds in solution were studied using cyclic voltammetry (CV) technique. Micro-Autolab III (Metrohm Autolab) potentiostat-galvanostat equipped with a standard three-electrode configuration consisting of a glassy carbon working electrode, an $Ag/Ag^{+}$ reference electrode, and a platinum wire counter electrode. Compounds and ferrocene were dissolved in a solution containing 0.1 M tetrabutylammonium hexafluorophosphate ($TBAF_6$) as the supporting electrolyte and dry dichloromethane solvent under nitrogen atmosphere at room temperature. CV measurements were performed with a scan rate of 0.1 V/s. The measurements were calibrated using ferrocene/ferrocenium (Fc) system, as an internal standard.

**OLEDs**

Electroluminescent devices were fabricated using vacuum deposition ($2\times10^{-6}$ mbar) of organic and metal layers onto pre-cleaned ITO coated glass substrates. Density-voltage and luminance-voltage characteristics were recorded using photodiode PH100-Si-HA-D0 together with the PC-based power and energy Monitor 11S-LINK and Keithley 2400C source meter. Electroluminescence (EL) spectra were recorded by Avantes AvaSpec-2048XL spectrometer.

## Synthetic Scheme




**Scheme S1**. Synthesis of intermediates **PTZ-(Br)$_2$** and **PTZO$_2$-(Br)$_2$**.

The intermediates **PTZO$_2$-(Br)$_2$** and **PTZ-(Br)$_2$** were synthesized according to the literature procedure. (Ref. S1 and Ref. S2). The boronate ester derivatives of phenothiazine and tetraphenylethylene (**PTZ-Bpin** and **TPE-Bpin)** were synthesized according to the literature procedure. (Ref. S3 and Ref. S4).

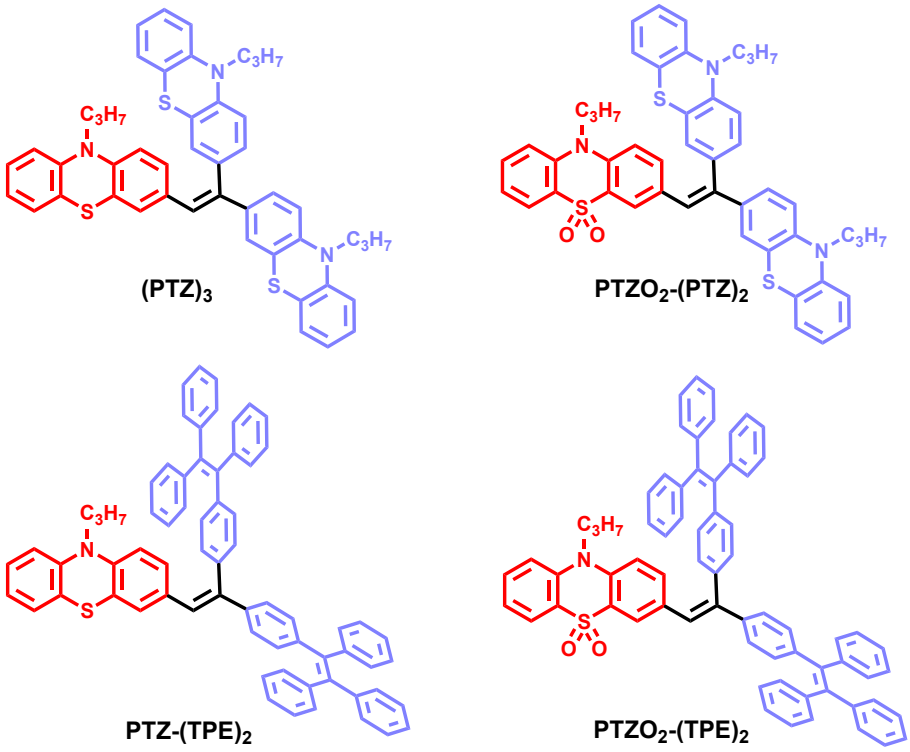


**Chart S1**. Chemical structures of phenothiazine and tetraphenylethylene based luminogens **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$**.

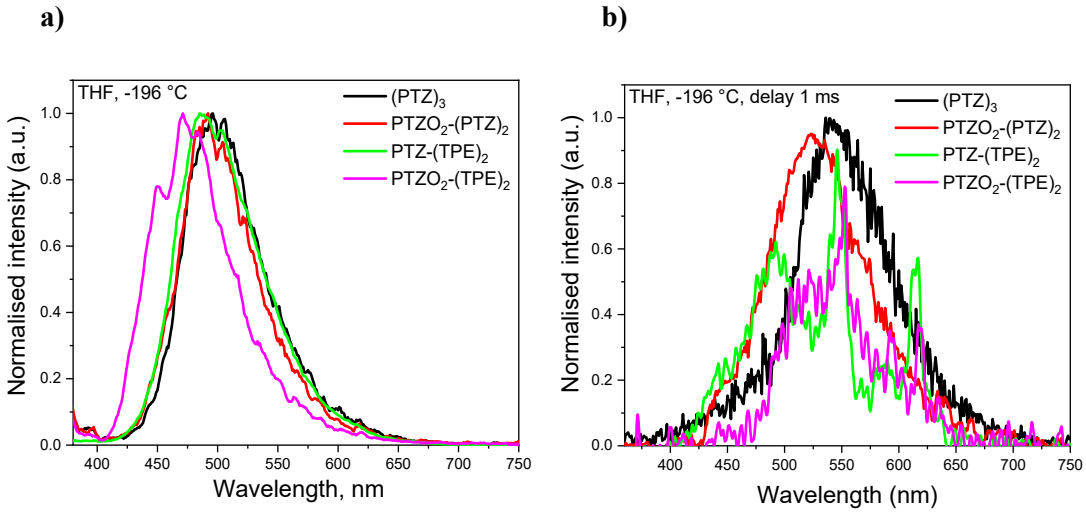



Fig. S1. Normalized PL (a) and phosphorescence (b) spectra of the frozen THF solutions of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** recorded at -196 °C ($\lambda_{ex}$ = 340 nm).

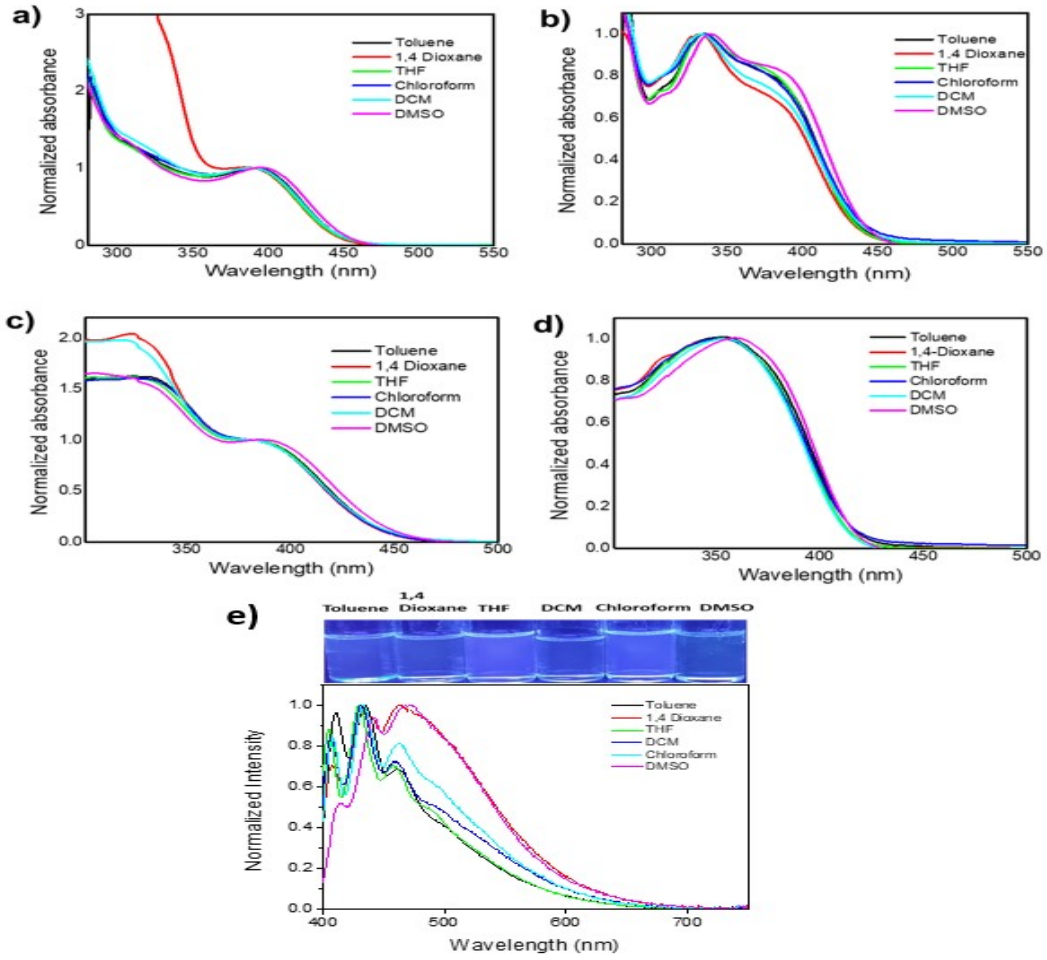


**Fig. S2** Normalized absorbance spectra of (a) **$(PTZ)_3$**, (b) **$PTZO_2$-$(PTZ)_2$**, (c) **PTZ-$(TPE)_2$** and (d) **$PTZO_2$-$(TPE)_2$** in different polarity solvents, (e) normalized emission spectra of **$PTZO_2$-$(TPE)_2$** in different polarity solvents.

**Table S1** Photophysical properties of compounds **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$**.

| Compounds | Solvent | $\lambda_{ab}$(nm)[a] | $\lambda_{em}$(nm)[a] | Stokes shift ($cm^{-1}$) | $\phi_f$[b] |
|---|---|---|---|---|---|
| **$(PTZ)_3$** | Toluene | 391 | 530 | 6708 | 0.38 |
| | 1,4-Dioxane | 387 | 533 | 7078 | 0.50 |
| | THF | 387 | 536 | 7183 | 0.37 |
| | Chloroform | 391 | 536 | 6919 | 0.34 |
| | DCM | 387 | 546 | 7524 | 0.36 |
| | DMSO | 394 | 563 | 7619 | 0.49 |
| **$PTZO_2$-$(PTZ)_2$** | Toluene | 334 | 512 | 10409 | 0.20 |
| | 1,4-Dioxane | 332 | 516 | 10741 | 0.18 |
| | THF | 333 | 532 | 11234 | 0.15 |
| | Chloroform | 334 | 532 | 11144 | 0.15 |
| | DCM | 333 | 545 | 11682 | 0.20 |
| | DMSO | 338 | 577 | 3060 | 0.24 |
| **PTZ-$(TPE)_2$** | Toluene | 383 | 536 | 7453 | 0.39 |
| | 1,4-Dioxane | 382 | 541 | 7694 | 0.31 |
| | THF | 382 | 559 | 8289 | 0.27 |
| | Chloroform | 385 | 547 | 7693 | 0.35 |
| | DCM | 385 | 563 | 8213 | 0.27 |
| | DMSO | 385 | 600 | 9308 | 0.19 |
| **$PTZO_2$-$(TPE)_2$** | Toluene | 354 | - | - | - |
| | 1,4-Dioxane | 352 | - | - | - |
| | THF | 354 | - | - | - |
| | Chloroform | 353 | - | - | - |
| | DCM | 354 | - | - | - |

| | | | | | |
|---|---|---|---|---|---|
| | DMSO | 360 | - | - | - |

([a] absorption and emission maxima were recorded in different polarity solvents, [b] the fluorescence quantum yields were measured using Quinine sulphate in 0.5 M $H_2SO_4$ as standard for **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$** and **$PTZO_2$-$(TPE)_2$**).

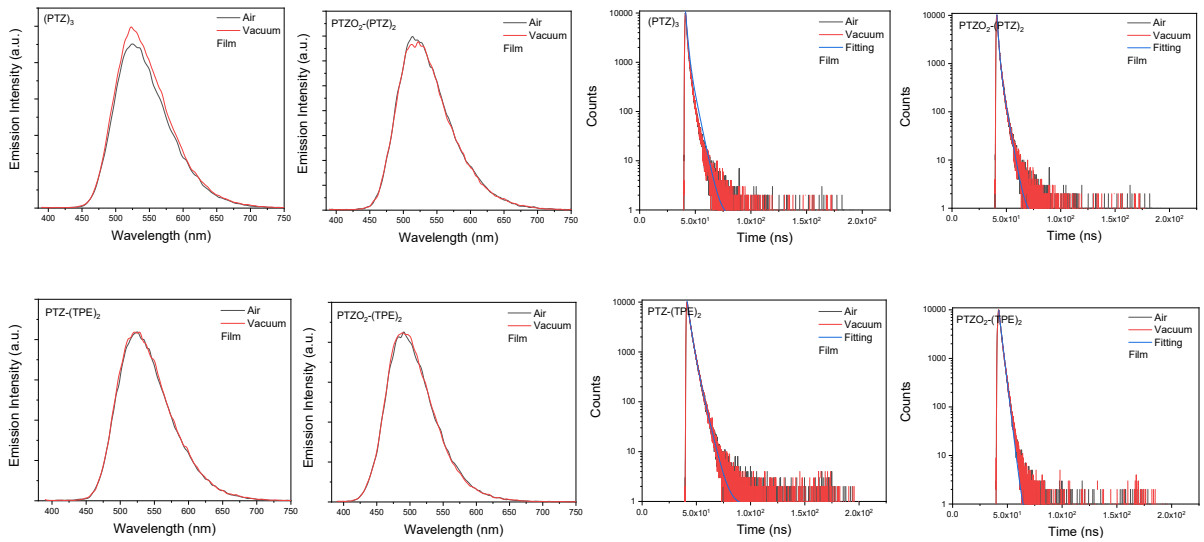
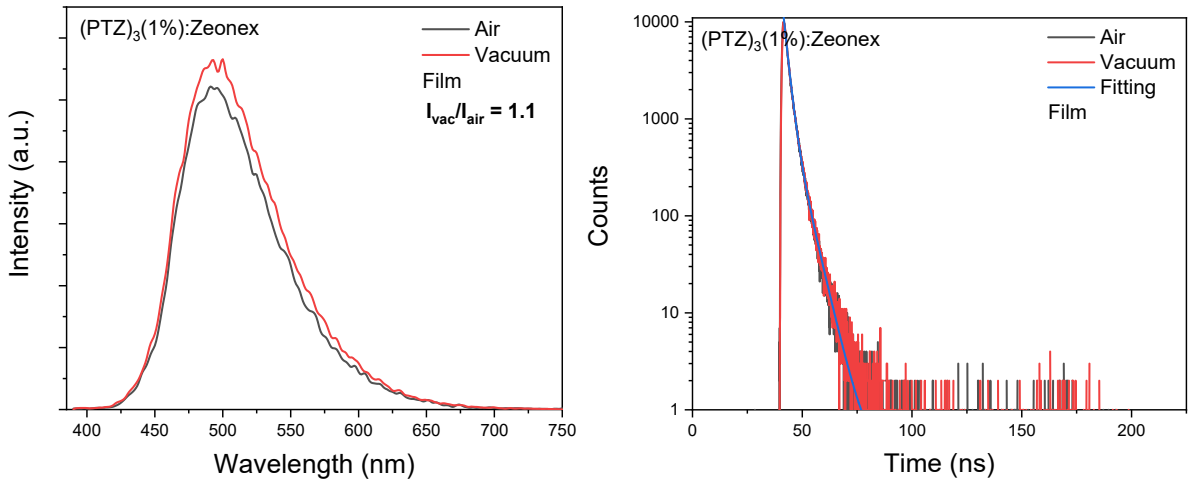



**Fig. S3** (a) PL spectra and (b) PL decay of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** on glass substrate in air and vacuum.



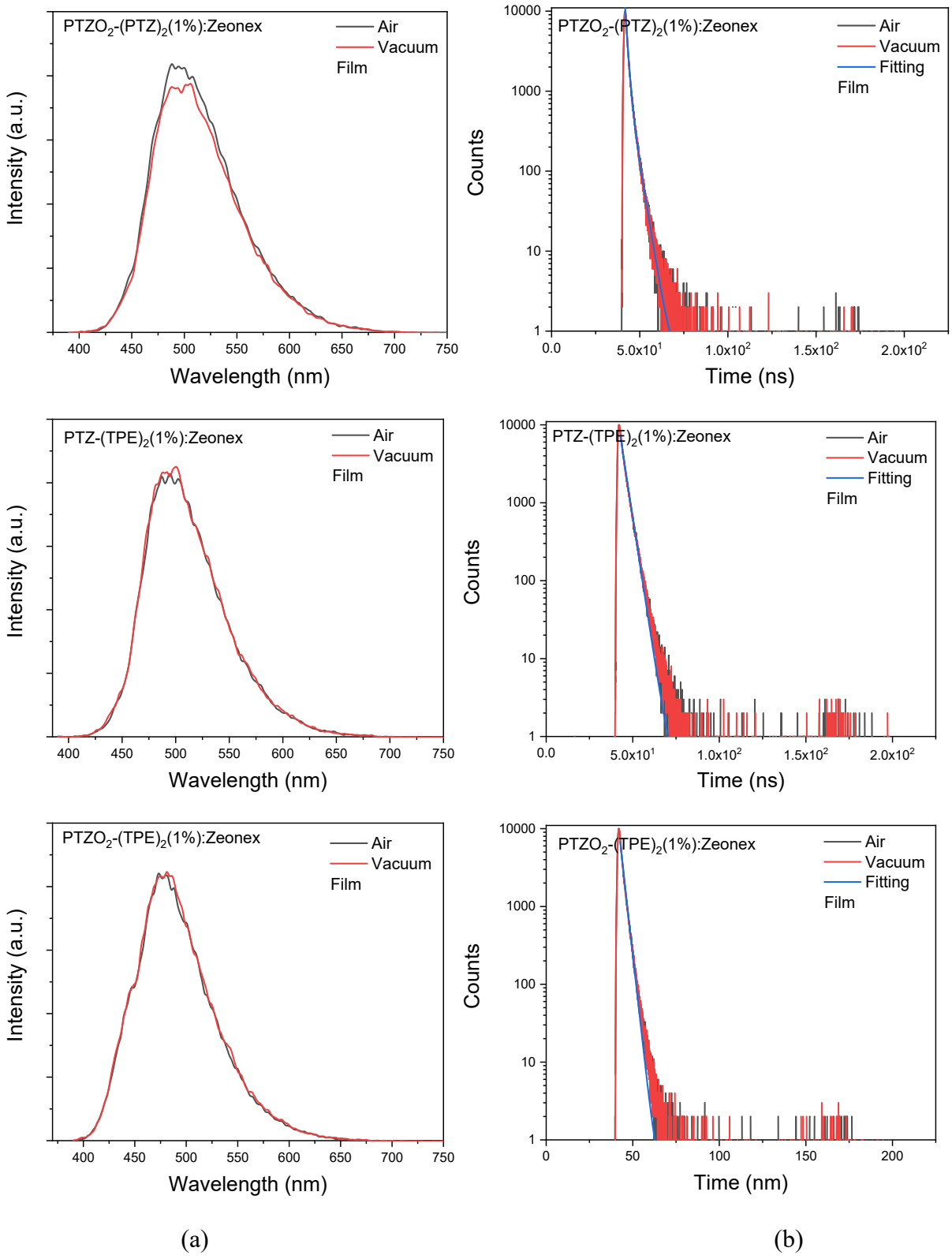
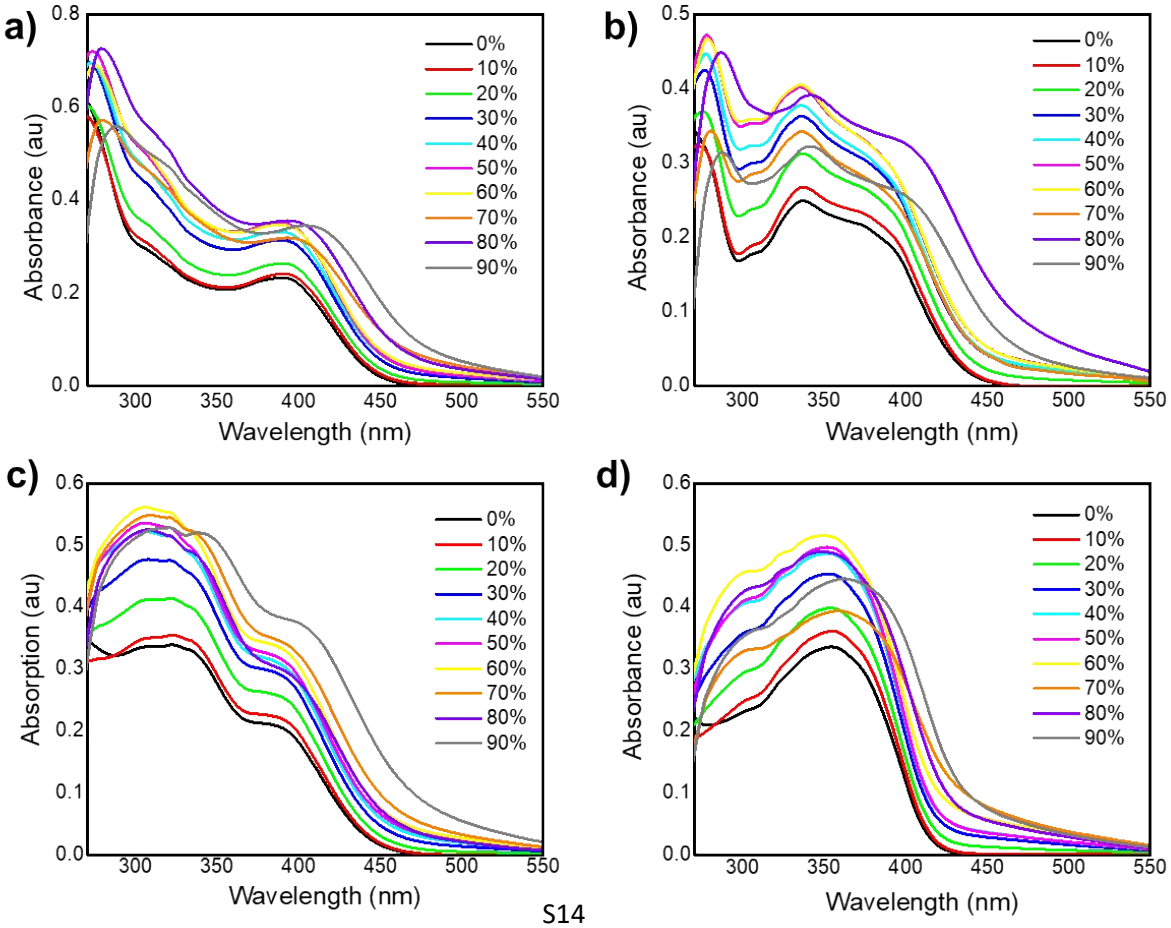



**Fig. S4** (a) PL spectra and (b) PL decay of the compounds (1wt%) in ZEONEX on glass substrate in air and vacuum.

**Table S2.** Intensity averaged lifetime.

| Parameters | Compounds | | | |
|---|---|---|---|---|
| | $(PTZ)_3$ | $PTZO_2(PTZ)_2$ | $PTZ(TPE)_2$ | $PTZO_2(TPE)_2$ |
| $A_1$ | 9017.233 | 9110.058 | 7823.938 | 9950.755 |
| $\tau_1$ (ns) | 1.3525 | 1.1106 | 2.4278 | 2.3012 |
| $A_2$ | 1985.008 | 1737.818 | 3000.473 | - |
| $\tau_2$ (ns) | 3.9742 | 3.375 | 4.8067 | - |
| $\sum A_i\tau_i^2$ | 47846.57 | 31031.47 | 115440 | - |
| $\sum A_i\tau_i$ | 20084.63 | 15982.77 | 33417.33 | - |
| $\tau_{avg}$ (ns) | 2.382249 | 1.941558 | 3.454494 | - |
| $X^2$ | 1.05 | 1.01 | 1.02 | 1.00 |
| | Compounds(1%) in ZEONEX | | | |
| $A_1$ | 9839.454 | 9992.021 | 7246.076 | 6920.84 |
| $\tau_1$ (ns) | 1.8284 | 1.1459 | 2.9773 | 2.1785 |
| $A_2$ | 1524.606 | 1636.245 | - | - |
| $\tau_2$ (ns) | 4.5609 | 3.2363 | - | - |
| $\sum A_i\tau_i^2$ | 64608.32 | 30257.83 | - | - |
| $\sum A_i\tau_i$ | 24944.03 | 16745.24 | - | - |
| $\tau_{avg}$ (ns) | 2.590131 | 1.806951 | - | - |
| $X^2$ | 1.08 | 1.00 | 1.19 | 1.00 |



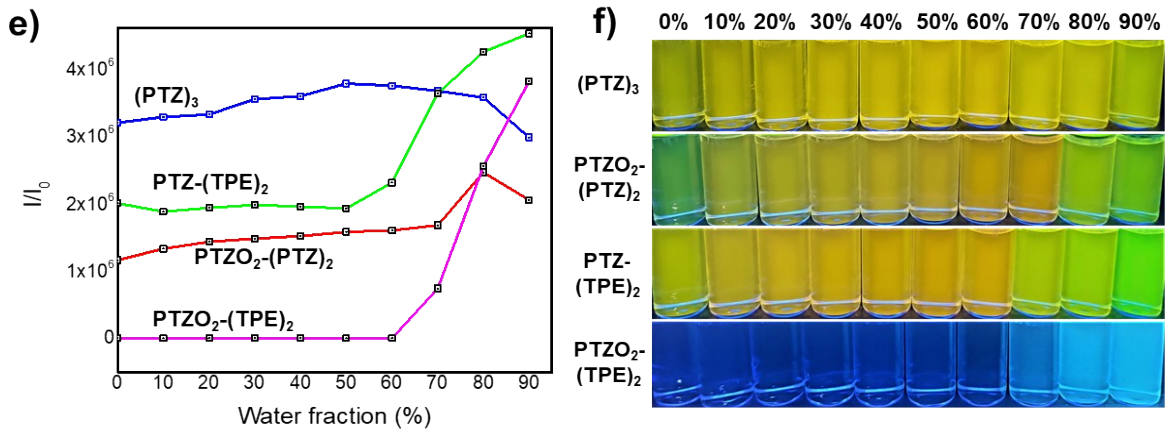



**Fig. S5**. Absorption spectra of (a) **$(PTZ)_3$** (b) **$PTZO_2$-$(PTZ)_2$** (c) **PTZ-$(TPE)_2$** and (d) **$PTZO_2$-$(TPE)_2$** in THF–water mixtures with different water fractions; (e) Plot of fluorescence intensity *vs.* % of water fraction for compounds **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$**; (f) Fluorescence images of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** in different THF–water binary mixtures.

**Table S3.** Fluorescence quantum yields of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** in different THF-water mixtures with increasing water percentage.

| Water Vol % | $\phi_f$[a] | | | |
|---|---|---|---|---|
| | **$(PTZ)_3$** | **PTZO-$(PTZ)_2$** | **PTZ-$(TPE)_2$** | **PTZO-$(TPE)_2$** |
| 0 % | 0.31 | 0.15 | 0.20 | - |
| 10 % | 0.30 | 0.15 | 0.18 | - |
| 20 % | 0.28 | 0.13 | 0.17 | - |
| 30 % | 0.25 | 0.12 | 0.15 | - |
| 40 % | 0.24 | 0.12 | 0.13 | - |
| 50 % | 0.24 | 0.12 | 0.13 | - |
| 60 % | 0.23 | 0.11 | 0.12 | - |
| 70 % | 0.23 | 0.12 | 0.19 | 0.04 |
| 80 % | 0.20 | 0.12 | 0.26 | 0.14 |
| 90 % | 0.16 | 0.12 | 0.22 | 0.21 |

([a] Fluorescence quantum yields recorded using quinine sulphate as a standard in 0.5 M $H_2SO_4$ solution.)

## Computational analysis

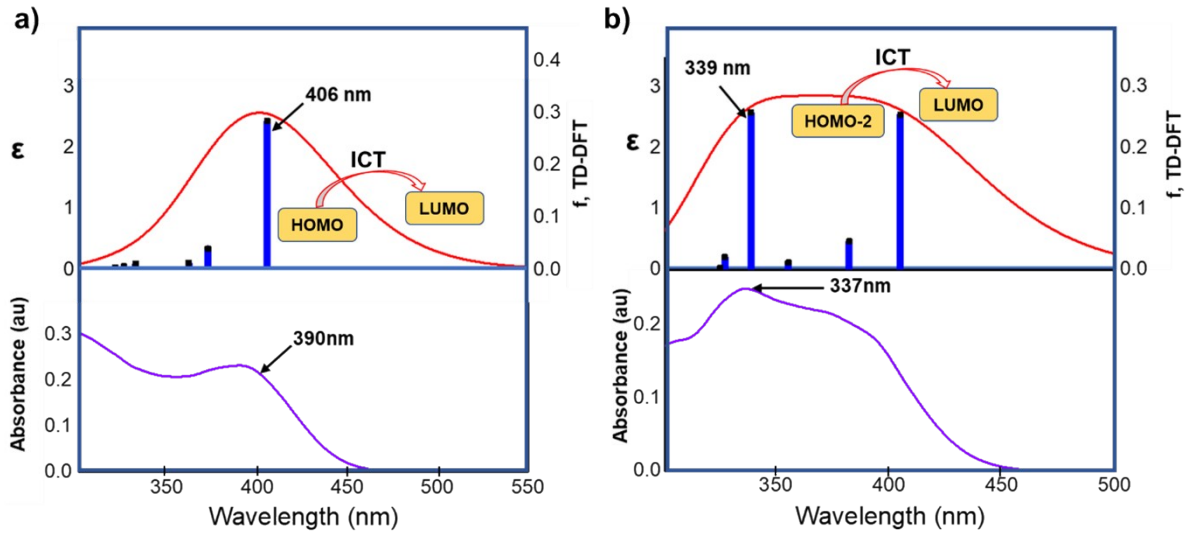



**Fig. S6**. Comparison of the simulated absorption spectra of (a) **$(PTZ)_3$** and (b) **$PTZO_2$-$(PTZ)_2$** generated from DFT and TD-DFT calculations (top) with their experimental absorption spectra recorded at room temperature in THF ($10^{-5}$ M) (bottom).

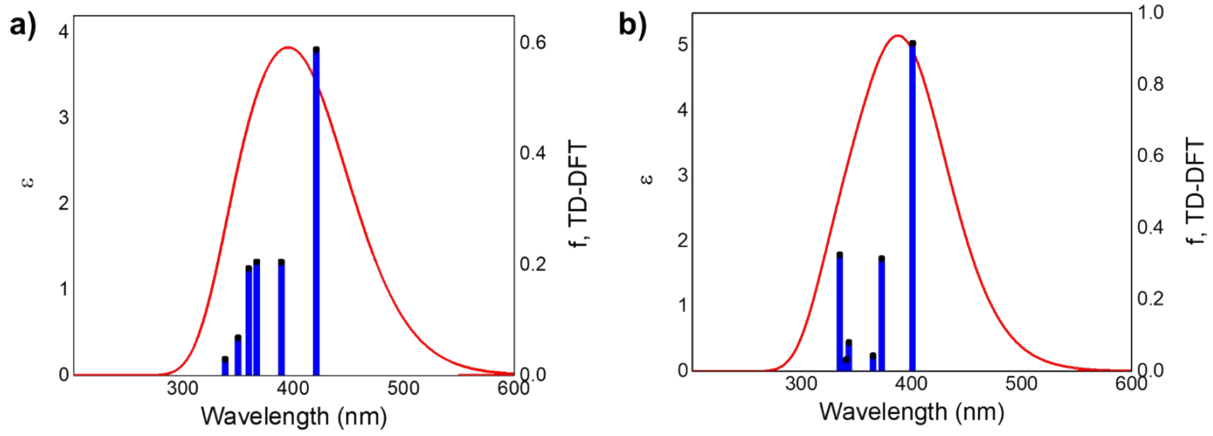


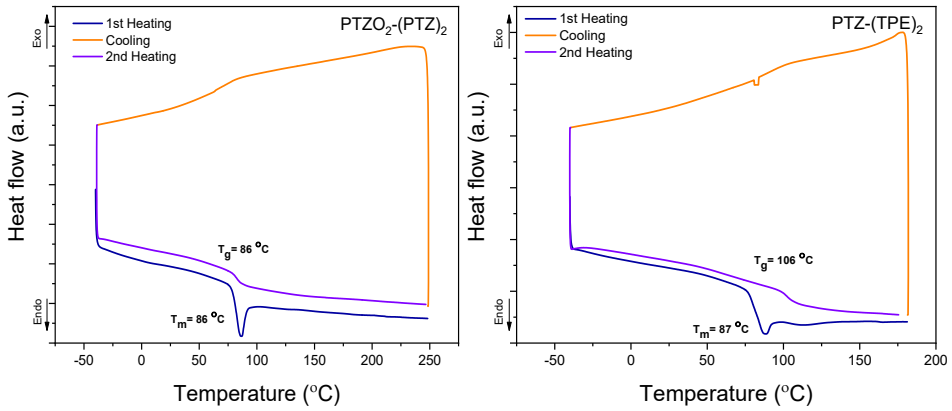

**Fig. S7**. Simulated absorption spectra of (a) **PTZ-$(TPE)_2$** and (b) and **$PTZO_2$-$(TPE)_2$** generated from DFT and TD-DFT calculations.

**Table S4**. Calculated major electronic transitions for **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** in the gas phase.

| Compounds | Wavelength (nm) | Composition | Assignment | $f^a$ |
|---|---|---|---|---|
| **$(PTZ)_3$** | 406 | HOMO→LUMO (0.70) | ICT | 0.57 |
| **$PTZO_2$-$(PTZ)_2$** | 339 | HOMO-2→LUMO (0.70) | ICT | 0.51 |
| **PTZ-$(TPE)_2$** | 421 | HOMO→LUMO (0.70) | ICT | 0.59 |
| **$PTZO_2$-$(TPE)_2$** | 401 | HOMO→LUMO (0.70) | ICT | 0.92 |

$f^a$ = Oscillatory strength

## Thermal properties



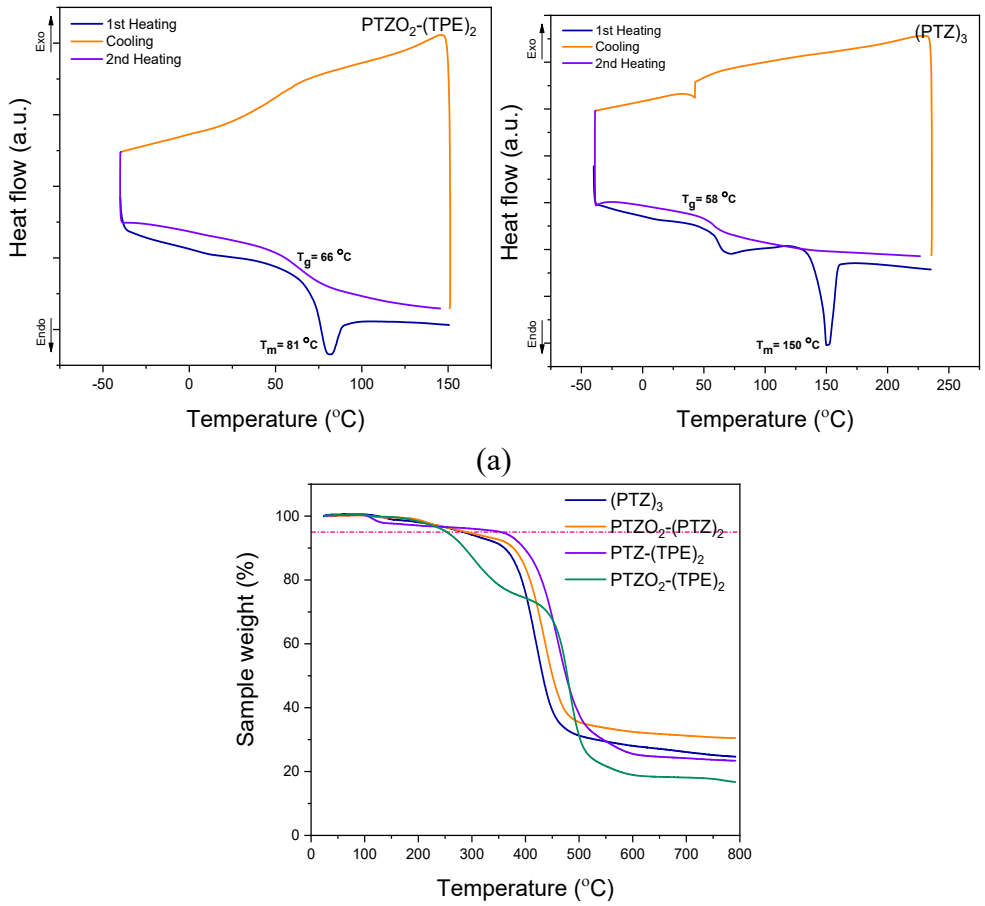



**Fig. S8**. DSC (a) and TGA (b) thermograms of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** recorded at 10 °C $min^{-1}$.

## Cyclic Voltammetry (CV)

The potentials of reduction and oxidation processes were obtained relative to an internal ferrocene reference ($Fc/Fc^+$) (Fig. S10). The $IP_{CV}$ vs Fc values were calculated using equation (1) where the values are 4.98, 5.0, 5.05, and 5.47 eV (vs $Fc/Fc^+$), respectively (Table 3). The and values of **$(PTZ)_3$** and **$PTZO_2$-$(PTZ)_2$** are almost equal because of the PTZ donor moiety.

$$IP_{CV} = -e(E_{ox} + 4.8) \quad (1)$$

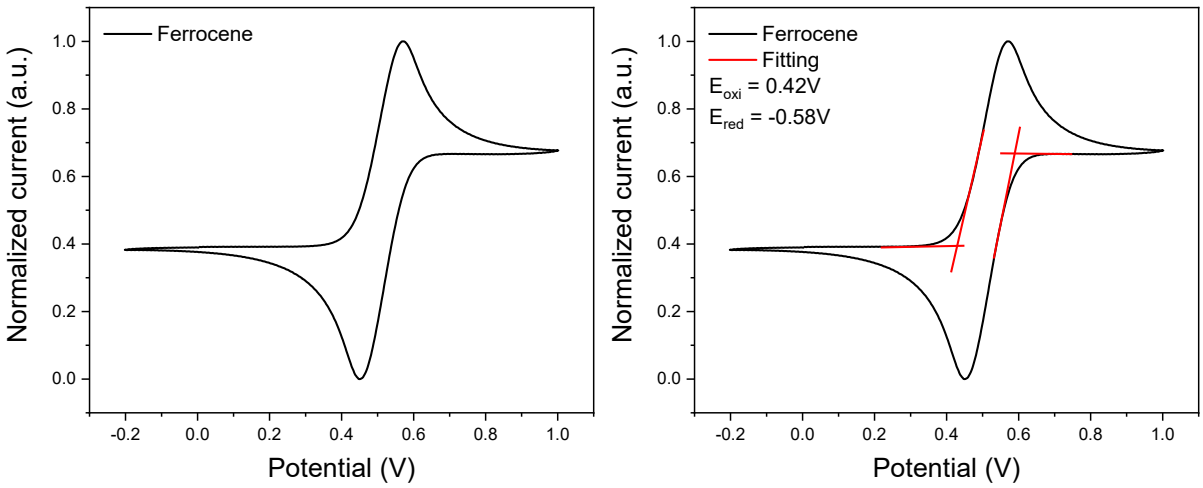
The CV spectra of the compounds indicates that only **$PTZO_2$-$(PTZ)_2$** and **$PTZO_2$-$(TPE)_2$** have reduction potential ($E_{red}$) which is due to the D-A-D structure containing the electron

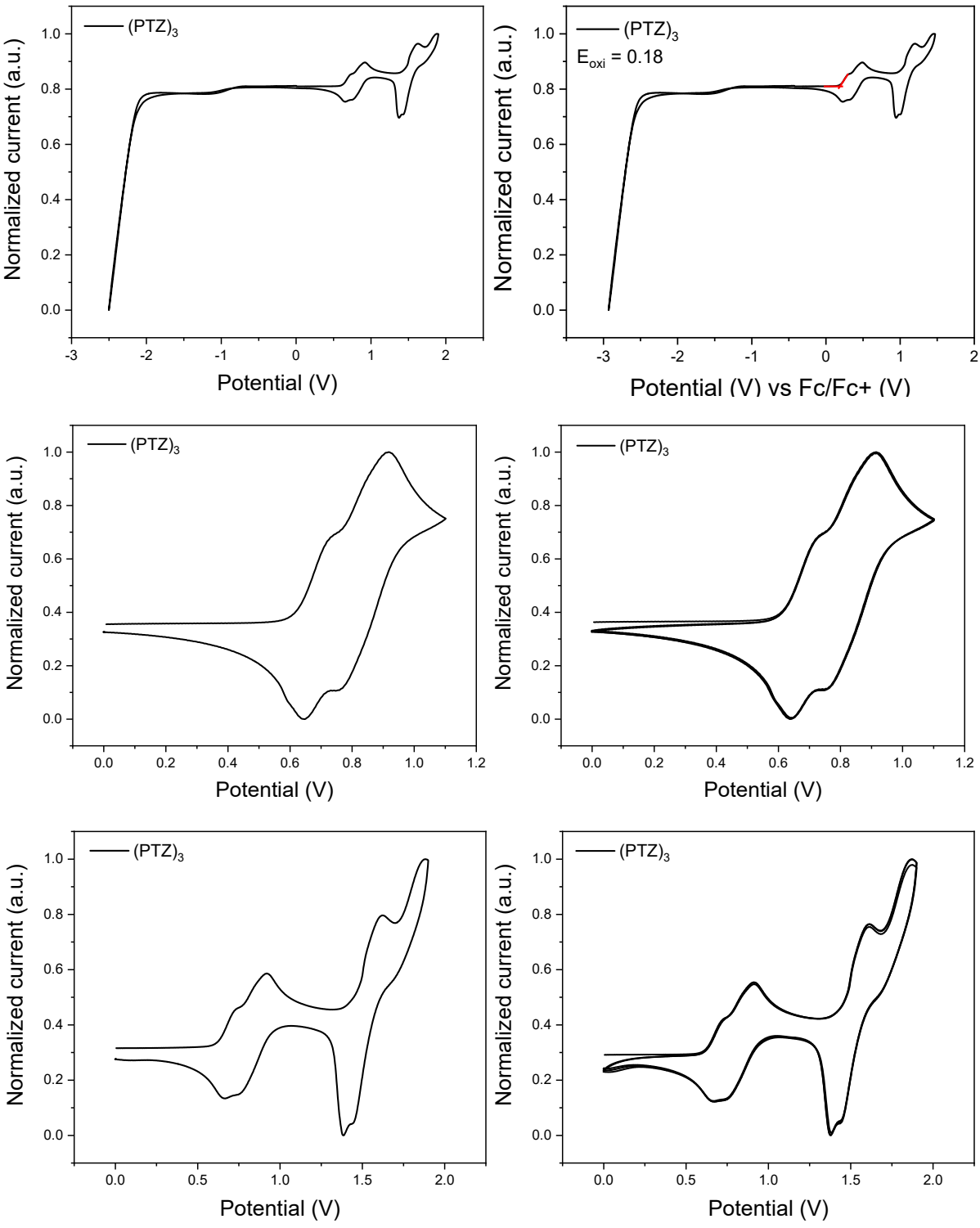
accepting moiety PTZ dioxide. The $EA_{CV}$ values were calculated using Equation (2) and are 3.40eV and 3.52eV, respectively (Table 3).

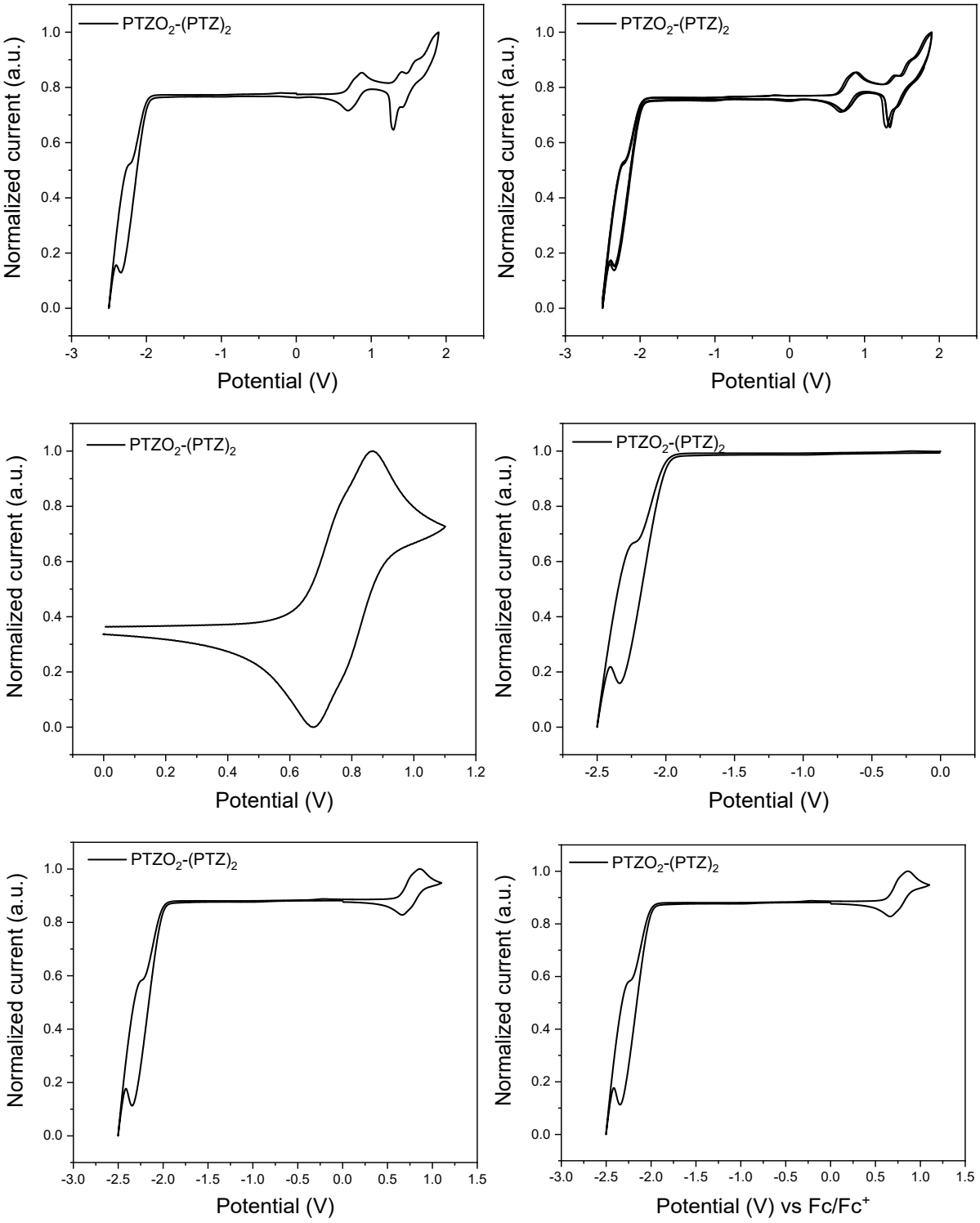
$$EA_{CV} = -e(E_{red} + 4.8) \quad (2)$$

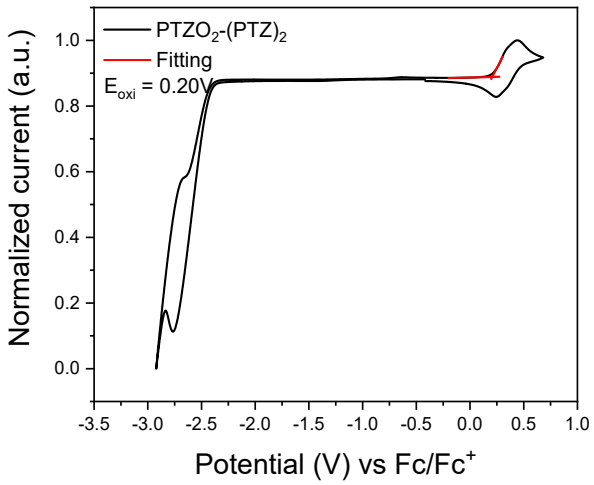
By subtracting $IP_{CV}$ from $EA_{CV}$ it is possible to calculate the gap ($E_{gCV}$). The CV spectra of all the compounds were ran for three cycles, the results indicate reversibility and the stability of the samples in solution.

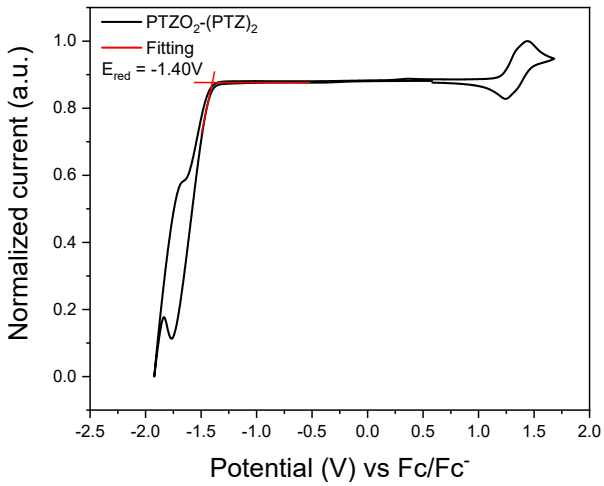
Employing different methods of IP measurements caused small differences between the obtained values that can be explained by different environments in the solution and the solid state. Such small margin of error indicates collaborative electron-donor effect of PTZ donor moiety on electron releasing energy. The absorption band gap of the derivatives has linear effect on the IP values.

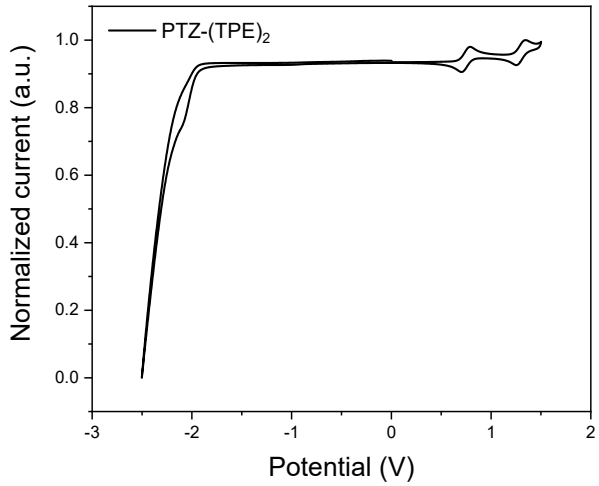


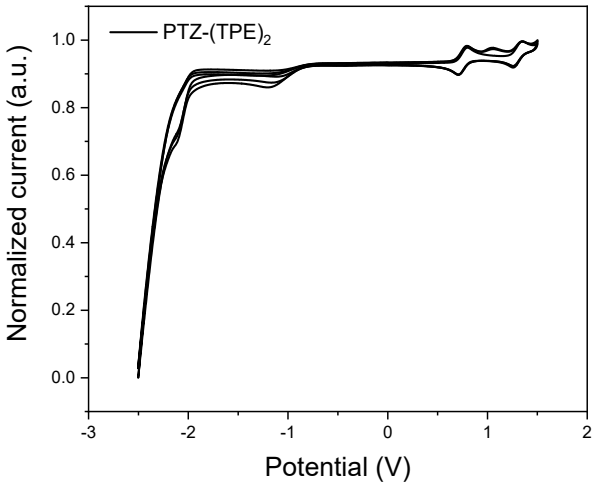

(PTZ)3
Normalized current (a.u.)
Potential (V)
(PTZ)3
Eoxi = 0.18
Normalized current (a.u.)
Potential (V) vs Fc/Fc+ (V)
(PTZ)3
Normalized current (a.u.)
Potential (V)
(PTZ)3
Normalized current (a.u.)
Potential (V)
(PTZ)3
Normalized current (a.u.)
Potential (V)
(PTZ)3
Normalized current (a.u.)
Potential (V)

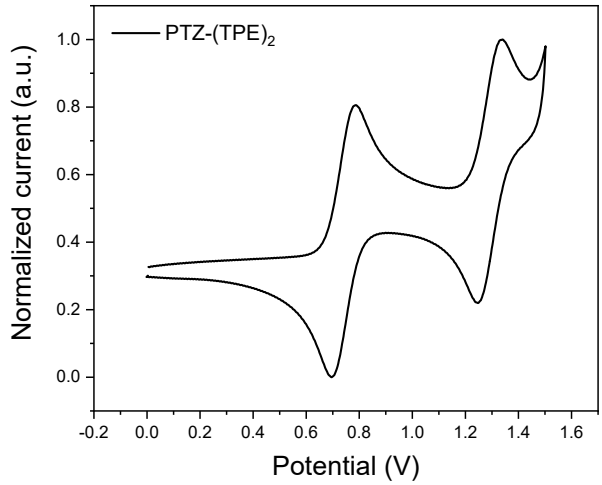

PTZO2-(PTZ)2
Normalized current (a.u.)
Potential (V)
Potential (V) vs Fc/Fc+

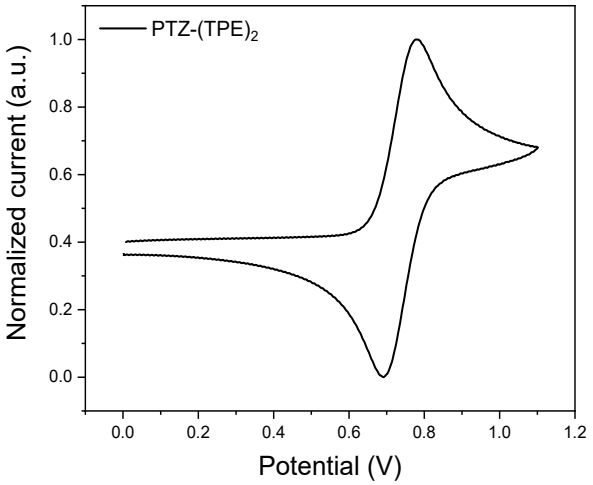

PTZO2-(PTZ)2
Fitting
Eoxi = 0.20V
Normalized current (a.u.)
Potential (V) vs Fc/Fc+


PTZO2-(PTZ)2
Fitting
Ered = -1.40V
Normalized current (a.u.)
Potential (V) vs Fc/Fc-


PTZ-(TPE)2
Normalized current (a.u.)
Potential (V)


PTZ-(TPE)2
Normalized current (a.u.)
Potential (V)


PTZ-(TPE)2
Normalized current (a.u.)
Potential (V)


PTZ-(TPE)2
Normalized current (a.u.)
Potential (V)

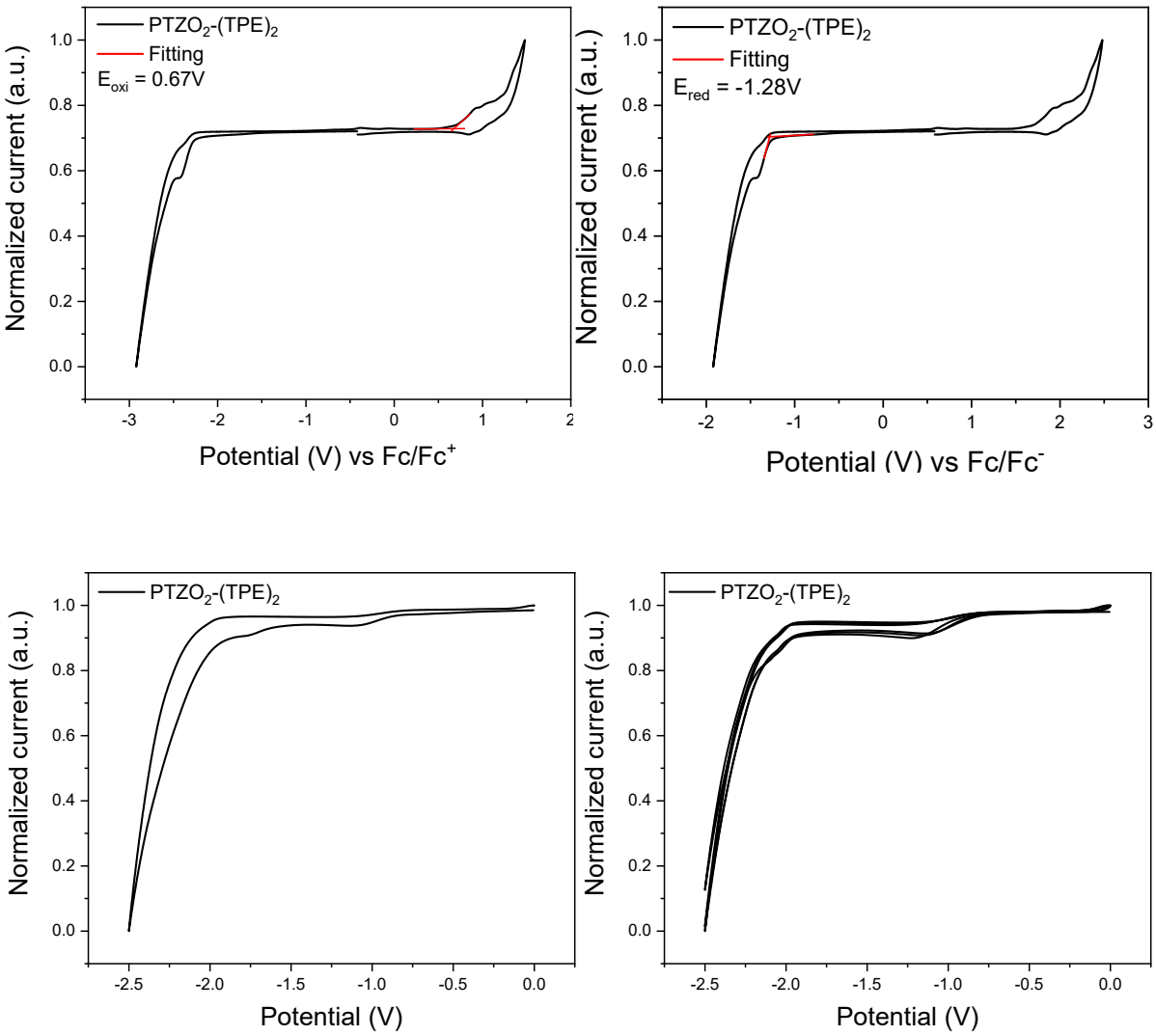



**Fig. S9** Cyclic voltammograms of the Ferrocene and the dilute solutions of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$**, and **$PTZO_2$-$(TPE)_2$** in dichloromethane recorded as sweep rate of 100 mV/s.

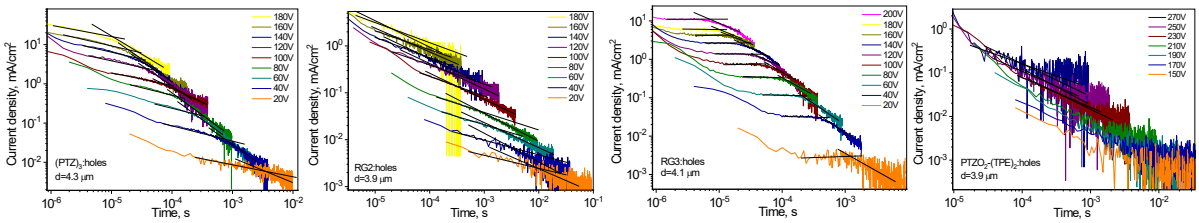



**Fig. S10** Time of flight (TOF) current transients of holes for deposited layers of **$(PTZ)_3$**, **$PTZO_2$-$(PTZ)_2$**, **PTZ-$(TPE)_2$** and **$PTZO_2$-$(TPE)_2$**.

## Device

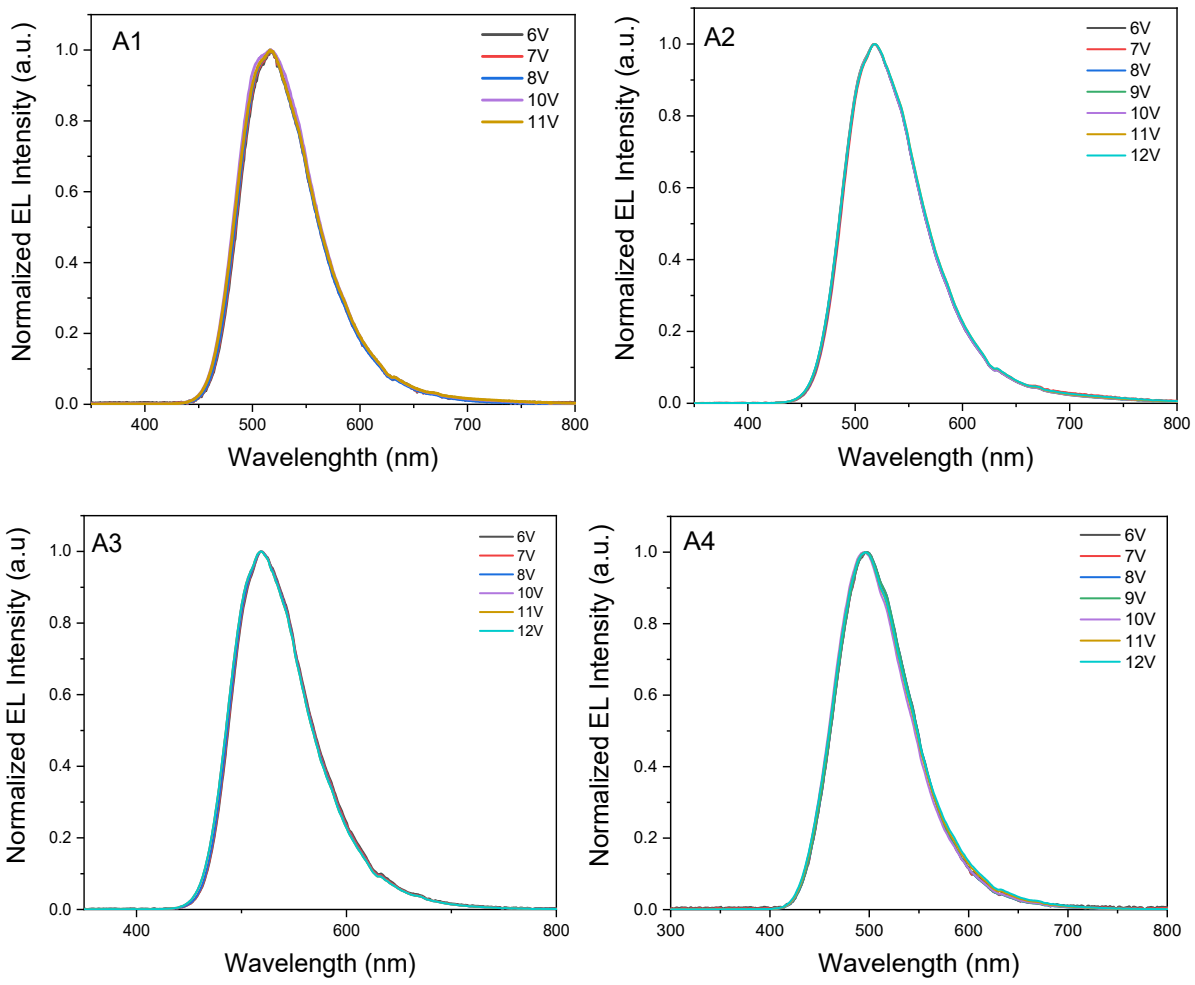



**Fig. S11** EL spectra of devices A1-A4 at different voltages.

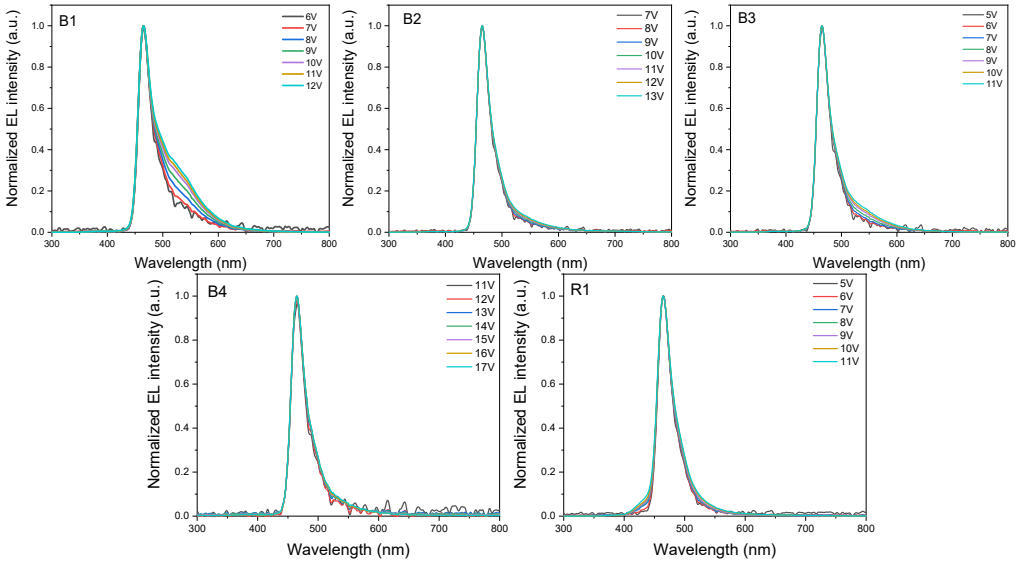



**Fig. S12** EL spectra of devices B1-B4 and R1 at different voltages.

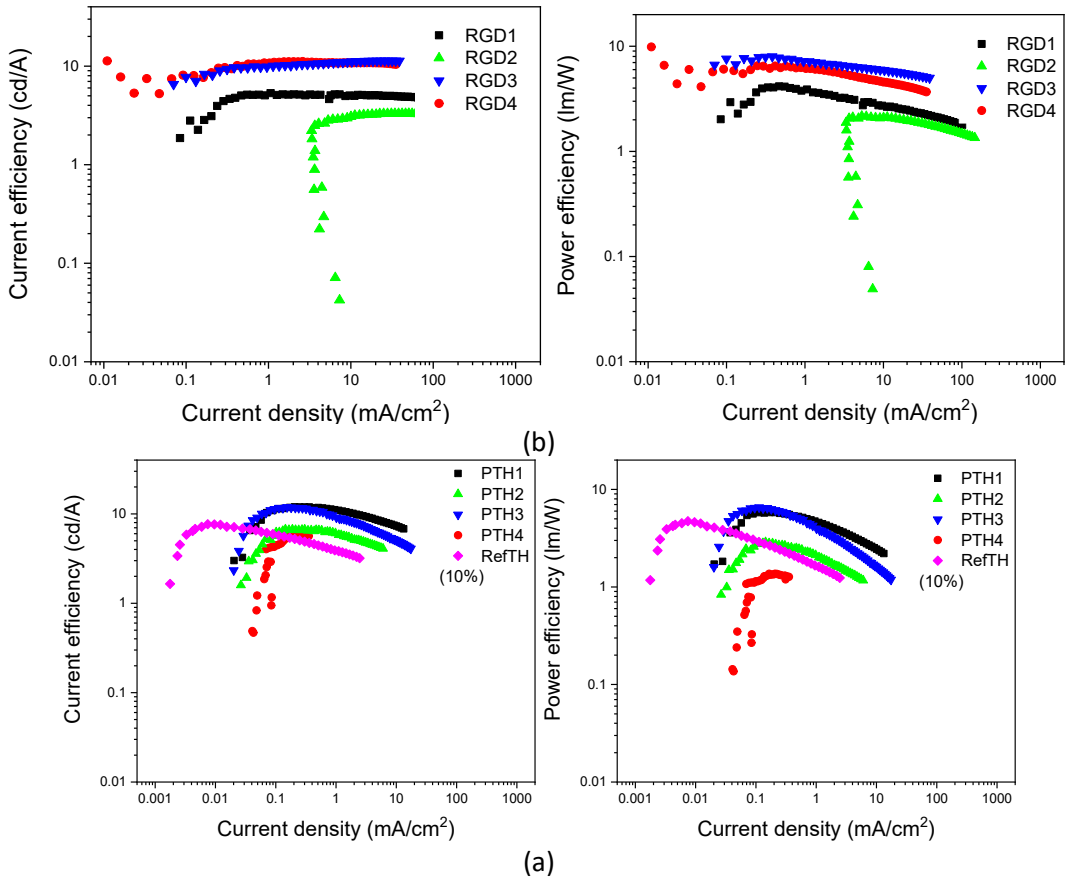



**Fig. S13** Current and power efficiencies of devices A1-A4 (a) and B1-B4, R1 (b).

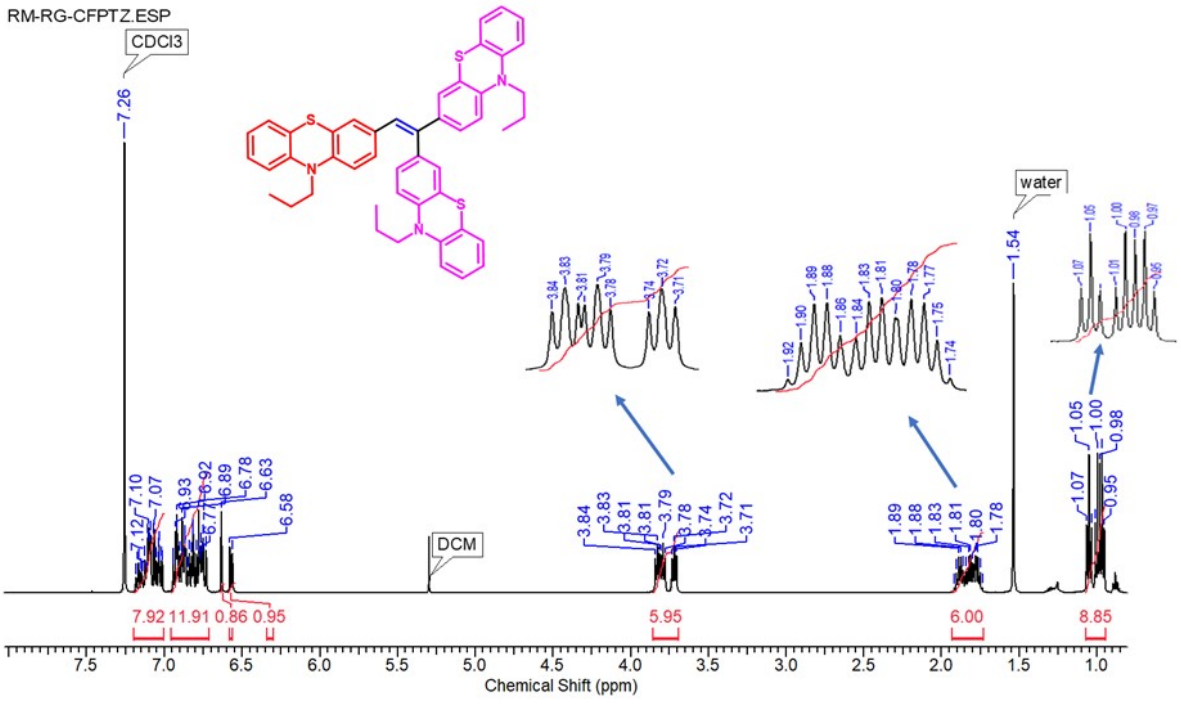


**Fig. S14** $^{1}$H NMR spectra of **(PTZ)$_3$** ($CDCl_3$, 500 MHz).

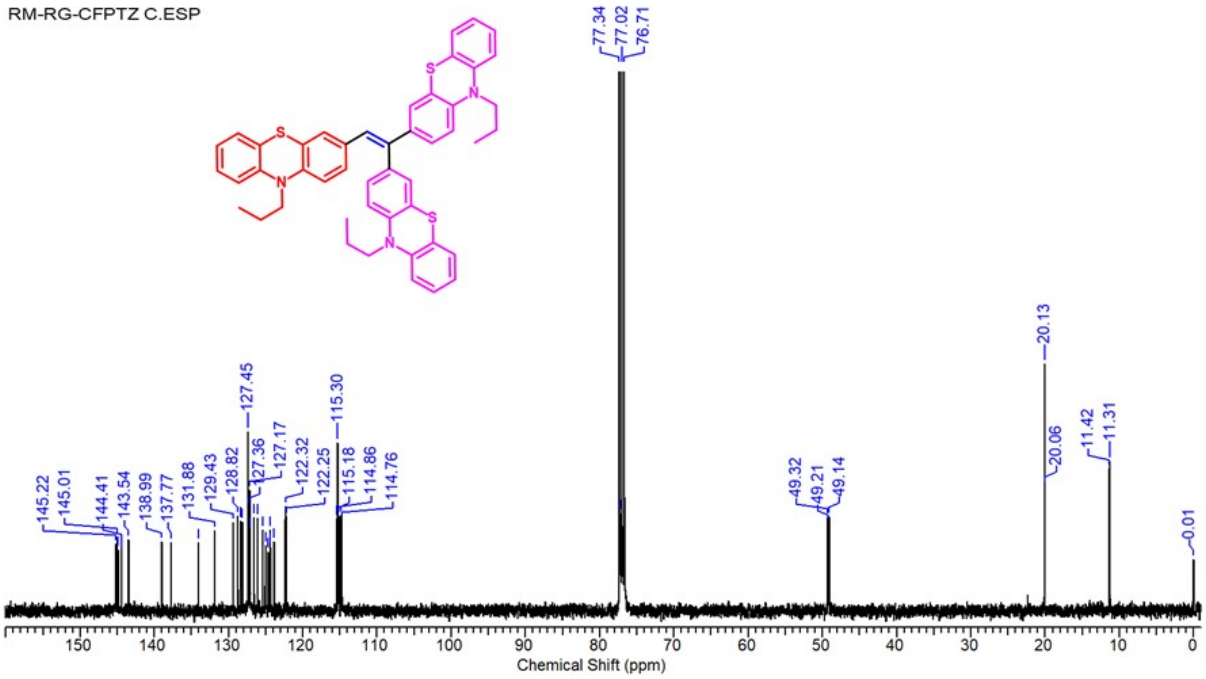



**Fig. S15**. $^{13}$C {$^{1}$H} NMR spectra of **(PTZ)$_3$** ($CDCl_3$, 126 MHz).

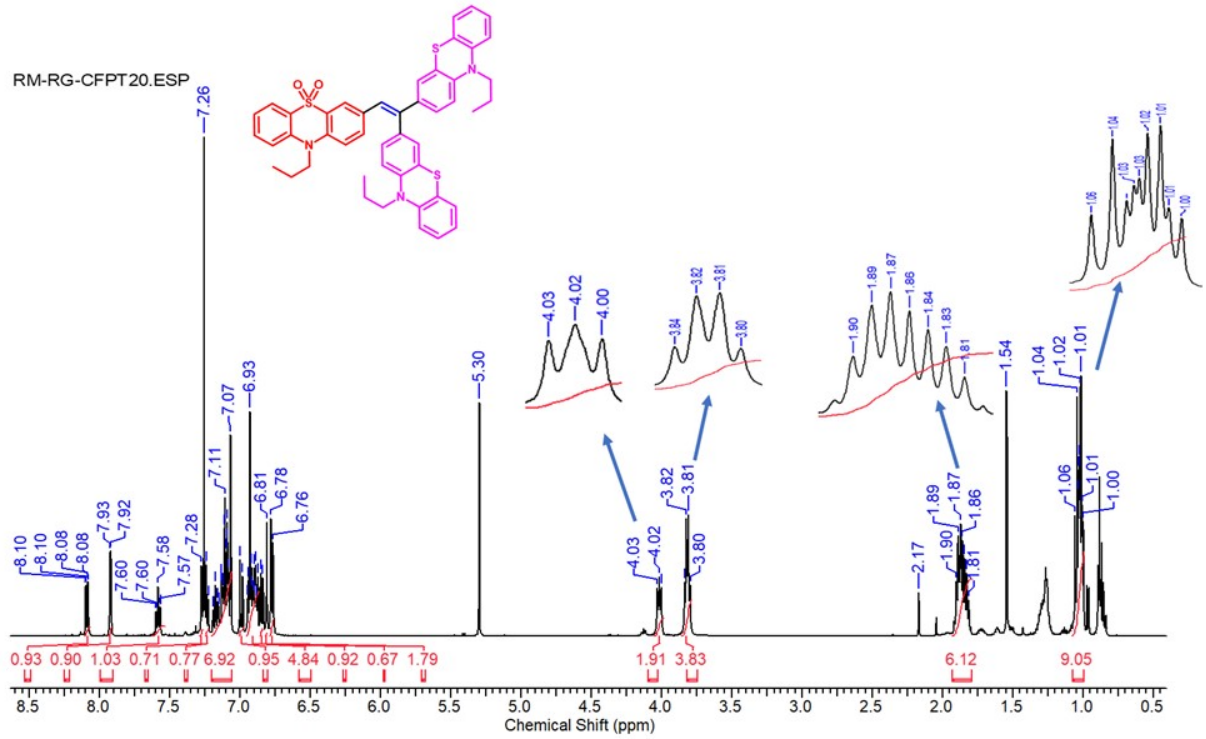



**Fig. S16**. $^{1}$H NMR spectra of **PTZO$_2$-(PTZ)$_2$** ($CDCl_3$, 500 MHz).

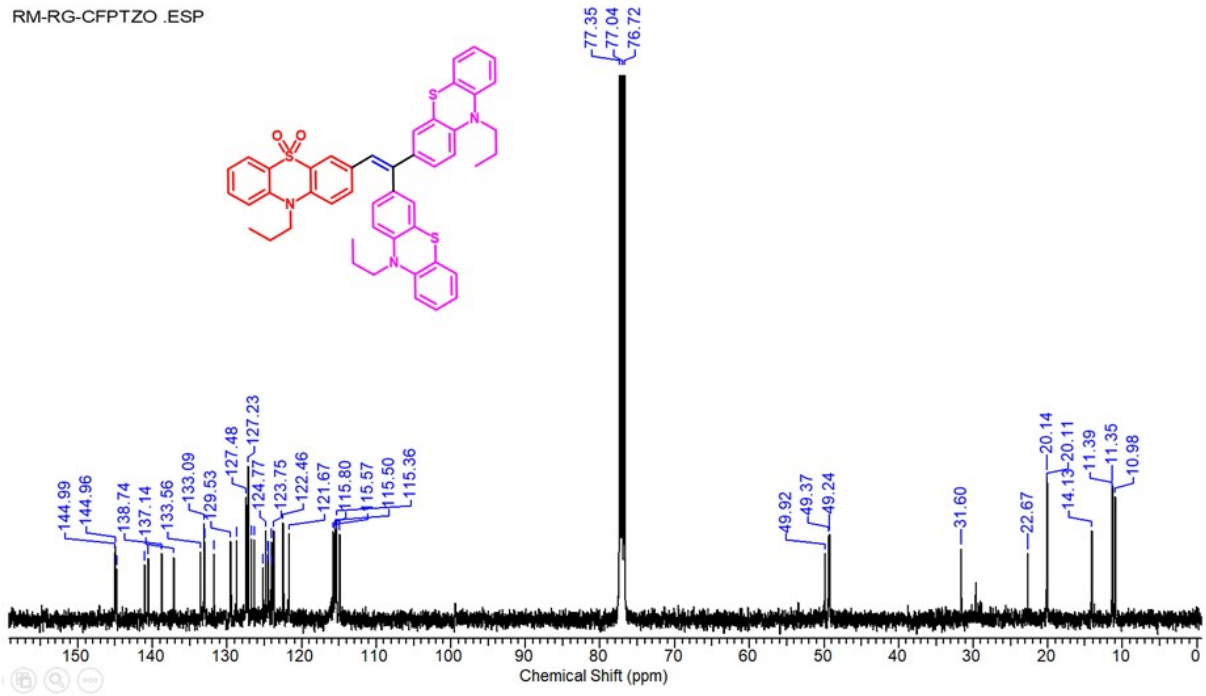



**Fig. S17**. $^{13}C$ {$^{1}H$} NMR spectra of **$PTZO_2$-$(PTZ)_2$** ($CDCl_3$, 126 MHz).

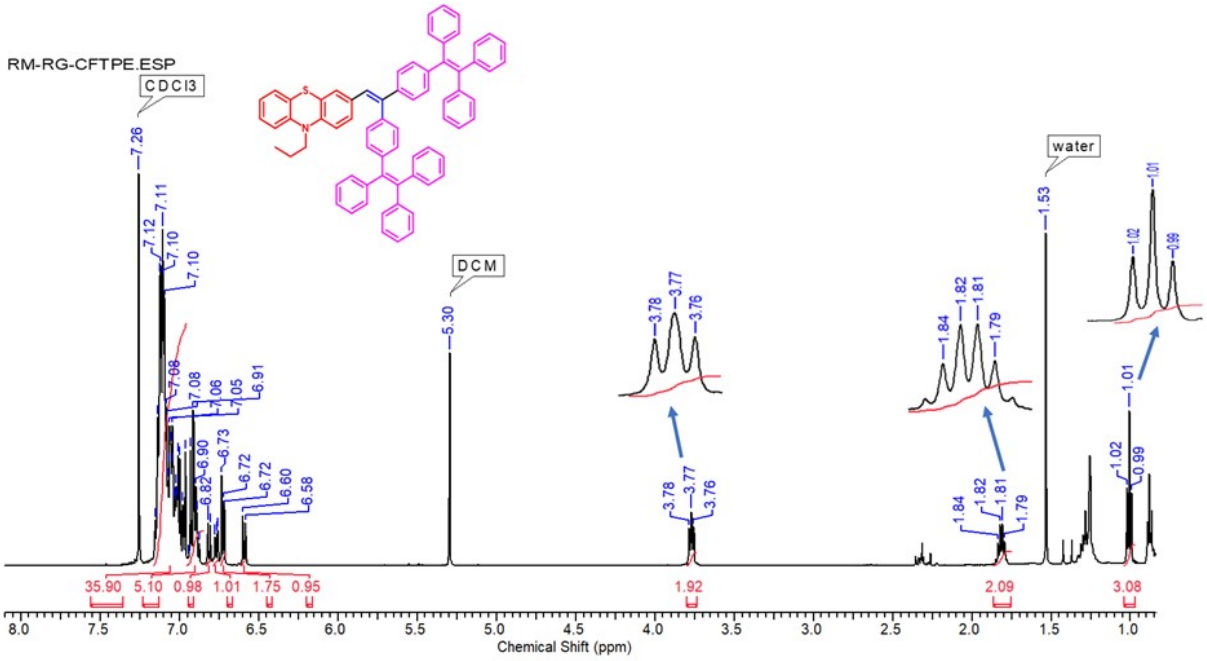



**Fig. S18**. $^{1}$H NMR spectra of **PTZ-(TPE)$_2$** ($CDCl_3$, 500 MHz).

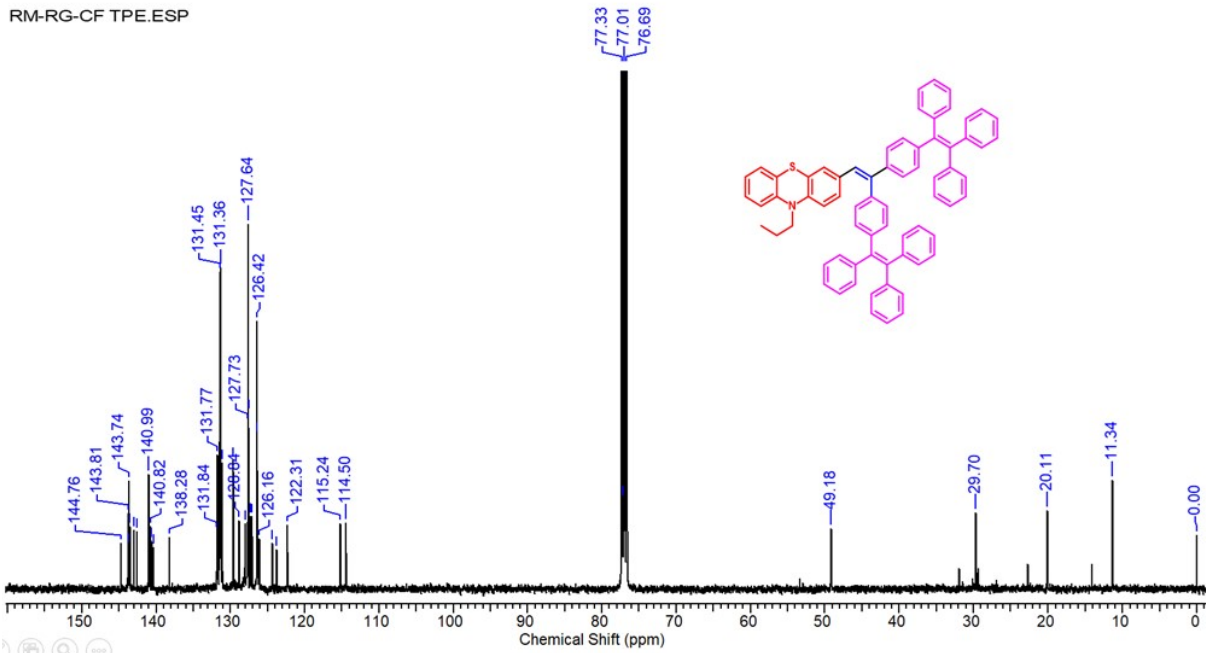



**Fig. S19**. $^{13}$C {$^{1}$H} NMR spectra of **PTZ-(TPE)$_2$** ($CDCl_3$, 126 MHz).

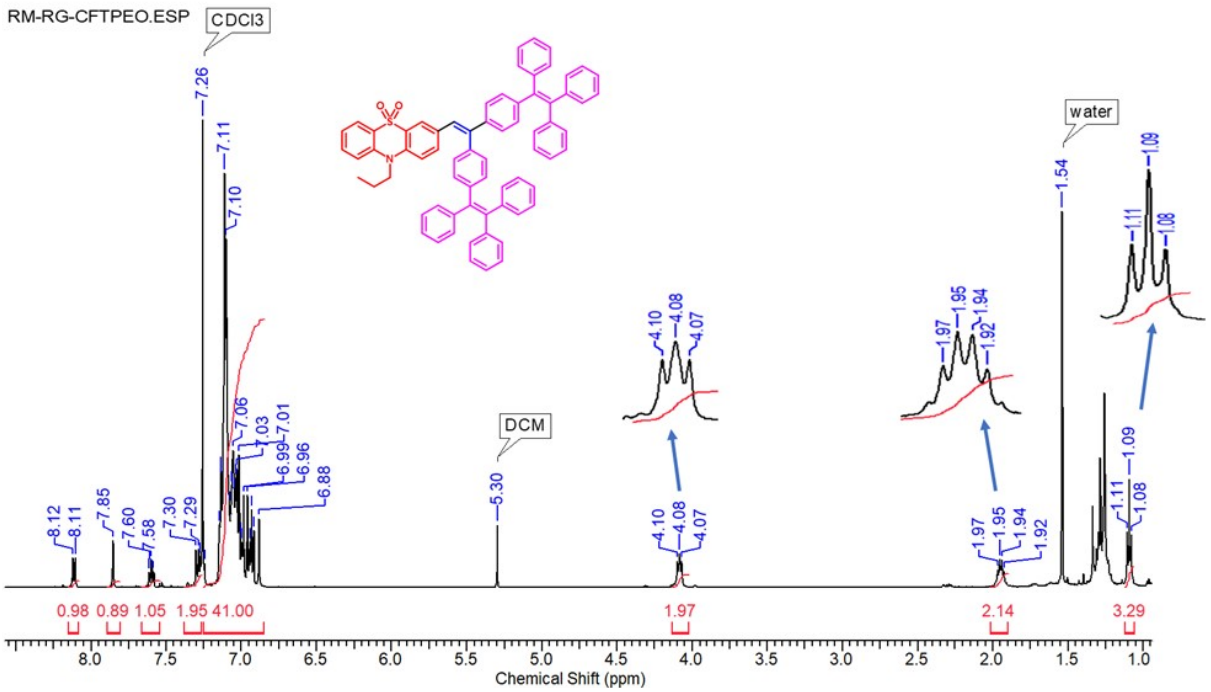



**Fig. S20**. $^{1}$H NMR spectra of **$PTZO_2$-$(TPE)_2$** ($CDCl_3$, 500 MHz).

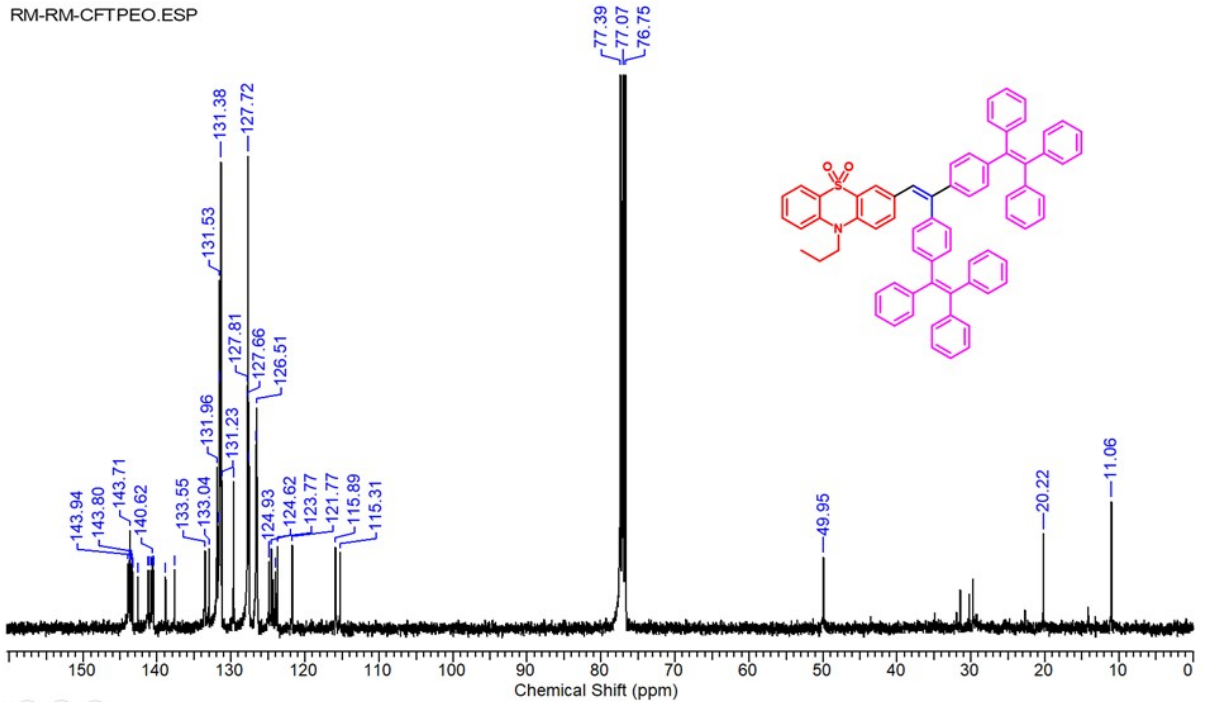



**Fig. S21**. $^{13}$C {$^{1}$H} NMR spectra of **$PTZO_2$-$(TPE)_2$** ($CDCl_3$, 126 MHz).

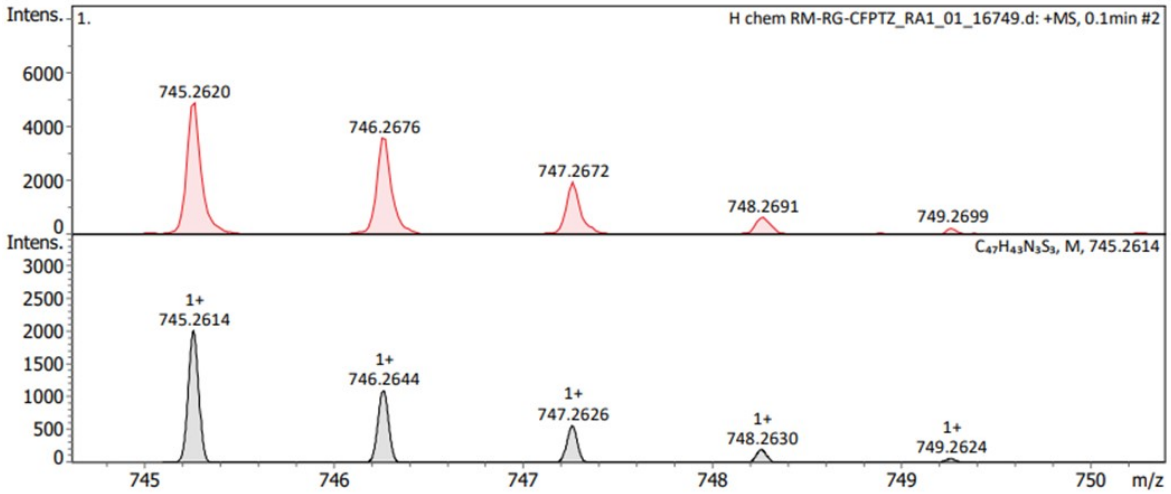



**Fig. S22**. HRMS of **$(PTZ)_3$**.

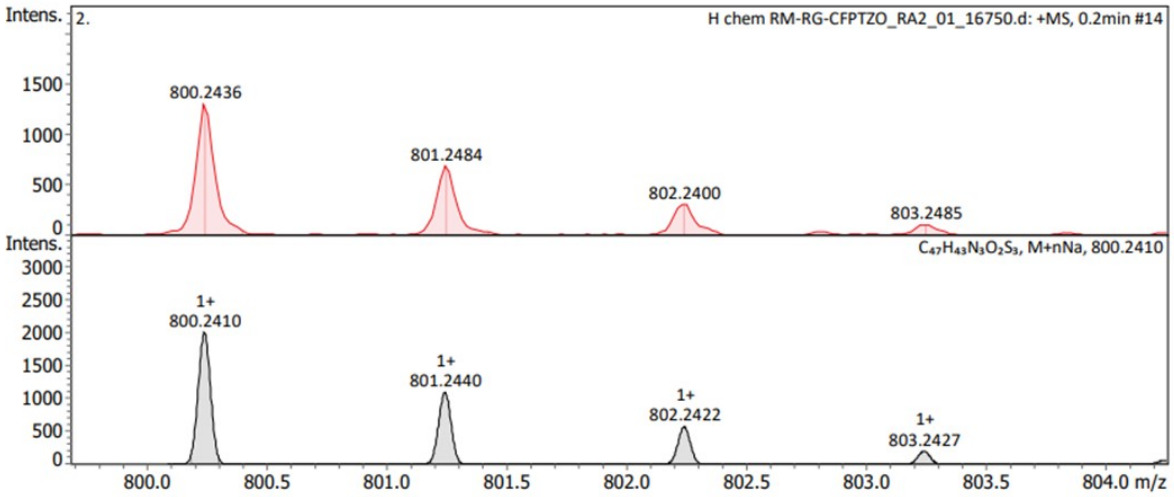



**Fig. S23**. HRMS of **$PTZO_2$-$(PTZ)_2$**.

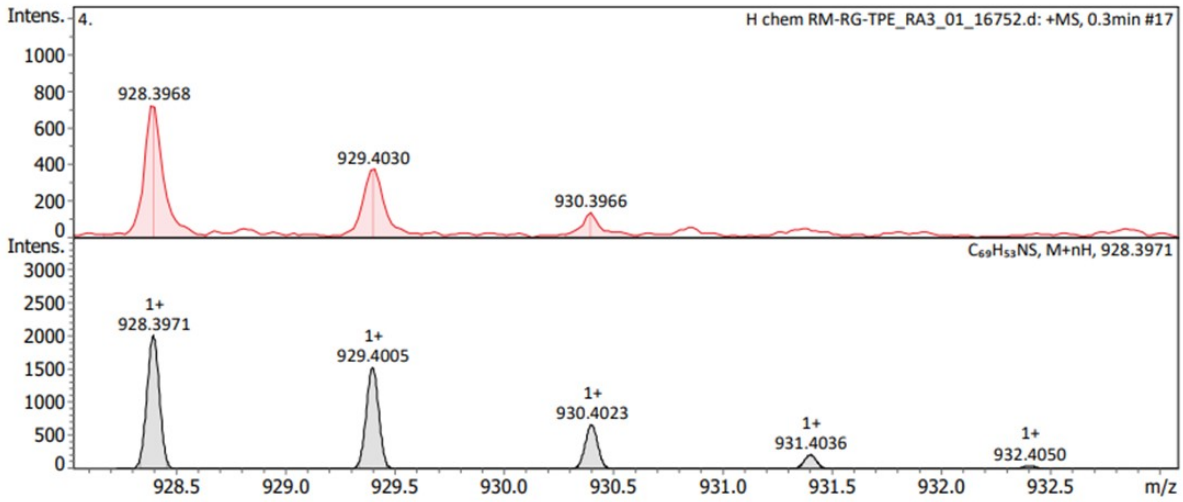



**Fig. S24**. HRMS of **PTZ-(TPE)$_2$**.

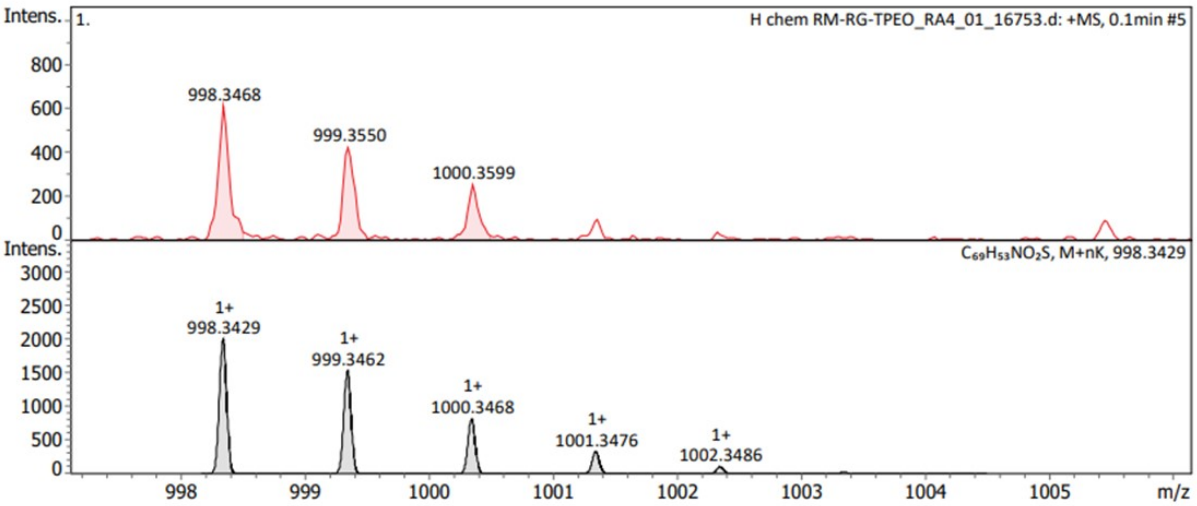



**Fig. S25**. HRMS of **PTZO$_2$-(TPE)$_2$**.

**DFT**

**$(PTZ)_3$**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 7.447878 | -5.844508 | 0.892078 |
| 2 | 6 | 0 | 6.371145 | -5.659044 | 0.024154 |
| 3 | 6 | 0 | 8.013233 | -4.738764 | 1.524132 |
| 4 | 6 | 0 | 5.888922 | -4.376625 | -0.237395 |
| 5 | 1 | 0 | 5.906248 | -6.508359 | -0.467121 |
| 6 | 6 | 0 | 7.510020 | -3.457538 | 1.295624 |
| 7 | 1 | 0 | 8.843428 | -4.867439 | 2.212193 |
| 8 | 6 | 0 | 6.450027 | -3.252123 | 0.399204 |
| 9 | 1 | 0 | 7.948493 | -2.614970 | 1.817769 |
| 10 | 7 | 0 | 5.924804 | -1.963828 | 0.129746 |
| 11 | 6 | 0 | 3.753004 | -2.784092 | -0.620032 |
| 12 | 6 | 0 | 4.519460 | -1.818156 | 0.059019 |
| 13 | 6 | 0 | 6.760549 | -0.783725 | 0.363217 |
| 14 | 6 | 0 | 2.368977 | -2.670831 | -0.697318 |
| 15 | 6 | 0 | 3.833742 | -0.751848 | 0.665017 |
| 16 | 1 | 0 | 7.036177 | -0.677900 | 1.424708 |
| 17 | 6 | 0 | 8.015749 | -0.757471 | -0.520304 |
| 18 | 1 | 0 | 6.153803 | 0.088884 | 0.114645 |
| 19 | 1 | 0 | 1.807834 | -3.446912 | -1.210518 |
| 20 | 6 | 0 | 2.454569 | -0.618749 | 0.545381 |
| 21 | 1 | 0 | 4.378983 | -0.024673 | 1.256397 |

| | | | | | |
|---|---|---|---|---|---|
| 22 | 1 | 0 | 7.697217 | -0.805776 | -1.567741 |
| 23 | 1 | 0 | 8.623028 | -1.649693 | -0.339726 |
| 24 | 1 | 0 | 1.965530 | 0.215121 | 1.034208 |
| 25 | 6 | 0 | 1.684898 | -1.567535 | -0.151994 |
| 26 | 6 | 0 | 8.856863 | 0.499217 | -0.276806 |
| 27 | 1 | 0 | 9.739126 | 0.511692 | -0.923547 |
| 28 | 1 | 0 | 8.284465 | 1.411595 | -0.479986 |
| 29 | 1 | 0 | 9.207023 | 0.553178 | 0.760421 |
| 30 | 16 | 0 | 4.594273 | -4.127493 | -1.438532 |
| 31 | 6 | 0 | 0.222350 | -1.530848 | -0.269155 |
| 32 | 6 | 0 | -0.645559 | -0.485010 | -0.229478 |
| 33 | 1 | 0 | -0.223570 | -2.514242 | -0.407775 |
| 34 | 1 | 0 | 7.833127 | -6.842598 | 1.074619 |
| 35 | 6 | 0 | -0.220087 | 0.943427 | -0.266621 |
| 36 | 6 | 0 | -0.704168 | 1.867171 | 0.674360 |
| 37 | 6 | 0 | 0.629602 | 1.424480 | -1.272836 |
| 38 | 6 | 0 | -0.296690 | 3.198857 | 0.653142 |
| 39 | 1 | 0 | -1.391478 | 1.537871 | 1.447301 |
| 40 | 6 | 0 | 1.003984 | 2.764868 | -1.325948 |
| 41 | 1 | 0 | 0.986022 | 0.741892 | -2.037133 |
| 42 | 6 | 0 | 0.575113 | 3.674181 | -0.346007 |
| 43 | 16 | 0 | -0.820225 | 4.320173 | 1.938517 |
| 44 | 1 | 0 | 1.624160 | 3.104650 | -2.147763 |
| 45 | 7 | 0 | 0.969774 | 5.032956 | -0.338181 |
| 46 | 6 | 0 | -0.964870 | 5.791328 | 0.940259 |
| 47 | 6 | 0 | -0.021157 | 6.013010 | -0.081715 |
| 48 | 6 | 0 | 2.210523 | 5.424486 | -1.011429 |
| 49 | 6 | 0 | -1.964035 | 6.728258 | 1.204041 |
| 50 | 6 | 0 | -0.110258 | 7.202081 | -0.821390 |

| | | | | | |
|---|---|---|---|---|---|
| 51 | 1 | 0 | 2.025296 | 5.801444 | -2.030054 |
| 52 | 6 | 0 | 3.034080 | 6.440065 | -0.207084 |
| 53 | 1 | 0 | 2.809467 | 4.518841 | -1.123341 |
| 54 | 6 | 0 | -2.019021 | 7.922107 | 0.483667 |
| 55 | 1 | 0 | -2.688402 | 6.521958 | 1.986086 |
| 56 | 6 | 0 | -1.088608 | 8.152761 | -0.527859 |
| 57 | 1 | 0 | 0.587004 | 7.390476 | -1.629613 |
| 58 | 1 | 0 | 3.249417 | 6.004379 | 0.775116 |
| 59 | 1 | 0 | 2.445852 | 7.344145 | -0.022408 |
| 60 | 6 | 0 | 4.336936 | 6.808014 | -0.923507 |
| 61 | 1 | 0 | -2.784821 | 8.657586 | 0.708494 |
| 62 | 1 | 0 | -1.126206 | 9.071069 | -1.106218 |
| 63 | 1 | 0 | 4.919874 | 7.521978 | -0.334324 |
| 64 | 1 | 0 | 4.965586 | 5.926222 | -1.092192 |
| 65 | 1 | 0 | 4.142134 | 7.266496 | -1.899804 |
| 66 | 6 | 0 | -2.108095 | -0.750354 | -0.202674 |
| 67 | 6 | 0 | -2.635419 | -1.869347 | 0.467172 |
| 68 | 6 | 0 | -3.018185 | 0.087689 | -0.867348 |
| 69 | 6 | 0 | -4.001963 | -2.128570 | 0.483046 |
| 70 | 1 | 0 | -1.972114 | -2.527037 | 1.019469 |
| 71 | 6 | 0 | -4.382699 | -0.187435 | -0.885710 |
| 72 | 1 | 0 | -2.649879 | 0.952031 | -1.409559 |
| 73 | 6 | 0 | -4.909321 | -1.288612 | -0.192705 |
| 74 | 16 | 0 | -4.645796 | -3.484643 | 1.447739 |
| 75 | 1 | 0 | -5.038643 | 0.458271 | -1.458309 |
| 76 | 7 | 0 | -6.292621 | -1.578196 | -0.148829 |
| 77 | 6 | 0 | -5.981903 | -3.944742 | 0.359389 |
| 78 | 6 | 0 | -6.695688 | -2.927905 | -0.304552 |
| 79 | 6 | 0 | -7.262017 | -0.505751 | -0.386103 |

| | | | | | |
|---|---|---|---|---|---|
| 80 | 6 | 0 | -6.343287 | -5.283670 | 0.210098 |
| 81 | 6 | 0 | -7.781106 | -3.297582 | -1.113230 |
| 82 | 1 | 0 | -7.610238 | -0.490060 | -1.431425 |
| 83 | 6 | 0 | -8.458555 | -0.554422 | 0.574700 |
| 84 | 1 | 0 | -6.737861 | 0.437519 | -0.222323 |
| 85 | 6 | 0 | -7.445972 | -5.633590 | -0.570191 |
| 86 | 1 | 0 | -5.763469 | -6.047391 | 0.719398 |
| 87 | 6 | 0 | -8.160856 | -4.635240 | -1.229224 |
| 88 | 1 | 0 | -8.335647 | -2.538975 | -1.653475 |
| 89 | 1 | 0 | -8.074983 | -0.515984 | 1.600454 |
| 90 | 1 | 0 | -8.985623 | -1.508384 | 0.476089 |
| 91 | 6 | 0 | -9.431485 | 0.602097 | 0.326233 |
| 92 | 1 | 0 | -7.735686 | -6.675220 | -0.665178 |
| 93 | 1 | 0 | -9.013401 | -4.892691 | -1.850603 |
| 94 | 1 | 0 | -10.272825 | 0.562658 | 1.024296 |
| 95 | 1 | 0 | -8.941025 | 1.573900 | 0.453028 |
| 96 | 1 | 0 | -9.842860 | 0.569267 | -0.689186 |

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Rotational constants (GHZ): 0.0413659 0.0266382 0.0168548

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## $PTZO_2$-$(PTZ)_2$

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 7.670149 | -5.225364 | 0.888669 |
| 2 | 6 | 0 | 6.572722 | -5.050012 | 0.053635 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 8.172432 | -4.124151 | 1.588967 |
| 4 | 6 | 0 | 5.997443 | -3.785885 | -0.075438 |
| 5 | 1 | 0 | 6.151195 | -5.872445 | -0.514861 |
| 6 | 6 | 0 | 7.580290 | -2.869510 | 1.484014 |
| 7 | 1 | 0 | 9.027937 | -4.246114 | 2.246757 |
| 8 | 6 | 0 | 6.461687 | -2.671125 | 0.651374 |
| 9 | 1 | 0 | 7.972089 | -2.049098 | 2.072828 |
| 10 | 7 | 0 | 5.801529 | -1.431093 | 0.586694 |
| 11 | 6 | 0 | 3.746301 | -2.345870 | -0.397522 |
| 12 | 6 | 0 | 4.412532 | -1.370954 | 0.369732 |
| 13 | 6 | 0 | 6.555443 | -0.201024 | 0.874304 |
| 14 | 6 | 0 | 2.362252 | -2.360189 | -0.547509 |
| 15 | 6 | 0 | 3.602096 | -0.385573 | 0.969633 |
| 16 | 1 | 0 | 6.917723 | -0.196160 | 1.911505 |
| 17 | 6 | 0 | 7.710887 | 0.037049 | -0.108556 |
| 18 | 1 | 0 | 5.859302 | 0.632559 | 0.786984 |
| 19 | 1 | 0 | 1.915851 | -3.161577 | -1.128515 |
| 20 | 6 | 0 | 2.227744 | -0.374650 | 0.785447 |
| 21 | 1 | 0 | 4.041504 | 0.351046 | 1.631852 |
| 22 | 1 | 0 | 7.300797 | 0.043316 | -1.124554 |
| 23 | 1 | 0 | 8.418885 | -0.796639 | -0.066617 |
| 24 | 1 | 0 | 1.644715 | 0.388136 | 1.287916 |
| 25 | 6 | 0 | 1.564613 | -1.355867 | 0.017238 |
| 26 | 6 | 0 | 8.439493 | 1.351818 | 0.184263 |
| 27 | 1 | 0 | 9.255340 | 1.511363 | -0.526458 |
| 28 | 1 | 0 | 7.763462 | 2.211234 | 0.110637 |
| 29 | 1 | 0 | 8.872597 | 1.356375 | 1.191145 |
| 30 | 16 | 0 | 4.728939 | -3.523758 | -1.289468 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 8 | 0 | 3.966135 | -4.766773 | -1.493588 |
| 32 | 8 | 0 | 5.328294 | -2.850857 | -2.456311 |
| 33 | 6 | 0 | 0.106687 | -1.424068 | -0.144430 |
| 34 | 6 | 0 | -0.815994 | -0.425596 | -0.147699 |
| 35 | 1 | 0 | -0.272093 | -2.435384 | -0.278499 |
| 36 | 1 | 0 | 8.132117 | -6.201542 | 0.990376 |
| 37 | 6 | 0 | -0.457564 | 1.020019 | -0.211235 |
| 38 | 6 | 0 | -1.021865 | 1.947362 | 0.680458 |
| 39 | 6 | 0 | 0.411638 | 1.510025 | -1.196617 |
| 40 | 6 | 0 | -0.674007 | 3.295092 | 0.634419 |
| 41 | 1 | 0 | -1.726104 | 1.609511 | 1.434260 |
| 42 | 6 | 0 | 0.726554 | 2.864154 | -1.276556 |
| 43 | 1 | 0 | 0.827740 | 0.823911 | -1.926801 |
| 44 | 6 | 0 | 0.216001 | 3.781186 | -0.344031 |
| 45 | 16 | 0 | -1.299871 | 4.427392 | 1.863012 |
| 46 | 1 | 0 | 1.362941 | 3.207777 | -2.084058 |
| 47 | 7 | 0 | 0.546311 | 5.156053 | -0.364130 |
| 48 | 6 | 0 | -1.472057 | 5.859707 | 0.813623 |
| 49 | 6 | 0 | -0.499888 | 6.094643 | -0.177943 |
| 50 | 6 | 0 | 1.791491 | 5.586298 | -1.005894 |
| 51 | 6 | 0 | -2.523827 | 6.755179 | 1.007910 |
| 52 | 6 | 0 | -0.615635 | 7.253718 | -0.960133 |
| 53 | 1 | 0 | 1.626583 | 5.916581 | -2.043942 |
| 54 | 6 | 0 | 2.531949 | 6.670465 | -0.210621 |
| 55 | 1 | 0 | 2.438528 | 4.708985 | -1.062180 |
| 56 | 6 | 0 | -2.606244 | 7.921564 | 0.246475 |
| 57 | 1 | 0 | -3.268417 | 6.538890 | 1.767927 |
| 58 | 6 | 0 | -1.648533 | 8.164740 | -0.736226 |

| | | | | | |
|---|---|---|---|---|---|
| 59 | 1 | 0 | 0.103578 | 7.450330 | -1.746786 |
| 60 | 1 | 0 | 2.729252 | 6.282617 | 0.795174 |
| 61 | 1 | 0 | 1.893307 | 7.549857 | -0.083641 |
| 62 | 6 | 0 | 3.842639 | 7.076832 | -0.891254 |
| 63 | 1 | 0 | -3.414157 | 8.625820 | 0.417243 |
| 64 | 1 | 0 | -1.706446 | 9.061246 | -1.346170 |
| 65 | 1 | 0 | 4.366578 | 7.839827 | -0.308183 |
| 66 | 1 | 0 | 4.519433 | 6.222021 | -1.002900 |
| 67 | 1 | 0 | 3.664355 | 7.489446 | -1.890816 |
| 68 | 6 | 0 | -2.263046 | -0.762924 | -0.144788 |
| 69 | 6 | 0 | -2.748037 | -1.888931 | 0.544814 |
| 70 | 6 | 0 | -3.198449 | 0.013330 | -0.847929 |
| 71 | 6 | 0 | -4.101274 | -2.210346 | 0.547976 |
| 72 | 1 | 0 | -2.063896 | -2.500560 | 1.124050 |
| 73 | 6 | 0 | -4.547883 | -0.325925 | -0.880490 |
| 74 | 1 | 0 | -2.861158 | 0.878820 | -1.408040 |
| 75 | 6 | 0 | -5.035217 | -1.430497 | -0.163894 |
| 76 | 16 | 0 | -4.697228 | -3.563743 | 1.545661 |
| 77 | 1 | 0 | -5.222855 | 0.272398 | -1.481557 |
| 78 | 7 | 0 | -6.404242 | -1.777666 | -0.129292 |
| 79 | 6 | 0 | -6.001965 | -4.112224 | 0.460297 |
| 80 | 6 | 0 | -6.749898 | -3.147886 | -0.242573 |
| 81 | 6 | 0 | -7.416159 | -0.755392 | -0.408981 |
| 82 | 6 | 0 | -6.306125 | -5.469148 | 0.351703 |
| 83 | 6 | 0 | -7.811322 | -3.587969 | -1.047702 |
| 84 | 1 | 0 | -7.755835 | -0.789770 | -1.456445 |
| 85 | 6 | 0 | -8.617142 | -0.822552 | 0.545032 |
| 86 | 1 | 0 | -6.933755 | 0.214182 | -0.273536 |

| | | | | | |
|---|---|---|---|---|---|
| 87 | 6 | 0 | -7.385675 | -5.889412 | -0.426055 |
| 88 | 1 | 0 | -5.700134 | -6.191294 | 0.890269 |
| 89 | 6 | 0 | -8.134675 | -4.943238 | -1.123022 |
| 90 | 1 | 0 | -8.391346 | -2.871011 | -1.617301 |
| 91 | 1 | 0 | -8.243730 | -0.733965 | 1.571448 |
| 92 | 1 | 0 | -9.102821 | -1.800647 | 0.474900 |
| 93 | 6 | 0 | -9.635341 | 0.283386 | 0.251776 |
| 94 | 1 | 0 | -7.631055 | -6.944673 | -0.489813 |
| 95 | 1 | 0 | -8.969899 | -5.255560 | -1.742700 |
| 96 | 1 | 0 | -10.479577 | 0.231885 | 0.945506 |
| 97 | 1 | 0 | -9.186635 | 1.278482 | 0.349169 |
| 98 | 1 | 0 | -10.037301 | 0.199864 | -0.764498 |

---

Rotational constants (GHZ): 0.0399669 0.0253272 0.0162355

**********

## PTZ-(TPE)$_2$

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

---

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.704010 | -8.133584 | -0.018669 |
| 2 | 6 | 0 | 5.620439 | -7.641445 | -0.747117 |
| 3 | 6 | 0 | 7.521366 | -7.242736 | 0.674267 |
| 4 | 6 | 0 | 5.378551 | -6.269244 | -0.811667 |
| 5 | 1 | 0 | 4.962613 | -8.319256 | -1.282569 |
| 6 | 6 | 0 | 7.261612 | -5.872122 | 0.644006 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 1 | 0 | 8.361431 | -7.610435 | 1.255899 |
| 8 | 6 | 0 | 6.195741 | -5.360033 | -0.111702 |
| 9 | 1 | 0 | 7.895018 | -5.199609 | 1.210894 |
| 10 | 7 | 0 | 5.912862 | -3.973083 | -0.178196 |
| 11 | 6 | 0 | 3.571993 | -4.272561 | -0.799222 |
| 12 | 6 | 0 | 4.562129 | -3.562676 | -0.093407 |
| 13 | 6 | 0 | 6.976707 | -3.008297 | 0.110715 |
| 14 | 6 | 0 | 2.236269 | -3.890918 | -0.731698 |
| 15 | 6 | 0 | 4.146346 | -2.474940 | 0.692869 |
| 16 | 1 | 0 | 7.341927 | -3.097437 | 1.146424 |
| 17 | 6 | 0 | 8.148439 | -3.091853 | -0.877937 |
| 18 | 1 | 0 | 6.534960 | -2.013962 | 0.024785 |
| 19 | 1 | 0 | 1.496971 | -4.473552 | -1.274474 |
| 20 | 6 | 0 | 2.816695 | -2.069146 | 0.719867 |
| 21 | 1 | 0 | 4.865481 | -1.946136 | 1.308187 |
| 22 | 1 | 0 | 7.753446 | -2.943858 | -1.889335 |
| 23 | 1 | 0 | 8.588437 | -4.093683 | -0.860508 |
| 24 | 1 | 0 | 2.539301 | -1.227894 | 1.343276 |
| 25 | 6 | 0 | 1.826645 | -2.756340 | -0.005286 |
| 26 | 6 | 0 | 9.225214 | -2.047439 | -0.569046 |
| 27 | 1 | 0 | 10.047501 | -2.108685 | -1.287889 |
| 28 | 1 | 0 | 8.821679 | -1.029447 | -0.613189 |
| 29 | 1 | 0 | 9.649458 | -2.191834 | 0.431243 |
| 30 | 16 | 0 | 4.068422 | -5.633047 | -1.841047 |
| 31 | 6 | 0 | 0.398588 | -2.419862 | 0.014816 |
| 32 | 6 | 0 | -0.226216 | -1.235560 | 0.247026 |
| 33 | 1 | 0 | -0.250284 | -3.268914 | -0.193255 |
| 34 | 1 | 0 | 6.900134 | -9.200650 | 0.009801 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 6 | 0 | 0.486900 | 0.071289 | 0.352011 |
| 36 | 6 | 0 | 0.313202 | 0.901040 | 1.472183 |
| 37 | 6 | 0 | 1.320060 | 0.528647 | -0.681730 |
| 38 | 6 | 0 | 0.969123 | 2.124835 | 1.567047 |
| 39 | 1 | 0 | -0.336245 | 0.575253 | 2.279441 |
| 40 | 6 | 0 | 1.955179 | 1.763810 | -0.598040 |
| 41 | 1 | 0 | 1.467690 | -0.094906 | -1.557806 |
| 42 | 6 | 0 | 1.789127 | 2.592118 | 0.524901 |
| 43 | 1 | 0 | 0.837502 | 2.735937 | 2.454935 |
| 44 | 1 | 0 | 2.587548 | 2.097135 | -1.414175 |
| 45 | 6 | 0 | 2.497574 | 3.902174 | 0.640701 |
| 46 | 6 | 0 | 2.493949 | 4.833007 | -0.359663 |
| 47 | 6 | 0 | 3.208258 | 4.113981 | 1.939019 |
| 48 | 6 | 0 | 3.406156 | 6.017131 | -0.364444 |
| 49 | 6 | 0 | 1.575601 | 4.746530 | -1.536225 |
| 50 | 6 | 0 | 4.029932 | 3.107358 | 2.475764 |
| 51 | 6 | 0 | 3.029584 | 5.291297 | 2.684825 |
| 52 | 6 | 0 | 2.908075 | 7.301159 | -0.647441 |
| 53 | 6 | 0 | 4.787037 | 5.874831 | -0.146595 |
| 54 | 6 | 0 | 2.067087 | 4.926743 | -2.841002 |
| 55 | 6 | 0 | 0.195631 | 4.539835 | -1.369959 |
| 56 | 6 | 0 | 4.674953 | 3.284268 | 3.698491 |
| 57 | 1 | 0 | 4.163392 | 2.182423 | 1.922663 |
| 58 | 6 | 0 | 3.664943 | 5.463837 | 3.913346 |
| 59 | 1 | 0 | 2.385562 | 6.072490 | 2.294758 |
| 60 | 6 | 0 | 3.754977 | 8.407546 | -0.678216 |
| 61 | 1 | 0 | 1.846946 | 7.428006 | -0.839691 |
| 62 | 6 | 0 | 5.636098 | 6.979222 | -0.189678 |

| | | | | | |
|---|---|---|---|---|---|
| 63 | 1 | 0 | 5.192131 | 4.888773 | 0.055393 |
| 64 | 6 | 0 | 1.214915 | 4.866807 | -3.942237 |
| 65 | 1 | 0 | 3.127386 | 5.109024 | -2.988223 |
| 66 | 6 | 0 | -0.658674 | 4.491998 | -2.470211 |
| 67 | 1 | 0 | -0.204571 | 4.418983 | -0.368684 |
| 68 | 6 | 0 | 4.494705 | 4.463818 | 4.423350 |
| 69 | 1 | 0 | 5.315310 | 2.497970 | 4.088314 |
| 70 | 1 | 0 | 3.507809 | 6.380256 | 4.475030 |
| 71 | 6 | 0 | 5.123547 | 8.251328 | -0.449905 |
| 72 | 1 | 0 | 3.346118 | 9.392287 | -0.886206 |
| 73 | 1 | 0 | 6.701191 | 6.844462 | -0.023831 |
| 74 | 6 | 0 | -0.152228 | 4.648740 | -3.761668 |
| 75 | 1 | 0 | 1.618843 | 4.994767 | -4.942531 |
| 76 | 1 | 0 | -1.723007 | 4.336913 | -2.317759 |
| 77 | 1 | 0 | 4.990669 | 4.599309 | 5.380058 |
| 78 | 1 | 0 | 5.785360 | 9.111926 | -0.481999 |
| 79 | 1 | 0 | -0.817915 | 4.608701 | -4.618873 |
| 80 | 6 | 0 | -1.708730 | -1.198469 | 0.354541 |
| 81 | 6 | 0 | -2.431045 | -2.256755 | 0.936836 |
| 82 | 6 | 0 | -2.444907 | -0.098892 | -0.124676 |
| 83 | 6 | 0 | -3.819026 | -2.226821 | 1.014283 |
| 84 | 1 | 0 | -1.892406 | -3.097585 | 1.362716 |
| 85 | 6 | 0 | -3.833328 | -0.076694 | -0.060208 |
| 86 | 1 | 0 | -1.919043 | 0.743270 | -0.562569 |
| 87 | 6 | 0 | -4.555034 | -1.144732 | 0.500062 |
| 88 | 1 | 0 | -4.345423 | -3.049272 | 1.489057 |
| 89 | 1 | 0 | -4.372455 | 0.780839 | -0.448840 |
| 90 | 6 | 0 | -6.042943 | -1.108161 | 0.617238 |

| | | | | | |
|---|---|---|---|---|---|
| 91 | 6 | 0 | -6.858529 | -0.769957 | -0.426365 |
| 92 | 6 | 0 | -6.572660 | -1.472558 | 1.967664 |
| 93 | 6 | 0 | -8.313467 | -0.475214 | -0.249849 |
| 94 | 6 | 0 | -6.367806 | -0.668916 | -1.834632 |
| 95 | 6 | 0 | -6.020236 | -0.903778 | 3.128710 |
| 96 | 6 | 0 | -7.589414 | -2.430439 | 2.118014 |
| 97 | 6 | 0 | -9.268214 | -1.056377 | -1.102934 |
| 98 | 6 | 0 | -8.761580 | 0.428149 | 0.728602 |
| 99 | 6 | 0 | -6.708612 | 0.438144 | -2.631824 |
| 100 | 6 | 0 | -5.606606 | -1.696114 | -2.417843 |
| 101 | 6 | 0 | -6.490142 | -1.255767 | 4.392707 |
| 102 | 1 | 0 | -5.219213 | -0.176855 | 3.033420 |
| 103 | 6 | 0 | -8.051465 | -2.791625 | 3.382446 |
| 104 | 1 | 0 | -8.015553 | -2.893118 | 1.233994 |
| 105 | 6 | 0 | -10.624793 | -0.770648 | -0.960607 |
| 106 | 1 | 0 | -8.939003 | -1.740685 | -1.879075 |
| 107 | 6 | 0 | -10.117027 | 0.723449 | 0.863395 |
| 108 | 1 | 0 | -8.037373 | 0.900203 | 1.384184 |
| 109 | 6 | 0 | -6.275322 | 0.530429 | -3.953223 |
| 110 | 1 | 0 | -7.314097 | 1.232466 | -2.205753 |
| 111 | 6 | 0 | -5.182939 | -1.609508 | -3.742714 |
| 112 | 1 | 0 | -5.349287 | -2.566816 | -1.823854 |
| 113 | 6 | 0 | -7.508133 | -2.202154 | 4.525171 |
| 114 | 1 | 0 | -6.057300 | -0.793821 | 5.275575 |
| 115 | 1 | 0 | -8.835001 | -3.538372 | 3.474679 |
| 116 | 6 | 0 | -11.055453 | 0.121240 | 0.023534 |
| 117 | 1 | 0 | -11.346094 | -1.241703 | -1.622445 |
| 118 | 1 | 0 | -10.439770 | 1.428728 | 1.623995 |

| | | | | | |
|---|---|---|---|---|---|
| 119 | 6 | 0 | -5.510122 | -0.493474 | -4.514845 |
| 120 | 1 | 0 | -6.539954 | 1.401197 | -4.546514 |
| 121 | 1 | 0 | -4.599210 | -2.417943 | -4.173632 |
| 122 | 1 | 0 | -7.869572 | -2.482703 | 5.510228 |
| 123 | 1 | 0 | -12.111813 | 0.350208 | 0.130130 |
| 124 | 1 | 0 | -5.178239 | -0.425774 | -5.546794 |

---

Rotational constants (GHZ): 0.0276765 0.0165274 0.0121838

**********

## $PTZO_2$-$(TPE)_2$

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.971095 | -7.624615 | 0.203597 |
| 2 | 6 | 0 | 5.860741 | -7.159949 | -0.491773 |
| 3 | 6 | 0 | 7.773094 | -6.708365 | 0.891233 |
| 4 | 6 | 0 | 5.568353 | -5.796142 | -0.494809 |
| 5 | 1 | 0 | 5.213550 | -7.830702 | -1.047227 |
| 6 | 6 | 0 | 7.465127 | -5.351720 | 0.913031 |
| 7 | 1 | 0 | 8.643690 | -7.056576 | 1.439216 |
| 8 | 6 | 0 | 6.337698 | -4.860838 | 0.226147 |
| 9 | 1 | 0 | 8.087694 | -4.676991 | 1.487899 |
| 10 | 7 | 0 | 5.962362 | -3.507397 | 0.298385 |
| 11 | 6 | 0 | 3.670198 | -3.887708 | -0.495487 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | 4.606909 | -3.136235 | 0.239934 |
| 13 | 6 | 0 | 6.994503 | -2.488864 | 0.548366 |
| 14 | 6 | 0 | 2.310173 | -3.592417 | -0.492948 |
| 15 | 6 | 0 | 4.096227 | -2.046104 | 0.973890 |
| 16 | 1 | 0 | 7.462902 | -2.638555 | 1.530707 |
| 17 | 6 | 0 | 8.055957 | -2.428454 | -0.559502 |
| 18 | 1 | 0 | 6.492096 | -1.523019 | 0.589806 |
| 19 | 1 | 0 | 1.643620 | -4.234300 | -1.061064 |
| 20 | 6 | 0 | 2.747244 | -1.726576 | 0.944231 |
| 21 | 1 | 0 | 4.750796 | -1.470734 | 1.617924 |
| 22 | 1 | 0 | 7.545502 | -2.261472 | -1.514434 |
| 23 | 1 | 0 | 8.564793 | -3.393743 | -0.646159 |
| 24 | 1 | 0 | 2.399965 | -0.895147 | 1.545725 |
| 25 | 6 | 0 | 1.812283 | -2.483738 | 0.205461 |
| 26 | 6 | 0 | 9.081887 | -1.321940 | -0.298306 |
| 27 | 1 | 0 | 9.828349 | -1.286945 | -1.096817 |
| 28 | 1 | 0 | 8.605490 | -0.336368 | -0.247014 |
| 29 | 1 | 0 | 9.614829 | -1.482312 | 0.646030 |
| 30 | 16 | 0 | 4.276688 | -5.182269 | -1.546653 |
| 31 | 8 | 0 | 3.241357 | -6.214469 | -1.724503 |
| 32 | 8 | 0 | 4.894103 | -4.572235 | -2.738073 |
| 33 | 6 | 0 | 0.367284 | -2.228346 | 0.191210 |
| 34 | 6 | 0 | -0.318031 | -1.069812 | 0.376487 |
| 35 | 1 | 0 | -0.229752 | -3.117388 | -0.001766 |
| 36 | 1 | 0 | 7.214256 | -8.681756 | 0.206446 |
| 37 | 6 | 0 | 0.334274 | 0.270912 | 0.442594 |
| 38 | 6 | 0 | 0.115848 | 1.130095 | 1.532453 |

| | | | | | |
|---|---|---|---|---|---|
| 39 | 6 | 0 | 1.156044 | 0.726472 | -0.600931 |
| 40 | 6 | 0 | 0.720556 | 2.382326 | 1.589499 |
| 41 | 1 | 0 | -0.527051 | 0.805492 | 2.345417 |
| 42 | 6 | 0 | 1.738486 | 1.989437 | -0.555575 |
| 43 | 1 | 0 | 1.334645 | 0.081337 | -1.455398 |
| 44 | 6 | 0 | 1.529242 | 2.847398 | 0.537259 |
| 45 | 1 | 0 | 0.556472 | 3.017854 | 2.454546 |
| 46 | 1 | 0 | 2.361920 | 2.321147 | -1.379108 |
| 47 | 6 | 0 | 2.181314 | 4.189598 | 0.611694 |
| 48 | 6 | 0 | 2.140319 | 5.085214 | -0.419640 |
| 49 | 6 | 0 | 2.878793 | 4.473167 | 1.903352 |
| 50 | 6 | 0 | 2.998636 | 6.307867 | -0.464038 |
| 51 | 6 | 0 | 1.229427 | 4.917037 | -1.593154 |
| 52 | 6 | 0 | 3.739869 | 3.519268 | 2.473605 |
| 53 | 6 | 0 | 2.650535 | 5.666087 | 2.609882 |
| 54 | 6 | 0 | 2.444770 | 7.556149 | -0.798822 |
| 55 | 6 | 0 | 4.383017 | 6.236853 | -0.233693 |
| 56 | 6 | 0 | 1.717675 | 5.062541 | -2.903392 |
| 57 | 6 | 0 | -0.141981 | 4.665121 | -1.419889 |
| 58 | 6 | 0 | 4.374650 | 3.762213 | 3.690299 |
| 59 | 1 | 0 | 3.912523 | 2.583243 | 1.950721 |
| 60 | 6 | 0 | 3.276014 | 5.904607 | 3.832373 |
| 61 | 1 | 0 | 1.976203 | 6.407138 | 2.193642 |
| 62 | 6 | 0 | 3.240925 | 8.697885 | -0.867760 |
| 63 | 1 | 0 | 1.380482 | 7.626900 | -1.001817 |
| 64 | 6 | 0 | 5.181475 | 7.376219 | -0.315097 |
| 65 | 1 | 0 | 4.831022 | 5.278643 | 0.007651 |

| | | | | | |
|---|---|---|---|---|---|
| 66 | 6 | 0 | 0.871587 | 4.924174 | -4.002204 |
| 67 | 1 | 0 | 2.770694 | 5.279039 | -3.056507 |
| 68 | 6 | 0 | -0.990886 | 4.539621 | -2.518308 |
| 69 | 1 | 0 | -0.540009 | 4.571184 | -0.414812 |
| 70 | 6 | 0 | 4.144867 | 4.956642 | 4.375697 |
| 71 | 1 | 0 | 5.046025 | 3.016237 | 4.106377 |
| 72 | 1 | 0 | 3.080748 | 6.831888 | 4.363384 |
| 73 | 6 | 0 | 4.613564 | 8.612755 | -0.626841 |
| 74 | 1 | 0 | 2.789495 | 9.654317 | -1.115787 |
| 75 | 1 | 0 | 6.250455 | 7.296577 | -0.139095 |
| 76 | 6 | 0 | -0.486779 | 4.661634 | -3.814367 |
| 77 | 1 | 0 | 1.273127 | 5.025435 | -5.006450 |
| 78 | 1 | 0 | -2.048977 | 4.350455 | -2.361085 |
| 79 | 1 | 0 | 4.632936 | 5.143953 | 5.327690 |
| 80 | 1 | 0 | 5.235992 | 9.500640 | -0.689020 |
| 81 | 1 | 0 | -1.147757 | 4.560142 | -4.670093 |
| 82 | 6 | 0 | -1.801576 | -1.099707 | 0.462667 |
| 83 | 6 | 0 | -2.482115 | -2.177997 | 1.058189 |
| 84 | 6 | 0 | -2.579820 | -0.046374 | -0.052140 |
| 85 | 6 | 0 | -3.870845 | -2.211919 | 1.113714 |
| 86 | 1 | 0 | -1.912091 | -2.983586 | 1.510493 |
| 87 | 6 | 0 | -3.968558 | -0.088438 | -0.009110 |
| 88 | 1 | 0 | -2.087001 | 0.809469 | -0.501617 |
| 89 | 6 | 0 | -4.648263 | -1.177553 | 0.563196 |
| 90 | 1 | 0 | -4.365612 | -3.048282 | 1.597889 |
| 91 | 1 | 0 | -4.540849 | 0.733864 | -0.425299 |
| 92 | 6 | 0 | -6.137960 | -1.210769 | 0.654068 |

| | | | | | |
|---|---|---|---|---|---|
| 93 | 6 | 0 | -6.949693 | -0.930407 | -0.409575 |
| 94 | 6 | 0 | -6.673779 | -1.579152 | 2.000967 |
| 95 | 6 | 0 | -8.420112 | -0.704513 | -0.263572 |
| 96 | 6 | 0 | -6.438043 | -0.830126 | -1.810483 |
| 97 | 6 | 0 | -6.177656 | -0.959472 | 3.161279 |
| 98 | 6 | 0 | -7.638780 | -2.589422 | 2.149442 |
| 99 | 6 | 0 | -9.329406 | -1.337805 | -1.129179 |
| 100 | 6 | 0 | -8.929887 | 0.185025 | 0.697319 |
| 101 | 6 | 0 | -6.815902 | 0.245550 | -2.633523 |
| 102 | 6 | 0 | -5.618269 | -1.829878 | -2.361078 |
| 103 | 6 | 0 | -6.653127 | -1.314462 | 4.422377 |
| 104 | 1 | 0 | -5.416868 | -0.190237 | 3.067570 |
| 105 | 6 | 0 | -8.105825 | -2.953140 | 3.411324 |
| 106 | 1 | 0 | -8.020558 | -3.090553 | 1.266071 |
| 107 | 6 | 0 | -10.700531 | -1.115585 | -1.015693 |
| 108 | 1 | 0 | -8.953368 | -2.012488 | -1.892282 |
| 109 | 6 | 0 | -10.300128 | 0.416460 | 0.803462 |
| 110 | 1 | 0 | -8.242256 | 0.697970 | 1.361398 |
| 111 | 6 | 0 | -6.362531 | 0.335431 | -3.948340 |
| 112 | 1 | 0 | -7.466323 | 1.017370 | -2.233059 |
| 113 | 6 | 0 | -5.174025 | -1.746101 | -3.679386 |
| 114 | 1 | 0 | -5.332172 | -2.677476 | -1.747193 |
| 115 | 6 | 0 | -7.619482 | -2.313788 | 4.552926 |
| 116 | 1 | 0 | -6.265088 | -0.813151 | 5.304600 |
| 117 | 1 | 0 | -8.848386 | -3.740731 | 3.502548 |
| 118 | 6 | 0 | -11.192285 | -0.236985 | -0.048392 |
| 119 | 1 | 0 | -11.385455 | -1.626087 | -1.686819 |

| | | | | | |
|---|---|---|---|---|---|
| 120 | 1 | 0 | -10.670727 | 1.112360 | 1.550757 |
| 121 | 6 | 0 | -5.539181 | -0.660389 | -4.477309 |
| 122 | 1 | 0 | -6.656949 | 1.182068 | -4.562147 |
| 123 | 1 | 0 | -4.544838 | -2.533179 | -4.084987 |
| 124 | 1 | 0 | -7.984963 | -2.596301 | 5.535913 |
| 125 | 1 | 0 | -12.260205 | -0.057712 | 0.035711 |
| 126 | 1 | 0 | -5.191477 | -0.594929 | -5.504146 |

---

Rotational constants (GHZ): 0.0262281 0.0161129 0.0117663

## TD-DFT

### $(PTZ)_3$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0572 eV 405.55 nm f=0.5688 <S**2>=0.000

197 -> 198 0.69607

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3175.68858448

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3267 eV 372.69 nm f=0.0794 <S**2>=0.000

196 -> 198 0.68590

Excited State 3: Singlet-A 3.4258 eV 361.91 nm f=0.0247 <S**2>=0.000

195 -> 198 0.68463

Excited State 4: Singlet-A 3.7283 eV 332.55 nm f=0.0218 <S**2>=0.000

194 -> 198 0.16289

195 -> 199 0.10151

197 -> 199 0.63624

Excited State 5: Singlet-A 3.8030 eV 326.02 nm f=0.0115 <S**2>=0.000

195 -> 200 0.12948

196 -> 199 0.16244

196 -> 200 0.12868

196 -> 201 0.19770

197 -> 200 0.51404

197 -> 201 0.27769

Excited State 6: Singlet-A 3.8580 eV 321.37 nm f=0.0069 <S**2>=0.000

194 -> 198 -0.10996

195 -> 199 0.23662

195 -> 200 -0.12541

196 -> 200 0.19202

197 -> 200 -0.22056

197 -> 201 0.45226

197 -> 202 -0.19745

197 -> 203 -0.11893

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

**********

**$PTZO_2$-$(PTZ)_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0606 eV 405.10 nm f=0.5077 <S**2>=0.000

205 -> 206 0.69892

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3326.06923826

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2418 eV 382.46 nm f=0.0922 <S**2>=0.000

204 -> 206 0.69717

Excited State 3: Singlet-A 3.4877 eV 355.49 nm f=0.0220 <S**2>=0.000

203 -> 207 0.12046

204 -> 207 0.10778

205 -> 207 0.66990

Excited State 4: Singlet-A 3.6586 eV 338.89 nm f=0.5148 <S**2>=0.000

203 -> 206 0.68264

Excited State 5: Singlet-A 3.7872 eV 327.37 nm f=0.0406 <S**2>=0.000

204 -> 207 0.61010

204 -> 208 -0.23619

205 -> 207 -0.11951

205 -> 208 -0.12195

205 -> 209 -0.11073

Excited State 6: Singlet-A 3.8104 eV 325.39 nm f=0.0053 <S**2>=0.000

202 -> 206 0.11135

204 -> 210 -0.12671

205 -> 208 -0.35953

205 -> 210 0.45025

205 -> 211 -0.16269

205 -> 212 -0.20282

205 -> 214 -0.11360

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

**********

**PTZ-(TPE)$_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9453 eV 420.96 nm f=0.5884 <S**2>=0.000

245 -> 246 0.69657

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3114.17269158

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1865 eV 389.09 nm f=0.2043 <S**2>=0.000

245 -> 247 0.69204

Excited State 3: Singlet-A 3.3790 eV 366.93 nm f=0.2047 <S**2>=0.000

243 -> 246 -0.19117

244 -> 246 0.65524

Excited State 4: Singlet-A 3.4482 eV 359.57 nm f=0.1927 <S**2>=0.000

243 -> 246 0.65637

244 -> 246 0.20184

Excited State 5: Singlet-A 3.5410 eV 350.13 nm f=0.0674 <S**2>=0.000

245 -> 248 0.66817

Excited State 6: Singlet-A 3.6642 eV 338.37 nm f=0.0289 <S**2>=0.000

243 -> 246 0.11877

243 -> 247 0.14951

244 -> 247 0.66292

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

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**$PTZO_2$-$(TPE)_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0914 eV 401.06 nm f=0.9157 <S**2>=0.000

253 -> 254 0.70067

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3264.54798096

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3250 eV 372.88 nm f=0.3138 <S**2>=0.000

252 -> 254 0.59157

253 -> 255 0.37011

Excited State 3: Singlet-A 3.3958 eV 365.11 nm f=0.0426 <S**2>=0.000

252 -> 254 -0.37289

253 -> 255 0.58693

Excited State 4: Singlet-A 3.6113 eV 343.33 nm f=0.0796 <S**2>=0.000

251 -> 254 0.65862

253 -> 257 0.23072

Excited State 5: Singlet-A 3.6355 eV 341.04 nm f=0.0323 <S**2>=0.000

251 -> 256 -0.15018

252 -> 255 -0.10519

253 -> 256 0.66049

Excited State 6: Singlet-A 3.7023 eV 334.89 nm f=0.3243 <S**2>=0.000

252 -> 255 0.66970

253 -> 257 -0.12772

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 6 LETran= 118.

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S3. J. Huang, X. Yang, J. Wang, C. Zhong, L. Wang, J. Qin and Z. Li, *J. Mater. Chem.*, 2012, **22**, 2478–2484.

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