# Supporting Information

# Phenothiazine and Anthracene Derivatives as Emitters for Vacuum-Deposited and Solution-Processed Optoelectronic Devices

**Ramakant Gavale[a], Melika Ghasemi[b], Dmytro Volyniuk[b], Asta Dabuliene[b], Juozas Vidas Grazulevicius[b], Rajneesh Misra[a]***

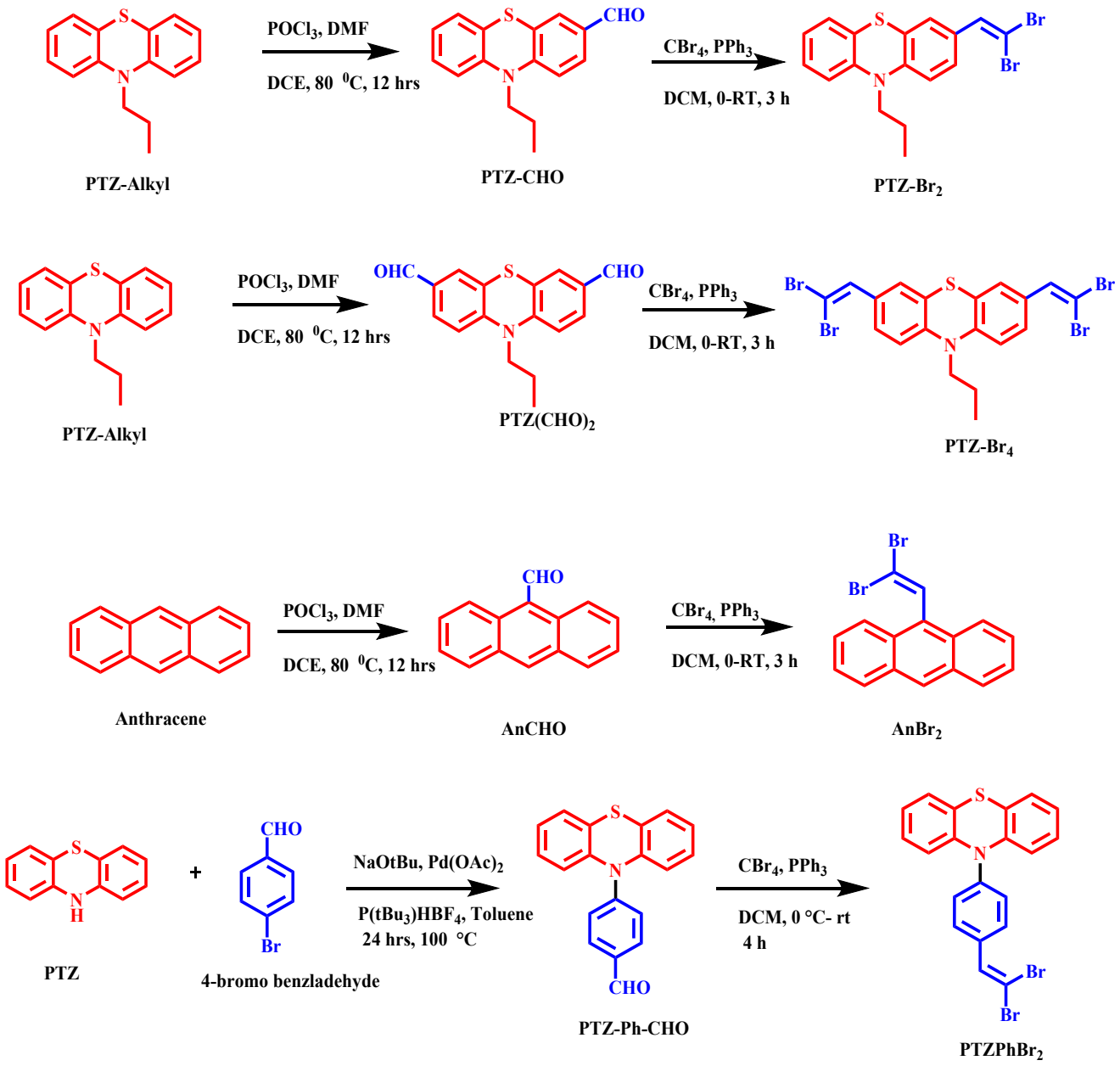
[a] Department of Chemistry, Indian Institute of Technology Indore,

Indore- 453552, India

[b] Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Barsausko g. 59, Kaunas 51423, Lithuania;

Email: rajneeshmisra@iiti.ac.in

## Experimental Section




**Scheme S1.** Synthetic scheme for Intermediate Intermediates.

## Solvatochromism

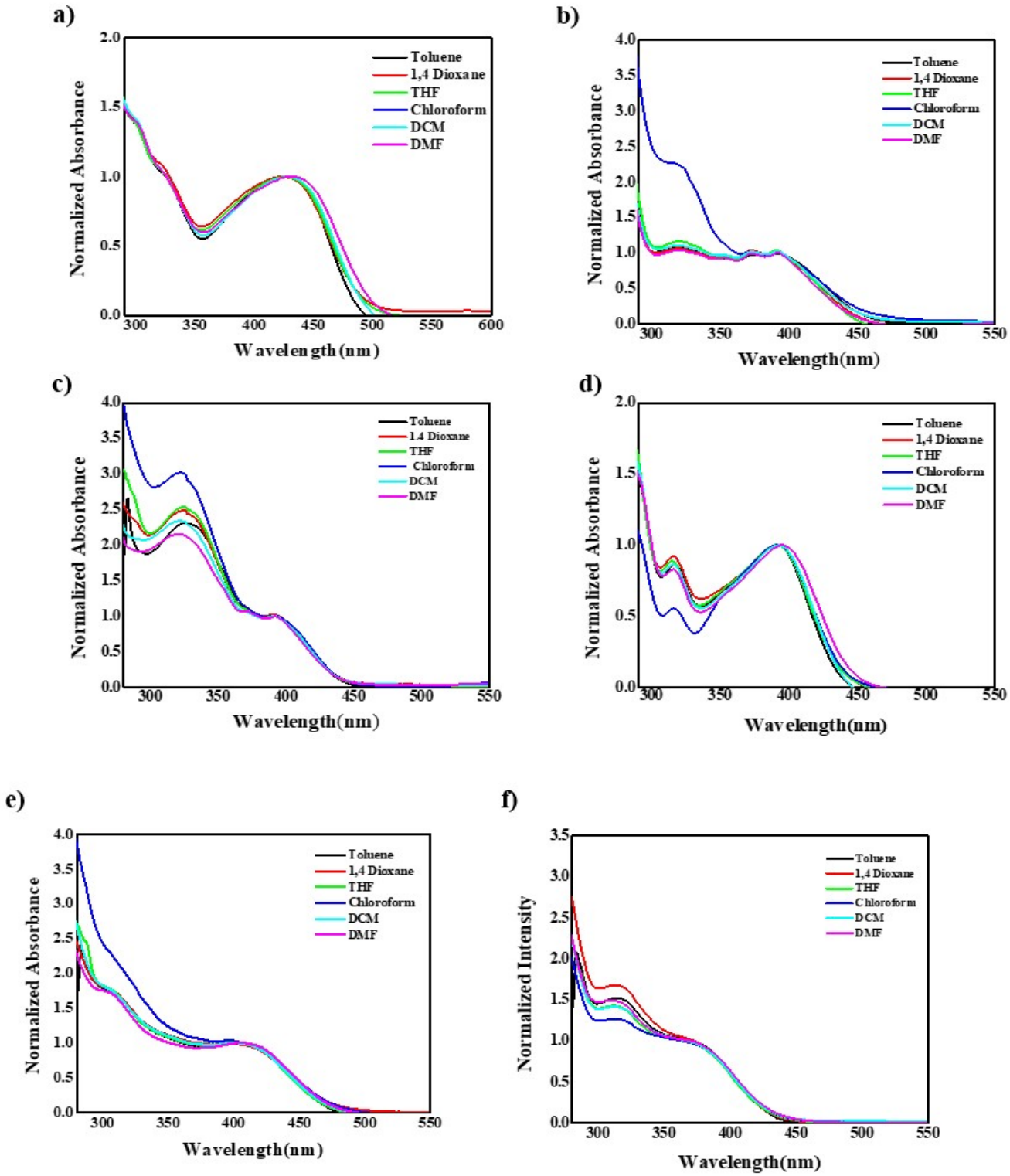



**Fig. S1.** UV- vis absorption Spectra of (a) **$(PTZ)_3$**, b) **$An(PTZ)_2$**, c) **$An(TPE)_2$**, d) **$(PTZ)_4$**, e) **$(PTZ)_5$** and f) **PTZ-Ph-$(PTZ)_2$** in different polarity of solvents respectively.

## Lippert Mataga Plot

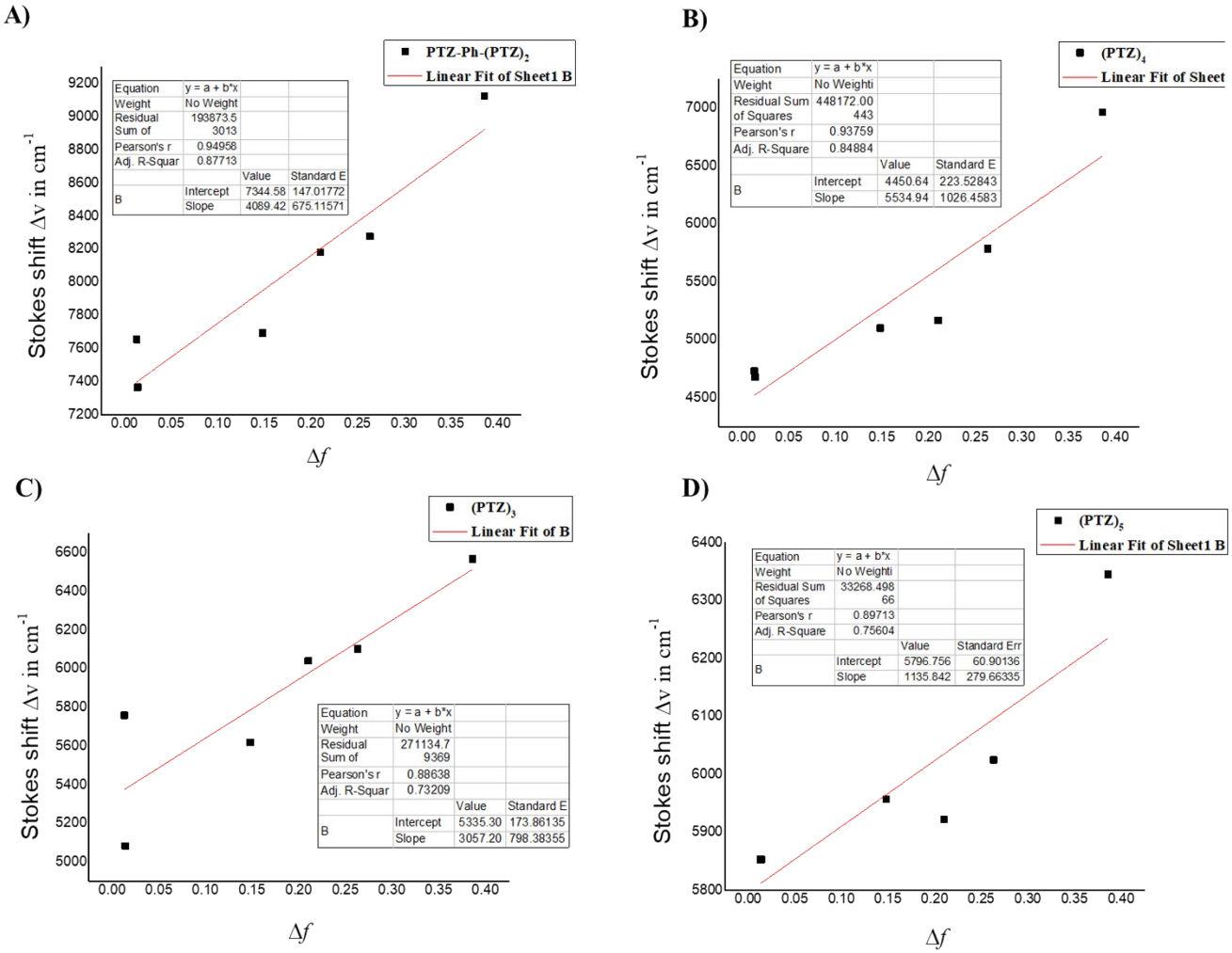



**Fig. S2.** Stokes Shift ($\Delta\nu$) of **(a) PTZ-Ph-$(PTZ)_2$, (b) $(PTZ)_4$, (c) $(PTZ)_3$,** and **d) $(PTZ)_5$** as a function of the solvent polarity parameter ($\Delta f$).

**Table S1** Photophysical properties of the compounds **PTZ-Ph-$(PTZ)_2$, $(PTZ)_4$, $(PTZ)_3$,** and **$(PTZ)_5$**

| Compound | Solvent | $\lambda_{abs}$ (nm)[a] | $\lambda_{em}$ (nm) [a] | Stokes shift ($cm^{-1}$) | $\phi$[b] |
|---|---|---|---|---|---|
| $(PTZ)_3$ | Toluene | 428 | 547 | 5083 | 0.43 |
| | 1,4 Dioxane | 424 | 561 | 5759 | 0.33 |
| | Tetrahydrofuran | 424 | 570 | 6041 | 0.32 |
| | Chloroform | 430 | 567 | 5619 | 0.35 |
| | Dichloromethane | 430 | 583 | 6103 | 0.45 |
| | DMF | 435 | 609 | 6568 | 0.27 |
| $(PTZ)_4$ | Toluene | 390 | 477 | 4677 | 0.42 |
| | 1,4 Dioxane | 390 | 483 | 4731 | 0.32 |
| | Tetrahydrofuran | 391 | 490 | 5167 | 0.31 |
| | Chloroform | 392 | 490 | 5102 | 0.33 |
| | Dichloromethane | 392 | 507 | 5787 | 0.46 |
| | DMF | 394 | 530 | 6963 | 0.41 |
| $(PTZ)_5$ | Toluene | 408 | 536 | 5853 | 0.29 |
| | 1,4 Dioxane | 408 | 536 | 5853 | 0.19 |
| | Tetrahydrofuran | 408 | 538 | 5922 | 0.24 |
| | Chloroform | 408 | 539 | 5957 | 0.25 |
| | Dichloromethane | 408 | 541 | 6025 | 0.23 |
| | DMF | 411 | 556 | 6345 | 0.21 |
| PTZ-Ph-$(PTZ)_2$ | Toluene | 376 | 520 | 7365 | 0.39 |
| | 1,4 Dioxane | 375 | 526 | 7655 | 0.24 |
| | Tetrahydrofuran | 375 | 541 | 8182 | 0.31 |
| | Chloroform | 378 | 533 | 7694 | 0.25 |
| | Dichloromethane | 377 | 548 | 8277 | 0.23 |
| | DMF | 375 | 570 | 9123 | 0.27 |

**(**[a]absorption and emission maxima values recorded in different polarity solvents, [b]the fluorescence quantum yields were measured using quinine sulphate as a standard in 0.5 M H2SO4**).**

## Aggregation Induced Emission (AIE)

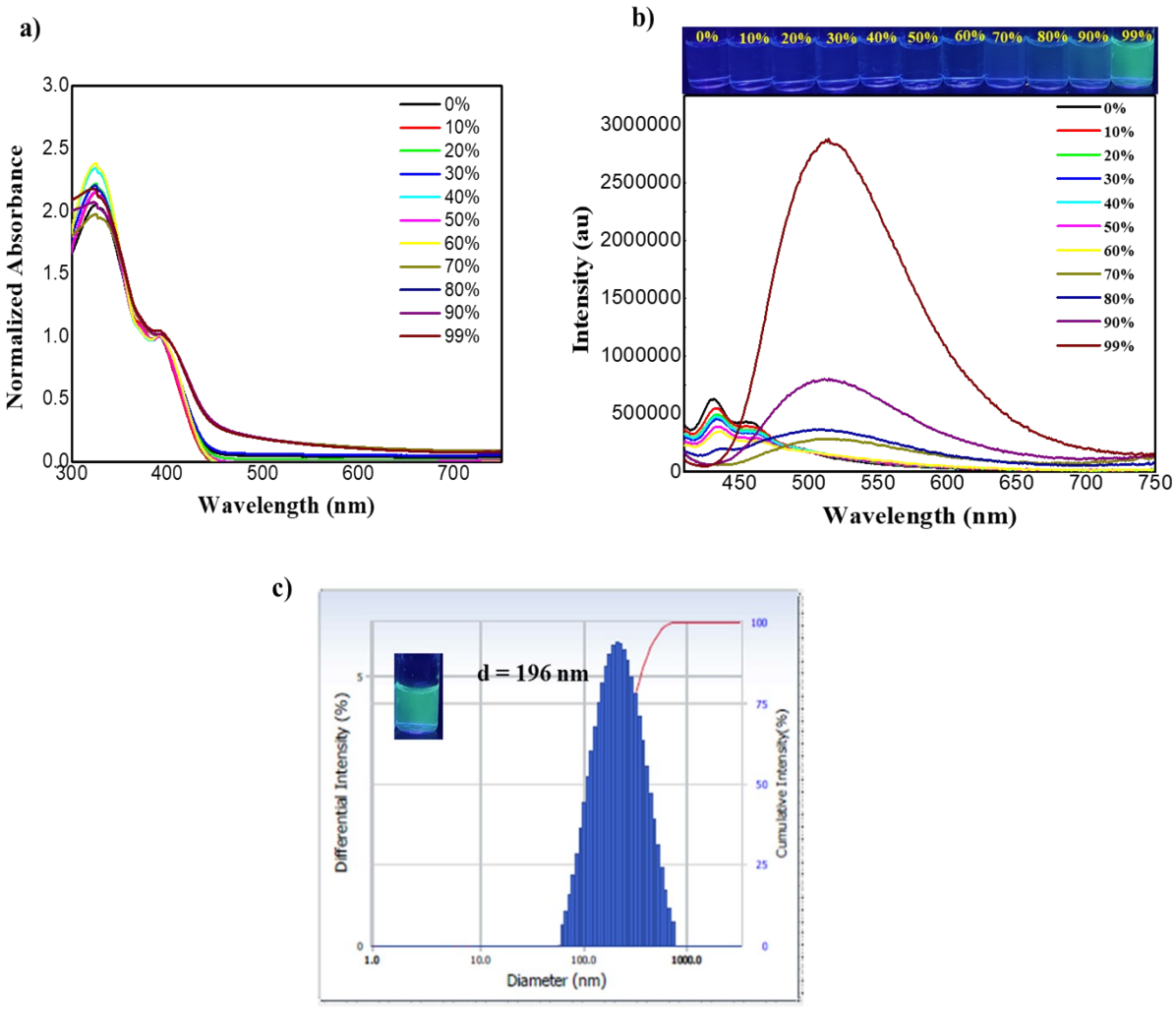



**Fig. S3.** Absorption spectra (a) and Emission spectra (b) of **An(TPE)$_2$** in different THF- Water Mixture with increasing water percentage (Inset: Photographs under 365 nm UV illuminations) c) Dynamic light scattering(DLS) analysis.

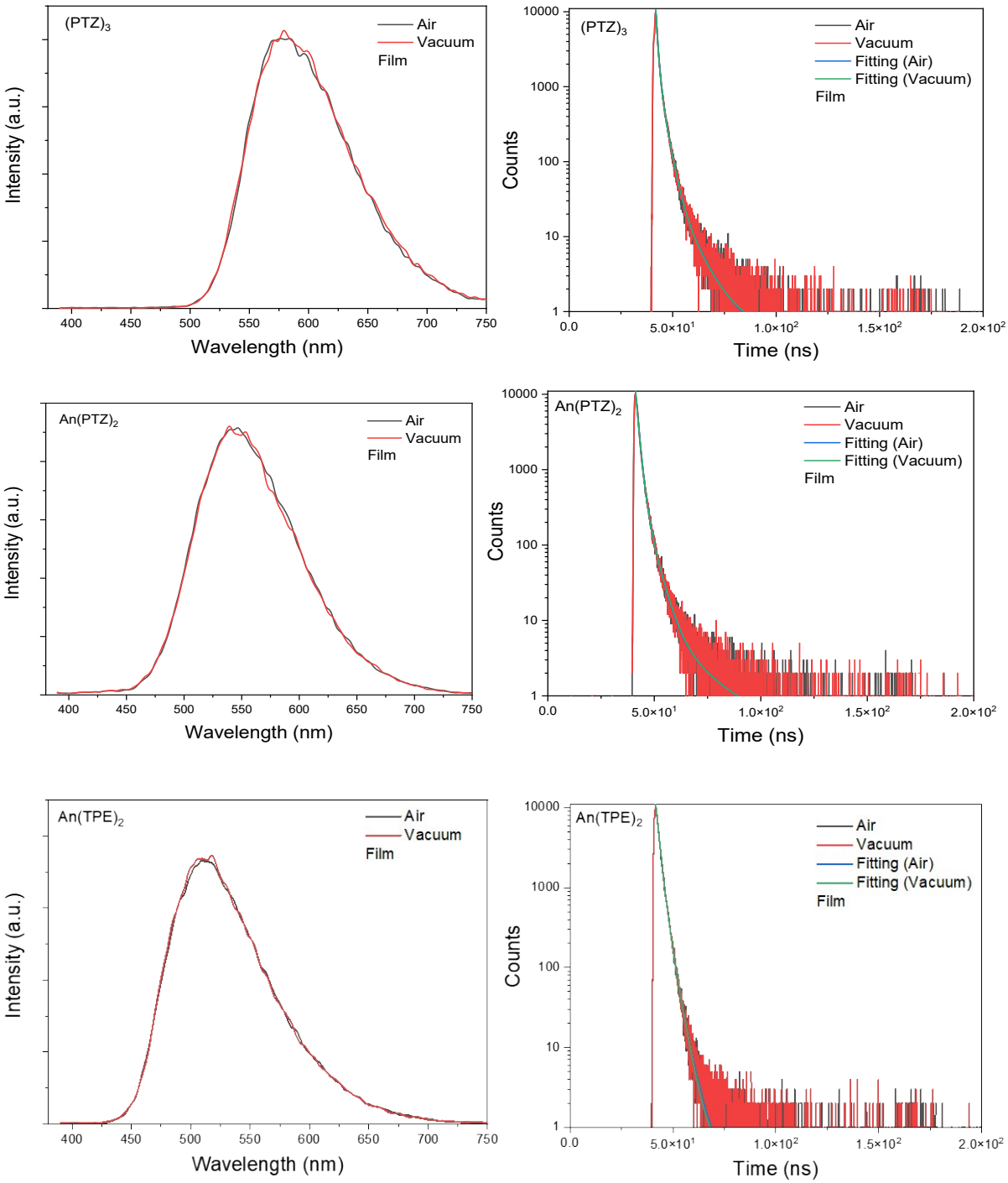
**Table S2** Fluorescence quantum yields of **An(TPE)$_2$** in different THF-water mixtures with increasing water percentage**.**

| **Water Vol %** | $\phi_f$[a] |
|---|---|
| | **An(TPE)$_2$** |
| 0% | 0.02 |
| 10% | 0.03 |
| 20% | 0.01 |
| 30% | 0.01 |
| 40% | 0.01 |
| 50% | 0.02 |
| 60% | 0.01 |
| 70% | 0.01 |
| 80% | 0.01 |
| 90% | 0.07 |
| 99% | 0.21 |

( [a] Fluorescence quantum yields recorded using quinine sulphate as a standard in 0.5 M H2SO4 solution.)

## Photophysical properties

a) b)



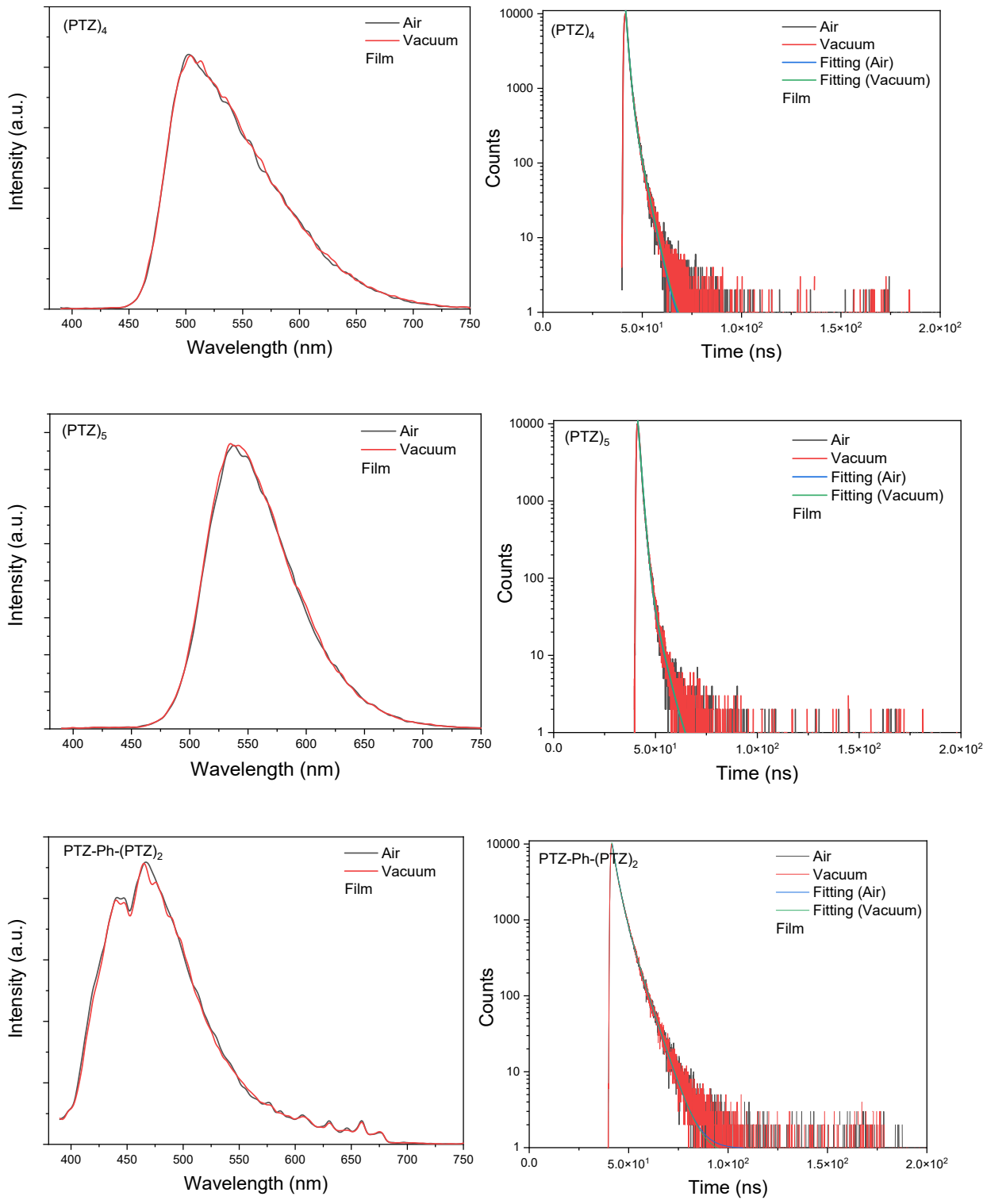
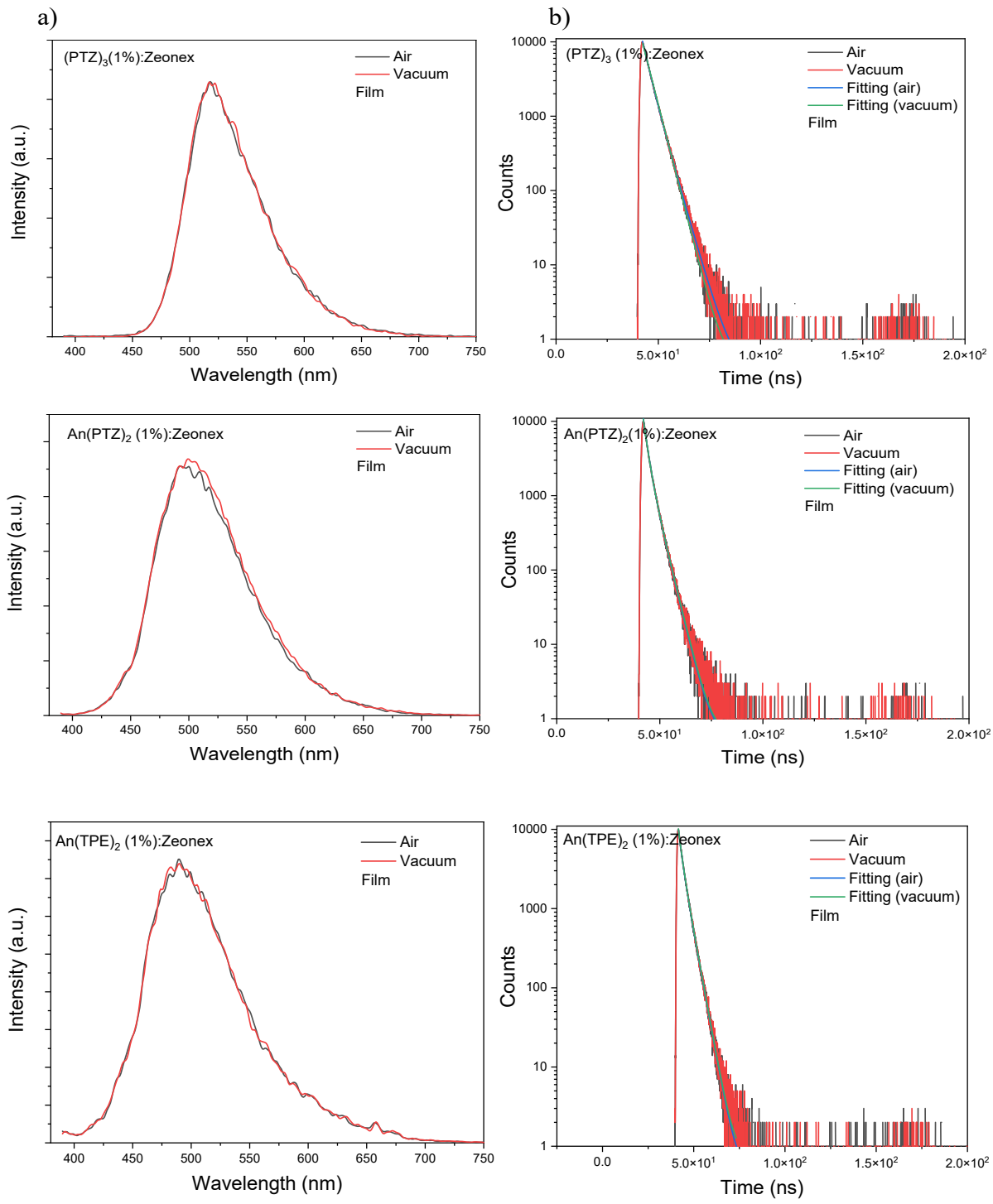



**Fig. S4.** Emission spectra (a) and PL decay curves (b) of neat films of **(PTZ)$_3$**, **An(PTZ)$_2$**, **An(TPE)$_2$**, **(PTZ)$_4$**, **(PTZ)$_5$**, and **PTZ-Ph-(PTZ)$_2$** recorded in air and vacuum at 25 °C ($\lambda_{ex}$ = 340 nm).


a)
b)
(PTZ)3(1%):Zeonex
Air
Vacuum
Film
Intensity (a.u.)
Wavelength (nm)
(PTZ)3 (1%):Zeonex
Fitting (air)
Fitting (vacuum)
Counts
Time (ns)
An(PTZ)2 (1%):Zeonex
An(PTZ)2(1%):Zeonex
An(TPE)2 (1%):Zeonex
An(TPE)2 (1%):Zeonex

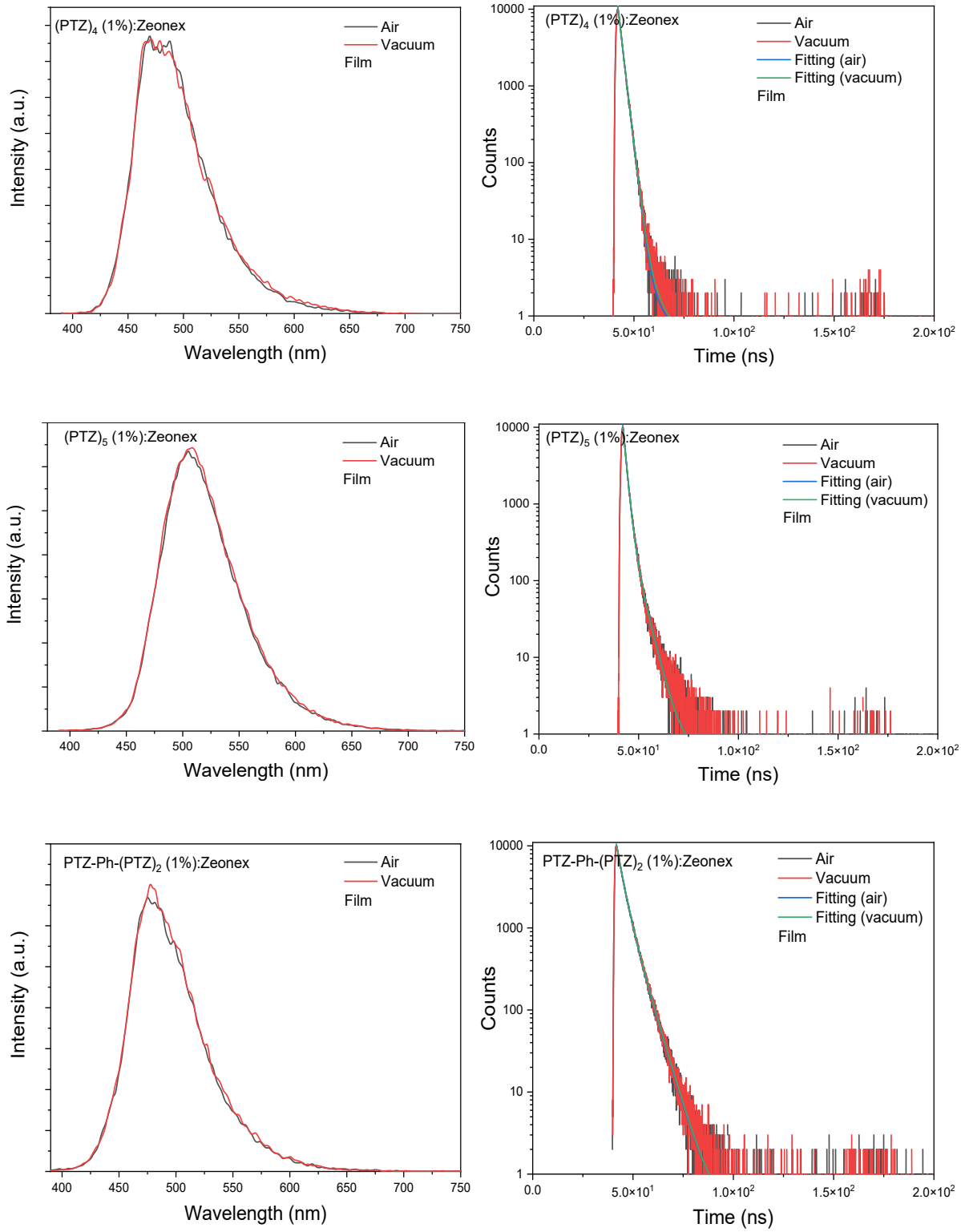



**Fig. S5.** Emission spectra (a) and PL decay curves (b) of **$(PTZ)_3$**, **$An(PTZ)_2$**, **$An(TPE)_2$**, **$(PTZ)_4$**, **$(PTZ)_5$**, and **PTZ-Ph-$(PTZ)_2$** with 1wt% dispersed in Zeonex recorded in air and vacuum at 25 °C ($\lambda_{ex}$ = 340 nm).

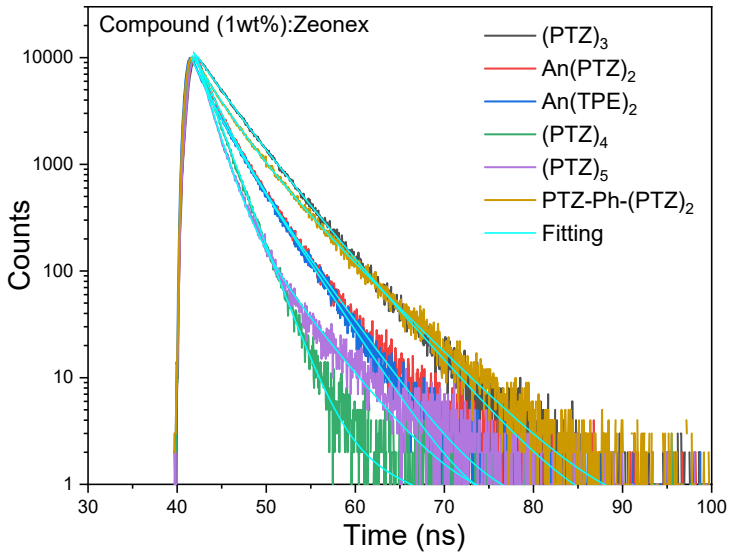



**Fig. S6.** PL decay curves of **(PTZ)$_3$**, **An(PTZ)$_2$**, **An(TPE)$_2$**, **(PTZ)$_4$**, **(PTZ)$_5$**, and **PTZ-Ph-(PTZ)$_2$** with 1wt% dispersed in Zeonex recorded in air.

**Determination and analysis of fluorescence lifetimes**

The fittings of their PL decay curves were provided using software of the Edinburgh Instruments FLS980 spectrometer, according to the following formulas

$$R(t) = B1 \cdot \exp(-t/\tau 1) \quad (1)$$

$$R(t) = B1 \cdot \exp(-t/\tau 1) + B2 \cdot \exp(-x/\tau 2) \quad (2)$$

$$R(t) = B1 \cdot \exp(-t/\tau 1) + B2 \cdot \exp(-t/\tau 2) + B3 \cdot \exp(-t/\tau 3) \quad (3)$$

Here, t is time, B1, B2, and B3 are the fractional intensities of the time components τ1, τ2, and τ3, respectively. If the error fitting factor $\chi^2$ was not in the range $1 \geq \chi 2 < 1.3$ using formula (1), formula (2) or even formula (3) was selected. The fitting data are collected in Table S3. In addition, the formula (4)[1].

$$\tau = \frac{\sum A_i \tau_i^2}{\sum A_i \tau_i} \#(4)$$

was used to calculate the average prompt and delayed fluorescence lifetimes. The results are also collected in Table S3.

**Table S3**. Fitting parameters of PL decay curves and the corresponding intensity-averaged emission lifetimes.

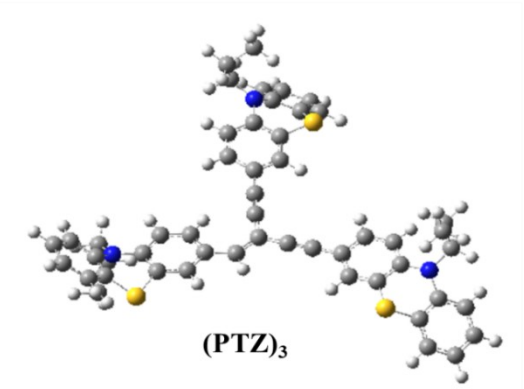
| Parameters | Neat Film | | | | | |
|---|---|---|---|---|---|---|
| | **$(PTZ)_3$** | **$An(PTZ)_2$** | **$An(TPE)_2$** | **$(PTZ)_4$** | **$(PTZ)_5$** | **PTZ-Ph-$(PTZ)_2$** |
| **Air** | | | | | | |
| **B1** | 8746.48 | 10216.80 | 10589.84 | 10334.37 | 11822.28 | 7123.62 |
| **$\tau_1$ (ns)**<br>**Rel (%)** | 0.77<br>(51.45%) | 1.26<br>(77.70%) | 1.66<br>(81.33%) | 1.14<br>(74.18%) | 1.23<br>(93.25%) | 2.26<br>(50.38%) |
| **B2** | 2283.70 | 939.59 | 1134.55 | 1205.37 | 265.28 | 2931.27 |
| **$\tau_2$ (ns)**<br>**Rel (%)** | 2.47<br>(42.98%) | 3.71<br>(20.96%) | 3.55<br>(18.67%) | 3.39<br>(25.82%) | 2.2<br>(6.75%) | 5.40<br>(49.62%) |
| **B3** | 94.61 | 14.06 | - | - | - | - |
| **$\tau_3$ (ns)**<br>**Rel (%)** | 7.74<br>(5.57%) | 15.83<br>(1.34%) | - | - | - | - |
| $\sum B_i\tau_i^2$ | 24786.27 | 32676.08 | 43479.53 | 27282.78 | 22045.94 | 121860.43 |
| $\sum B\tau_i$ | 13107.8100 | 16581.6167 | 21606.7869 | 15867.3861 | 15591.9132 | 31928.2392 |
| **$\tau_{avg}$ (ns)** | 1.89 | 1.97 | 2.01 | 1.71 | 1.41 | 3.81 |
| $\chi^2$ | 1.04 | 1.07 | 1.07 | 1.07 | 1.06 | 1.06 |
| **Vacuum** | | | | | | |
| **B1** | 8869.19 | 10594.73 | 9855.84 | 10439.70 | 11859.65 | 7639.19 |
| **$\tau_1$ (ns)**<br>**Rel (%)** | 0.79<br>(53.56%) | 1.29<br>(79.67%) | 1.57<br>(74.27%) | 1.14<br>(74.96%) | 1.23<br>(92.76%) | 2.32<br>(52.23%) |
| **B2** | 2086.58 | 847.94 | 1646.45 | 1147.89 | 289.51 | 2954.67 |
| **$\tau_2$ (ns)**<br>**Rel (%)** | 2.59<br>(41.34%) | 3.88<br>(19.12%) | 3.25<br>(25.73%) | 3.47<br>(25.04%) | 3.92<br>(7.24%) | 5.48<br>(47.77%) |
| **B3** | 84.43 | 12.75 | - | - | - | - |
| **$\tau_3$ (ns)**<br>**Rel (%)** | 7.89<br>(5.10%) | 16.33<br>(1.21%) | - | - | - | - |
| $\sum B_i\tau_i^2$ | 24788.19 | 33795.95 | 41684.29 | 27389.06 | 22391.19 | 129847.10 |
| $\sum B\tau_i$ | 13077.0550 | 17165.4164 | 20824.6313 | 15884.4363 | 15722.2487 | 33914.5124 |
| **$\tau_{avg}$ (ns)** | 1.89 | 1.96 | 2.00 | 1.72 | 1.42 | 3.82 |
| $\chi^2$ | 1.03 | 1.08 | 1.07 | 1.07 | 1.02 | 1.04 |
| **Compound (1%):Zeonex (air)** | | | | | | |
| **B1** | 5314.36 | 7164.07 | 4410.02 | 7366.16 | 10205.24 | 6925.96 |
| **$\tau_1$ (ns)**<br>**Rel (%)** | 3.01<br>(40.33%) | 1.75<br>(45.97%) | 1.62<br>(26.40%) | 2.12<br>(57.60%) | 1.45<br>(82.16%) | 2.64<br>(48.77%) |
| **B2** | 5029.86 | 3873.91 | 5777.38 | 3054.95 | 771.08 | 3633.68 |
| **$\tau_2$ (ns)**<br>**Rel (%)** | 4.71<br>(59.67%) | 3.80<br>(54.03%) | 3.45<br>(73.60%) | 3.76<br>(42.40%) | 4.18<br>(17.84%) | 5.28<br>(51.23%) |
| $\sum B_i\tau_i^2$ | 159731.55 | 77879.22 | 80338.92 | 76296.13 | 34929.14 | 48271.17 |
| $\sum B\tau_i$ | 39686.8642 | 27257.9805 | 27076.1934 | 27102.8712 | 18020.7124 | 18284.5344 |
| **$\tau_{avg}$ (ns)** | 4.02 | 2.85 | 2.96 | 2.81 | 1.93 | 2.64 |
| $\chi^2$ | 1.01 | 1.09 | 1.05 | 1.04 | 1.07 | 1.02 |
| **Compound (1%):Zeonex (vacuum)** | | | | | | |
| **B1** | 9653.27 | 7171.38 | 4293.60 | 7322.91 | 10257.07 | 7057.07 |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\tau_1$ (ns)<br>Rel (%) | 4.03<br>(100%) | 1.75<br>(46.12%) | 1.56<br>(24.37%) | 2.11<br>(55.98%) | 1.48<br>(82.80%) | 2.63<br>(49.02%) |
| B2 | - | 3804.03 | 6066.78 | 3244.34 | 749.04 | 3633.81 |
| $\tau_2$ (ns)<br>Rel (%) | - | 3.85<br>(53.88%) | 3.42<br>(75.63%) | 3.74<br>(44.02%) | 4.20<br>(17.20%) | 5.32<br>(50.98%) |
| $\sum B_i\tau_i^2$ | - | 78347.59 | 81408.39 | 77982.86 | 35680.15 | 151658.59 |
| $\sum B\tau_i$ | - | 27195.4305 | 27446.4036 | 27585.1717 | 18326.4316 | 37891.9633 |
| $\tau_{avg}$ (ns) | - | 2.88 | 2.96 | 2.82 | 1.94 | 4.00 |
| $\chi^2$ | 1.00 | 1.03 | 1.00 | 1.02 | 1.04 | 1.00 |

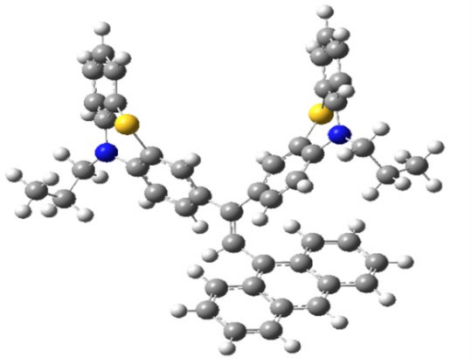
**Table S4**. Photophysical parameters of the compounds under air and vacuum

| Compounds | $\lambda_{ems}$ (nm) (Air/Vac) | $\tau_{avg}$ (ns) (Air/Vac) | $\lambda_{ems}$ (nm) (Air/Vac) Zeonex +(1%) | $\tau_{avg}$ (ns) (Air/Vac) Zeonex +(1%) |
|---|---|---|---|---|
| **$(PTZ)_3$** | 584/579 | 1.89/1.89 | 518/517 | 4.02/4.03 |
| **$An(PTZ)_2$** | 547/546 | 1.97/1.96 | 499/499 | 2.85/2.88 |
| **$An(TPE)_2$** | 510/510 | 2.01/2.00 | 490/490 | 2.96/2.96 |
| **$(PTZ)_4$** | 502/504 | 1.71/1.72 | 470/471 | 2.81/2.82 |
| **$(PTZ)_5$** | 538/535 | 1.41/1.42 | 505/508 | 1.93/1.94 |
| **PTZ-Ph-$(PTZ)_2$** | 508 / 508 | 3.81/3.82 | 475/478 | 2.64/4.00 |

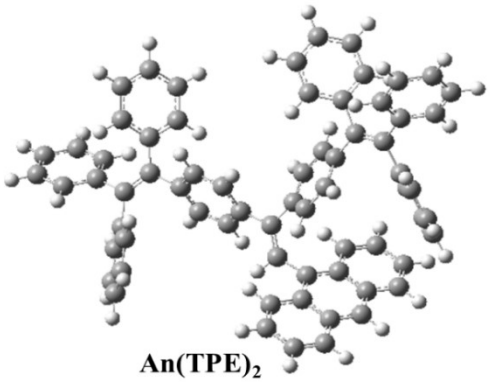
DFT Optimized Structures of **$(PTZ)_3$**, **$An(PTZ)_2$**, **$An(TPE)_2$**, **$(PTZ)_4$**, **$(PTZ)_5$** and **PTZ-Ph-$(PTZ)_2$**.



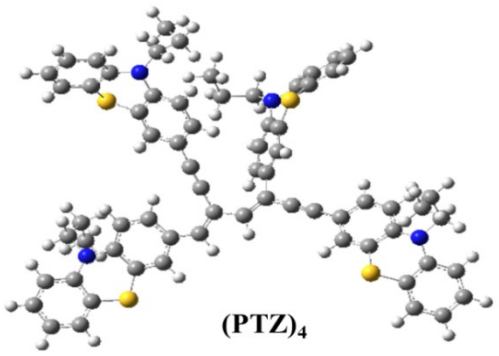
$(PTZ)_3$



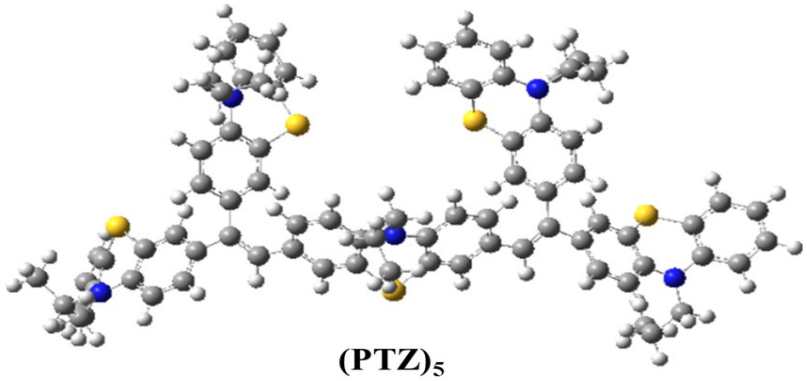
$An(PTZ)_2$



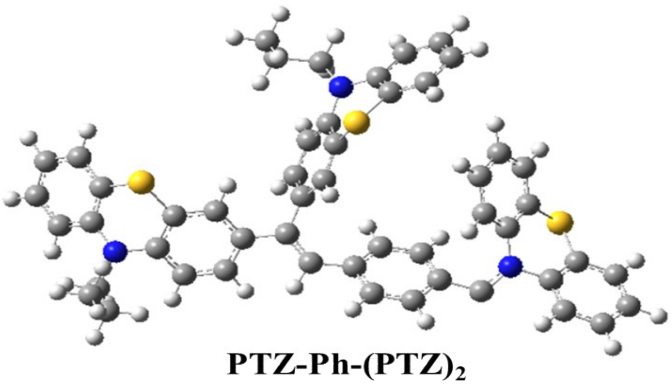
$An(TPE)_2$



$(PTZ)_4$

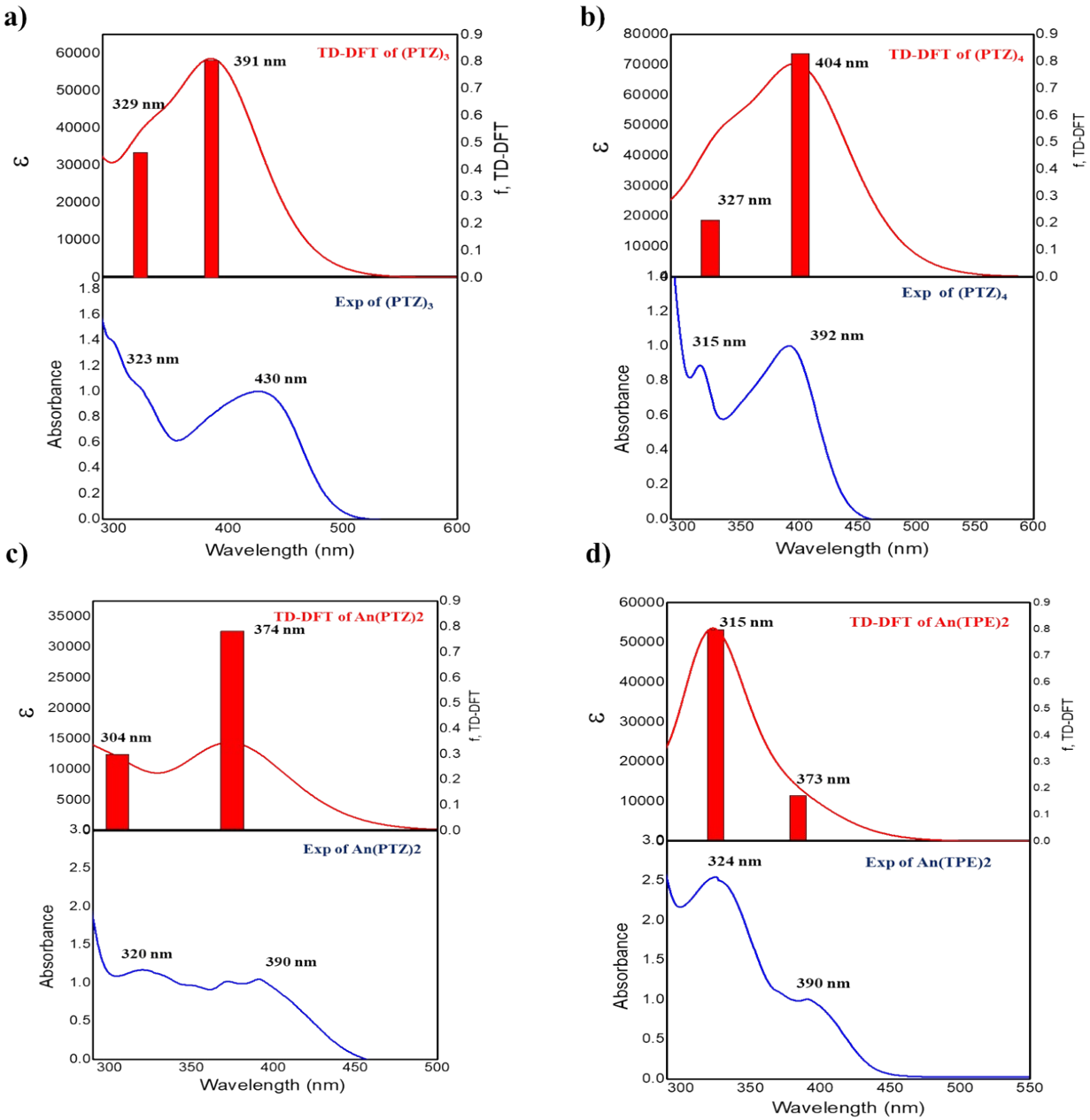


$(PTZ)_5$



$PTZ\text{-}Ph\text{-}(PTZ)_2$

## TD-DFT Calculation



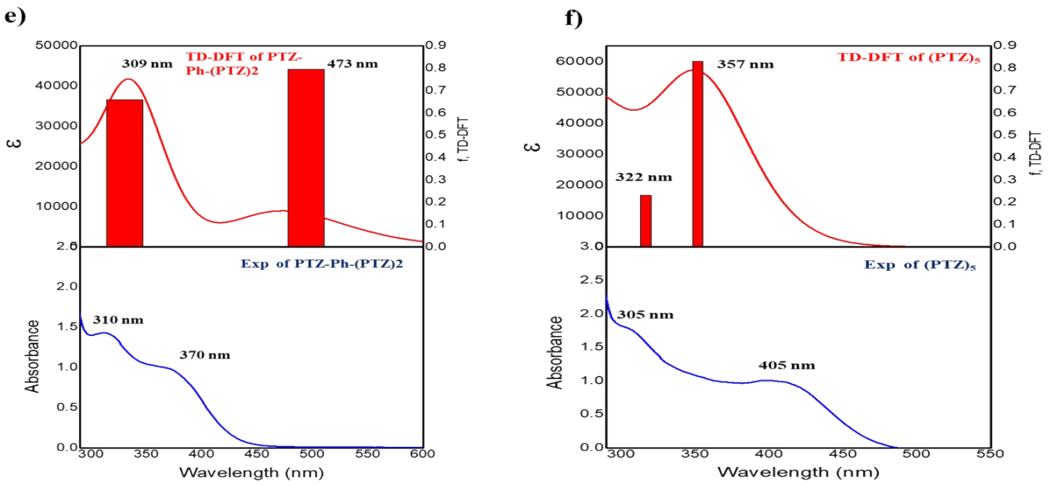



**Fig. S7.** UV-vis absorption spectra of a) **(PTZ)$_3$**, b) **(PTZ)$_4$**, c) **An(PTZ)$_2$**, d) **An(TPE)$_2$**, e) **PTZ-Ph-(PTZ)$_2$**, f) **(PTZ)$_5$**. Experimental (bottom) and TD-DFT predicted (top) in the gas phase.

**Table S5** The computed vertical transitions; oscillator strengths and configurations of **(PTZ)$_3$**, **(PTZ)$_4$**, **An(PTZ)$_2$**, **An(TPE)$_2$**, **PTZ-Ph-(PTZ)$_2$**, **(PTZ)$_5$**.

| Compound | Wavelength (nm) | *f*[a] | Configuration | Assignment |
|---|---|---|---|---|
| **(PTZ)$_3$** | 391 | 1.3402 | HOMO → LUMO (44%) | ICT |
| | 329 | 0.7733 | (HOMO-1) → LUMO (27%) | π–π* |
| **(PTZ)$_4$** | 404 | 1.5677 | HOMO → LUMO (45%) | ICT |
| | 327 | 0.4010 | (HOMO-2) → LUMO (26%) | π–π* |
| **An(PTZ)$_2$** | 374 | 0.3481 | HOMO → LUMO (40%) | ICT |
| | 304 | 0.1330 | (HOMO-1) → (LUMO+1)(15%) | π–π* |
| **An(TPE)$_2$** | 373 | 0.2502 | HOMO → LUMO (44%) | ICT |
| | 315 | 1.1534 | (HOMO-1) → (LUMO+2)(17%) | π–π* |
| **(PTZ)$_5$** | 357 | 1.2012 | HOMO → LUMO (36%) | ICT |
| | 322 | 0.3359 | HOMO → (LUMO+1) (26%) | π–π* |
| **PTZ-Ph-(PTZ)$_2$** | 473 | 0.2211 | HOMO → LUMO (17%) | ICT |
| | 309 | 0.1836 | (HOMO-1) → LUMO (20%) | π–π* |

[a]Oscillator strength.

## Thermal properties

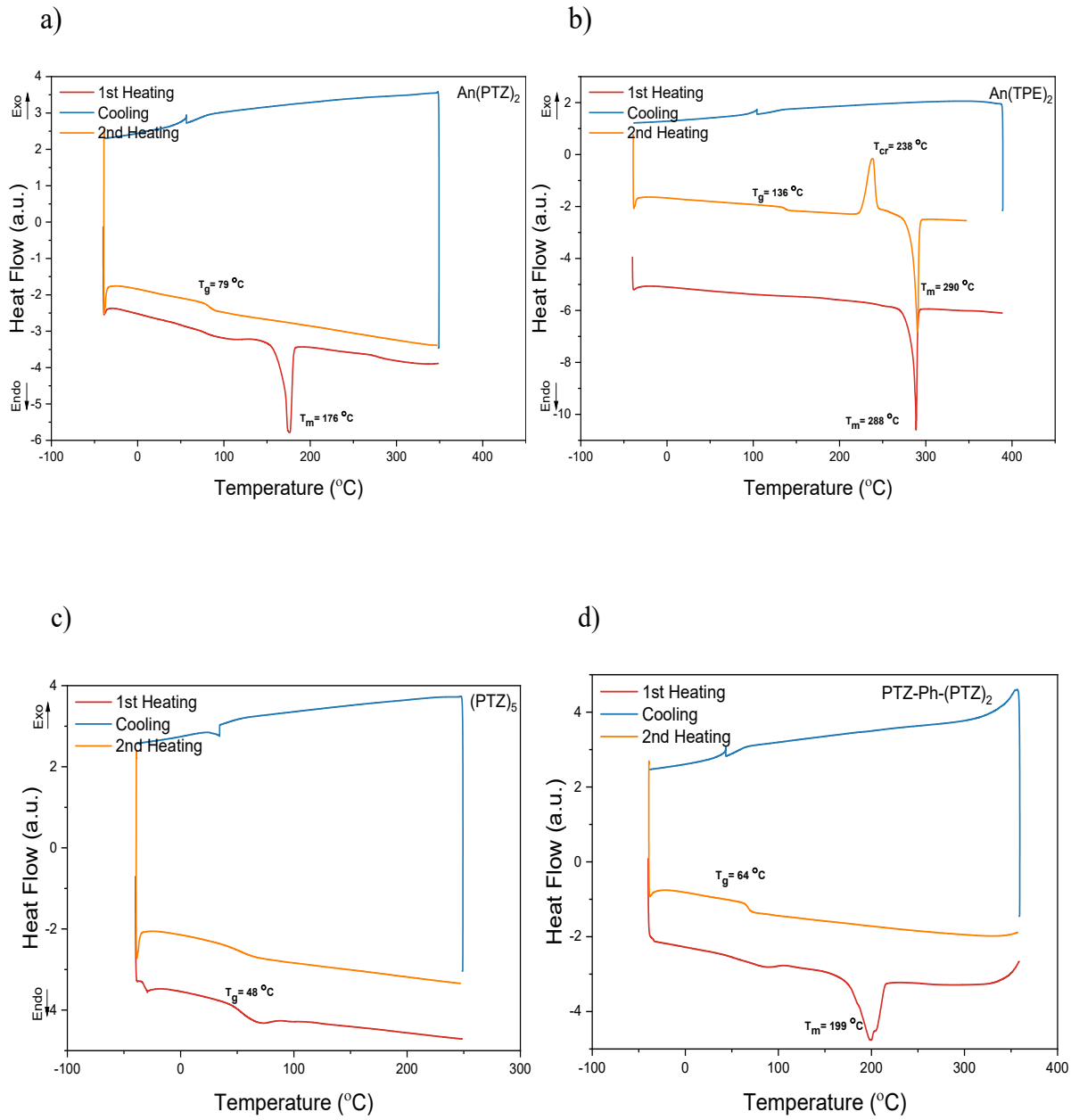



**Fig. S8.** Differential scanning calorimetry (DSC) plots of compounds. Photoelectron emission spectra for vacuum-deposited films of **An(PTZ)$_2$** (a), **An(TPE)$_2$** (b), **(PTZ)$_5$** (c), and **PTZ-Ph-(PTZ)$_2$** (d)

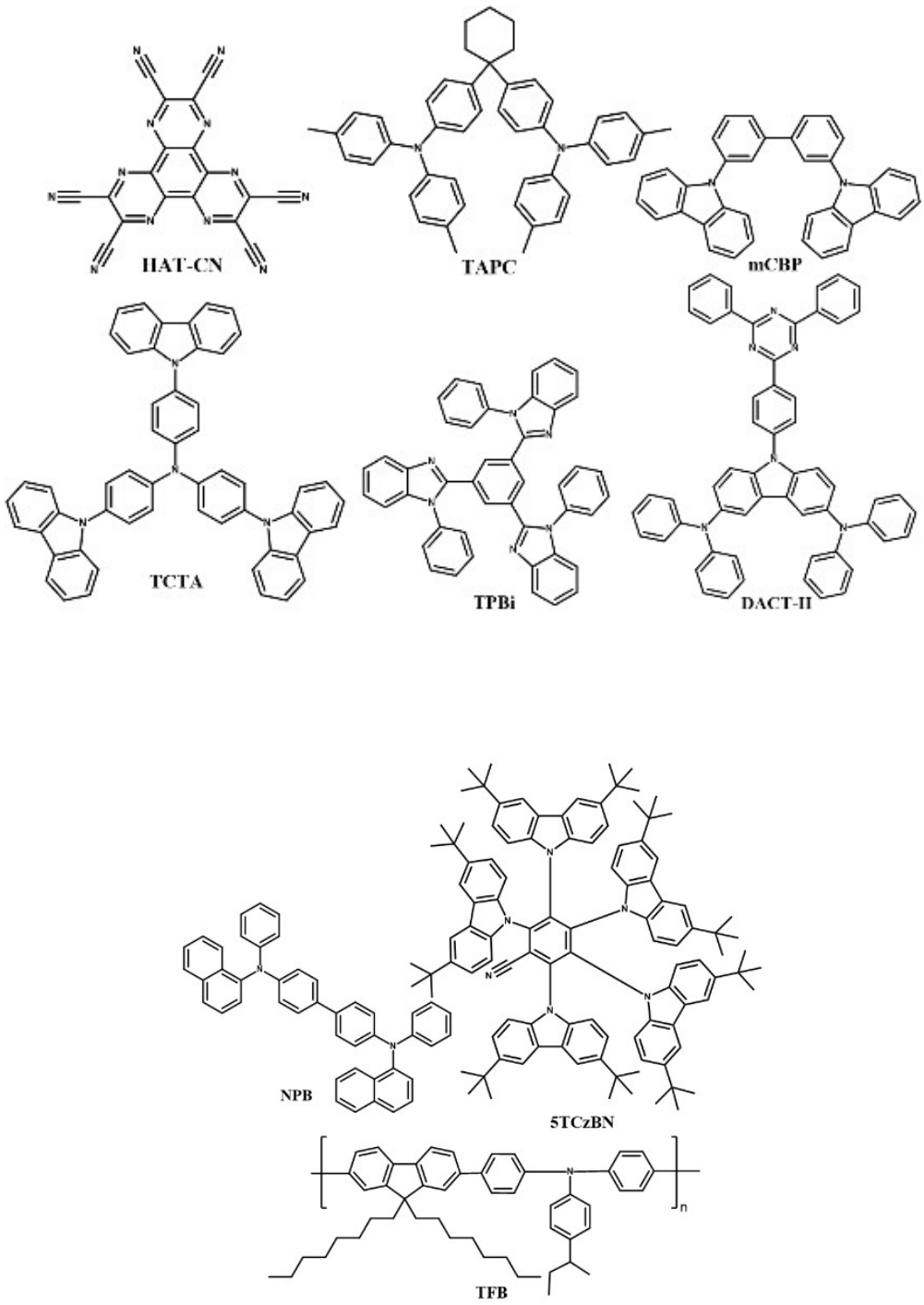



**Fig. S9.** The chemical structure of compounds used for fabrication of OLEDs.

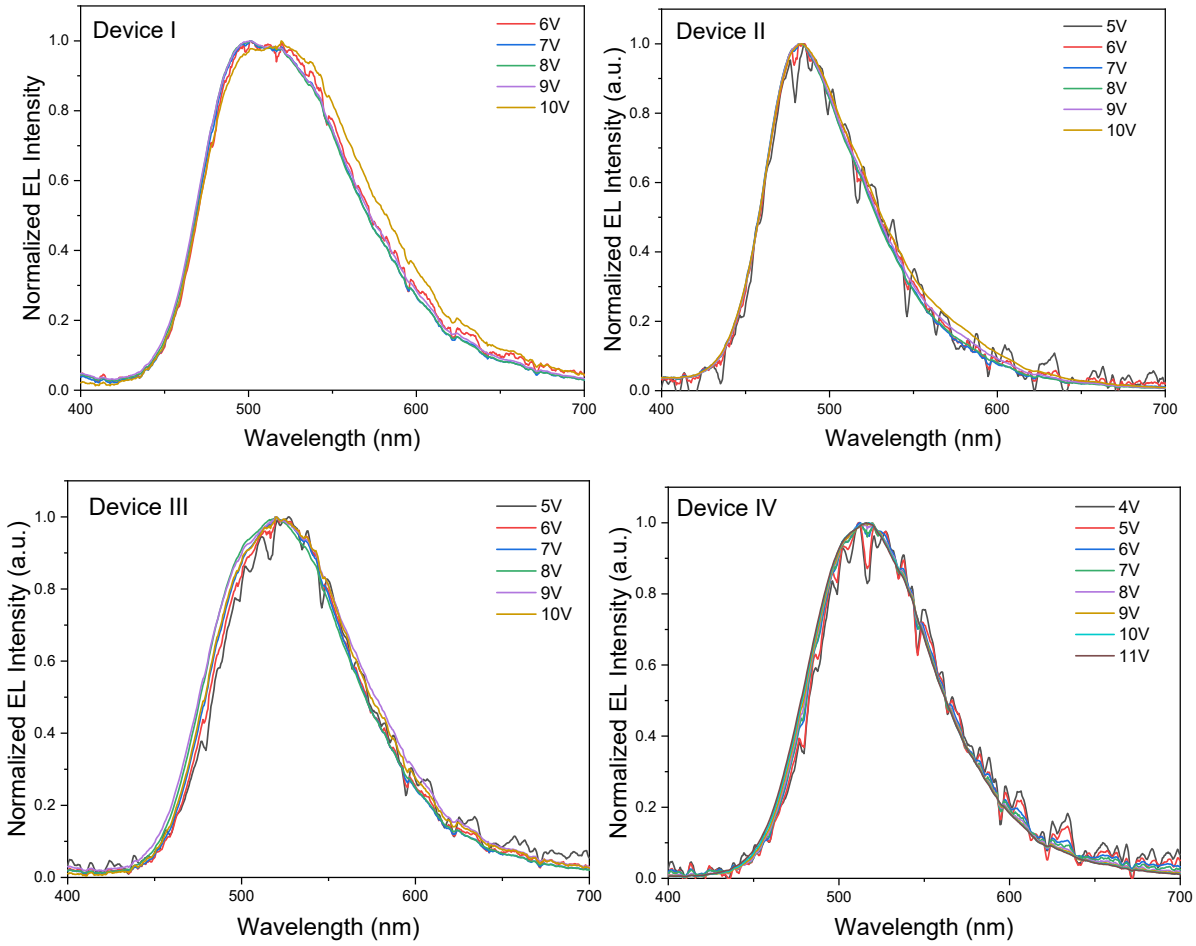



**Fig. S10.** Normalized EL spectra of devices I-IV.

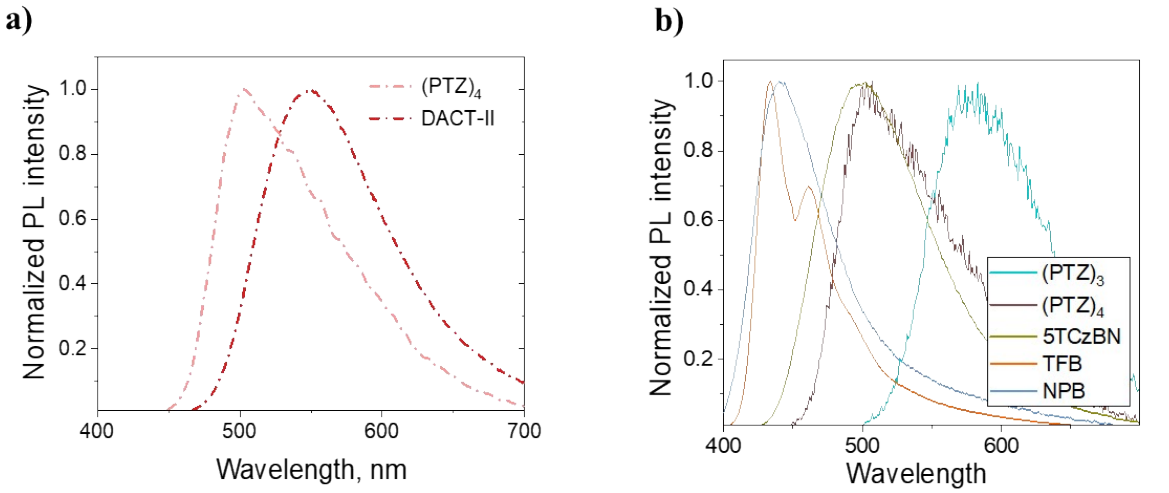



**Fig. S11.** The chemical structure of compounds used for fabrication of OLEDs.

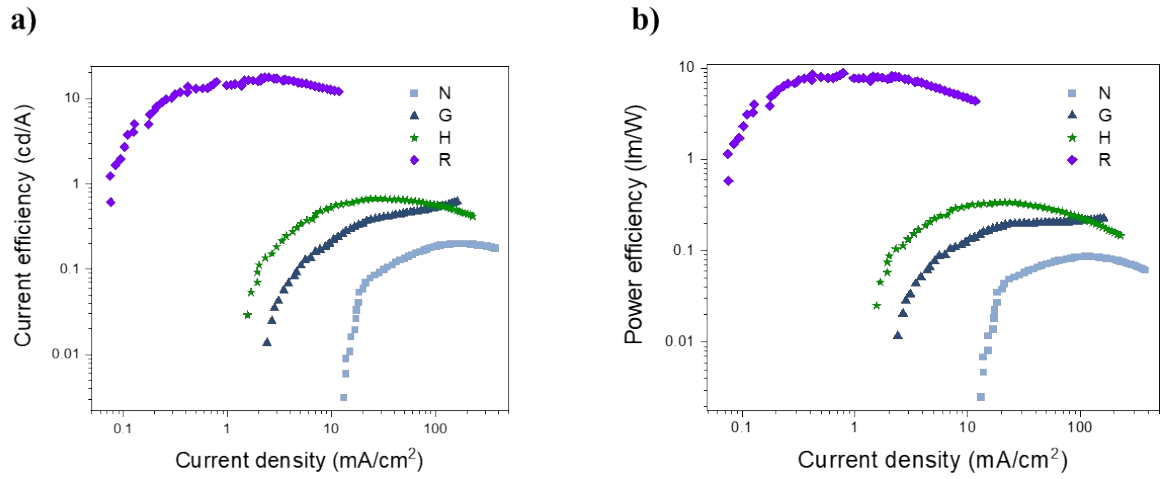



**Fig. S12.** Current density (a) and power efficiency (b)as a function of current density of devices I-IV.

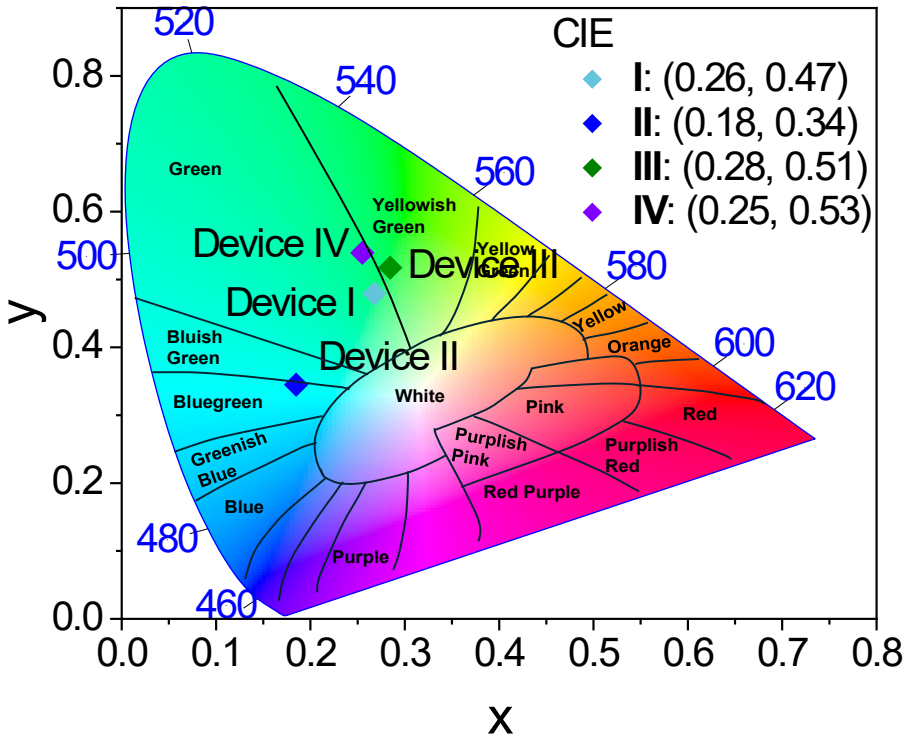
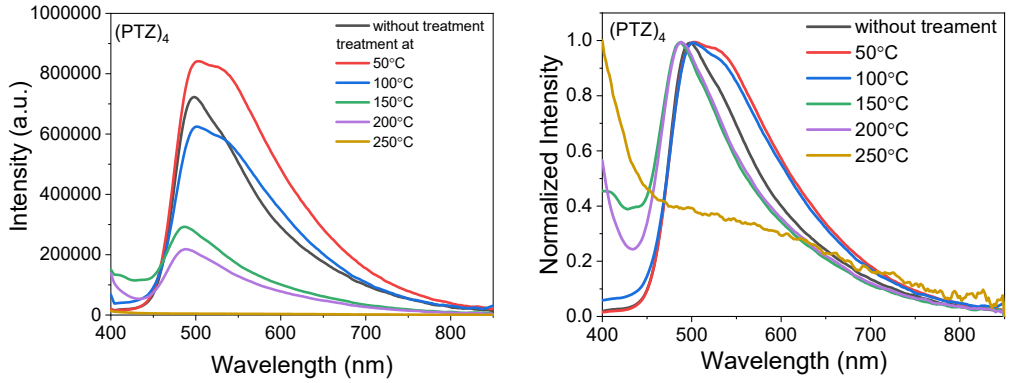
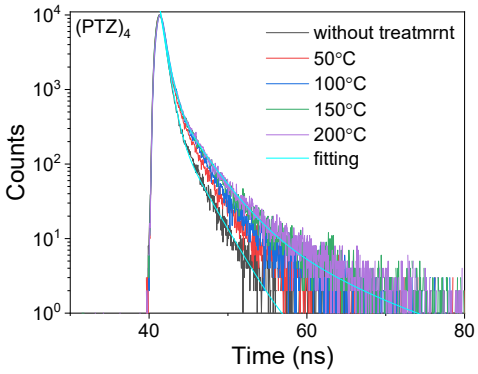



**Fig. S13.** CIE coordinates of devices I-IV.

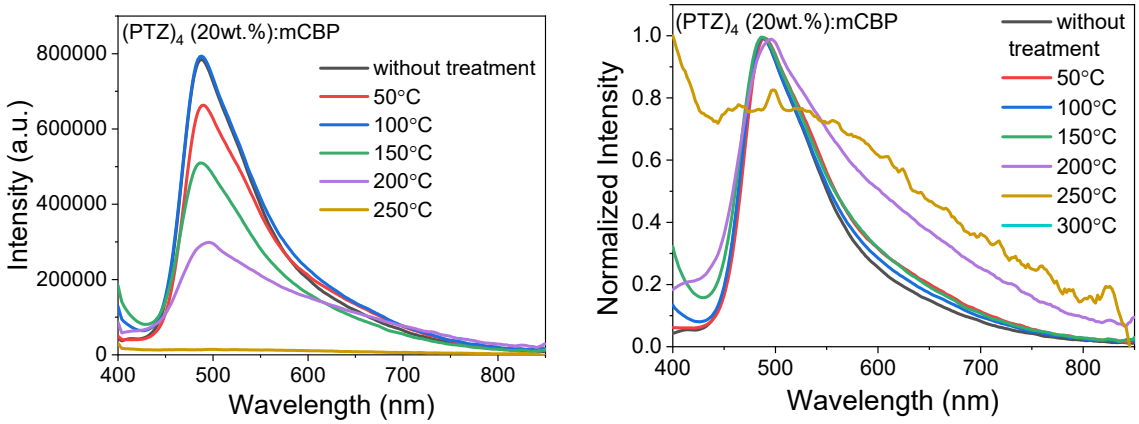



a) b)

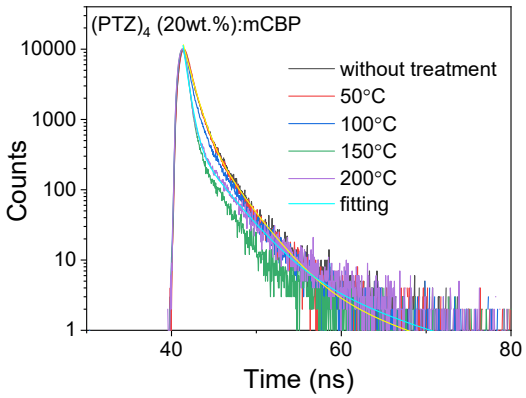



c)

**Figure S14.** Non-normalised (a) and normalised (b) PL spectra and PL decay curves (c) of the spin-coated film $(PTZ)_4$ before and after thermal treatments at different temperatures.

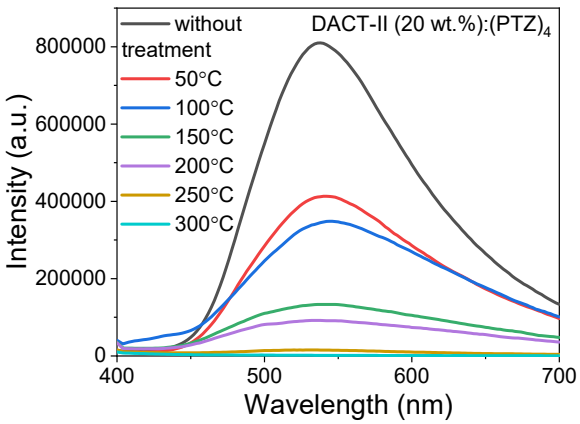



a) b)

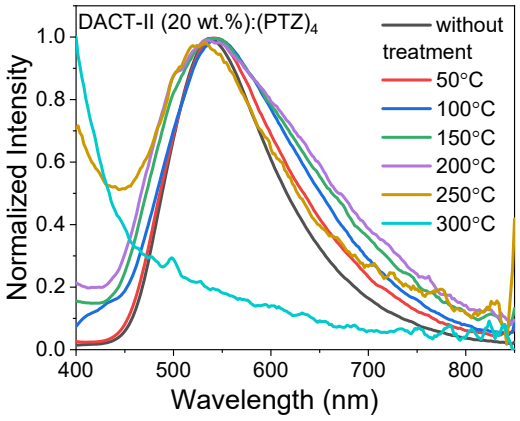



c)

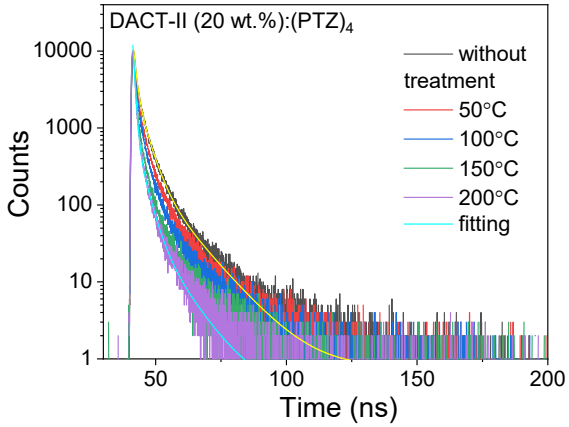
**Figure S15.** Non-normalised (a) and normalised (b) PL spectra and PL decay curves (c) of the spin-coated film of 20% solid solution of $(PTZ)_4$ in mCBP before and after thermal treatments at the different temperatures.




a)




b)




c)

**Figure S16.** Non-normalised (a) and normalised (b) PL spectra and PL decay curves (c) of the spin-coated film of 20% solid solution of DACT-II dispersed in $(PTZ)_4$ as the host before and after thermal treatments at the different temperatures.

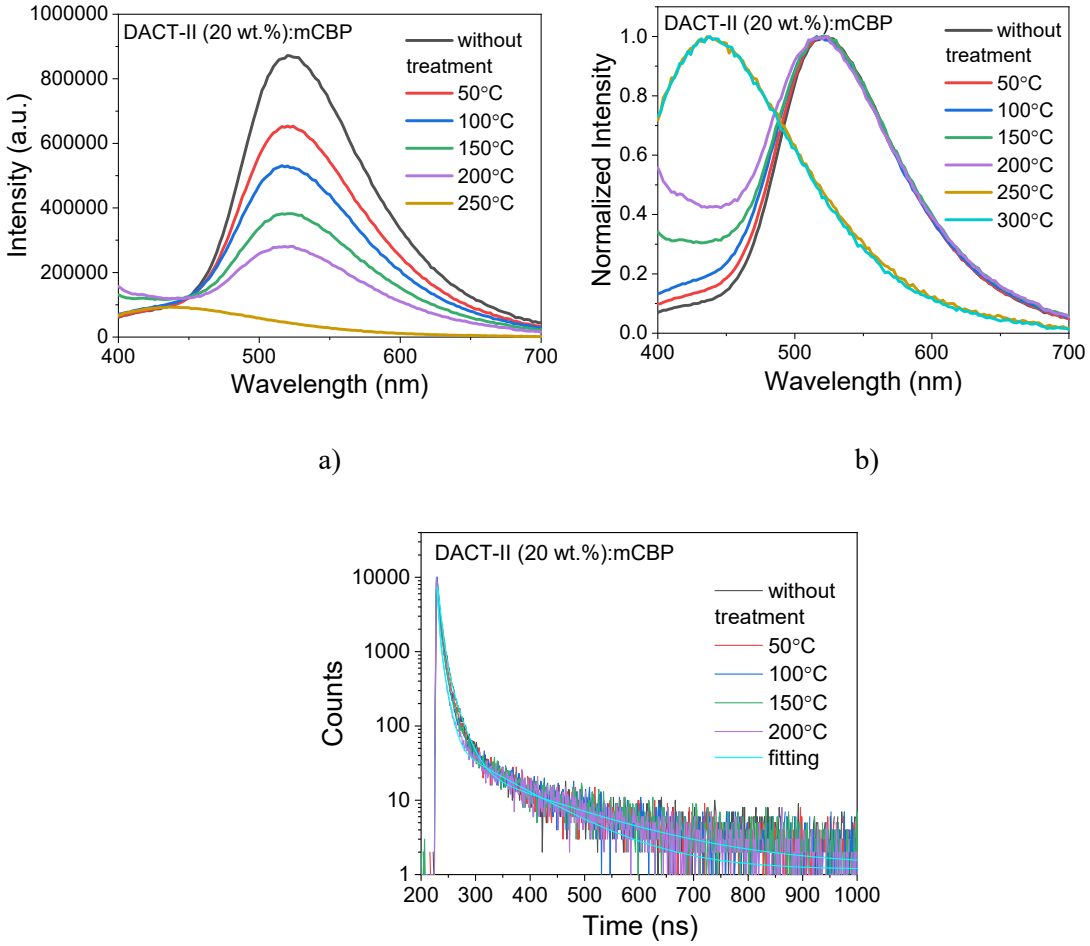



**Figure S17.** Non-normalised (a) and normalised (b) PL spectra and PL decay curves (c) of the spin-coated film of the 20% solid solution od DACT-II mCBP before and after thermal treatments at the different temperatures.

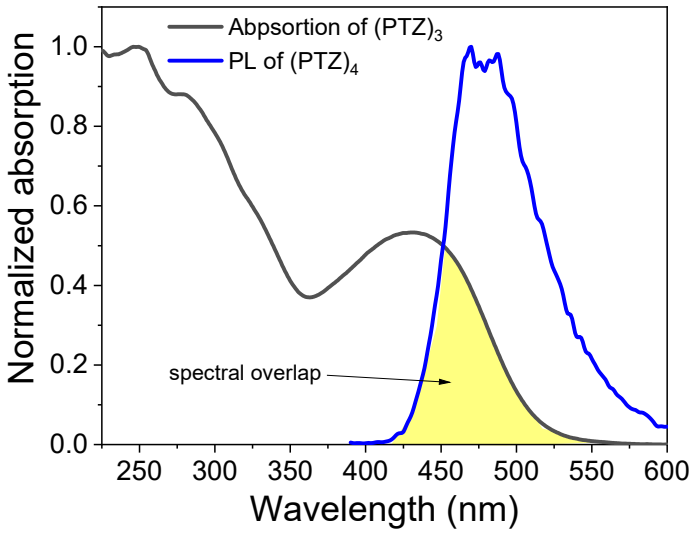



**Figure S18.** Normalised absorption spectrum of neat films of (PTZ)3 and PL spectrum of 1% solid dispersion of compound **$(PTZ)_4$** in Zeonex. The yellow area is related to the spectral overlap.

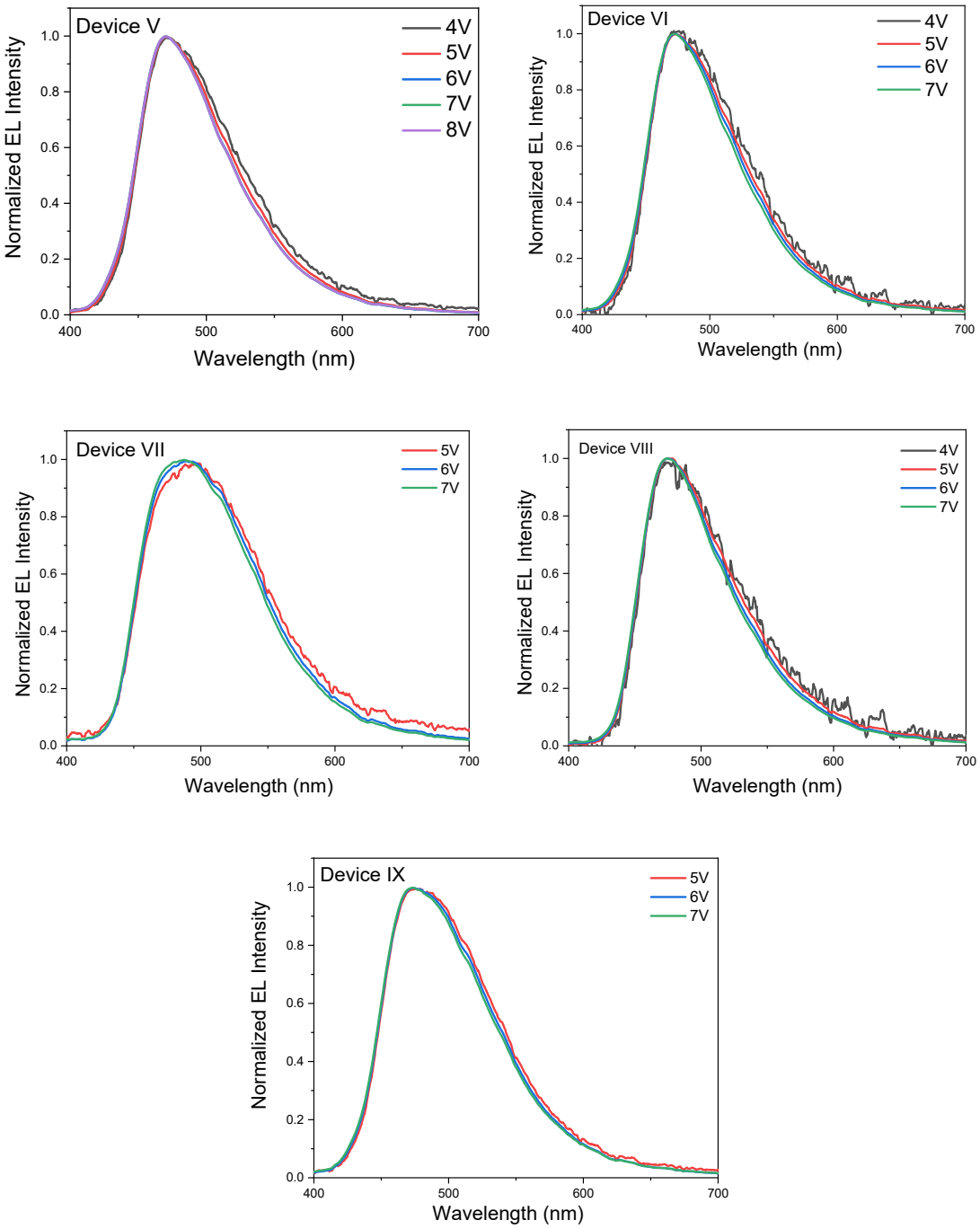



**Fig. S19.** Normalized EL spectra of devices V-IX.

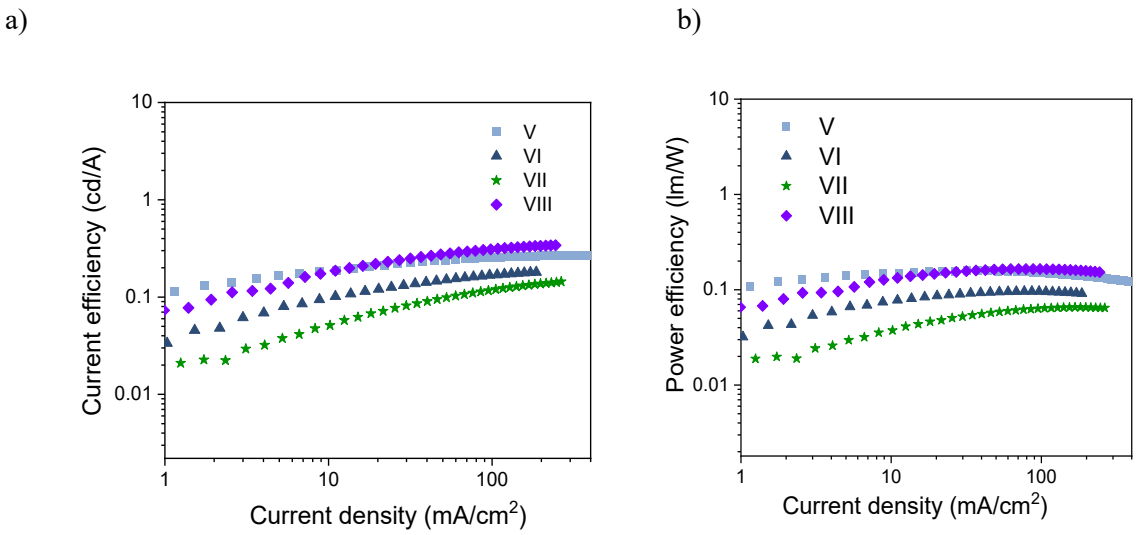



**Fig. S20.** Current density (a) and power efficiency (b)as a function of current density of devices V-VIII.

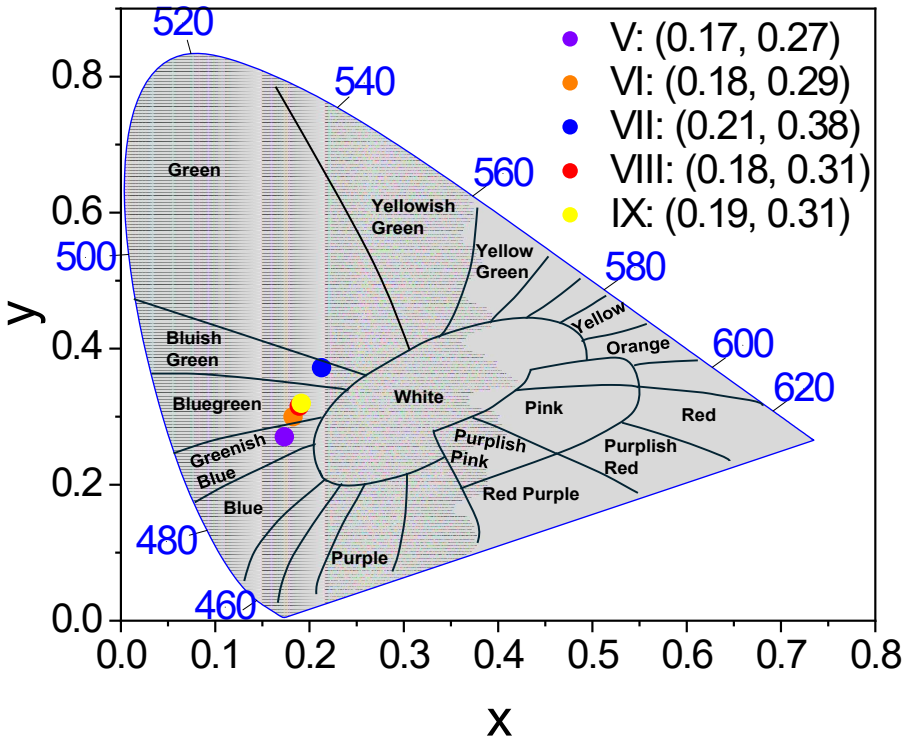



**Fig. S21.** CIE coordinates of devices V-IX.

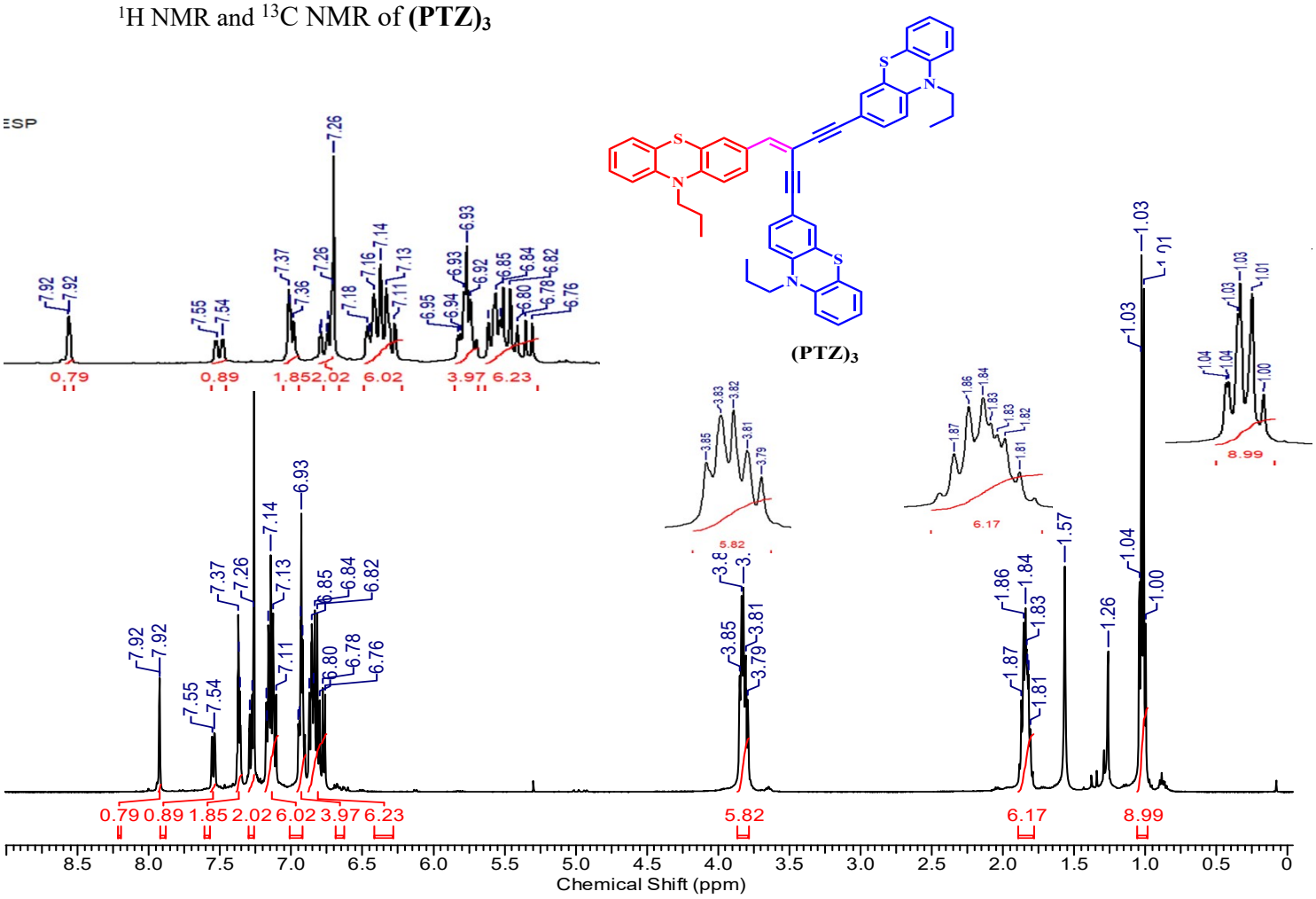
**Table S6**. Different ratios of each compound dissolved and mixed for EMLs of devices V-IX.

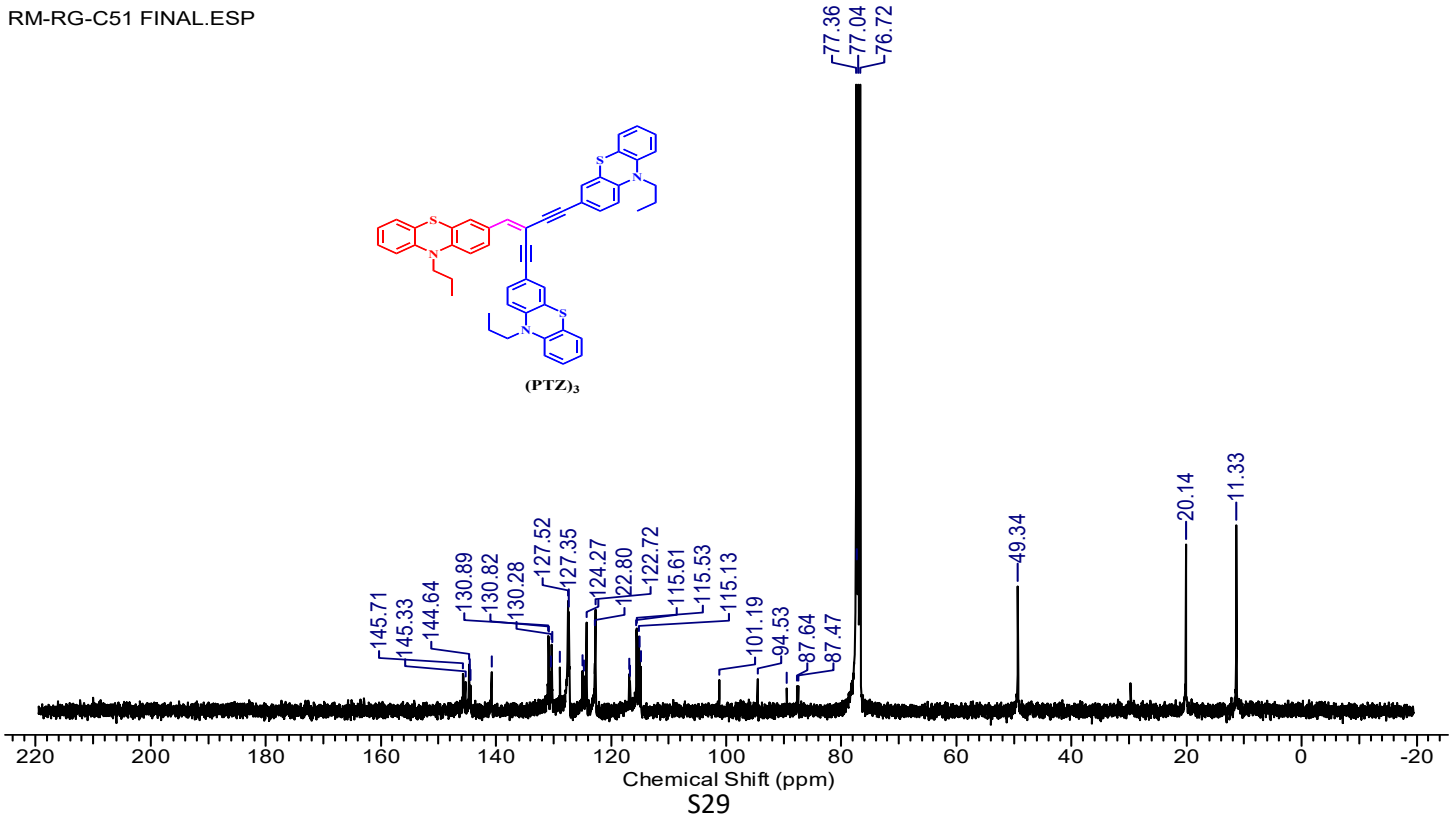
| Compounds | $(PTZ)_3$ (orange) | $(PTZ)_4$ (Blue) | 5TCzBN | NPB |
|---|---|---|---|---|
| **V** | (1%) | (5 %) | (10 %) | (84 %) |
| **VI** | (3 %) | (15 %) | (20 %) | (72 %) |
| **VII** | (10 %) | - | (20 %) | (70 %) |
| **VIII** | - | (10 %) | (20 %) | (70 %) |
| **IX** | (10 %) | (10 %) | (10 %) | (70 %) |


**Fig. S22.** Photos of solution-processable OLEDs V-IX at 7V.

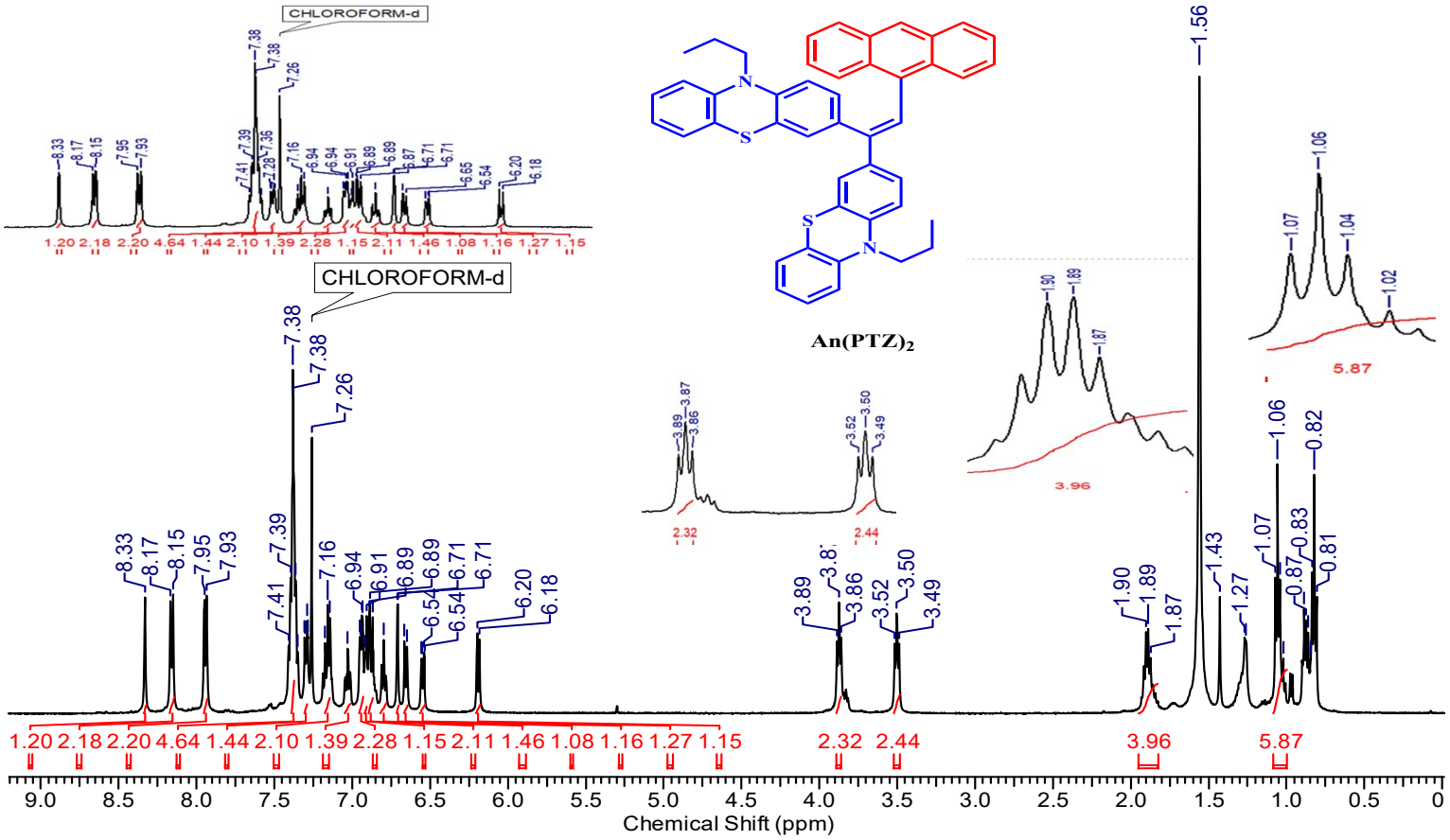
## Copies of NMR and HRMS spectra of new compounds

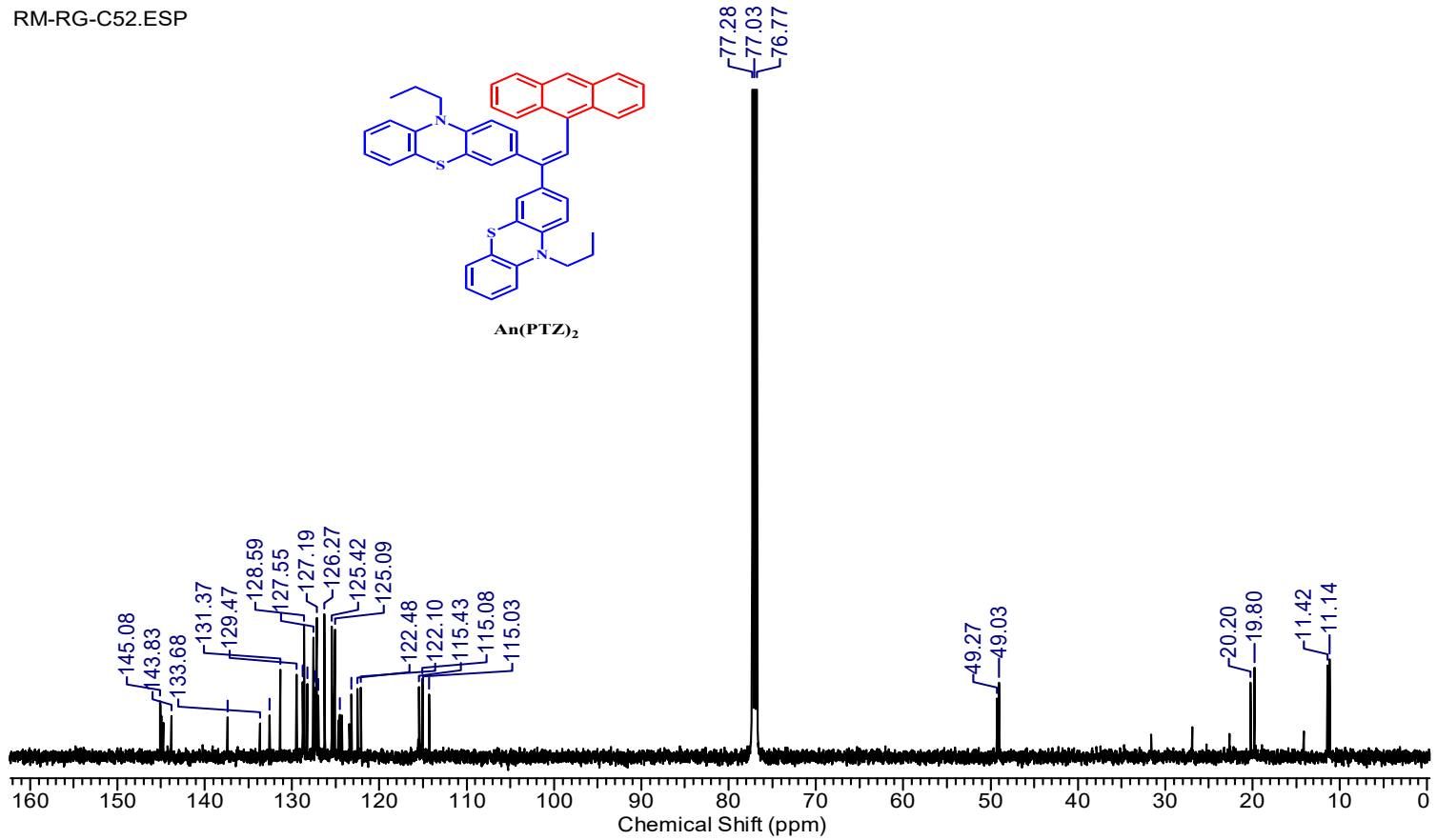
$^{1}$H NMR and $^{13}$C NMR of **(PTZ)$_3$**



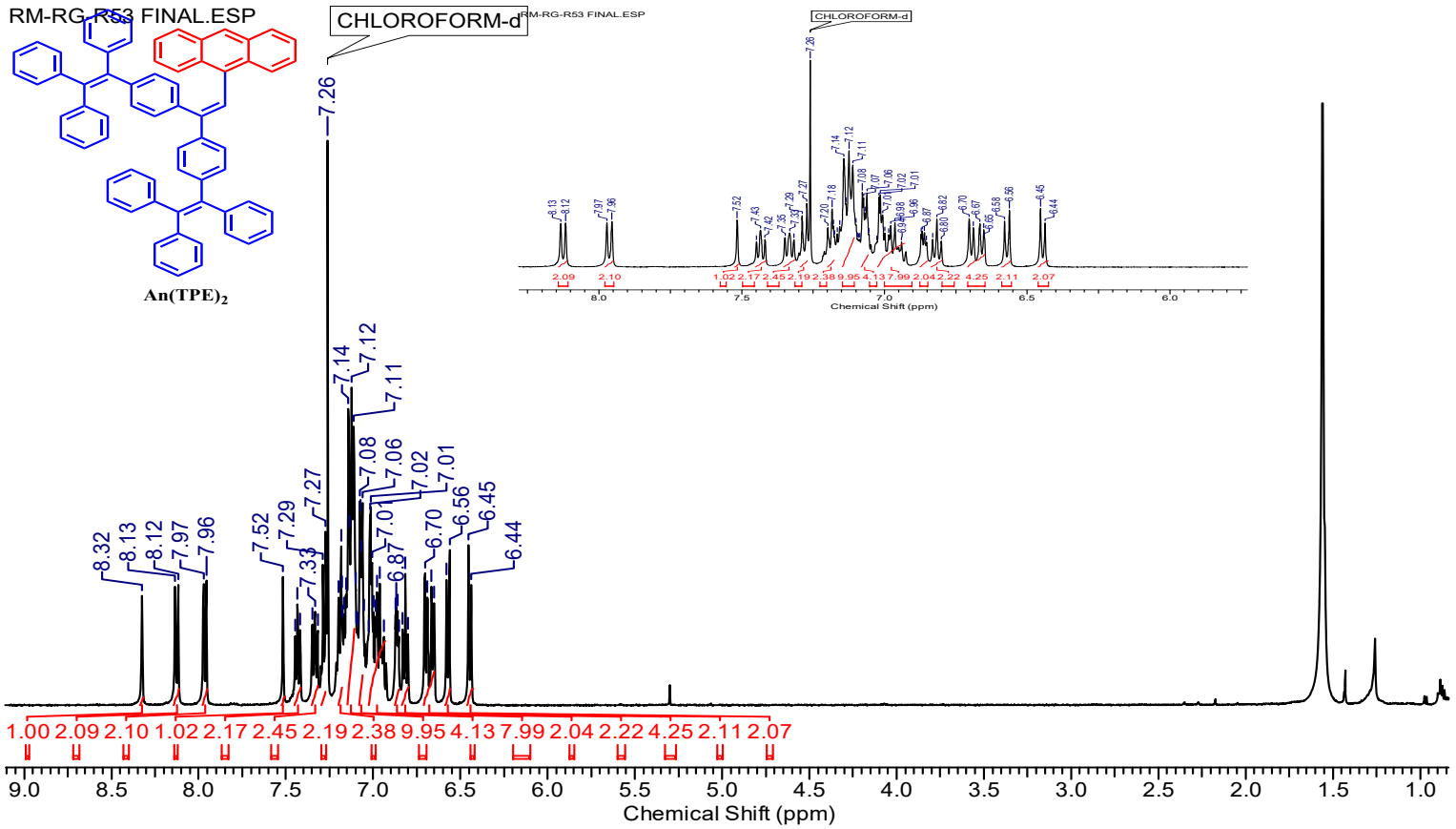



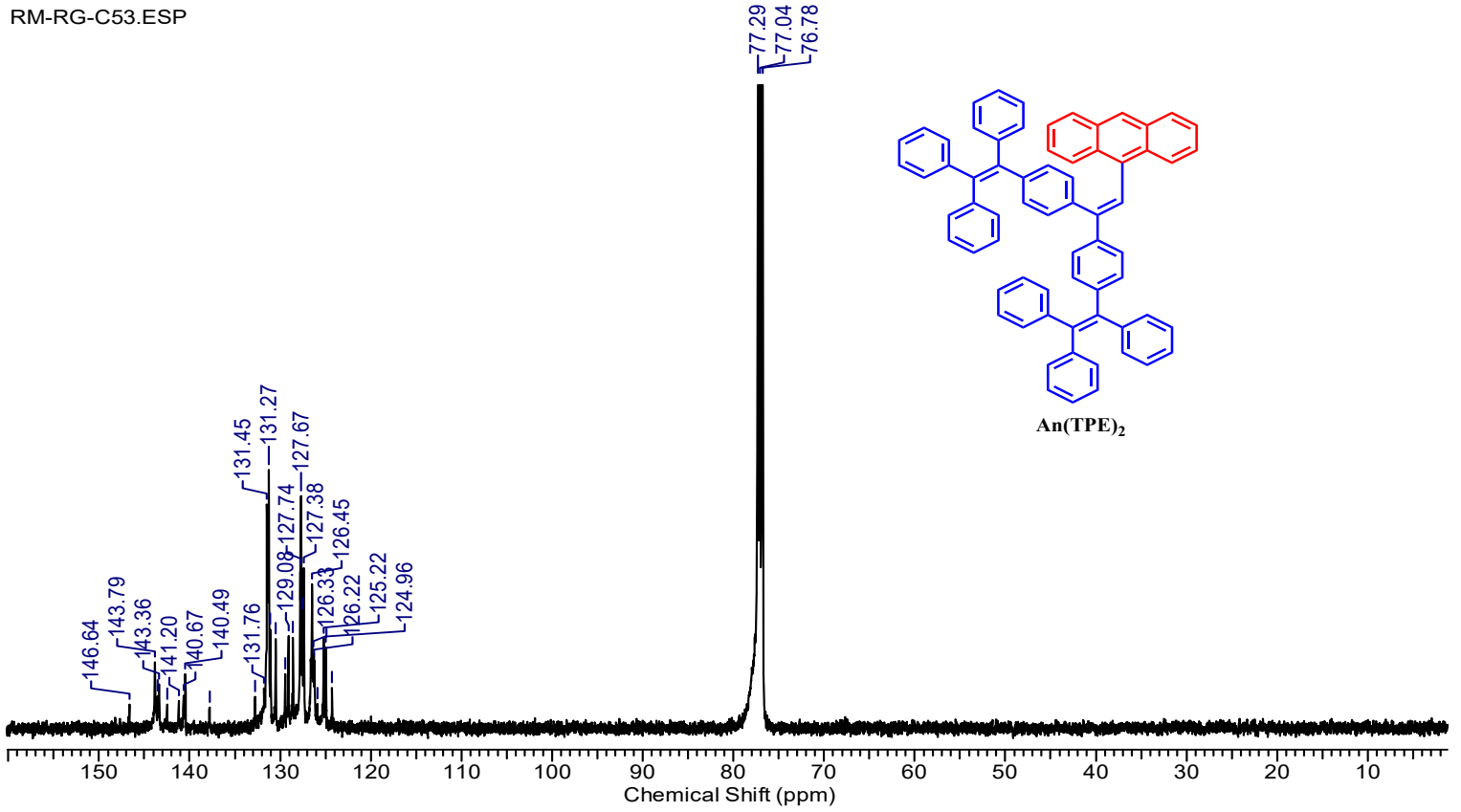
$^{1}$H NMR and $^{13}$C NMR of **An(PTZ)$_2$**



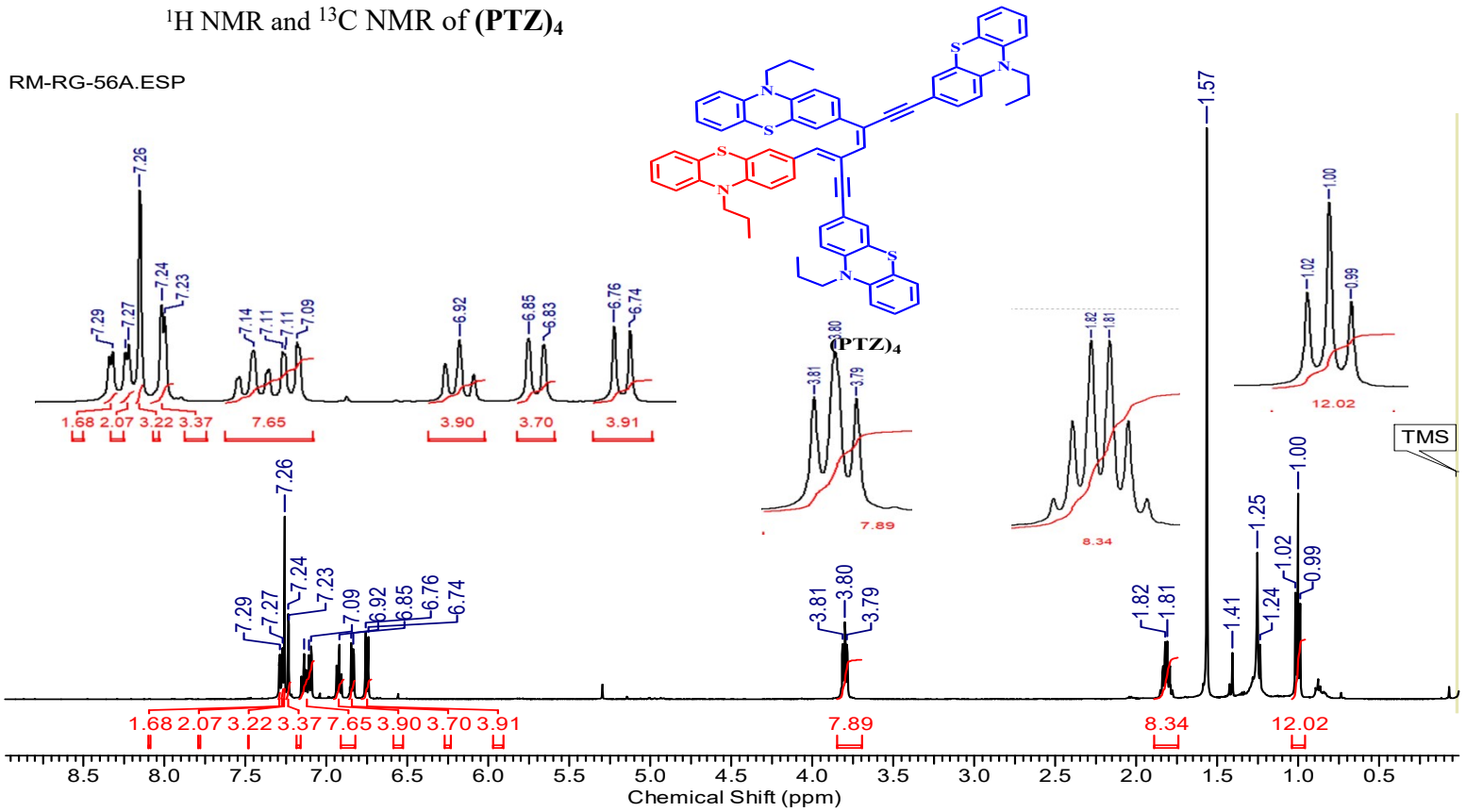



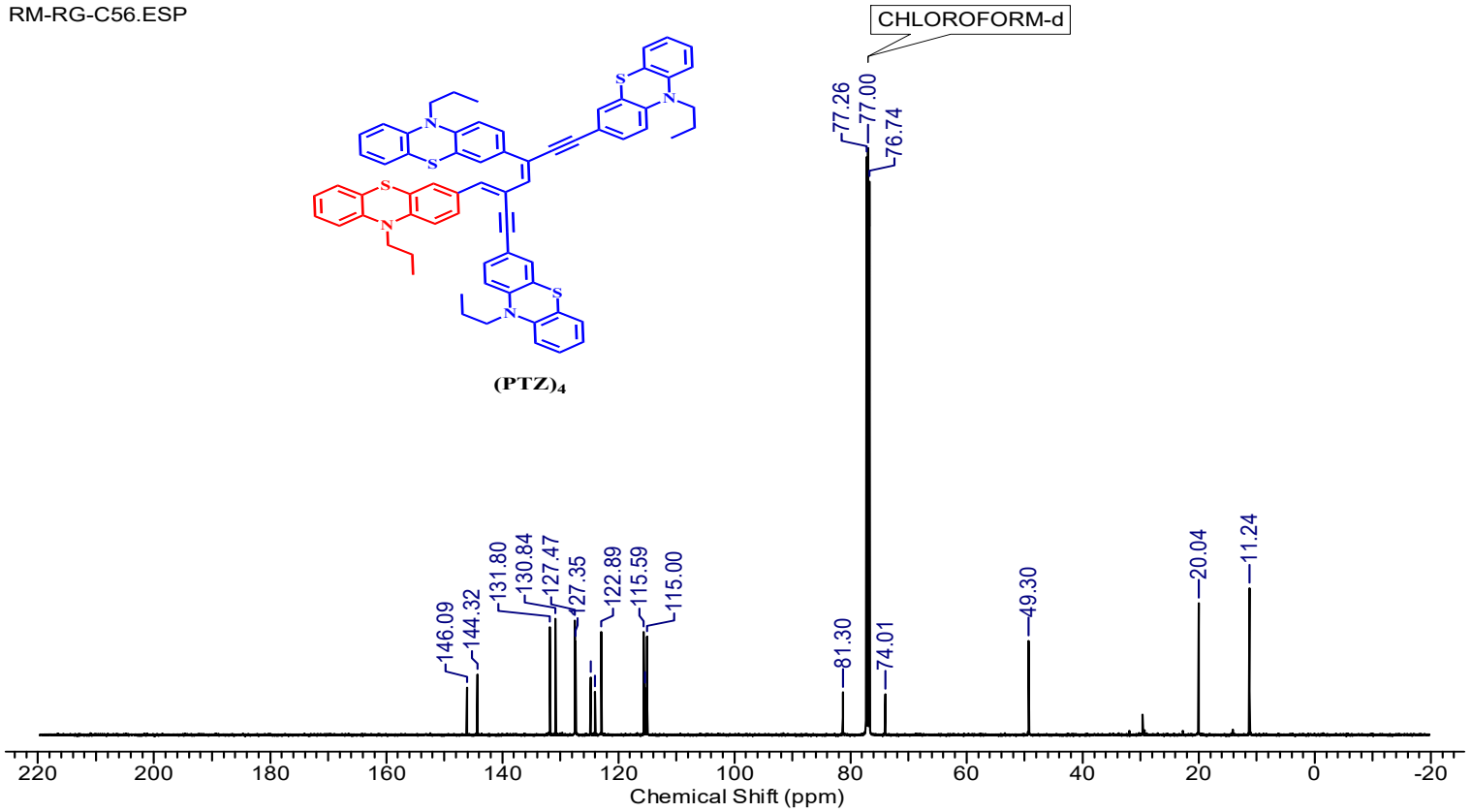
$^{1}$H NMR and $^{13}$C NMR of **An(TPE)$_2$**



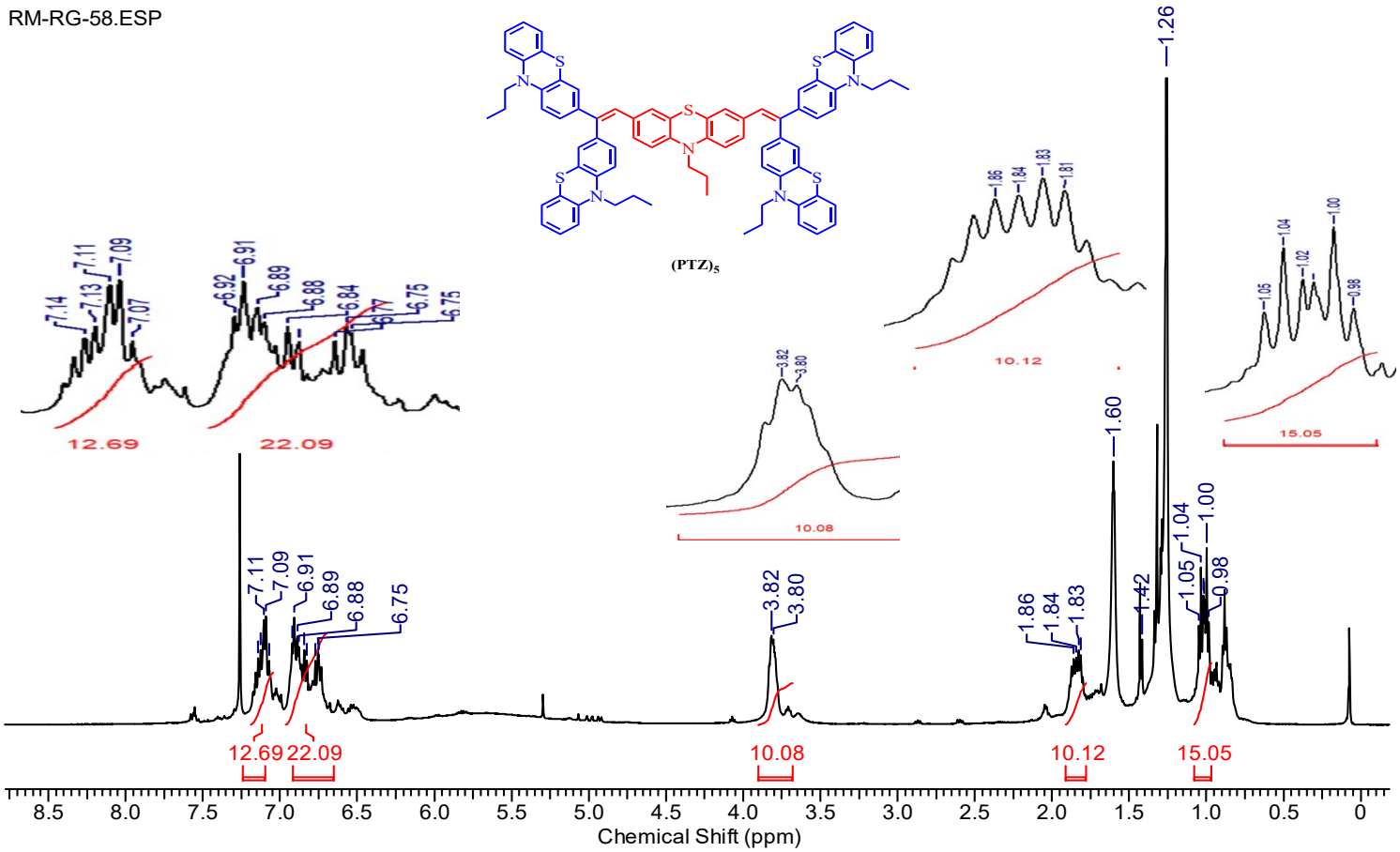
$^{1}$H NMR and $^{13}$C NMR of **(PTZ)$_4$**



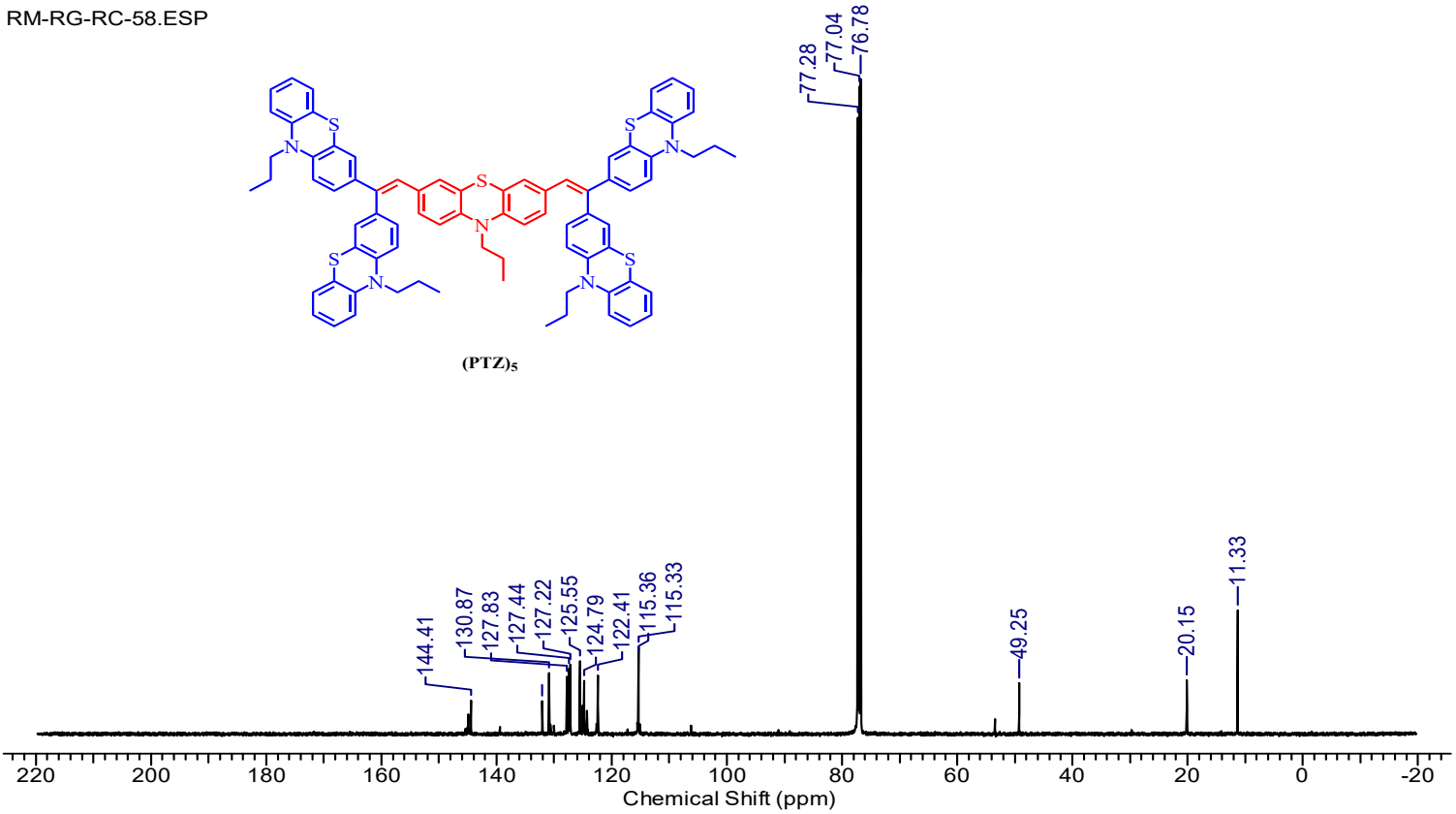



$^{1}$H NMR and $^{13}$C NMR of **$(PTZ)_5$**

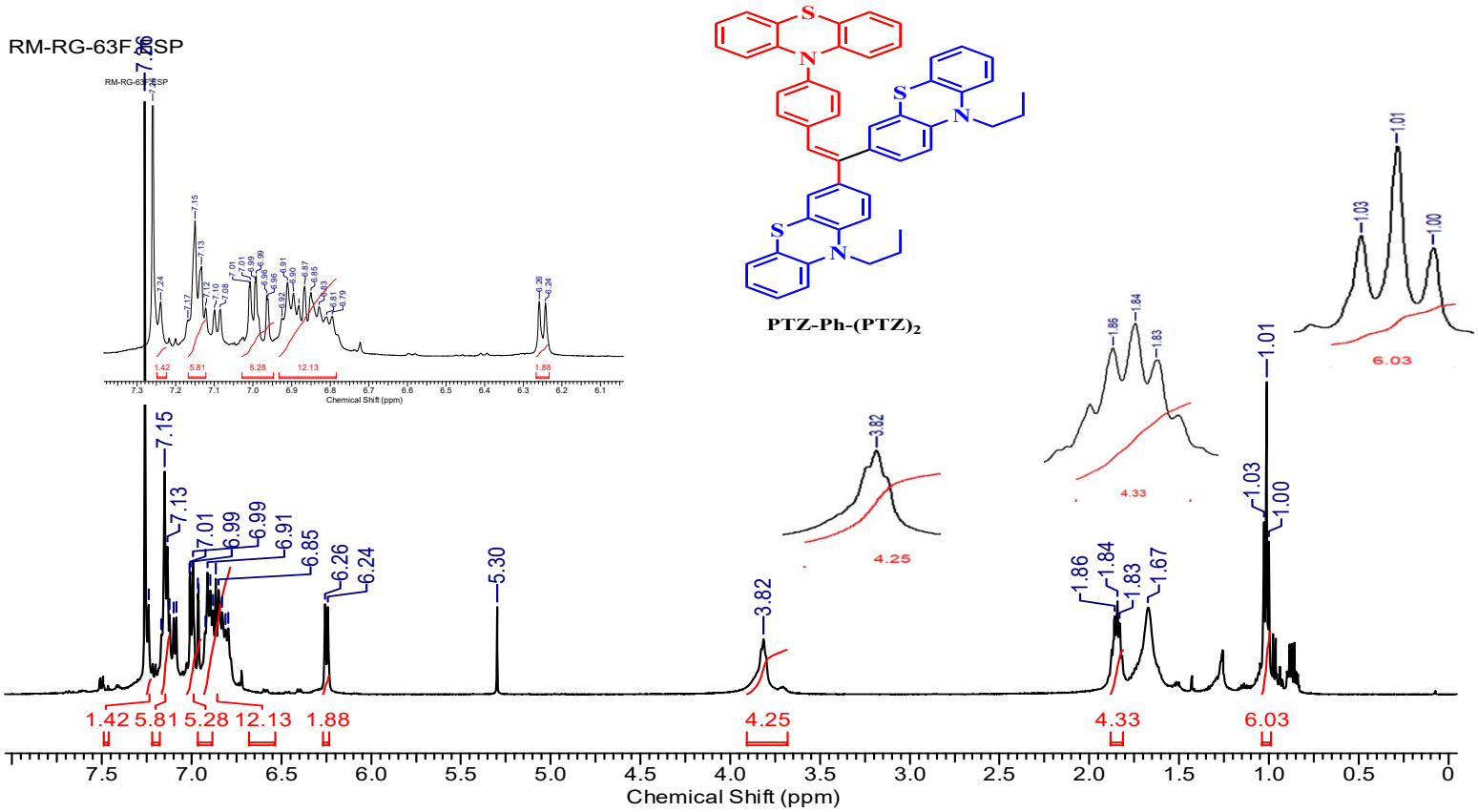
RM-RG-58.ESP

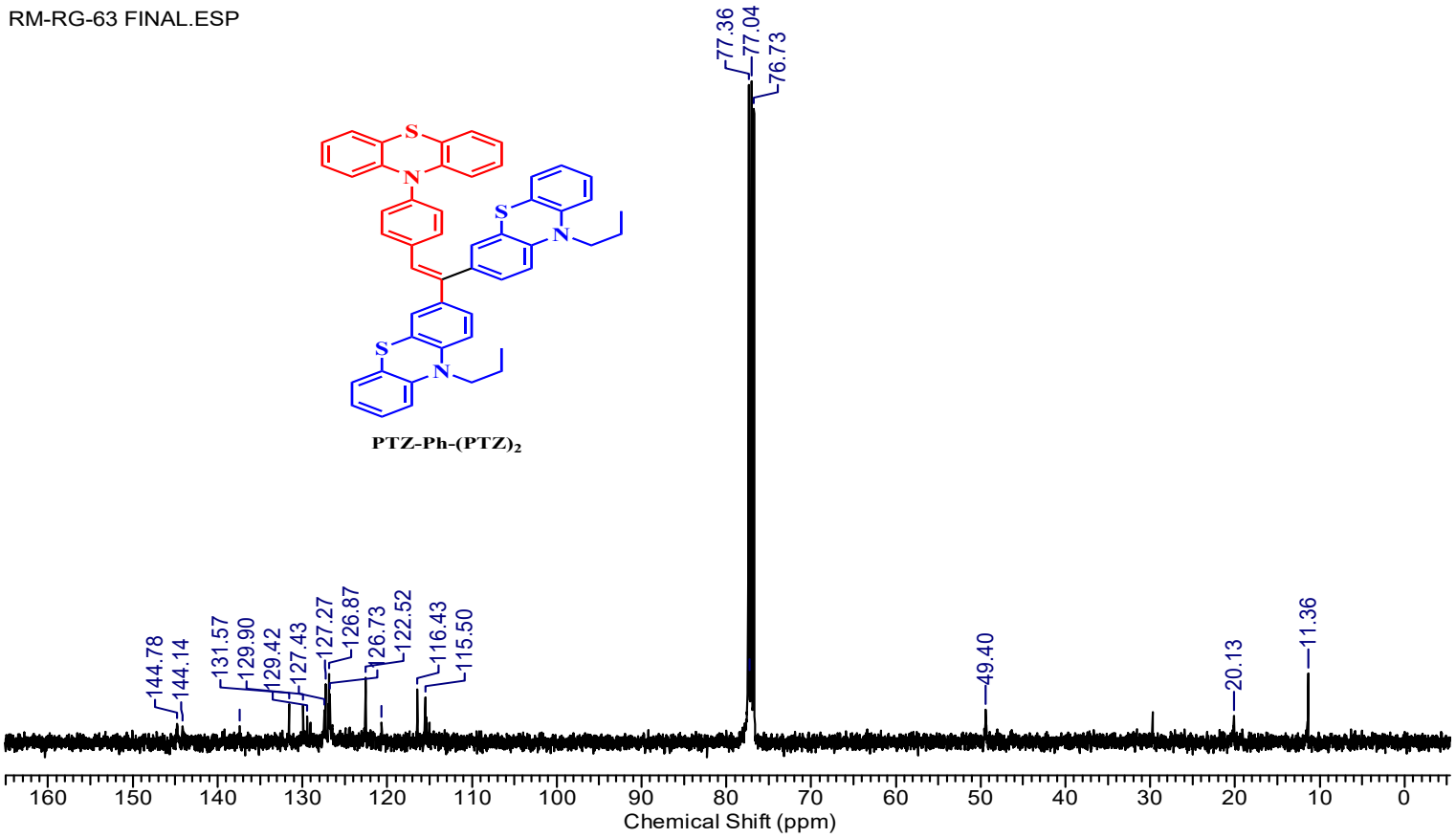



RM-RG-RC-58.ESP

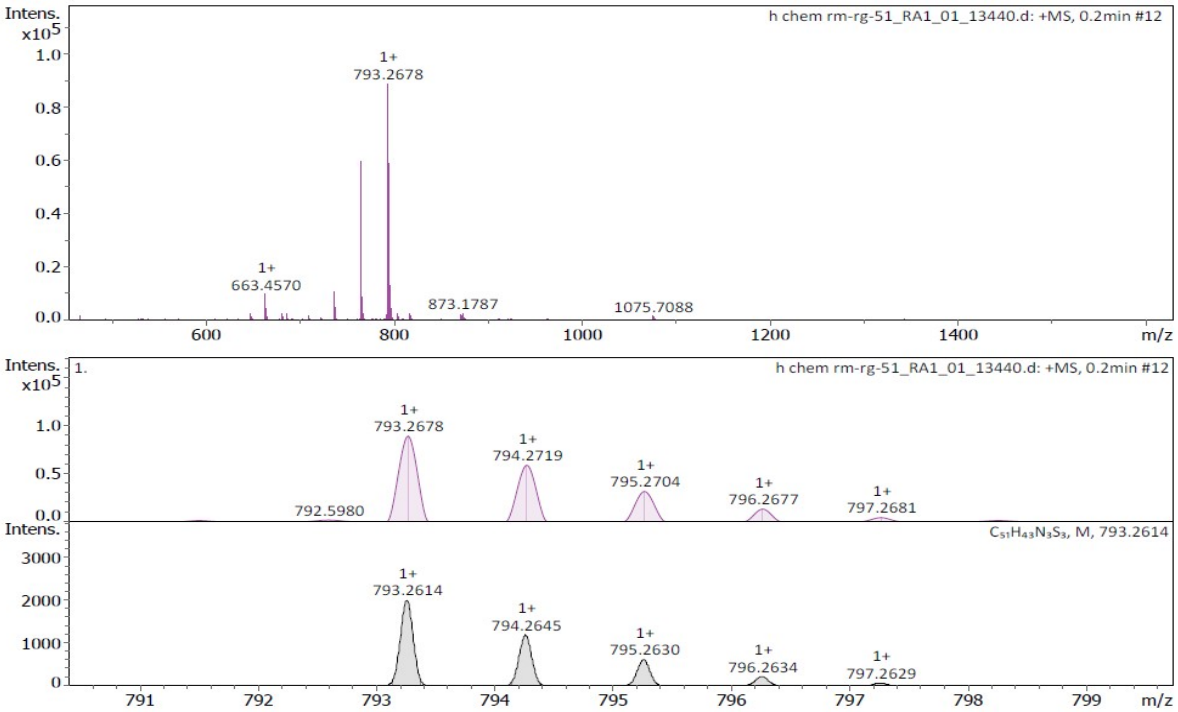


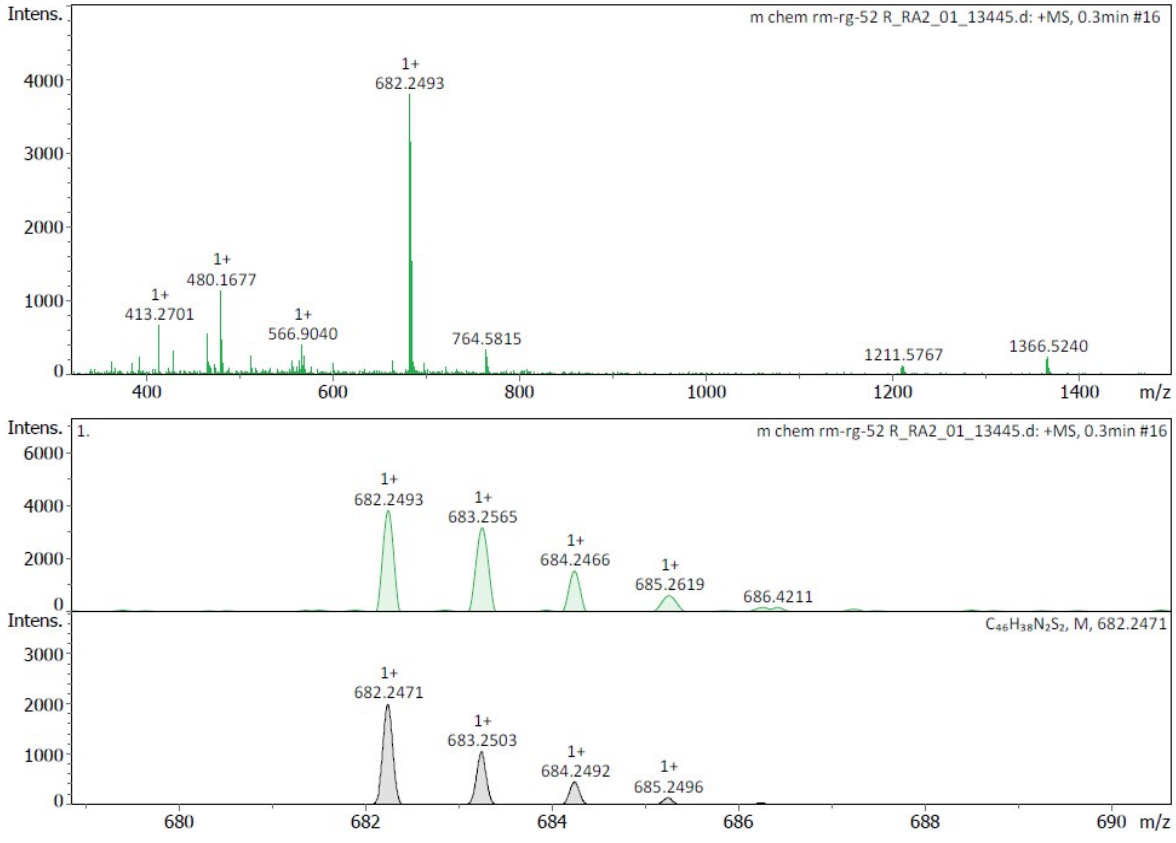
$^{1}$H NMR and $^{13}$C NMR of **PTZ-Ph-(PTZ)$_2$**



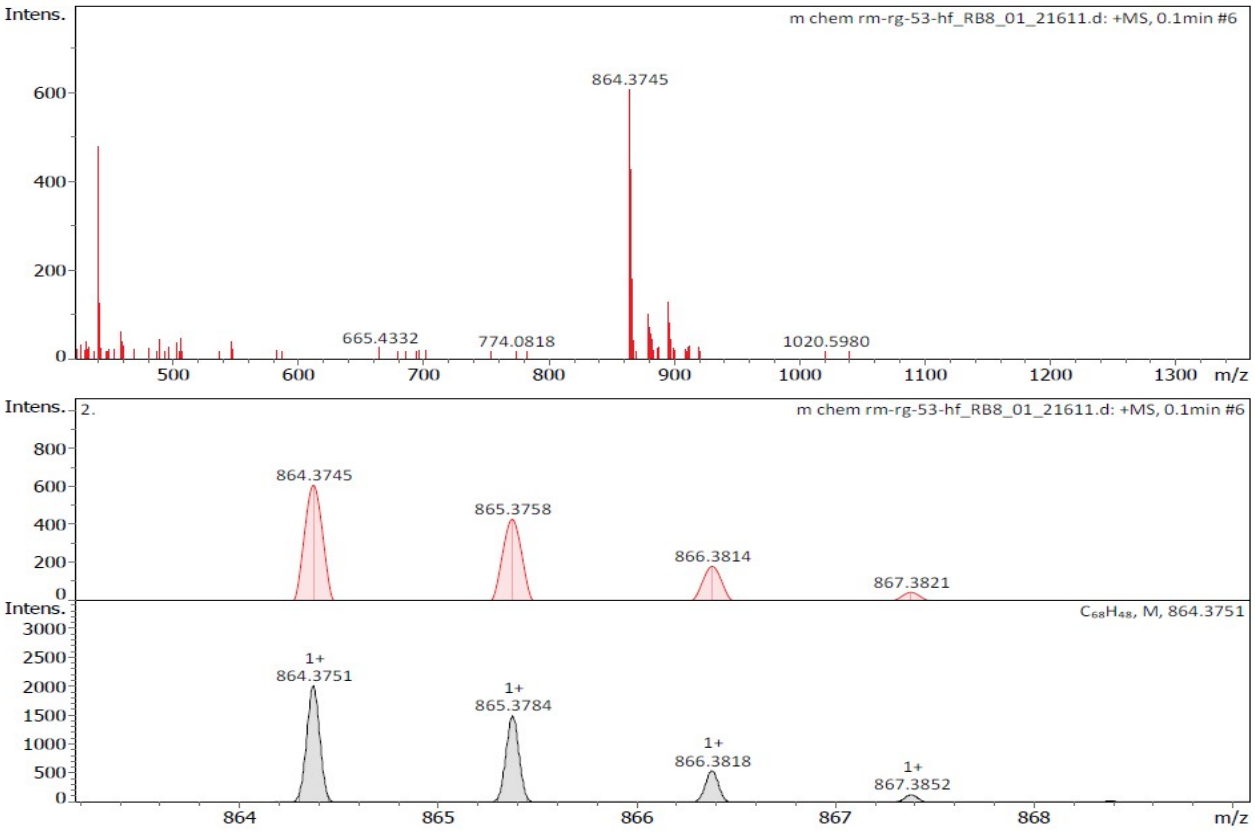



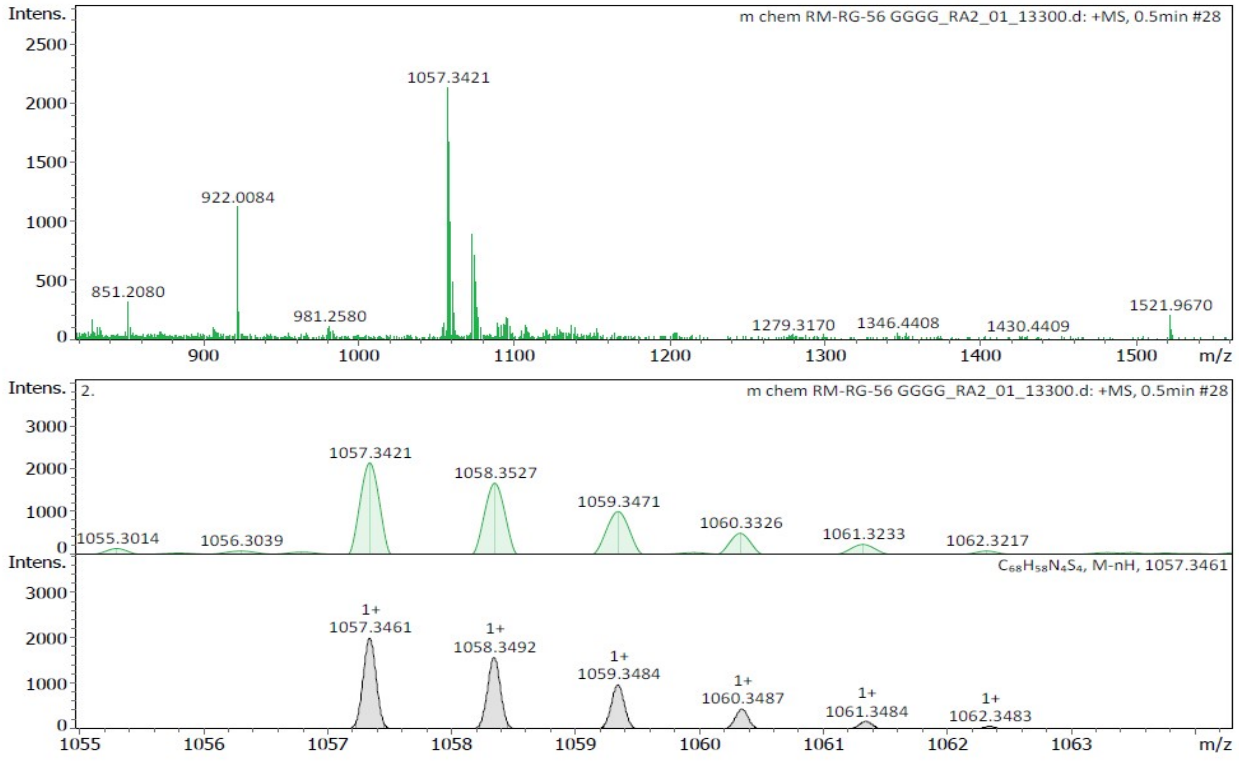
HRMS of **(PTZ)$_3$**, and **An(PTZ)$_2$**



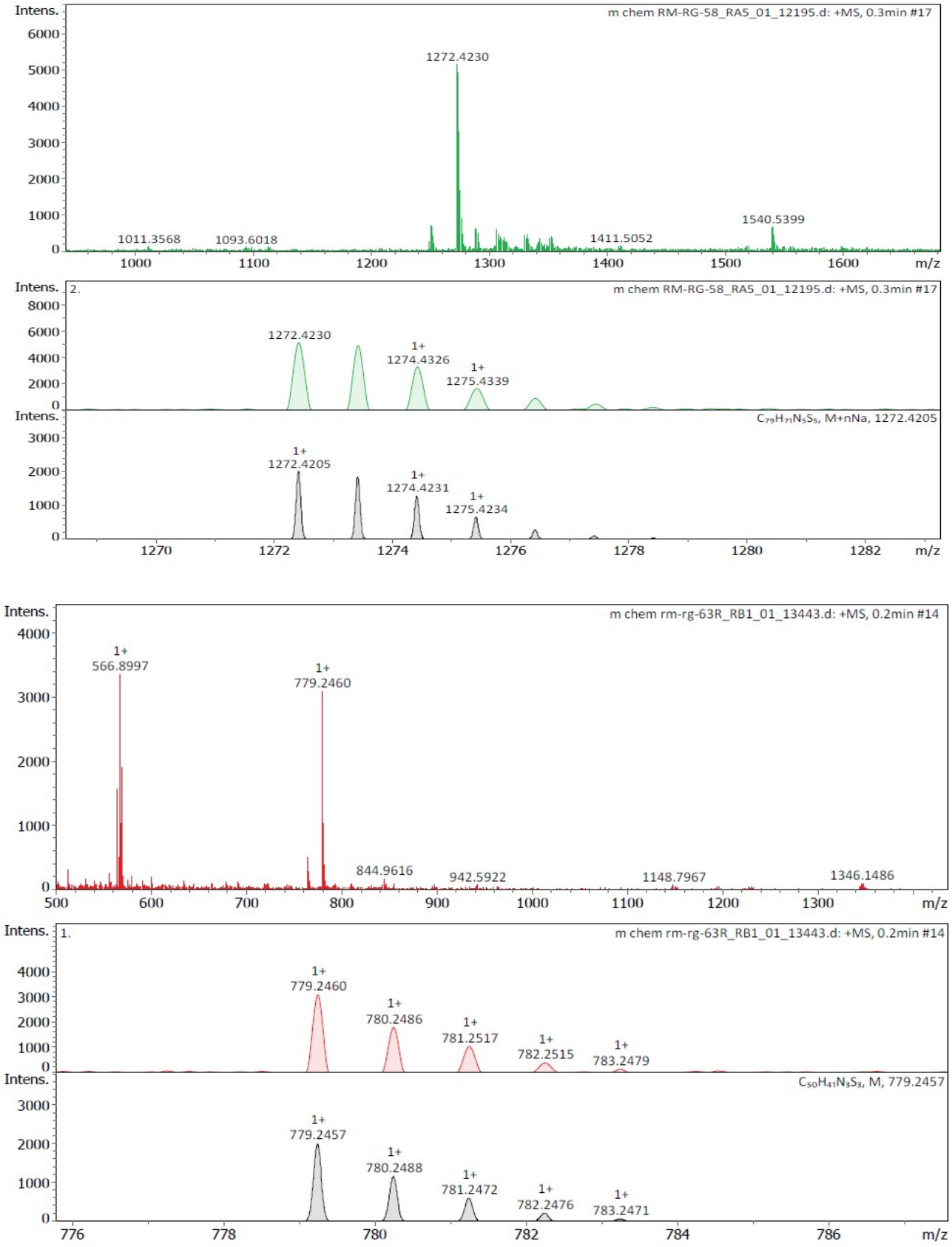



HRMS of **An(TPE)$_2$**, and **(PTZ)$_4$,**



HRMS of **$(PTZ)_5$** and **PTZ-Ph-$(PTZ)_2$**.



**DFT Calculation data of $(PTZ)_3$, $An(PTZ)_2$, $An(TPE)_2$, $(PTZ)_4$, $(PTZ)_5$ and PTZ-Ph-$(PTZ)_2$**
Calculation method: B3LYP/6-31G (d,p) with Gaussian 09

## 1. $(PTZ)_3$,

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -7.151640 | -7.014231 | 1.877112 |
| 2 | 6 | 0 | -6.894841 | -5.910693 | 1.063862 |
| 3 | 6 | 0 | -5.665164 | -5.780152 | 0.403898 |
| 4 | 6 | 0 | -4.680783 | -6.761875 | 0.622361 |
| 5 | 6 | 0 | -4.928364 | -7.841697 | 1.468217 |
| 6 | 6 | 0 | -6.172596 | -7.983927 | 2.082537 |
| 7 | 6 | 0 | -2.967785 | -4.871099 | -0.226451 |
| 8 | 6 | 0 | -4.122129 | -4.078632 | -0.380554 |
| 9 | 6 | 0 | -3.956448 | -2.686544 | -0.456583 |
| 10 | 1 | 0 | -4.824702 | -2.048493 | -0.570928 |
| 11 | 6 | 0 | -2.698134 | -2.104404 | -0.392284 |
| 12 | 6 | 0 | -1.539607 | -2.888226 | -0.216270 |
| 13 | 6 | 0 | -1.714218 | -4.286336 | -0.127998 |
| 14 | 1 | 0 | -8.117078 | -7.100075 | 2.365691 |
| 15 | 1 | 0 | -7.652182 | -5.143776 | 0.950779 |
| 16 | 1 | 0 | -4.145667 | -8.576166 | 1.628867 |
| 17 | 1 | 0 | -6.367066 | -8.837837 | 2.722828 |
| 18 | 1 | 0 | -2.609471 | -1.030864 | -0.477507 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 1 | 0 | -0.845945 | -4.924539 | 0.006133 |
| 20 | 7 | 0 | -5.385559 | -4.690682 | -0.451045 |
| 21 | 16 | 0 | -3.137818 | -6.644709 | -0.259532 |
| 22 | 6 | 0 | -6.479042 | -4.005604 | -1.141183 |
| 23 | 6 | 0 | -6.158502 | -3.737133 | -2.617502 |
| 24 | 6 | 0 | -5.829418 | -5.015253 | -3.389743 |
| 25 | 1 | 0 | -7.342852 | -4.670683 | -1.094784 |
| 26 | 1 | 0 | -6.765502 | -3.075784 | -0.628208 |
| 27 | 1 | 0 | -5.326398 | -3.031258 | -2.700161 |
| 28 | 1 | 0 | -7.032669 | -3.239415 | -3.054895 |
| 29 | 1 | 0 | -5.627549 | -4.795127 | -4.442006 |
| 30 | 1 | 0 | -4.949282 | -5.509122 | -2.969451 |
| 31 | 1 | 0 | -6.661381 | -5.727217 | -3.347727 |
| 32 | 6 | 0 | -0.187680 | -2.375357 | -0.129135 |
| 33 | 1 | 0 | 0.587825 | -3.136463 | -0.120649 |
| 34 | 6 | 0 | 0.273512 | -1.085129 | -0.042179 |
| 35 | 6 | 0 | 1.676375 | -0.843386 | 0.016988 |
| 36 | 6 | 0 | 2.869523 | -0.612808 | 0.069410 |
| 37 | 6 | 0 | 4.262365 | -0.347721 | 0.132740 |
| 38 | 6 | 0 | 4.743064 | 0.965564 | 0.285490 |
| 39 | 6 | 0 | 5.199171 | -1.395655 | 0.039325 |
| 40 | 6 | 0 | 6.106934 | 1.222382 | 0.342046 |
| 41 | 1 | 0 | 4.034863 | 1.784377 | 0.344824 |
| 42 | 6 | 0 | 6.560096 | -1.138337 | 0.136122 |
| 43 | 1 | 0 | 4.851780 | -2.414608 | -0.089486 |
| 44 | 6 | 0 | 7.041722 | 0.177582 | 0.283433 |
| 45 | 1 | 0 | 6.448976 | 2.246105 | 0.433406 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 16 | 0 | 7.728431 | -2.483228 | 0.163478 |
| 47 | 7 | 0 | 8.428530 | 0.406452 | 0.360760 |
| 48 | 6 | 0 | 9.049530 | -1.682989 | -0.724078 |
| 49 | 6 | 0 | 9.284225 | -0.313278 | -0.502140 |
| 50 | 6 | 0 | 8.922030 | 1.601707 | 1.045267 |
| 51 | 6 | 0 | 9.871658 | -2.417411 | -1.576778 |
| 52 | 6 | 0 | 10.359603 | 0.294673 | -1.164196 |
| 53 | 6 | 0 | 8.489468 | 1.651626 | 2.516317 |
| 54 | 1 | 0 | 10.011772 | 1.551738 | 1.011454 |
| 55 | 1 | 0 | 8.629446 | 2.523682 | 0.521082 |
| 56 | 6 | 0 | 10.965456 | -1.810497 | -2.194271 |
| 57 | 1 | 0 | 9.657898 | -3.468813 | -1.740257 |
| 58 | 6 | 0 | 11.203697 | -0.453924 | -1.984319 |
| 59 | 1 | 0 | 10.534248 | 1.357811 | -1.046588 |
| 60 | 6 | 0 | 8.946633 | 0.425386 | 3.307187 |
| 61 | 1 | 0 | 7.402005 | 1.751768 | 2.586325 |
| 62 | 1 | 0 | 8.913621 | 2.566152 | 2.948662 |
| 63 | 1 | 0 | 11.615170 | -2.391513 | -2.840222 |
| 64 | 1 | 0 | 12.038563 | 0.036566 | -2.474843 |
| 65 | 1 | 0 | 8.644618 | 0.501980 | 4.355770 |
| 66 | 1 | 0 | 8.514369 | -0.489700 | 2.893660 |
| 67 | 1 | 0 | 10.036977 | 0.320286 | 3.277505 |
| 68 | 6 | 0 | -0.547780 | 0.074528 | 0.018441 |
| 69 | 6 | 0 | -1.203197 | 1.097027 | 0.089985 |
| 70 | 6 | 0 | -2.016535 | 2.257254 | 0.170258 |
| 71 | 6 | 0 | -3.393166 | 2.152899 | 0.441043 |
| 72 | 6 | 0 | -1.468638 | 3.539293 | -0.028269 |

| | | | | | |
|---|---|---|---|---|---|
| 73 | 6 | 0 | -4.194376 | 3.285590 | 0.503373 |
| 74 | 1 | 0 | -3.830032 | 1.172065 | 0.594078 |
| 75 | 6 | 0 | -2.265447 | 4.671632 | 0.074955 |
| 76 | 1 | 0 | -0.411646 | 3.641546 | -0.246614 |
| 77 | 6 | 0 | -3.647030 | 4.566707 | 0.333344 |
| 78 | 1 | 0 | -5.255678 | 3.173688 | 0.688803 |
| 79 | 16 | 0 | -1.537957 | 6.294320 | -0.031560 |
| 80 | 7 | 0 | -4.430522 | 5.732719 | 0.407732 |
| 81 | 6 | 0 | -2.881226 | 7.112851 | -0.867503 |
| 82 | 6 | 0 | -4.202103 | 6.764816 | -0.530158 |
| 83 | 6 | 0 | -5.670442 | 5.717082 | 1.184891 |
| 84 | 6 | 0 | -2.625093 | 8.120461 | -1.795717 |
| 85 | 6 | 0 | -5.252748 | 7.449859 | -1.155372 |
| 86 | 6 | 0 | -5.427446 | 5.387238 | 2.663241 |
| 87 | 1 | 0 | -6.088414 | 6.723274 | 1.123969 |
| 88 | 1 | 0 | -6.416840 | 5.036089 | 0.749702 |
| 89 | 6 | 0 | -3.679267 | 8.825549 | -2.376574 |
| 90 | 1 | 0 | -1.596373 | 8.357664 | -2.047283 |
| 91 | 6 | 0 | -4.990898 | 8.485054 | -2.052751 |
| 92 | 1 | 0 | -6.278883 | 7.169411 | -0.948199 |
| 93 | 6 | 0 | -4.464456 | 6.367187 | 3.334544 |
| 94 | 1 | 0 | -5.045922 | 4.366530 | 2.764186 |
| 95 | 1 | 0 | -6.402900 | 5.405059 | 3.164513 |
| 96 | 1 | 0 | -3.474437 | 9.623585 | -3.082319 |
| 97 | 1 | 0 | -5.821427 | 9.010961 | -2.512902 |
| 98 | 1 | 0 | -4.331554 | 6.122089 | 4.392238 |
| 99 | 1 | 0 | -3.483352 | 6.342844 | 2.852830 |

| | | | | | |
|---|---|---|---|---|---|
| 100 | 1 | 0 | -4.839756 | 7.394749 | 3.271158 |

---

Rotational constants (GHZ): 0.0278786 0.0183732 0.0118181

2. **An(PTZ)$_2$**,

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.675357 | -1.101258 | 2.886927 |
| 2 | 6 | 0 | -5.104143 | -2.046600 | 1.995908 |
| 3 | 6 | 0 | -4.177951 | -2.750842 | 1.165477 |
| 4 | 6 | 0 | -2.771548 | -2.439235 | 1.258691 |
| 5 | 6 | 0 | -2.368863 | -1.474037 | 2.232788 |
| 6 | 6 | 0 | -3.285758 | -0.820513 | 3.011526 |
| 7 | 6 | 0 | -4.610905 | -3.734681 | 0.272806 |
| 8 | 6 | 0 | -1.852113 | -3.086364 | 0.395989 |
| 9 | 6 | 0 | -2.310802 | -4.085296 | -0.497791 |
| 10 | 6 | 0 | -3.712280 | -4.422874 | -0.546103 |
| 11 | 6 | 0 | -4.152736 | -5.433700 | -1.454215 |
| 12 | 1 | 0 | -5.210258 | -5.682456 | -1.472538 |
| 13 | 6 | 0 | -3.271114 | -6.070291 | -2.285267 |
| 14 | 6 | 0 | -1.892598 | -5.718554 | -2.263502 |
| 15 | 6 | 0 | -1.431747 | -4.754577 | -1.405047 |
| 16 | 1 | 0 | -5.670641 | -3.969968 | 0.214569 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 1 | 0 | -5.387723 | -0.573121 | 3.512592 |
| 18 | 1 | 0 | -6.159904 | -2.286526 | 1.905461 |
| 19 | 1 | 0 | -1.314061 | -1.265147 | 2.348673 |
| 20 | 1 | 0 | -2.952405 | -0.085604 | 3.737421 |
| 21 | 1 | 0 | -3.619508 | -6.836348 | -2.971062 |
| 22 | 1 | 0 | -1.203659 | -6.214558 | -2.940313 |
| 23 | 1 | 0 | -0.383650 | -4.478139 | -1.416592 |
| 24 | 6 | 0 | -0.416025 | -2.738766 | 0.393970 |
| 25 | 6 | 0 | 0.113862 | -1.510645 | 0.170604 |
| 26 | 1 | 0 | 0.276524 | -3.563985 | 0.545627 |
| 27 | 6 | 0 | 1.570188 | -1.281441 | 0.290514 |
| 28 | 6 | 0 | 2.355282 | -1.990160 | 1.212333 |
| 29 | 6 | 0 | 2.214909 | -0.343759 | -0.533202 |
| 30 | 6 | 0 | 3.729677 | -1.794128 | 1.293328 |
| 31 | 1 | 0 | 1.875916 | -2.677225 | 1.901608 |
| 32 | 6 | 0 | 3.593455 | -0.173973 | -0.483454 |
| 33 | 1 | 0 | 1.634299 | 0.236479 | -1.241833 |
| 34 | 6 | 0 | 4.379625 | -0.897038 | 0.433415 |
| 35 | 1 | 0 | 4.300008 | -2.333288 | 2.040358 |
| 36 | 16 | 0 | 4.408751 | 0.903181 | -1.645146 |
| 37 | 7 | 0 | 5.772361 | -0.691889 | 0.473027 |
| 38 | 6 | 0 | 5.690461 | 1.508667 | -0.565987 |
| 39 | 6 | 0 | 6.267614 | 0.626128 | 0.366199 |
| 40 | 6 | 0 | 6.640224 | -1.757671 | 0.973506 |
| 41 | 6 | 0 | 6.153104 | 2.817701 | -0.687670 |
| 42 | 6 | 0 | 7.313374 | 1.097434 | 1.171542 |
| 43 | 6 | 0 | 6.501447 | -3.052898 | 0.162998 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | 7.665723 | -1.398393 | 0.869797 |
| 45 | 1 | 0 | 6.477578 | -1.949906 | 2.044676 |
| 46 | 6 | 0 | 7.224571 | 3.260303 | 0.088447 |
| 47 | 1 | 0 | 5.678938 | 3.480467 | -1.404437 |
| 48 | 6 | 0 | 7.800303 | 2.395334 | 1.016429 |
| 49 | 1 | 0 | 7.743977 | 0.452561 | 1.928663 |
| 50 | 6 | 0 | 6.793587 | -2.852612 | -1.324504 |
| 51 | 1 | 0 | 5.497645 | -3.470040 | 0.289122 |
| 52 | 1 | 0 | 7.197211 | -3.782557 | 0.595094 |
| 53 | 1 | 0 | 7.595161 | 4.273514 | -0.025827 |
| 54 | 1 | 0 | 8.621152 | 2.732299 | 1.641639 |
| 55 | 1 | 0 | 6.705968 | -3.796606 | -1.870353 |
| 56 | 1 | 0 | 6.096001 | -2.136254 | -1.766493 |
| 57 | 1 | 0 | 7.807466 | -2.466992 | -1.479596 |
| 58 | 6 | 0 | -0.748802 | -0.359581 | -0.193178 |
| 59 | 6 | 0 | -1.762628 | -0.487057 | -1.150432 |
| 60 | 6 | 0 | -0.627705 | 0.861269 | 0.486690 |
| 61 | 6 | 0 | -2.668605 | 0.541948 | -1.373933 |
| 62 | 1 | 0 | -1.849436 | -1.407494 | -1.715366 |
| 63 | 6 | 0 | -1.559259 | 1.876381 | 0.298160 |
| 64 | 1 | 0 | 0.168245 | 0.997291 | 1.211573 |
| 65 | 6 | 0 | -2.611230 | 1.723832 | -0.622253 |
| 66 | 1 | 0 | -3.439349 | 0.418299 | -2.125092 |
| 67 | 16 | 0 | -1.512436 | 3.341879 | 1.308775 |
| 68 | 7 | 0 | -3.569520 | 2.744902 | -0.767297 |
| 69 | 6 | 0 | -2.133977 | 4.503102 | 0.108167 |
| 70 | 6 | 0 | -3.139553 | 4.087239 | -0.785294 |

| | | | | | |
|---|---|---|---|---|---|
| 71 | 6 | 0 | -4.920889 | 2.393578 | -1.204084 |
| 72 | 6 | 0 | -1.677911 | 5.819989 | 0.103136 |
| 73 | 6 | 0 | -3.669058 | 5.028959 | -1.678112 |
| 74 | 6 | 0 | -5.595277 | 1.393367 | -0.254816 |
| 75 | 1 | 0 | -5.501251 | 3.318221 | -1.197759 |
| 76 | 1 | 0 | -4.932771 | 2.018440 | -2.238196 |
| 77 | 6 | 0 | -2.243037 | 6.757333 | -0.762081 |
| 78 | 1 | 0 | -0.890912 | 6.108525 | 0.792615 |
| 79 | 6 | 0 | -3.239341 | 6.355649 | -1.649357 |
| 80 | 1 | 0 | -4.412788 | 4.722697 | -2.404605 |
| 81 | 6 | 0 | -5.682071 | 1.913401 | 1.179991 |
| 82 | 1 | 0 | -5.063130 | 0.437128 | -0.264205 |
| 83 | 1 | 0 | -6.598816 | 1.195956 | -0.651761 |
| 84 | 1 | 0 | -1.899315 | 7.786243 | -0.746878 |
| 85 | 1 | 0 | -3.675014 | 7.069626 | -2.341291 |
| 86 | 1 | 0 | -6.207516 | 1.198805 | 1.818495 |
| 87 | 1 | 0 | -4.684259 | 2.068453 | 1.598744 |
| 88 | 1 | 0 | -6.216764 | 2.869178 | 1.223726 |

---

Rotational constants (GHZ): 0.0651621 0.0391239 0.0273535

3. **An(TPE)$_2$**,

Standard orientation:

---

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

---

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.356798 | 3.503656 | 3.957314 |
| 2 | 6 | 0 | 3.755416 | 4.301478 | 2.919427 |
| 3 | 6 | 0 | 3.041786 | 4.314361 | 1.681202 |
| 4 | 6 | 0 | 1.869077 | 3.483027 | 1.538446 |
| 5 | 6 | 0 | 1.488981 | 2.668709 | 2.650482 |
| 6 | 6 | 0 | 2.209997 | 2.672103 | 3.814713 |
| 7 | 6 | 0 | 3.452421 | 5.120979 | 0.617884 |
| 8 | 6 | 0 | 1.129878 | 3.521675 | 0.332815 |
| 9 | 6 | 0 | 1.556962 | 4.350701 | -0.729299 |
| 10 | 6 | 0 | 2.744160 | 5.156017 | -0.586007 |
| 11 | 6 | 0 | 3.164973 | 5.969207 | -1.681802 |
| 12 | 1 | 0 | 4.060890 | 6.571872 | -1.560957 |
| 13 | 6 | 0 | 2.463692 | 5.988356 | -2.857373 |
| 14 | 6 | 0 | 1.297531 | 5.186175 | -3.006224 |
| 15 | 6 | 0 | 0.861082 | 4.393545 | -1.976920 |
| 16 | 1 | 0 | 4.340211 | 5.738039 | 0.731265 |
| 17 | 1 | 0 | 3.909606 | 3.502260 | 4.891683 |
| 18 | 1 | 0 | 4.628679 | 4.941044 | 3.015222 |
| 19 | 1 | 0 | 0.609254 | 2.045162 | 2.557827 |
| 20 | 1 | 0 | 1.900673 | 2.042746 | 4.643433 |
| 21 | 1 | 0 | 2.796555 | 6.609352 | -3.683257 |
| 22 | 1 | 0 | 0.755739 | 5.200608 | -3.946955 |
| 23 | 1 | 0 | -0.017021 | 3.768958 | -2.101203 |
| 24 | 6 | 0 | -0.278011 | 1.422699 | 0.146626 |
| 25 | 6 | 0 | -1.627303 | 0.809229 | 0.139222 |
| 26 | 6 | 0 | -1.881424 | -0.361352 | -0.594679 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 6 | 0 | -2.691568 | 1.377505 | 0.859801 |
| 28 | 6 | 0 | -3.152318 | -0.921615 | -0.629215 |
| 29 | 1 | 0 | -1.072423 | -0.826083 | -1.147740 |
| 30 | 6 | 0 | -3.963068 | 0.821618 | 0.818447 |
| 31 | 1 | 0 | -2.506787 | 2.248115 | 1.480708 |
| 32 | 6 | 0 | -4.224041 | -0.330496 | 0.059325 |
| 33 | 1 | 0 | -3.326995 | -1.825930 | -1.202954 |
| 34 | 1 | 0 | -4.768301 | 1.274311 | 1.385906 |
| 35 | 6 | 0 | -5.576480 | -0.945052 | 0.021859 |
| 36 | 6 | 0 | -6.710513 | -0.206465 | -0.153189 |
| 37 | 6 | 0 | -5.604109 | -2.424256 | 0.185107 |
| 38 | 6 | 0 | -8.071730 | -0.767283 | 0.060334 |
| 39 | 6 | 0 | -6.673117 | 1.220444 | -0.573865 |
| 40 | 6 | 0 | -4.836014 | -3.041373 | 1.185063 |
| 41 | 6 | 0 | -6.359671 | -3.236361 | -0.674939 |
| 42 | 6 | 0 | -9.096858 | -0.509369 | -0.863763 |
| 43 | 6 | 0 | -8.376027 | -1.527351 | 1.200731 |
| 44 | 6 | 0 | -7.470762 | 2.173709 | 0.078725 |
| 45 | 6 | 0 | -5.874557 | 1.640242 | -1.649276 |
| 46 | 6 | 0 | -4.850482 | -4.425300 | 1.343235 |
| 47 | 1 | 0 | -4.231067 | -2.424509 | 1.841858 |
| 48 | 6 | 0 | -6.366813 | -4.620091 | -0.523439 |
| 49 | 1 | 0 | -6.945906 | -2.771207 | -1.459568 |
| 50 | 6 | 0 | -10.376496 | -1.025446 | -0.672420 |
| 51 | 1 | 0 | -8.879594 | 0.095247 | -1.738441 |
| 52 | 6 | 0 | -9.657089 | -2.034962 | 1.397142 |
| 53 | 1 | 0 | -7.596888 | -1.720637 | 1.929482 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 6 | 0 | -7.441491 | 3.512064 | -0.306649 |
| 55 | 1 | 0 | -8.109260 | 1.856681 | 0.897087 |
| 56 | 6 | 0 | -5.852669 | 2.975743 | -2.041215 |
| 57 | 1 | 0 | -5.266740 | 0.909730 | -2.171427 |
| 58 | 6 | 0 | -5.617298 | -5.220252 | 0.490110 |
| 59 | 1 | 0 | -4.259793 | -4.883691 | 2.130728 |
| 60 | 1 | 0 | -6.955847 | -5.231806 | -1.200111 |
| 61 | 6 | 0 | -10.661652 | -1.791723 | 0.458537 |
| 62 | 1 | 0 | -11.152530 | -0.826101 | -1.405388 |
| 63 | 1 | 0 | -9.872981 | -2.618599 | 2.286983 |
| 64 | 6 | 0 | -6.630542 | 3.918978 | -1.367182 |
| 65 | 1 | 0 | -8.054508 | 4.237520 | 0.219749 |
| 66 | 1 | 0 | -5.229958 | 3.280500 | -2.876969 |
| 67 | 1 | 0 | -5.624760 | -6.299422 | 0.608953 |
| 68 | 1 | 0 | -11.660189 | -2.189604 | 0.611503 |
| 69 | 1 | 0 | -6.610987 | 4.961023 | -1.671351 |
| 70 | 6 | 0 | 0.892879 | 0.513213 | 0.068743 |
| 71 | 6 | 0 | 0.980327 | -0.620779 | 0.890118 |
| 72 | 6 | 0 | 1.924131 | 0.748854 | -0.852682 |
| 73 | 6 | 0 | 2.076469 | -1.472608 | 0.814102 |
| 74 | 1 | 0 | 0.180788 | -0.830275 | 1.593755 |
| 75 | 6 | 0 | 3.015451 | -0.104785 | -0.931040 |
| 76 | 1 | 0 | 1.856670 | 1.599136 | -1.521329 |
| 77 | 6 | 0 | 3.124856 | -1.219745 | -0.084865 |
| 78 | 1 | 0 | 2.131136 | -2.342576 | 1.460388 |
| 79 | 1 | 0 | 3.800437 | 0.092171 | -1.651817 |
| 80 | 6 | 0 | 4.298443 | -2.129608 | -0.159626 |

| | | | | | |
|---|---|---|---|---|---|
| 81 | 6 | 0 | 5.575728 | -1.653485 | -0.230410 |
| 82 | 6 | 0 | 3.980387 | -3.582628 | -0.145809 |
| 83 | 6 | 0 | 6.741031 | -2.512987 | -0.566448 |
| 84 | 6 | 0 | 5.888498 | -0.220456 | 0.020887 |
| 85 | 6 | 0 | 2.933632 | -4.087051 | -0.934076 |
| 86 | 6 | 0 | 4.683272 | -4.473780 | 0.680380 |
| 87 | 6 | 0 | 7.941409 | -2.388740 | 0.151406 |
| 88 | 6 | 0 | 6.689769 | -3.430221 | -1.628421 |
| 89 | 6 | 0 | 6.709363 | 0.497370 | -0.862554 |
| 90 | 6 | 0 | 5.374163 | 0.441494 | 1.146070 |
| 91 | 6 | 0 | 2.621557 | -5.444612 | -0.922705 |
| 92 | 1 | 0 | 2.369244 | -3.404343 | -1.561111 |
| 93 | 6 | 0 | 4.366799 | -5.829185 | 0.697894 |
| 94 | 1 | 0 | 5.483384 | -4.093484 | 1.305432 |
| 95 | 6 | 0 | 9.043770 | -3.181952 | -0.158603 |
| 96 | 1 | 0 | 7.999982 | -1.666553 | 0.959235 |
| 97 | 6 | 0 | 7.794157 | -4.216056 | -1.944445 |
| 98 | 1 | 0 | 5.774362 | -3.523133 | -2.201827 |
| 99 | 6 | 0 | 6.962599 | 1.851959 | -0.654846 |
| 100 | 1 | 0 | 7.131581 | -0.011380 | -1.723417 |
| 101 | 6 | 0 | 5.636554 | 1.790139 | 1.361374 |
| 102 | 1 | 0 | 4.748297 | -0.106339 | 1.841665 |
| 103 | 6 | 0 | 3.338269 | -6.321835 | -0.107605 |
| 104 | 1 | 0 | 1.816244 | -5.817427 | -1.548608 |
| 105 | 1 | 0 | 4.921076 | -6.501979 | 1.345378 |
| 106 | 6 | 0 | 8.974166 | -4.100399 | -1.207034 |
| 107 | 1 | 0 | 9.959153 | -3.080174 | 0.416711 |

| | | | | | |
|---|---|---|---|---|---|
| 108 | 1 | 0 | 7.735469 | -4.917353 | -2.771418 |
| 109 | 6 | 0 | 6.420930 | 2.503957 | 0.453954 |
| 110 | 1 | 0 | 7.580599 | 2.398567 | -1.361050 |
| 111 | 1 | 0 | 5.219247 | 2.285491 | 2.229810 |
| 112 | 1 | 0 | 3.092478 | -7.379313 | -0.094073 |
| 113 | 1 | 0 | 9.834700 | -4.714985 | -1.453276 |
| 114 | 1 | 0 | 6.610215 | 3.561203 | 0.613254 |
| 115 | 6 | 0 | -0.136771 | 2.766309 | 0.193094 |
| 116 | 1 | 0 | -1.039066 | 3.372045 | 0.120562 |

---

Rotational constants (GHZ): 0.0479464 0.0187044 0.0146920

4. **$(PTZ)_4$,**

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -8.271396 | 8.005230 | -1.584423 |
| 2 | 6 | 0 | -8.020719 | 6.724290 | -1.092888 |
| 3 | 6 | 0 | -6.917901 | 6.480481 | -0.262743 |
| 4 | 6 | 0 | -6.044661 | 7.547613 | 0.019378 |
| 5 | 6 | 0 | -6.277866 | 8.816764 | -0.507309 |
| 6 | 6 | 0 | -7.404378 | 9.056412 | -1.294172 |
| 7 | 6 | 0 | -4.275732 | 5.610926 | 0.612156 |
| 8 | 6 | 0 | -5.327709 | 4.732409 | 0.288092 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | -4.999037 | 3.404293 | -0.026267 |
| 10 | 1 | 0 | -5.782113 | 2.709415 | -0.305173 |
| 11 | 6 | 0 | -3.685475 | 2.957847 | 0.006895 |
| 12 | 6 | 0 | -2.624984 | 3.832048 | 0.321510 |
| 13 | 6 | 0 | -2.959292 | 5.174732 | 0.602217 |
| 14 | 1 | 0 | -9.140218 | 8.171039 | -2.213578 |
| 15 | 1 | 0 | -8.681644 | 5.910053 | -1.365711 |
| 16 | 1 | 0 | -5.579570 | 9.616956 | -0.283765 |
| 17 | 1 | 0 | -7.592637 | 10.051179 | -1.683986 |
| 18 | 1 | 0 | -3.473150 | 1.926551 | -0.235964 |
| 19 | 1 | 0 | -2.170357 | 5.882490 | 0.839121 |
| 20 | 7 | 0 | -6.653149 | 5.202428 | 0.277862 |
| 21 | 16 | 0 | -4.674891 | 7.270632 | 1.124099 |
| 22 | 6 | 0 | -7.751103 | 4.256401 | 0.480892 |
| 23 | 6 | 0 | -7.660657 | 3.540273 | 1.834621 |
| 24 | 6 | 0 | -7.648449 | 4.512749 | 3.014554 |
| 25 | 1 | 0 | -8.673006 | 4.840109 | 0.465391 |
| 26 | 1 | 0 | -7.820123 | 3.529281 | -0.341433 |
| 27 | 1 | 0 | -6.768512 | 2.907486 | 1.867333 |
| 28 | 1 | 0 | -8.522635 | 2.865380 | 1.903215 |
| 29 | 1 | 0 | -7.605527 | 3.973863 | 3.965560 |
| 30 | 1 | 0 | -6.784405 | 5.180612 | 2.961190 |
| 31 | 1 | 0 | -8.549501 | 5.136393 | 3.020976 |
| 32 | 6 | 0 | -1.224452 | 3.463408 | 0.372613 |
| 33 | 1 | 0 | -0.555935 | 4.294656 | 0.588238 |
| 34 | 6 | 0 | -0.603935 | 2.250735 | 0.214450 |
| 35 | 6 | 0 | 1.140972 | -0.116824 | 1.209907 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | 0.294070 | -0.056174 | 2.321140 |
| 37 | 6 | 0 | 1.520539 | -1.377966 | 0.734115 |
| 38 | 6 | 0 | -0.180147 | -1.212661 | 2.927343 |
| 39 | 1 | 0 | 0.013900 | 0.911741 | 2.721022 |
| 40 | 6 | 0 | 0.991911 | -2.536866 | 1.294952 |
| 41 | 1 | 0 | 2.202088 | -1.452206 | -0.107261 |
| 42 | 6 | 0 | 0.137059 | -2.477699 | 2.411361 |
| 43 | 1 | 0 | -0.808734 | -1.125283 | 3.803961 |
| 44 | 16 | 0 | 1.292192 | -4.113753 | 0.526334 |
| 45 | 7 | 0 | -0.366768 | -3.665781 | 2.980200 |
| 46 | 6 | 0 | 1.333244 | -5.114640 | 1.996628 |
| 47 | 6 | 0 | 0.476500 | -4.795942 | 3.068542 |
| 48 | 6 | 0 | -1.550295 | -3.578591 | 3.839255 |
| 49 | 6 | 0 | 2.167197 | -6.229926 | 2.054116 |
| 50 | 6 | 0 | 0.505995 | -5.622478 | 4.201859 |
| 51 | 6 | 0 | -2.793060 | -3.091545 | 3.084380 |
| 52 | 1 | 0 | -1.757988 | -4.587129 | 4.197617 |
| 53 | 1 | 0 | -1.355343 | -2.960419 | 4.727521 |
| 54 | 6 | 0 | 2.144663 | -7.072046 | 3.165332 |
| 55 | 1 | 0 | 2.824342 | -6.438816 | 1.215843 |
| 56 | 6 | 0 | 1.313779 | -6.758729 | 4.238279 |
| 57 | 1 | 0 | -0.095945 | -5.375854 | 5.067744 |
| 58 | 6 | 0 | -3.202078 | -4.056449 | 1.975002 |
| 59 | 1 | 0 | -2.625391 | -2.094942 | 2.665499 |
| 60 | 1 | 0 | -3.600158 | -2.991047 | 3.820795 |
| 61 | 1 | 0 | 2.779612 | -7.951192 | 3.195045 |
| 62 | 1 | 0 | 1.302527 | -7.387442 | 5.123058 |

| | | | | | |
|---|---|---|---|---|---|
| 63 | 1 | 0 | -4.130657 | -3.743012 | 1.494232 |
| 64 | 1 | 0 | -2.430301 | -4.111565 | 1.204337 |
| 65 | 1 | 0 | -3.355946 | -5.065663 | 2.371209 |
| 66 | 6 | 0 | -1.274942 | 1.041752 | -0.115633 |
| 67 | 6 | 0 | -1.737651 | -0.029982 | -0.458590 |
| 68 | 6 | 0 | -2.157259 | -1.316073 | -0.886553 |
| 69 | 6 | 0 | -1.198593 | -2.228961 | -1.361987 |
| 70 | 6 | 0 | -3.506646 | -1.716175 | -0.867690 |
| 71 | 6 | 0 | -1.566776 | -3.496929 | -1.784410 |
| 72 | 1 | 0 | -0.160198 | -1.926555 | -1.398833 |
| 73 | 6 | 0 | -3.868090 | -2.997401 | -1.266596 |
| 74 | 1 | 0 | -4.268598 | -1.028080 | -0.518104 |
| 75 | 6 | 0 | -2.904345 | -3.915768 | -1.728470 |
| 76 | 1 | 0 | -0.800229 | -4.169860 | -2.144528 |
| 77 | 16 | 0 | -5.553623 | -3.545105 | -1.092825 |
| 78 | 7 | 0 | -3.298116 | -5.211815 | -2.116752 |
| 79 | 6 | 0 | -5.622017 | -4.602290 | -2.524220 |
| 80 | 6 | 0 | -4.484389 | -5.354967 | -2.872499 |
| 81 | 6 | 0 | -2.291233 | -6.276898 | -2.139683 |
| 82 | 6 | 0 | -6.804973 | -4.717715 | -3.251951 |
| 83 | 6 | 0 | -4.570185 | -6.211666 | -3.979055 |
| 84 | 6 | 0 | -1.702081 | -6.559387 | -0.751629 |
| 85 | 1 | 0 | -2.797151 | -7.180560 | -2.482768 |
| 86 | 1 | 0 | -1.496224 | -6.062607 | -2.868520 |
| 87 | 6 | 0 | -6.890484 | -5.610581 | -4.319972 |
| 88 | 1 | 0 | -7.660320 | -4.113409 | -2.967113 |
| 89 | 6 | 0 | -5.768013 | -6.352913 | -4.679479 |

| | | | | | |
|---|---|---|---|---|---|
| 90 | 1 | 0 | -3.697576 | -6.765123 | -4.304200 |
| 91 | 6 | 0 | -2.744945 | -7.110645 | 0.220497 |
| 92 | 1 | 0 | -1.242731 | -5.656667 | -0.338768 |
| 93 | 1 | 0 | -0.887564 | -7.282475 | -0.882321 |
| 94 | 1 | 0 | -7.820028 | -5.712600 | -4.869927 |
| 95 | 1 | 0 | -5.810822 | -7.034617 | -5.523064 |
| 96 | 1 | 0 | -2.313912 | -7.253019 | 1.215584 |
| 97 | 1 | 0 | -3.590398 | -6.424089 | 0.311469 |
| 98 | 1 | 0 | -3.132661 | -8.076689 | -0.122544 |
| 99 | 6 | 0 | 3.053481 | 1.205215 | 0.391839 |
| 100 | 6 | 0 | 4.259284 | 1.193255 | 0.220932 |
| 101 | 6 | 0 | 5.663391 | 1.182288 | 0.020230 |
| 102 | 6 | 0 | 6.453034 | 0.123594 | 0.505721 |
| 103 | 6 | 0 | 6.302968 | 2.231770 | -0.668820 |
| 104 | 6 | 0 | 7.827940 | 0.113120 | 0.309943 |
| 105 | 1 | 0 | 5.976939 | -0.683562 | 1.051183 |
| 106 | 6 | 0 | 7.672477 | 2.198589 | -0.894375 |
| 107 | 1 | 0 | 5.715243 | 3.062291 | -1.043459 |
| 108 | 6 | 0 | 8.463426 | 1.139885 | -0.405169 |
| 109 | 1 | 0 | 8.413901 | -0.701712 | 0.717549 |
| 110 | 16 | 0 | 8.449240 | 3.455704 | -1.890230 |
| 111 | 7 | 0 | 9.851282 | 1.143229 | -0.638917 |
| 112 | 6 | 0 | 9.997648 | 3.544637 | -1.014140 |
| 113 | 6 | 0 | 10.558564 | 2.358643 | -0.505132 |
| 114 | 6 | 0 | 10.581345 | -0.124769 | -0.648503 |
| 115 | 6 | 0 | 10.668384 | 4.760001 | -0.889208 |
| 116 | 6 | 0 | 11.802770 | 2.430619 | 0.135905 |

| | | | | | |
|---|---|---|---|---|---|
| 117 | 6 | 0 | 10.057287 | -1.093626 | -1.716449 |
| 118 | 1 | 0 | 11.618752 | 0.116316 | -0.886932 |
| 119 | 1 | 0 | 10.585317 | -0.602232 | 0.342718 |
| 120 | 6 | 0 | 11.926596 | 4.810441 | -0.288865 |
| 121 | 1 | 0 | 10.205413 | 5.661049 | -1.278626 |
| 122 | 6 | 0 | 12.488121 | 3.642389 | 0.222357 |
| 123 | 1 | 0 | 12.234787 | 1.540099 | 0.577319 |
| 124 | 6 | 0 | 10.100108 | -0.499044 | -3.124594 |
| 125 | 1 | 0 | 9.035324 | -1.403306 | -1.477516 |
| 126 | 1 | 0 | 10.675503 | -1.998213 | -1.664060 |
| 127 | 1 | 0 | 12.454083 | 5.755429 | -0.213305 |
| 128 | 1 | 0 | 13.456999 | 3.670256 | 0.710885 |
| 129 | 1 | 0 | 9.750143 | -1.223848 | -3.865396 |
| 130 | 1 | 0 | 9.468277 | 0.390448 | -3.192558 |
| 131 | 1 | 0 | 11.119297 | -0.203325 | -3.397603 |
| 132 | 6 | 0 | 1.650999 | 1.135732 | 0.592301 |
| 133 | 6 | 0 | 0.861992 | 2.203193 | 0.275742 |
| 134 | 1 | 0 | 1.367548 | 3.123529 | -0.004890 |

---

Rotational constants (GHZ): 0.0205247 0.0125857 0.0088272

## 5. **$(PTZ)_5$**

Standard orientation:

---

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

---

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.129723 | 0.233912 | 3.014496 |
| 2 | 6 | 0 | 1.960987 | 0.732153 | 3.574797 |
| 3 | 6 | 0 | 0.869577 | -0.109629 | 3.837621 |
| 4 | 6 | 0 | 0.991409 | -1.471731 | 3.506170 |
| 5 | 6 | 0 | 2.149693 | -1.957253 | 2.909684 |
| 6 | 6 | 0 | 3.243703 | -1.116114 | 2.641595 |
| 7 | 6 | 0 | -1.691023 | -1.470135 | 3.540895 |
| 8 | 6 | 0 | -1.547666 | -0.107507 | 3.859336 |
| 9 | 6 | 0 | -2.629737 | 0.746760 | 3.604389 |
| 10 | 1 | 0 | -2.551603 | 1.802537 | 3.830371 |
| 11 | 6 | 0 | -3.804672 | 0.258559 | 3.050388 |
| 12 | 6 | 0 | -3.941876 | -1.093152 | 2.692951 |
| 13 | 6 | 0 | -2.863533 | -1.949794 | 2.962259 |
| 14 | 1 | 0 | 3.957808 | 0.909325 | 2.841288 |
| 15 | 1 | 0 | 1.895417 | 1.790588 | 3.796078 |
| 16 | 1 | 0 | 2.203769 | -3.008470 | 2.642555 |
| 17 | 1 | 0 | -4.622126 | 0.943662 | 2.863306 |
| 18 | 1 | 0 | -2.929090 | -3.000471 | 2.695927 |
| 19 | 7 | 0 | -0.332602 | 0.359623 | 4.404011 |
| 20 | 16 | 0 | -0.345758 | -2.575235 | 3.926054 |
| 21 | 6 | 0 | -0.330345 | 1.595003 | 5.186201 |
| 22 | 6 | 0 | -1.227302 | 1.502894 | 6.427222 |
| 23 | 6 | 0 | -0.832855 | 0.351688 | 7.353229 |
| 24 | 1 | 0 | 0.696145 | 1.749782 | 5.522766 |
| 25 | 1 | 0 | -0.598763 | 2.467023 | 4.571093 |
| 26 | 1 | 0 | -2.274816 | 1.394641 | 6.130345 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | -1.151306 | 2.461745 | 6.954605 |
| 28 | 1 | 0 | -1.476742 | 0.321171 | 8.237201 |
| 29 | 1 | 0 | -0.914659 | -0.608163 | 6.836512 |
| 30 | 1 | 0 | 0.203166 | 0.457005 | 7.694387 |
| 31 | 6 | 0 | -5.154053 | -1.600128 | 2.028754 |
| 32 | 1 | 0 | -5.512938 | -2.573593 | 2.357241 |
| 33 | 6 | 0 | -5.828271 | -0.965188 | 1.036628 |
| 34 | 6 | 0 | 4.436138 | -1.685918 | 2.007080 |
| 35 | 1 | 0 | 4.606573 | -2.737578 | 2.228438 |
| 36 | 6 | 0 | 5.321987 | -1.089315 | 1.168515 |
| 37 | 6 | 0 | -7.117323 | -1.463009 | 0.518047 |
| 38 | 6 | 0 | -8.001486 | -2.208512 | 1.313576 |
| 39 | 6 | 0 | -7.495966 | -1.204257 | -0.810416 |
| 40 | 6 | 0 | -9.196582 | -2.701147 | 0.801008 |
| 41 | 1 | 0 | -7.755657 | -2.396205 | 2.353104 |
| 42 | 6 | 0 | -8.708887 | -1.659371 | -1.313832 |
| 43 | 1 | 0 | -6.835116 | -0.634348 | -1.454022 |
| 44 | 6 | 0 | -9.581082 | -2.426250 | -0.519191 |
| 45 | 1 | 0 | -9.844326 | -3.289450 | 1.439807 |
| 46 | 16 | 0 | -9.223423 | -1.215449 | -2.961134 |
| 47 | 7 | 0 | -10.798038 | -2.885528 | -1.062168 |
| 48 | 6 | 0 | -10.062579 | -2.731026 | -3.377125 |
| 49 | 6 | 0 | -10.799176 | -3.395745 | -2.378711 |
| 50 | 6 | 0 | -11.920888 | -3.168360 | -0.169205 |
| 51 | 6 | 0 | -10.036765 | -3.214858 | -4.683865 |
| 52 | 6 | 0 | -11.500099 | -4.557627 | -2.729607 |
| 53 | 6 | 0 | -12.359355 | -1.929417 | 0.622697 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | -12.752818 | -3.480357 | -0.803124 |
| 55 | 1 | 0 | -11.705195 | -4.007912 | 0.508499 |
| 56 | 6 | 0 | -10.774911 | -4.347060 | -5.029555 |
| 57 | 1 | 0 | -9.447918 | -2.690010 | -5.429309 |
| 58 | 6 | 0 | -11.504393 | -5.014080 | -4.047695 |
| 59 | 1 | 0 | -12.037054 | -5.113574 | -1.969833 |
| 60 | 6 | 0 | -12.748024 | -0.760727 | -0.283713 |
| 61 | 1 | 0 | -11.562798 | -1.618470 | 1.305686 |
| 62 | 1 | 0 | -13.208361 | -2.226820 | 1.250397 |
| 63 | 1 | 0 | -10.768628 | -4.707342 | -6.052868 |
| 64 | 1 | 0 | -12.066764 | -5.908245 | -4.297683 |
| 65 | 1 | 0 | -13.076105 | 0.100294 | 0.306058 |
| 66 | 1 | 0 | -11.902225 | -0.449794 | -0.902796 |
| 67 | 1 | 0 | -13.566493 | -1.039527 | -0.956923 |
| 68 | 6 | 0 | -5.239950 | 0.252714 | 0.414658 |
| 69 | 6 | 0 | -5.899234 | 1.486846 | 0.427913 |
| 70 | 6 | 0 | -3.940133 | 0.197234 | -0.105606 |
| 71 | 6 | 0 | -5.240465 | 2.648870 | 0.029995 |
| 72 | 1 | 0 | -6.921277 | 1.543203 | 0.789053 |
| 73 | 6 | 0 | -3.270565 | 1.354882 | -0.479869 |
| 74 | 1 | 0 | -3.423301 | -0.755008 | -0.146978 |
| 75 | 6 | 0 | -3.899893 | 2.608020 | -0.378361 |
| 76 | 1 | 0 | -5.759996 | 3.599739 | 0.066665 |
| 77 | 16 | 0 | -1.556222 | 1.280014 | -0.949592 |
| 78 | 7 | 0 | -3.171447 | 3.778248 | -0.670891 |
| 79 | 6 | 0 | -1.534057 | 2.657047 | -2.078789 |
| 80 | 6 | 0 | -2.308573 | 3.796168 | -1.784351 |

| | | | | | |
|---|---|---|---|---|---|
| 81 | 6 | 0 | -3.468755 | 5.010513 | 0.057348 |
| 82 | 6 | 0 | -0.662037 | 2.654133 | -3.166433 |
| 83 | 6 | 0 | -2.177073 | 4.924598 | -2.604258 |
| 84 | 6 | 0 | -3.379171 | 4.827264 | 1.579596 |
| 85 | 1 | 0 | -2.716387 | 5.740648 | -0.248399 |
| 86 | 1 | 0 | -4.447234 | 5.429316 | -0.220789 |
| 87 | 6 | 0 | -0.503031 | 3.802128 | -3.943378 |
| 88 | 1 | 0 | -0.080720 | 1.763043 | -3.375404 |
| 89 | 6 | 0 | -1.260528 | 4.934857 | -3.655839 |
| 90 | 1 | 0 | -2.790241 | 5.798810 | -2.417465 |
| 91 | 6 | 0 | -2.029793 | 4.272051 | 2.040297 |
| 92 | 1 | 0 | -4.183671 | 4.169766 | 1.923494 |
| 93 | 1 | 0 | -3.564537 | 5.807983 | 2.034639 |
| 94 | 1 | 0 | 0.205489 | 3.804607 | -4.764502 |
| 95 | 1 | 0 | -1.155069 | 5.830470 | -4.259669 |
| 96 | 1 | 0 | -1.994211 | 4.203809 | 3.132676 |
| 97 | 1 | 0 | -1.851370 | 3.273953 | 1.631649 |
| 98 | 1 | 0 | -1.200898 | 4.912369 | 1.721424 |
| 99 | 6 | 0 | 6.542278 | -1.815116 | 0.747655 |
| 100 | 6 | 0 | 7.211858 | -2.693812 | 1.613017 |
| 101 | 6 | 0 | 7.073148 | -1.642132 | -0.542382 |
| 102 | 6 | 0 | 8.348569 | -3.385909 | 1.207769 |
| 103 | 1 | 0 | 6.859803 | -2.804159 | 2.633073 |
| 104 | 6 | 0 | 8.185580 | -2.360260 | -0.963549 |
| 105 | 1 | 0 | 6.592853 | -0.958610 | -1.233503 |
| 106 | 6 | 0 | 8.849836 | -3.244970 | -0.093716 |
| 107 | 1 | 0 | 8.859184 | -4.027748 | 1.915912 |

| | | | | | |
|---|---|---|---|---|---|
| 108 | 16 | 0 | 8.752343 | -2.234906 | -2.648976 |
| 109 | 7 | 0 | 9.993247 | -3.937160 | -0.541001 |
| 110 | 6 | 0 | 10.500490 | -2.368490 | -2.332025 |
| 111 | 6 | 0 | 10.942832 | -3.242859 | -1.320969 |
| 112 | 6 | 0 | 10.356123 | -5.204066 | 0.092626 |
| 113 | 6 | 0 | 11.414607 | -1.665321 | -3.114599 |
| 114 | 6 | 0 | 12.322725 | -3.382028 | -1.117250 |
| 115 | 6 | 0 | 9.249008 | -6.258027 | -0.037690 |
| 116 | 1 | 0 | 11.240616 | -5.572669 | -0.430032 |
| 117 | 1 | 0 | 10.642830 | -5.068455 | 1.146305 |
| 118 | 6 | 0 | 12.785568 | -1.847686 | -2.931349 |
| 119 | 1 | 0 | 11.044356 | -0.988418 | -3.877979 |
| 120 | 6 | 0 | 13.233230 | -2.707262 | -1.930458 |
| 121 | 1 | 0 | 12.688376 | -4.013099 | -0.315636 |
| 122 | 6 | 0 | 8.875666 | -6.541147 | -1.493360 |
| 123 | 1 | 0 | 8.360472 | -5.940877 | 0.516770 |
| 124 | 1 | 0 | 9.610021 | -7.171795 | 0.450105 |
| 125 | 1 | 0 | 13.492622 | -1.314676 | -3.558302 |
| 126 | 1 | 0 | 14.296979 | -2.843390 | -1.762470 |
| 127 | 1 | 0 | 8.100512 | -7.310442 | -1.556251 |
| 128 | 1 | 0 | 8.501451 | -5.637946 | -1.982713 |
| 129 | 1 | 0 | 9.744535 | -6.890708 | -2.062428 |
| 130 | 6 | 0 | 5.116905 | 0.266688 | 0.596943 |
| 131 | 6 | 0 | 6.150312 | 1.212555 | 0.587539 |
| 132 | 6 | 0 | 3.880810 | 0.636443 | 0.045122 |
| 133 | 6 | 0 | 5.953959 | 2.492126 | 0.073613 |
| 134 | 1 | 0 | 7.116343 | 0.948649 | 1.004621 |

| | | | | | |
|---|---|---|---|---|---|
| 135 | 6 | 0 | 3.687571 | 1.902206 | -0.492813 |
| 136 | 1 | 0 | 3.062609 | -0.074332 | 0.037907 |
| 137 | 6 | 0 | 4.722568 | 2.857585 | -0.485531 |
| 138 | 1 | 0 | 6.765494 | 3.209147 | 0.109059 |
| 139 | 16 | 0 | 2.143744 | 2.321026 | -1.275094 |
| 140 | 7 | 0 | 4.492285 | 4.135104 | -1.034860 |
| 141 | 6 | 0 | 2.074625 | 4.030731 | -0.778883 |
| 142 | 6 | 0 | 3.267197 | 4.778465 | -0.756169 |
| 143 | 6 | 0 | 5.618746 | 4.903707 | -1.561709 |
| 144 | 6 | 0 | 0.852539 | 4.630519 | -0.484188 |
| 145 | 6 | 0 | 3.194351 | 6.142225 | -0.439387 |
| 146 | 6 | 0 | 6.351068 | 4.164848 | -2.689648 |
| 147 | 1 | 0 | 5.201034 | 5.825317 | -1.971496 |
| 148 | 1 | 0 | 6.322826 | 5.198326 | -0.768872 |
| 149 | 6 | 0 | 0.789119 | 5.998293 | -0.218105 |
| 150 | 1 | 0 | -0.045370 | 4.027796 | -0.488350 |
| 151 | 6 | 0 | 1.961941 | 6.750025 | -0.198080 |
| 152 | 1 | 0 | 4.102895 | 6.729675 | -0.373979 |
| 153 | 6 | 0 | 5.423059 | 3.784028 | -3.843867 |
| 154 | 1 | 0 | 6.839948 | 3.267481 | -2.298203 |
| 155 | 1 | 0 | 7.152467 | 4.824741 | -3.043992 |
| 156 | 1 | 0 | -0.170792 | 6.466502 | -0.026044 |
| 157 | 1 | 0 | 1.928690 | 7.811896 | 0.025445 |
| 158 | 1 | 0 | 5.978383 | 3.284247 | -4.642955 |
| 159 | 1 | 0 | 4.633011 | 3.109860 | -3.502653 |
| 160 | 1 | 0 | 4.940437 | 4.670249 | -4.271232 |

---

Rotational constants (GHZ): 0.0254834 0.0077479 0.0072951

6. **PTZ-Ph-(PTZ)$_2$**.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 9.186066 | -3.659623 | 0.463373 |
| 2 | 6 | 0 | 7.832909 | -3.404034 | 0.664104 |
| 3 | 6 | 0 | 7.185877 | -2.448227 | -0.115761 |
| 4 | 6 | 0 | 7.891698 | -1.731268 | -1.087691 |
| 5 | 6 | 0 | 9.253099 | -1.987430 | -1.281986 |
| 6 | 6 | 0 | 9.895403 | -2.952904 | -0.511563 |
| 7 | 6 | 0 | 5.876093 | 0.048244 | -0.931812 |
| 8 | 6 | 0 | 5.394571 | -0.805335 | 0.065114 |
| 9 | 6 | 0 | 4.534360 | -0.316375 | 1.048050 |
| 10 | 1 | 0 | 4.188288 | -0.983514 | 1.827895 |
| 11 | 6 | 0 | 4.081857 | 0.996873 | 0.983354 |
| 12 | 6 | 0 | 5.426614 | 1.371753 | -0.988217 |
| 13 | 1 | 0 | 9.687312 | -4.408179 | 1.068094 |
| 14 | 1 | 0 | 7.241722 | -3.953728 | 1.386743 |
| 15 | 1 | 0 | 9.799097 | -1.425895 | -2.032937 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 1 | 0 | 10.951887 | -3.146939 | -0.666414 |
| 17 | 1 | 0 | 3.387187 | 1.361536 | 1.729927 |
| 18 | 1 | 0 | 5.805382 | 2.030773 | -1.762933 |
| 19 | 7 | 0 | 5.773476 | -2.209842 | 0.052157 |
| 20 | 16 | 0 | 7.048860 | -0.554847 | -2.126158 |
| 21 | 6 | 0 | 4.512673 | 1.836906 | -0.047147 |
| 22 | 1 | 0 | 4.157023 | 2.858456 | -0.100849 |
| 23 | 6 | 0 | 3.539450 | -3.023917 | 0.208242 |
| 24 | 6 | 0 | 2.765297 | -3.747806 | 1.136036 |
| 25 | 6 | 0 | 2.857075 | -2.204559 | -0.719453 |
| 26 | 6 | 0 | 1.387077 | -3.592019 | 1.192209 |
| 27 | 1 | 0 | 3.271741 | -4.429129 | 1.812241 |
| 28 | 6 | 0 | 1.480365 | -2.072498 | -0.677481 |
| 29 | 1 | 0 | 3.419359 | -1.675990 | -1.481500 |
| 30 | 6 | 0 | 0.713146 | -2.738889 | 0.299113 |
| 31 | 1 | 0 | 0.811653 | -4.145502 | 1.929554 |
| 32 | 1 | 0 | 0.981509 | -1.446485 | -1.407770 |
| 33 | 6 | 0 | 4.977665 | -3.263610 | 0.180139 |
| 34 | 6 | 0 | -0.746353 | -2.639358 | 0.348265 |
| 35 | 1 | 0 | -1.259342 | -3.544795 | 0.666965 |
| 36 | 6 | 0 | -1.514105 | -1.564488 | 0.040998 |
| 37 | 6 | 0 | -0.945435 | -0.200590 | -0.140662 |
| 38 | 6 | 0 | -1.160710 | 0.538737 | -1.309102 |

| | | | | | |
|---|---|---|---|---|---|
| 39 | 6 | 0 | -0.254456 | 0.414363 | 0.912971 |
| 40 | 6 | 0 | -0.686734 | 1.842018 | -1.431923 |
| 41 | 1 | 0 | -1.698925 | 0.085007 | -2.134870 |
| 42 | 6 | 0 | 0.149649 | 1.743116 | 0.823838 |
| 43 | 1 | 0 | -0.079541 | -0.139746 | 1.828806 |
| 44 | 6 | 0 | -0.052183 | 2.480805 | -0.356877 |
| 45 | 1 | 0 | -0.837141 | 2.376183 | -2.362167 |
| 46 | 16 | 0 | 0.782650 | 2.572502 | 2.269387 |
| 47 | 7 | 0 | 0.353438 | 3.827362 | -0.428214 |
| 48 | 6 | 0 | 1.881875 | 3.721339 | 1.470344 |
| 49 | 6 | 0 | 1.542107 | 4.238197 | 0.205192 |
| 50 | 6 | 0 | -0.346142 | 4.740763 | -1.334361 |
| 51 | 6 | 0 | 3.037978 | 4.143909 | 2.125663 |
| 52 | 6 | 0 | 2.415339 | 5.162402 | -0.388118 |
| 53 | 6 | 0 | -1.847361 | 4.836083 | -1.028423 |
| 54 | 1 | 0 | 0.095117 | 5.727366 | -1.184984 |
| 55 | 1 | 0 | -0.179510 | 4.474563 | -2.387953 |
| 56 | 6 | 0 | 3.868158 | 5.104001 | 1.547081 |
| 57 | 1 | 0 | 3.278527 | 3.721665 | 3.096165 |
| 58 | 6 | 0 | 3.553835 | 5.605693 | 0.285716 |
| 59 | 1 | 0 | 2.205266 | 5.534563 | -1.384054 |
| 60 | 6 | 0 | -2.129801 | 5.257579 | 0.413985 |
| 61 | 1 | 0 | -2.337653 | 3.880146 | -1.235782 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -2.274703 | 5.562469 | -1.730546 |
| 63 | 1 | 0 | 4.756901 | 5.439447 | 2.070433 |
| 64 | 1 | 0 | 4.202864 | 6.333540 | -0.190679 |
| 65 | 1 | 0 | -3.205441 | 5.346969 | 0.590917 |
| 66 | 1 | 0 | -1.729170 | 4.526151 | 1.121148 |
| 67 | 1 | 0 | -1.668505 | 6.225430 | 0.640795 |
| 68 | 6 | 0 | -2.986065 | -1.678421 | -0.040482 |
| 69 | 6 | 0 | -3.613639 | -2.873168 | -0.429488 |
| 70 | 6 | 0 | -3.810975 | -0.580857 | 0.262576 |
| 71 | 6 | 0 | -4.998573 | -2.979325 | -0.488359 |
| 72 | 1 | 0 | -3.006049 | -3.719325 | -0.731599 |
| 73 | 6 | 0 | -5.195657 | -0.693216 | 0.237596 |
| 74 | 1 | 0 | -3.364854 | 0.364396 | 0.549653 |
| 75 | 6 | 0 | -5.819091 | -1.896713 | -0.139922 |
| 76 | 1 | 0 | -5.445501 | -3.906871 | -0.826085 |
| 77 | 16 | 0 | -6.217506 | 0.670402 | 0.761096 |
| 78 | 7 | 0 | -7.225403 | -1.973738 | -0.178110 |
| 79 | 6 | 0 | -7.559724 | 0.428801 | -0.385438 |
| 80 | 6 | 0 | -7.948982 | -0.884723 | -0.709972 |
| 81 | 6 | 0 | -7.876761 | -3.273344 | -0.019060 |
| 82 | 6 | 0 | -8.250785 | 1.523672 | -0.901309 |
| 83 | 6 | 0 | -9.043460 | -1.062769 | -1.567489 |
| 84 | 6 | 0 | -7.525503 | -3.941541 | 1.316648 |

| | | | | | |
|---|---|---|---|---|---|
| 85 | 1 | 0 | -8.952123 | -3.086711 | -0.034348 |
| 86 | 1 | 0 | -7.658342 | -3.947477 | -0.860897 |
| 87 | 6 | 0 | -9.365444 | 1.331686 | -1.718022 |
| 88 | 1 | 0 | -7.919890 | 2.524984 | -0.644538 |
| 89 | 6 | 0 | -9.756577 | 0.035751 | -2.047490 |
| 90 | 1 | 0 | -9.335741 | -2.061940 | -1.868694 |
| 91 | 6 | 0 | -7.880535 | -3.069671 | 2.521648 |
| 92 | 1 | 0 | -6.460920 | -4.193376 | 1.343642 |
| 93 | 1 | 0 | -8.070605 | -4.892502 | 1.357467 |
| 94 | 1 | 0 | -9.913203 | 2.187245 | -2.098855 |
| 95 | 1 | 0 | -10.609762 | -0.128764 | -2.698091 |
| 96 | 1 | 0 | -7.634649 | -3.578116 | 3.458495 |
| 97 | 1 | 0 | -7.334331 | -2.122950 | 2.492731 |
| 98 | 1 | 0 | -8.950675 | -2.834396 | 2.536947 |

---

Rotational constants (GHZ): 0.0710291 0.0209390 0.0173231

TDDFT calculation data of (**PTZ**)$_3$, **An(PTZ)**$_2$, **An(TPE)**$_2$, (**PTZ**)$_4$, (**PTZ**)$_5$ and **PTZ-Ph-(PTZ)**$_2$

1 (**PTZ**)$_3$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1702 eV 391.10 nm f=1.3402 <S**2>=0.000

209 -> 210 0.66225

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

Total Energy, E(TD-HF/TD-KS) = -3326.74925789

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

Excited State 2: Singlet-A 3.7598 eV 329.76 nm f=0.7733 <S**2>=0.000

202 -> 210 0.11920

205 -> 210 -0.10015

207 -> 210 -0.15345

207 -> 211 -0.19896

208 -> 210 0.52074

208 -> 212 -0.12493

209 -> 211 -0.27128

Excited State 3: Singlet-A 3.9369 eV 314.93 nm f=0.0581 <S**2>=0.000

206 -> 210 0.17471

206 -> 212 0.11530

207 -> 210 0.53750

208 -> 210 0.13682

208 -> 211 -0.21601

209 -> 212 -0.11830

209 -> 213 -0.10372

Excited State 4: Singlet-A 4.2204 eV 293.77 nm f=0.0977 <S**2>=0.000

206 -> 210 0.43283

207 -> 211 -0.10222

207 -> 212 0.18652

207 -> 213 0.10171

208 -> 211 0.27961

208 -> 217 -0.10286

209 -> 212 0.14678

Excited State 5: Singlet-A 4.3425 eV 285.51 nm f=0.0591 <S**2>=0.000

203 -> 210 -0.14147

204 -> 210 0.15080

207 -> 213 -0.15086

207 -> 214 -0.14456

207 -> 215 -0.13248

207 -> 218 -0.11120

208 -> 212 -0.13532

208 -> 213 -0.10057

209 -> 213 0.11186

209 -> 214 0.15307

209 -> 215 0.33441

209 -> 217 0.21240

209 -> 218 0.11993

Excited State 6: Singlet-A 4.3708 eV 283.66 nm f=0.0893 <S**2>=0.000

202 -> 210 0.12221

207 -> 211 0.12702

207 -> 212 -0.22341

207 -> 217 -0.11222

208 -> 210 0.20452

208 -> 212 0.30160

208 -> 214 -0.10911

208 -> 215 -0.12308

208 -> 216 -0.11019

209 -> 211 0.19044

209 -> 213 0.18387

209 -> 214 0.14409

209 -> 216 -0.14747

Excited State 7: Singlet-A 4.4169 eV 280.71 nm f=0.0073 <S**2>=0.000

205 -> 211 -0.13613

206 -> 210 -0.23006

207 -> 210 0.14653

207 -> 212 0.14425

207 -> 213 -0.13297

208 -> 212 -0.12599

208 -> 213 0.17031

208 -> 215 -0.12934

208 -> 216 -0.22420

209 -> 212 0.24460

209 -> 215 -0.11767

209 -> 216 -0.18589

209 -> 218 0.12894

Excited State 8: Singlet-A 4.5134 eV 274.70 nm f=0.1267 <S**2>=0.000

202 -> 210 -0.12382

204 -> 210 -0.14919

204 -> 211 -0.10007

205 -> 210 0.32150

206 -> 211 0.16202

207 -> 211 -0.15935

207 -> 213 0.12808

208 -> 213 -0.17599

208 -> 216 -0.14351

208 -> 217 0.11887

209 -> 211 -0.10061

209 -> 213 0.11320

209 -> 216 -0.15530

Excited State 9: Singlet-A 4.6124 eV 268.81 nm f=0.2161 <S**2>=0.000

197 -> 210 -0.15830

199 -> 210 -0.13365

201 -> 210 0.12083

206 -> 211 0.16699

207 -> 210 -0.14890

207 -> 217 0.12662

208 -> 210 0.11796

208 -> 217 0.11315

209 -> 211 0.36409

209 -> 213 -0.12541

209 -> 214 -0.15794

209 -> 215 0.10687

Excited State 10: Singlet-A 4.6546 eV 266.37 nm f=0.3928 <S**2>=0.000

199 -> 210 0.10536

204 -> 210 -0.11160

206 -> 211 0.13934

207 -> 214 -0.18416

207 -> 215 0.14158

208 -> 210 0.21078

209 -> 211 0.32080

209 -> 212 0.10510

209 -> 215 -0.12133

209 -> 216 0.25184

209 -> 217 0.10408

Excited State 11: Singlet-A 4.6849 eV 264.64 nm f=0.0060 <S**2>=0.000

195 -> 211 -0.11086

197 -> 210 0.35315

198 -> 210 -0.17032

199 -> 210 0.16169

200 -> 210 -0.10166

201 -> 210 -0.22184

204 -> 210 -0.12670

207 -> 214 0.11527

207 -> 215 -0.13645

207 -> 216 0.10380

209 -> 211 0.10958

209 -> 215 0.19029

209 -> 216 -0.10208

Excited State 12: Singlet-A 4.7027 eV 263.65 nm f=0.0344 <S**2>=0.000

206 -> 210 0.16551

207 -> 213 -0.14386

207 -> 214 0.12953

207 -> 216 -0.15495

207 -> 218 -0.12306

208 -> 213 0.12122

208 -> 214 -0.13859

208 -> 216 -0.15937

208 -> 217 0.27201

208 -> 218 -0.12050

209 -> 213 -0.11349

209 -> 214 0.12304

209 -> 215 -0.14093

209 -> 217 0.18767

Excited State 13: Singlet-A 4.7361 eV 261.79 nm f=0.0084 <S**2>=0.000

205 -> 210 0.19195

207 -> 213 -0.14939

207 -> 214 0.18312

207 -> 217 -0.14423

208 -> 213 0.13803

208 -> 214 -0.18567

208 -> 216 0.13110

208 -> 217 -0.10606

208 -> 218 0.19315

209 -> 213 -0.10125

209 -> 214 0.11075

209 -> 217 -0.14931

Excited State 14: Singlet-A 4.7991 eV 258.35 nm f=0.0339 <S**2>=0.000

197 -> 210 0.20724

198 -> 210 -0.13299

204 -> 210 0.21231

207 -> 210 -0.22058

207 -> 219 -0.18891

208 -> 211 -0.13357

208 -> 220 -0.12968

209 -> 218 0.22772

Excited State 15: Singlet-A 4.9573 eV 250.10 nm f=0.0575 <S**2>=0.000

195 -> 210 0.10070

203 -> 210 0.13756

206 -> 210 0.34740

207 -> 218 0.11163

207 -> 221 -0.10882

208 -> 211 -0.13390

208 -> 219 0.11272

209 -> 210 -0.13687

209 -> 219 -0.21847

209 -> 220 -0.18911

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

2 **An(PTZ)$_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.3064 eV 374.98 nm f=0.3481 <S**2>=0.000

178 ->181 -0.28329

180 ->181 0.62838

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

Total Energy, E(TD-HF/TD-KS) = -2680.51835313

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

Excited State 2: Singlet-A 3.9751 eV 311.90 nm f=0.0389 <S**2>=0.000

175 ->181 -0.32914

177 ->181 0.12928

178 ->181 0.37083

178 ->184 -0.10506

179 ->181 -0.16937

180 ->181 0.14659

180 ->182 -0.24876

180 ->183 -0.15858

180 ->184 0.12530

Excited State 3: Singlet-A 4.0194 eV 308.46 nm f=0.0350 <S**2>=0.000

174 ->181 -0.19698

175 ->181 0.33098

177 ->181 0.10387

178 ->181 0.30055

178 ->182 -0.13395

178 ->183 -0.16527

178 ->185 -0.11967

179 ->184 -0.16079

180 ->181 0.10835

180 ->182 -0.14816

180 ->183 0.20238

180 ->184 -0.18300

180 ->185 0.14662

Excited State 4: Singlet-A 4.0766 eV 304.14 nm f=0.1330 <S**2>=0.000

178 ->184 0.24565

179 ->181 -0.38036

179 ->182 0.38350

180 ->184 0.15676

180 ->185 0.16057

Excited State 5: Singlet-A 4.1854 eV 296.23 nm f=0.0168 <S**2>=0.000

174 ->181 -0.10720

177 ->181 0.11885

178 ->181 0.21469

178 ->188 0.10104

179 ->181 -0.20149

179 ->183 0.12200

179 ->184 0.21769

179 ->185 0.10415

179 ->188 -0.11388

180 ->181 0.16068

180 ->182 0.41848

180 ->184 -0.12996

Excited State 6: Singlet-A 4.4028 eV 281.60 nm f=0.0526 <S**2>=0.000

178 ->182 -0.36052

179 ->181 0.12084

179 ->182 0.13131

179 ->183 -0.10976

179 ->184 -0.15957

179 ->188 0.12559

180 ->182 0.39561

180 ->188 -0.16581

Excited State 7: Singlet-A 4.4704 eV 277.34 nm f=0.0707 <S**2>=0.000

174 ->181 -0.10052

177 ->181 0.16206

178 ->181 0.13987

178 ->182 0.14872

178 ->183 0.17098

178 ->184 0.16968

179 ->181 0.24319

179 ->184 0.17980

179 ->188 0.23660

180 ->183 0.23116

180 ->184 0.16813

Excited State 8: Singlet-A 4.5354 eV 273.37 nm f=0.0070 <S**2>=0.000

177 ->181 -0.24729

177 ->182 0.16381

178 ->182 -0.13516

178 ->183 0.11044

178 ->185 -0.17277

178 ->188 0.12394

179 ->181 -0.15574

179 ->183 0.24746

179 ->185 -0.24663

180 ->185 -0.12949

180 ->188 0.15855

180 ->189 0.11290

Excited State 9: Singlet-A 4.6345 eV 267.53 nm f=0.0330 <S**2>=0.000

178 ->185 0.13644

179 ->181 0.32877

179 ->182 0.12320

179 ->183 0.16077

179 ->186 0.23352

180 ->183 -0.21215

180 ->185 0.19737

180 ->188 0.16561

Excited State 10: Singlet-A 4.7197 eV 262.70 nm f=0.0898 <S**2>=0.000

178 ->182 -0.11701

178 ->186 0.17231

178 ->187 -0.15070

179 ->181 0.10533

179 ->182 0.12887

179 ->186 -0.20320

179 ->187 0.35910

179 ->189 -0.11736

180 ->186 0.19532

180 ->187 -0.22888

180 ->189 0.10353

Excited State 11: Singlet-A 4.7360 eV 261.79 nm f=0.0456 <S**2>=0.000

177 ->181 -0.12782

178 ->185 0.10931

178 ->186 0.26183

178 ->187 0.20541

179 ->181 -0.14948

179 ->182 -0.10013

179 ->185 0.13356

179 ->186 0.28100

179 ->187 0.16100

179 ->189 0.11164

180 ->186 0.17621

180 ->187 0.16079

Excited State 12: Singlet-A 4.9606 eV 249.94 nm f=0.1932 <S**2>=0.000

177 ->181 0.37545

177 ->182 -0.20265

178 ->181 -0.20197

178 ->182 -0.29220

179 ->182 0.10627

179 ->183 0.11007

179 ->188 -0.11799

180 ->181 -0.15278

Excited State 13: Singlet-A 5.0294 eV 246.52 nm f=0.0368 <S**2>=0.000

174 ->181 -0.13326

177 ->181 0.30097

177 ->182 0.19311

178 ->181 -0.17729

178 ->182 0.21168

178 ->188 -0.10617

178 ->189 0.15293

179 ->182 -0.12169

179 ->184 -0.13351

179 ->185 -0.13631

179 ->187 0.10209

179 ->190 -0.14144

179 ->193 -0.10024

180 ->189 0.15475

Excited State 14: Singlet-A 5.0876 eV 243.70 nm f=0.4700 <S**2>=0.000

176 ->181 -0.18391

176 ->182 0.23133

177 ->182 -0.11159

177 ->184 -0.22872

178 ->182 -0.19617

179 ->181 -0.11296

179 ->182 -0.18924

179 ->188 0.15343

180 ->184 -0.10814

180 ->190 0.15221

Excited State 15: Singlet-A 5.1327 eV 241.56 nm f=0.0135 <S**2>=0.000

170 ->181 0.12096

171 ->181 0.47572

172 ->181 0.23444

173 ->181 -0.29987

178 ->190 0.10397

178 ->191 -0.10125

180 ->191 0.15766

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

3 **An(TPE)$_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.3231 eV 373.10 nm f=0.2502 <S**2>=0.000

227 -> 229 -0.15759

227 -> 230 -0.10154

228 -> 229 0.65953

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

Total Energy, E(TD-HF/TD-KS) = -2618.55286702

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

Excited State 2: Singlet-A 3.9264 eV 315.77 nm f=1.1534 <S**2>=0.000

226 -> 229 0.20256

226 -> 230 -0.36787

227 -> 229 -0.11321

227 -> 230 0.12307

227 -> 231 0.41180

228 -> 231 0.30206

Excited State 3: Singlet-A 3.9425 eV 314.48 nm f=0.0473 <S**2>=0.000

225 -> 229 0.11421

226 -> 229 -0.18138

226 -> 230 0.22357

226 -> 231 -0.28139

227 -> 229 -0.30006

227 -> 230 0.15092

227 -> 231 0.12669

228 -> 230 0.37958

Excited State 4: Singlet-A 4.0106 eV 309.14 nm f=0.0065 <S**2>=0.000

224 -> 229 0.46066

224 -> 230 0.13677

227 -> 231 0.11165

227 -> 233 0.15361

228 -> 233 -0.34982

228 -> 234 0.11547

228 -> 235 -0.16809

Excited State 5: Singlet-A 4.2298 eV 293.12 nm f=0.0099 <S**2>=0.000

225 -> 229 -0.25863

227 -> 229 0.48311

228 -> 229 0.11665

228 -> 230 0.31841

228 -> 231 0.11668

228 -> 232 -0.11210

Excited State 6: Singlet-A 4.2952 eV 288.66 nm f=0.1868 <S**2>=0.000

225 -> 229 -0.12811

226 -> 230 0.19317

226 -> 231 -0.19896

227 -> 230 0.31191

227 -> 231 0.20517

228 -> 229 0.11087

228 -> 230 -0.28277

228 -> 231 -0.12506

228 -> 232 0.29959

Excited State 7: Singlet-A 4.6521 eV 266.51 nm f=0.0423 <S**2>=0.000

223 -> 229 0.10089

225 -> 229 -0.15988

226 -> 229 0.49932

226 -> 231 -0.10765

226 -> 232 0.24160

227 -> 229 -0.18483

227 -> 231 -0.10316

228 -> 231 -0.11726

Excited State 8: Singlet-A 4.7803 eV 259.36 nm f=0.0387 <S**2>=0.000

225 -> 230 0.17839

225 -> 231 -0.14394

226 -> 229 -0.12413

226 -> 230 0.11273

226 -> 234 -0.15482

227 -> 230 -0.12823

227 -> 231 -0.12612

228 -> 230 -0.11150

228 -> 231 0.43431

228 -> 232 0.12155

228 -> 235 -0.10217

Excited State 9: Singlet-A 4.7967 eV 258.48 nm f=0.0610 <S**2>=0.000

223 -> 230 0.12484

223 -> 231 0.17519

225 -> 230 0.10942

225 -> 231 0.18179

226 -> 236 -0.10345

227 -> 230 -0.11000

227 -> 232 0.21517

227 -> 234 0.17113

227 -> 235 0.20309

227 -> 236 0.15988

228 -> 234 0.17440

228 -> 235 0.11692

228 -> 236 0.10085

Excited State 10: Singlet-A 4.8488 eV 255.70 nm f=0.0368 <S**2>=0.000

212 -> 230 0.10034

219 -> 229 -0.10878

219 -> 230 0.12524

225 -> 231 -0.10424

226 -> 232 0.10247

226 -> 234 0.24988

227 -> 231 -0.10500

227 -> 232 -0.13405

227 -> 235 -0.10572

228 -> 231 0.21114

228 -> 233 0.14679

228 -> 234 0.17017

228 -> 235 -0.10639

Excited State 11: Singlet-A 4.9397 eV 250.99 nm f=0.3218 <S**2>=0.000

226 -> 232 0.13004

226 -> 233 0.15579

226 -> 235 -0.15516

227 -> 230 -0.21433

227 -> 232 0.30262

227 -> 236 -0.18427

228 -> 232 0.18117

228 -> 236 -0.12536

Excited State 12: Singlet-A 4.9796 eV 248.98 nm f=0.0409 <S**2>=0.000

225 -> 229 0.18171

226 -> 229 -0.15036

226 -> 230 -0.17186

226 -> 232 0.26293

226 -> 234 -0.10263

226 -> 235 -0.12959

226 -> 237 -0.14605

227 -> 229 0.15492

227 -> 233 0.10248

227 -> 235 -0.14951

228 -> 231 -0.20247

228 -> 235 -0.10042

Excited State 13: Singlet-A 5.0605 eV 245.01 nm f=0.0242 <S**2>=0.000

220 -> 230 0.11338

221 -> 231 0.13094

223 -> 231 -0.11624

225 -> 230 0.10408

225 -> 232 -0.12207

226 -> 231 -0.11571

226 -> 235 0.12971

226 -> 239 -0.14044

227 -> 230 -0.13145

227 -> 235 -0.10723

227 -> 236 -0.11456

227 -> 237 0.18499

227 -> 239 0.12053

Excited State 14: Singlet-A 5.0777 eV 244.18 nm f=0.0106 <S**2>=0.000

219 -> 230 -0.17528

219 -> 231 0.14775

223 -> 230 0.10676

225 -> 229 0.23475

225 -> 230 -0.17276

226 -> 234 0.10446

226 -> 240 0.10475

226 -> 241 0.10553

227 -> 230 0.10845

228 -> 232 0.16531

Excited State 15: Singlet-A 5.0949 eV 243.35 nm f=0.0403 <S**2>=0.000

219 -> 230 0.12604

220 -> 231 0.14667

221 -> 230 0.12516

221 -> 231 0.19718

225 -> 230 -0.11739

225 -> 234 -0.10540

226 -> 236 0.16003

227 -> 236 -0.15952

227 -> 238 0.10323

227 -> 242 0.11395

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

4 **(PTZ)$_4$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0666 eV 404.30 nm f=1.5677 <S**2>=0.000

279 -> 280 0.66779

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

Total Energy, E(TD-HF/TD-KS) = -4436.14229150

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

Excited State 2: Singlet-A 3.5784 eV 346.48 nm f=0.6285 <S**2>=0.000

270 -> 280 0.10244

274 -> 280 -0.15591

276 -> 281 0.12763

277 -> 280 -0.10911

278 -> 280 0.54427

279 -> 281 0.26243

Excited State 3: Singlet-A 3.7839 eV 327.66 nm f=0.4010 <S**2>=0.000

269 -> 280 -0.11862

277 -> 280 0.50857

277 -> 281 -0.18285

278 -> 280 0.21478

278 -> 282 0.11587

279 -> 281 -0.21024

279 -> 282 -0.11403

Excited State 4: Singlet-A 3.9246 eV 315.92 nm f=0.1380 <S**2>=0.000

275 -> 280 -0.17294

275 -> 283 -0.10091

276 -> 280 0.53736

276 -> 281 0.14810

278 -> 280 -0.13246

278 -> 281 0.14954

278 -> 282 -0.11397

Excited State 5: Singlet-A 4.1197 eV 300.95 nm f=0.0761 <S**2>=0.000

274 -> 280 0.11060

275 -> 280 0.23941

276 -> 282 -0.15058

277 -> 280 0.14156

277 -> 281 -0.20123

278 -> 280 -0.20235

278 -> 281 0.14013

278 -> 283 -0.12439

279 -> 281 0.36654

279 -> 282 -0.16553

Excited State 6: Singlet-A 4.1807 eV 296.56 nm f=0.0200 <S**2>=0.000

275 -> 280 0.32494

276 -> 283 -0.11989

277 -> 280 -0.12461

277 -> 282 -0.23313

277 -> 283 0.12456

278 -> 281 0.21555

278 -> 282 -0.10445

279 -> 281 -0.30579

Excited State 7: Singlet-A 4.2991 eV 288.39 nm f=0.0992 <S**2>=0.000

271 -> 280 -0.11173

274 -> 280 0.22921

275 -> 281 0.14332

276 -> 281 0.14350

276 -> 286 -0.15888

277 -> 282 0.18565

278 -> 282 -0.12786

278 -> 283 -0.16314

279 -> 283 -0.18792

279 -> 287 -0.21192

Excited State 8: Singlet-A 4.3167 eV 287.22 nm f=0.0055 <S**2>=0.000

275 -> 280 0.10491

276 -> 280 0.12842

276 -> 283 0.13309

277 -> 280 -0.24075

277 -> 281 -0.10678

277 -> 283 -0.10228

277 -> 285 -0.11914

277 -> 287 0.13348

277 -> 288 -0.10268

278 -> 281 -0.12612

278 -> 282 0.24329

278 -> 283 -0.13790

278 -> 284 -0.10677

278 -> 290 -0.11655

278 -> 291 0.11103

279 -> 281 -0.15377

279 -> 282 -0.13446

279 -> 287 -0.10705

Excited State 9: Singlet-A 4.3698 eV 283.73 nm f=0.1332 <S**2>=0.000

266 -> 280 -0.10066

272 -> 280 -0.10865

275 -> 281 -0.14474

276 -> 282 0.13994

276 -> 283 0.20331

276 -> 287 0.11603

276 -> 290 -0.11397

278 -> 283 0.20078

278 -> 286 0.14565

279 -> 281 0.17254

279 -> 284 -0.13866

279 -> 286 0.21166

279 -> 287 -0.14025

279 -> 289 -0.11909

279 -> 291 0.11738

Excited State 10: Singlet-A 4.4155 eV 280.79 nm f=0.0443 <S**2>=0.000

274 -> 281 0.12653

275 -> 280 0.22425

276 -> 280 0.14987

276 -> 284 -0.10578

276 -> 286 0.10179

277 -> 285 0.30588

277 -> 290 -0.11537

278 -> 284 -0.10393

278 -> 285 -0.14194

279 -> 282 0.12261

279 -> 283 0.10336

279 -> 285 0.23888

279 -> 290 -0.12138

Excited State 11: Singlet-A 4.4586 eV 278.08 nm f=0.0252 <S**2>=0.000

272 -> 281 0.12131

274 -> 280 0.32251

275 -> 281 0.14774

276 -> 281 0.10198

276 -> 284 -0.18958

277 -> 285 -0.18110

278 -> 283 0.12462

278 -> 284 -0.17150

279 -> 283 0.14715

279 -> 284 -0.11334

279 -> 285 -0.16253

Excited State 12: Singlet-A 4.5739 eV 271.07 nm f=0.0221 <S**2>=0.000

262 -> 280 0.18619

264 -> 280 -0.10217

266 -> 280 -0.12794

269 -> 280 -0.14747

272 -> 280 -0.15812

273 -> 280 -0.12188

276 -> 280 0.20332

276 -> 286 0.12014

278 -> 281 -0.11853

278 -> 284 0.15396

279 -> 284 0.15377

279 -> 287 -0.12150

Excited State 13: Singlet-A 4.6113 eV 268.87 nm f=0.0724 <S**2>=0.000

267 -> 280 -0.10457

268 -> 280 -0.12579

273 -> 280 0.29656

276 -> 280 0.12290

276 -> 289 -0.11265

277 -> 289 0.17557

278 -> 289 0.24476

279 -> 286 -0.12350

279 -> 289 -0.12573

Excited State 14: Singlet-A 4.6773 eV 265.07 nm f=0.0416 <S**2>=0.000

262 -> 280 0.17207

263 -> 280 -0.12783

275 -> 280 0.16971

275 -> 288 0.14588

276 -> 287 -0.18483

276 -> 288 -0.16747

277 -> 287 -0.11907

279 -> 286 0.10180

279 -> 287 0.19459

279 -> 288 0.25238

Excited State 15: Singlet-A 4.7035 eV 263.60 nm f=0.0287 <S**2>=0.000

262 -> 280 -0.17226

275 -> 285 -0.10048

277 -> 285 -0.18082

277 -> 287 -0.20128

277 -> 288 0.27816

277 -> 290 -0.15600

278 -> 288 -0.10835

279 -> 285 -0.11240

279 -> 287 -0.12570

279 -> 288 0.11501

279 -> 290 -0.14145

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

5 **$(PTZ)_5$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.4705 eV 357.25 nm f=1.2012 <S**2>=0.000

325 -> 332 -0.13232

329 -> 332 0.24922

330 -> 331 0.59926

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

Total Energy, E(TD-HF/TD-KS) = -5315.93964017

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

Excited State 2: Singlet-A 3.8412 eV 322.78 nm f=0.3359 <S**2>=0.000

325 -> 331 -0.12316

327 -> 335 0.10978

328 -> 336 0.11629

329 -> 331 0.39052

330 -> 332 0.50920

Excited State 3: Singlet-A 4.0960 eV 302.70 nm f=0.1737 <S**2>=0.000

326 -> 331 0.25683

326 -> 336 -0.15315

327 -> 331 0.21473

327 -> 332 0.11819

328 -> 331 0.15138

328 -> 332 -0.24653

329 -> 332 0.19218

329 -> 335 0.13726

329 -> 336 0.17505

330 -> 335 0.10235

330 -> 336 -0.11905

Excited State 4: Singlet-A 4.1070 eV 301.88 nm f=0.1399 <S**2>=0.000

| | |
|---|---|
| 326 -> 331 | -0.10017 |
| 326 -> 336 | -0.12394 |
| 327 -> 331 | -0.16386 |
| 327 -> 332 | -0.16600 |
| 328 -> 331 | 0.28412 |
| 328 -> 332 | -0.24502 |
| 328 -> 334 | 0.12190 |
| 328 -> 336 | 0.14762 |
| 329 -> 332 | -0.15311 |
| 329 -> 335 | -0.12658 |
| 329 -> 336 | 0.19126 |
| 330 -> 335 | -0.10175 |
| 330 -> 336 | -0.12150 |

Excited State 5: Singlet-A 4.1302 eV 300.19 nm f=0.0533 <S**2>=0.000

| | |
|---|---|
| 326 -> 331 | 0.26197 |
| 326 -> 335 | -0.15068 |
| 327 -> 331 | -0.23403 |
| 327 -> 332 | -0.22625 |
| 327 -> 333 | -0.15485 |
| 327 -> 335 | 0.17118 |
| 328 -> 336 | -0.14537 |
| 329 -> 332 | 0.20179 |
| 329 -> 335 | -0.16615 |
| 330 -> 333 | 0.11554 |

330 -> 335 -0.11511

Excited State 6: Singlet-A 4.2816 eV 289.58 nm f=0.0679 <S**2>=0.000

325 -> 331 0.15675

326 -> 332 0.32338

327 -> 335 0.22097

328 -> 336 0.22413

329 -> 331 0.13655

329 -> 333 0.11067

330 -> 332 -0.26187

Excited State 7: Singlet-A 4.3567 eV 284.58 nm f=0.0136 <S**2>=0.000

324 -> 332 -0.10614

326 -> 331 -0.10915

326 -> 332 -0.12511

327 -> 333 -0.14740

329 -> 331 -0.12865

329 -> 333 0.23995

330 -> 333 0.33320

330 -> 334 -0.13833

330 -> 339 -0.12188

330 -> 341 -0.15538

Excited State 8: Singlet-A 4.3824 eV 282.91 nm f=0.0910 <S**2>=0.000

321 -> 331 0.10116

324 -> 331 -0.12352

326 -> 331 -0.14417

326 -> 342 0.11639

329 -> 334 -0.21627

330 -> 333 0.11955

330 -> 334 0.32766

330 -> 342 -0.21967

330 -> 345 0.13893

Excited State 9: Singlet-A 4.4185 eV 280.60 nm f=0.2569 <S**2>=0.000

325 -> 332 -0.11790

326 -> 333 -0.17819

326 -> 334 -0.12227

326 -> 337 -0.10368

327 -> 335 -0.13147

328 -> 334 0.13770

328 -> 336 0.13776

328 -> 346 0.10835

329 -> 332 0.10921

329 -> 333 -0.11715

329 -> 334 0.18010

329 -> 339 -0.10262

330 -> 339 -0.13017

330 -> 341 -0.12096

330 -> 342 -0.19188

330 -> 345 0.16931

Excited State 10: Singlet-A 4.4790 eV 276.81 nm f=0.0306 <S**2>=0.000

327 -> 331 -0.17045

327 -> 332 -0.12532

327 -> 333 0.30509

327 -> 339 0.16725

329 -> 333 0.10898

329 -> 335 0.11317

329 -> 339 0.15845

329 -> 344 0.13810

330 -> 339 0.16342

330 -> 344 0.10443

Excited State 11: Singlet-A 4.4939 eV 275.90 nm f=0.0157 <S**2>=0.000

325 -> 331 0.10332

326 -> 334 0.15098

328 -> 331 -0.10189

328 -> 334 0.21929

328 -> 340 -0.14253

328 -> 342 0.10006

329 -> 334 -0.14131

329 -> 336 0.11088

329 -> 338 -0.10986

329 -> 340 0.10994

329 -> 342 -0.12425

330 -> 338 0.10743

330 -> 340 -0.13840

330 -> 342 0.13478

Excited State 12: Singlet-A 4.5364 eV 273.31 nm f=0.1053 <S**2>=0.000

324 -> 332 0.12674

325 -> 331 -0.12099

326 -> 333 0.11507

327 -> 333 -0.12646

327 -> 335 -0.10831

328 -> 331 -0.10863

328 -> 332 0.10001

328 -> 334 0.24892

329 -> 345 -0.11959

330 -> 339 0.10925

330 -> 341 0.16420

330 -> 344 -0.10450

330 -> 346 -0.20922

Excited State 13: Singlet-A 4.5654 eV 271.57 nm f=0.3900 <S**2>=0.000

324 -> 331 0.30693

325 -> 332 -0.17971

326 -> 337 -0.11456

327 -> 335 -0.17228

328 -> 334 -0.14536

328 -> 336 0.14206

329 -> 338 -0.10723

329 -> 346 -0.12892

330 -> 345 -0.10346

330 -> 349 -0.12067

Excited State 14: Singlet-A 4.6694 eV 265.53 nm f=0.0210 <S**2>=0.000

326 -> 332 0.19027

326 -> 338 -0.22097

327 -> 335 -0.12101

327 -> 339 0.10109

328 -> 336 -0.13404

329 -> 331 0.27996

329 -> 337 -0.21317

330 -> 332 -0.17523

330 -> 334 -0.10281

Excited State 15: Singlet-A 4.6894 eV 264.39 nm f=0.1015 <S**2>=0.000

326 -> 339 -0.16530

327 -> 331 -0.12758

327 -> 333 -0.10512

327 -> 335 -0.11395

327 -> 337 0.28710

327 -> 338 0.22294

327 -> 339 0.10090

329 -> 339 -0.18463

329 -> 341 0.13586

330 -> 339 -0.11515

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

6 **PTZ-Ph-(PTZ)$_2$**

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.6173 eV 473.70 nm f=0.2211 <S**2>=0.000

204 -> 209 -0.14988

204 -> 210 -0.12002

206 -> 209 0.37107

206 -> 210 0.20413

208 -> 209 0.42126

208 -> 210 0.15285

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

Total Energy, E(TD-HF/TD-KS) = -3325.61744030

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

Excited State 2: Singlet-A 3.6557 eV 339.15 nm f=0.9049 <S**2>=0.000

202 -> 209 0.14115

204 -> 209 0.20709

205 -> 209 -0.13445

206 -> 209 -0.16677

208 -> 209 0.47913

208 -> 210 -0.30292

Excited State 3: Singlet-A 4.0077 eV 309.36 nm f=0.1836 <S**2>=0.000

206 -> 213 -0.12992

207 -> 209 0.44124

207 -> 210 -0.25993

207 -> 211 -0.14879

207 -> 212 -0.19304

208 -> 211 0.11877

208 -> 212 0.16652

208 -> 213 0.16519

Excited State 4: Singlet-A 4.2289 eV 293.18 nm f=0.1651 <S**2>=0.000

202 -> 209 -0.10120

204 -> 209 -0.15758

205 -> 209 0.16836

206 -> 209 -0.24816

206 -> 210 0.25247

206 -> 213 -0.13334

207 -> 211 0.16336

207 -> 212 0.21601

207 -> 213 0.18515

208 -> 211 -0.12289

208 -> 213 0.14027

208 -> 215 -0.11325

Excited State 5: Singlet-A 4.4352 eV 279.55 nm f=0.0786 <S**2>=0.000

206 -> 209 0.25848

206 -> 210 -0.18166

207 -> 209 0.21616

207 -> 211 0.12099

207 -> 216 -0.10122

207 -> 218 -0.13951

207 -> 219 -0.10980

208 -> 210 -0.21093

208 -> 211 -0.24741

208 -> 213 0.15395

208 -> 214 -0.16307

Excited State 6: Singlet-A 4.4552 eV 278.29 nm f=0.0689 <S**2>=0.000

206 -> 213 0.15046

206 -> 218 -0.14836

206 -> 219 -0.11051

207 -> 209 0.27845

207 -> 211 0.18942

207 -> 212 0.15612

207 -> 214 0.10888

207 -> 215 0.14496

208 -> 213 -0.27792

208 -> 218 0.17795

208 -> 219 0.13763

Excited State 7: Singlet-A 4.4978 eV 275.65 nm f=0.0389 <S**2>=0.000

205 -> 209 0.36831

205 -> 210 0.18457

206 -> 209 0.10758

206 -> 210 -0.19090

208 -> 210 -0.32782

208 -> 211 0.12629

208 -> 213 -0.11704

Excited State 8: Singlet-A 4.5267 eV 273.90 nm f=0.0264 <S**2>=0.000

199 -> 209 -0.11988

200 -> 209 0.14686

201 -> 209 0.29497

205 -> 209 -0.16430

206 -> 211 0.19122

206 -> 220 0.15232

207 -> 209 0.10584

207 -> 213 0.12737

208 -> 211 0.16761

208 -> 212 -0.11669

208 -> 218 -0.17751

208 -> 220 0.20602

208 -> 222 -0.12474

Excited State 9: Singlet-A 4.5901 eV 270.11 nm f=0.0327 <S**2>=0.000

204 -> 209 -0.11672

205 -> 209 -0.22084

205 -> 210 -0.15660

206 -> 209 0.11775

207 -> 211 -0.11026

207 -> 213 0.28520

207 -> 215 0.18121

208 -> 213 -0.12706

208 -> 214 0.12910

208 -> 215 -0.11323

208 -> 220 -0.15758

208 -> 222 0.10134

Excited State 10: Singlet-A 4.6408 eV 267.16 nm f=0.1143 <S**2>=0.000

204 -> 209 0.17860

205 -> 209 0.13918

205 -> 210 0.12025

206 -> 209 -0.13038

206 -> 216 0.23860

207 -> 209 0.10518

207 -> 215 0.34187

208 -> 210 0.12770

208 -> 215 -0.14166

208 -> 216 -0.21140

Excited State 11: Singlet-A 4.6917 eV 264.26 nm f=0.0248 <S**2>=0.000

206 -> 215 0.10572

206 -> 216 -0.21029

207 -> 209 -0.14496

207 -> 215 0.26945

207 -> 216 0.22708

207 -> 218 -0.20516

208 -> 215 -0.18466

208 -> 216 0.18926

208 -> 218 0.12968

Excited State 12: Singlet-A 4.7466 eV 261.20 nm f=0.0700 <S**2>=0.000

202 -> 209 0.10126

204 -> 209 0.28002

205 -> 209 0.14082

205 -> 210 0.14339

206 -> 216 -0.16485

206 -> 219 0.14700

207 -> 209 0.21577

207 -> 215 -0.10131

207 -> 218 0.10950

207 -> 219 -0.10798

208 -> 210 0.15896

208 -> 216 0.17102

208 -> 218 -0.13381

208 -> 219 -0.11453

Excited State 13: Singlet-A 4.8781 eV 254.17 nm f=0.0263 <S**2>=0.000

201 -> 209 0.14778

204 -> 211 0.11605

204 -> 212 -0.13546

205 -> 211 0.15032

205 -> 212 -0.18736

205 -> 223 -0.11151

206 -> 211 -0.18848

206 -> 212 0.24326

206 -> 213 -0.10967

208 -> 211 -0.22203

208 -> 212 0.31479

Excited State 14: Singlet-A 4.9119 eV 252.42 nm f=0.0691 <S**2>=0.000

200 -> 209 -0.14263

201 -> 209 0.12376

202 -> 209 0.13043

203 -> 209 -0.20739

204 -> 210 0.11809

204 -> 213 -0.11675

206 -> 209 0.23399

206 -> 219 -0.11389

206 -> 220 0.10105

207 -> 213 0.11476

208 -> 219 0.15105

208 -> 220 -0.13143

Excited State 15: Singlet-A 5.0209 eV 246.94 nm f=0.0228 <S**2>=0.000

204 -> 210 -0.12997

205 -> 211 0.19516

205 -> 212 -0.22980

205 -> 223 -0.10124

206 -> 212 -0.12748

206 -> 214 0.21068

208 -> 210 -0.10861

208 -> 214 0.32113

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

**References**

1 A. Sillen and Y. Engelborghs, *Photochem. Photobiol.*, 1998, 67, 475–486.