

*Supplementary Materials*

# Phenyl Derivatives Modulate the Luminescent Properties and Stability of CzBTM-type Radicals

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## 1. Synthetic procedures and structure characterization.

### 1.1 Synthetic procedures.

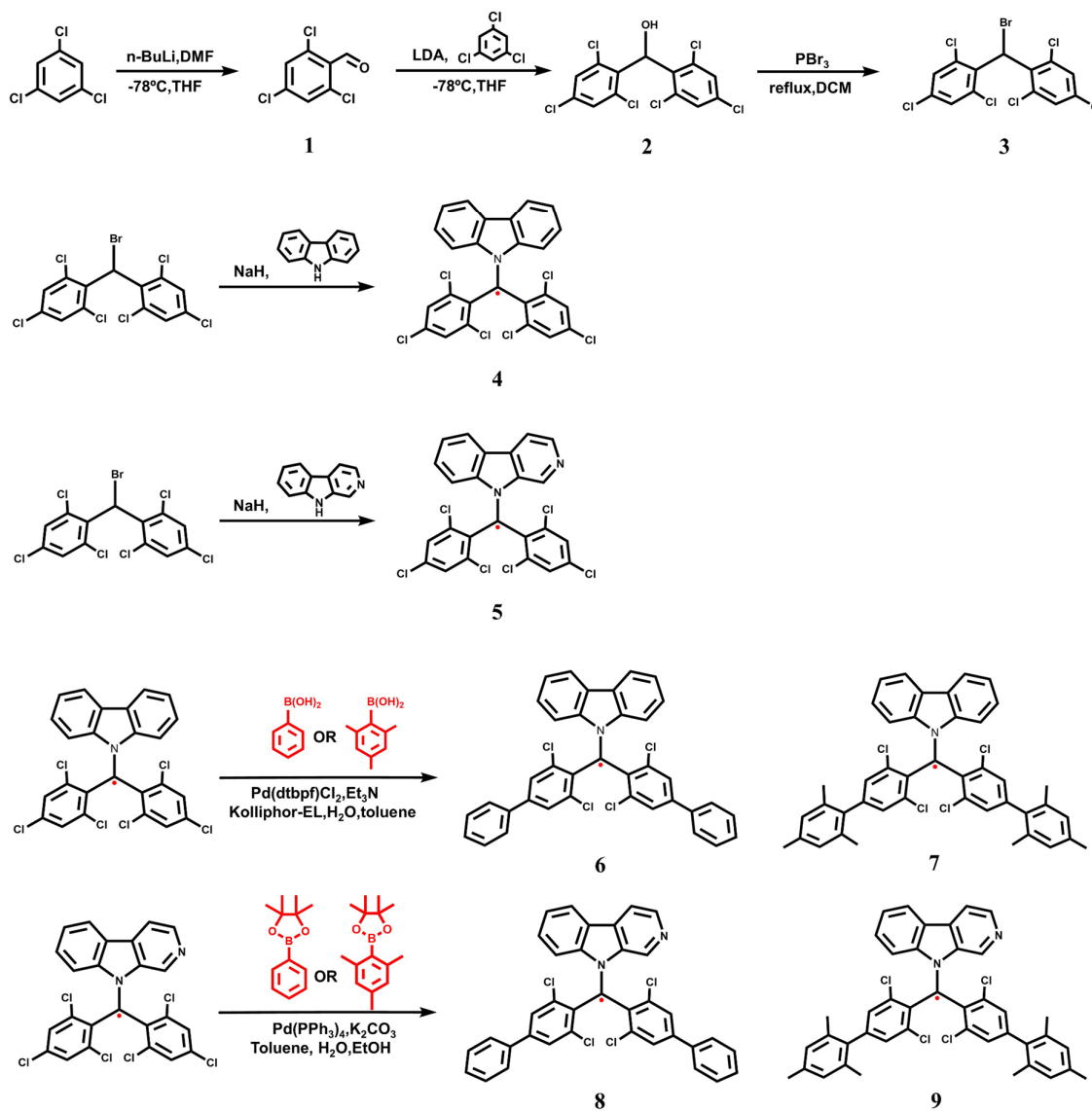


Figure S1. The synthetic routes of radicals

### Synthesis of compound 1

Under argon atmosphere, 1,3,5-trichlorobenzene (10.0 g, 55.1 mmol) was mixed in anhydrous THF (100 mL). After *n*-BuLi in hexane (2.4 M, 23 mL) was added dropwise at  $-78^\circ\text{C}$ . The mixture was stirred at  $-78^\circ\text{C}$  for 0.5 h and the anhydrous DMF (7.44 mL, 107.3 mmol) was added slowly, then stirred for 1.5 h. After warmed slowly to room temperature, the mixture was poured into 3 M HCl solution and extracted with ethyl acetate by three times. The

combined organic layer was washed with sodium bicarbonate solution and dried over anhydrous sodium sulfate. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography using petroleum ether/dichloromethane (silica gel, 3:1, v/v) as eluent. White solid **compound 1** was obtained in 86% yield (10.0 g, 48 mmol).  $^1\text{H NMR}$  (400 MHz, Chloroform-*d*)  $\delta$  7.43 (s, 2H), 10.44 (s, 1H).  $^{13}\text{C NMR}$  (101 MHz, Chloroform-*d*)  $\delta$  127.78, 136.79, 138.34, 186.68.

### Synthesis of compound 2

Under argon atmosphere, 1,3,5-trichlorobenzene (9.5 g, 52.4 mmol) was mixed in anhydrous THF (100 mL). After lithium diisopropyl amide (LDA) in THF/n-hexane (2 M, 26.3 mL) was added dropwise at  $-78^\circ\text{C}$ . The mixture was stirred at  $-78^\circ\text{C}$  for 0.5 h and the compound 1 (10.0 g, 47.7 mmol) dissolved in anhydrous THF (60 mL) was added slowly, then stirred for 2 h. After warmed slowly to room temperature, the mixture was poured into saturated  $\text{NH}_4\text{Cl}$  solution and extracted with diethyl ether by three times. The combined organic solution was washed with sodium bicarbonate solution and dried over anhydrous sodium sulfate. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography used petroleum ether/dichloromethane (silica gel, 2:1, v/v) as eluent. White solid **compound 2** was obtained in 80% yield (15.0 g, 38 mmol).  $^1\text{H NMR}$  (400 MHz, Chloroform-*d*)  $\delta$  3.50 (s, 1H), 6.74 (s, 1H), 7.31 (s, 4H).  $^{13}\text{C NMR}$  (101 MHz, Chloroform-*d*)  $\delta$  72.96, 129.84, 134.49, 135.99.

### Synthesis of compound 3 (HBTM-Br)

**Compound 2** (4.0 g, 10.2 mmol) was mixed in anhydrous dichloromethane (100 mL). After phosphorus tribromide (2 mL, 21.3 mmol) dissolved in dichloromethane (10 mL) was added dropwise at  $0^\circ\text{C}$ . Then the mixture warmed slowly to  $45^\circ\text{C}$  and refluxed overnight. Next, cooled to room temperature, the mixture was poured into water and extracted with dichloromethane by three times. The combined organic solution was washed with brine and dried over anhydrous sodium sulfate. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography used petroleum ether (silica gel) as eluent. White solid **compound 3** was obtained in 80% yield (3.7 g, 8.2 mmol).  $^1\text{H NMR}$  (400 MHz, Chloroform-*d*)  $\delta$  7.08 (s, 1H), 7.37 (s, 4H).  $^{13}\text{C NMR}$  (101 MHz, Chloroform-*d*)  $\delta$  41.97, 130.01, 132.16, 134.91, 137.08.

### Synthesis of compound 4 (CzBTM) and compound 4 (PyIDBTM)

**(a). compound 4 (CzBTM):** Under argon atmosphere, sodium hydride (60% in oil, 0.44 g, 11.0 mmol) was dispersed in anhydrous DMF (90 mL). After carbazole (1.1 g, 6.6 mmol) dissolved in anhydrous DMF (10 mL) was added dropwise

and stirred for 30 min in the dark. Then **compound 3 (HBTM-Br)** (2.0 g, 4.4 mmol) was added and warmed slowly to 50 °C and stirred for 2 h. After that, the mixture was tardily cooled to room temperature and continue stirring for 3 h. And then the the mixture was poured into saturated NH<sub>4</sub>Cl solution (400 mL). The precipitate was collected by suction filtration and purified by flash column chromatography used petroleum ether/dichloromethane (silica gel, 8:1, v/v) as eluent. Atropurpureus solid **compound 4 (CzBTM)** was obtained in 17% yield (0.4 g, 0.7 mmol). **LC-MS** (m/z): [M]<sup>+</sup> calcd. for C<sub>25</sub>H<sub>12</sub>C<sub>16</sub>N<sup>+</sup>, 537.925; found, 537.909.

**(b). compound 5 (PyIDBTM):** The β-Carboline (0.9 g, 4.8 mmol) was added dissolved in anhydrous DMF (10 mL) was added dropwise and stirred for 30 min in the dark. Then **compound 3 (HBTM-Br)** (1.7 g, 3.8 mmol) was added and warmed slowly to 65 °C and stirred for 4 h. Used petroleum ether/ ethyl acetate (silica gel, 8:1, v/v) as eluent. Atropurpureus solid **compound 5 (PyIDBTM)** was obtained in 13% yield (0.25 g, 0.4 mmol). **MALDI-TOF** (m/z): [M]<sup>+</sup> calcd. for C<sub>24</sub>H<sub>11</sub>Cl<sub>6</sub>N<sub>2</sub><sup>+</sup>, 538.90; found, 538.88.

### Synthesis of compound 6 and 7

**(a). compound 6 (Ph<sub>2</sub>CzBTM):** Under argon atmosphere, **compound 4 (CzBTM)** (0.4 g, 0.74 mmol), phenylboronic acid (0.2 g, 1.55 mmol) and Pd(dtbpf)Cl<sub>2</sub> (0.04 g, 0.06 mmol) were mixed degassed K-EL 2 wt%: toluene (9:1, v/v) emulsion (10 mL) in the dark. Next, the mixture was tardily warmed to 60 °C and degassed triethylamine (2 mL, 14 mmol) was added finally. After the reaction mixture was stirred for 12 h at 60 °C. And then the mixture was slowly cooled to room temperature, dichloromethane was added, and filtered on a celite pad. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography used petroleum ether/dichloromethane (silica gel, 24:1, v/v) as eluent. Black solid **compound 6 (Ph<sub>2</sub>CzBTM)** was obtained in 30% yield (0.14 g, 0.22 mmol). **MALDI-TOF** (m/z): [M]<sup>+</sup> calcd. for C<sub>37</sub>H<sub>22</sub>Cl<sub>4</sub>N<sup>+</sup>, 622.05; found, 622.05. **Elem. Anal.** calcd. for C<sub>37</sub>H<sub>22</sub>Cl<sub>4</sub>N<sup>+</sup> (%): C, 71.40; H, 3.56; N, 2.25. Found (%): C, 71.22; H, 3.41; N, 2.08. **IR (KBr)** 2924 (m), 2853 (w), 2369 (w), 2341 (w), 1635 (s), 1446 (m), 1386 (m), 1051(m), 880 (w), 757 (w), 565 (w), 478 (w).

**(b). compound 7 (Mes<sub>2</sub>CzBTM):** Under argon atmosphere, **compound 4 (CzBTM)** (0.4 g, 0.74 mmol), 2,4,6-trimethylphenylboronic acid (0.25 g, 1.55 mmol) and Pd(dtbpf)Cl<sub>2</sub> (0.04 g, 0.06 mmol) were mixed degassed K-EL 2 wt%: toluene (9:1, v/v) emulsion (10 mL) in the dark. Next, the mixture was tardily warmed to 70 °C and degassed triethylamine (2 mL, 14 mmol) was added finally. After the reaction mixture was stirred for 48 h at 70 °C. And then the mixture was slowly cooled to room temperature, dichloromethane was added, and filtered on a celite pad. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography used

petroleum ether/dichloromethane (silica gel, 24:1, v/v) as eluent. Atropurpureus **compound 7 (Mes<sub>2</sub>CzBTM)** was obtained in 23% yield (0.12 g, 0.17 mmol). **MALDI-TOF** (m/z): [M]<sup>+</sup> calcd. for C<sub>43</sub>H<sub>34</sub>Cl<sub>4</sub>N<sup>+</sup>, 706.14; found, 706.14. **Elem. Anal.** calcd. for C<sub>43</sub>H<sub>34</sub>Cl<sub>4</sub>N<sup>+</sup> (%): C, 73.10; H, 4.85; N, 1.98. Found (%): C, 73.11; H, 4.59; N, 1.96. **IR (KBr)** 2922 (m), 2857 (w), 2346 (w), 1699 (m), 1633 (m), 1494 (m), 1447 (s), 1390(m), 1338 (w), 1192 (w), 1084 (w), 855 (w), 802 (w), 750 (m), 720 (m), 673(w).

### Synthesis of compound 8 and 9

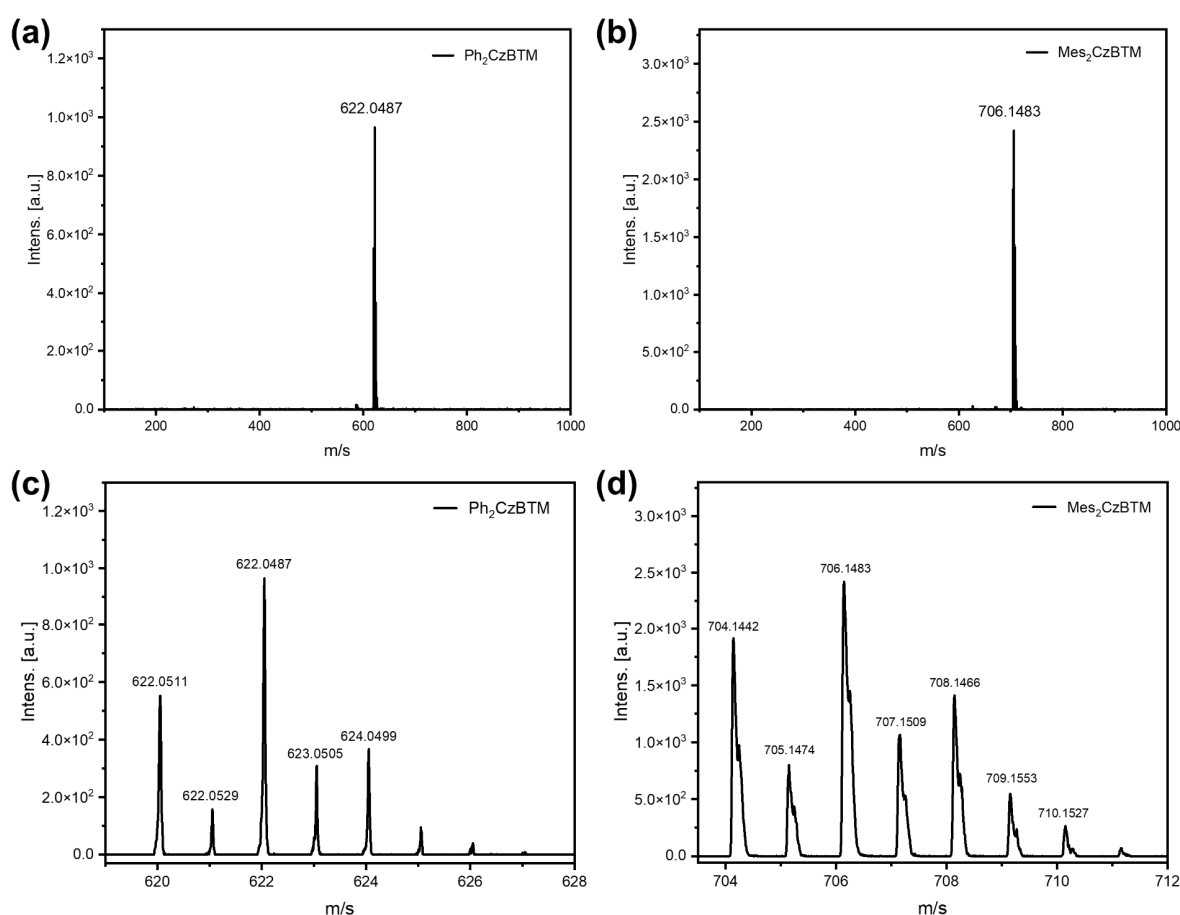
**(a). compound 8 (Ph<sub>2</sub>PyIDBTM):** Under argon atmosphere, **compound 5 (PyIDBTM)** (0.2 g, 0.4 mmol), phenylboronic acid pinacol ester (0.2 g, 0.9 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.04 g, 0.03 mmol), toluene (15 mL), ethanol (5 mL) and potassium carbonate solution (5 mL, 2 M) were added to a 250 mL two-necked flask. Then the mixture warmed slowly to 95 °C and stirred for 14 h. Next, cooled to room temperature, the mixture was poured into water and extracted with dichloromethane by three times. The combined organic solution was washed with brine and dried over anhydrous sodium sulfate. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (Purified twice. First: petroleum ether/ ethyl acetate (silica gel, 8:1, v/v) as eluent; Second: petroleum ether/dichloromethane (silica gel, 1:1, lack solid solid **compound 8 (Ph<sub>2</sub>PyIDBTM)** was obtained in 21% yield (0.05 g, 0.01 mmol). **MALDI-TOF** (m/z): [M]<sup>+</sup> calcd. for C<sub>36</sub>H<sub>21</sub>Cl<sub>4</sub>N<sub>2</sub><sup>+</sup>, 623.04; found, 623.05. **Elem. Anal.** calcd. for C<sub>36</sub>H<sub>21</sub>Cl<sub>4</sub>N<sub>2</sub><sup>+</sup> (%): C, 69.36; H, 3.40; N, 4.49. Found (%): C, 69.55; H, 3.43; N, 4.21. **IR (KBr)** 3053 (w), 2925 (s), 2854 (m), 2360 (w), 1618 (w), 1573 (w), 1515 (m), 1458(s), 1431 (s), 1388 (m), 1326 (w), 1274 (w), 1195 (w), 1080 (w), 968 (w), 869(w), 800(m), 757(m), 694(m), 601(w).

**(b). compound 9 (Mes<sub>2</sub>PyIDBTM):** Under argon atmosphere, **compound 5 (PyIDBTM)** (0.5 g, 0.9 mmol), 2,4,6-trimethylphenylboronic acid pinacol ester (0.7 g, 2.8 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.08 g, 0.06 mmol), toluene (15 mL), ethanol (5 mL) and potassium carbonate solution (5 mL, 2 M) were added to a 250 mL two-necked flask. Then the mixture warmed slowly to 95 °C and stirred for 48 h. Next, cooled to room temperature, the mixture was poured into water and extracted with dichloromethane by three times. The combined organic solution was washed with brine and dried over anhydrous sodium sulfate. After solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (Purified twice. First (normal phase): petroleum ether/ ethyl acetate (silica gel, 8:1, v/v) as eluent; Second (reverse phase): water: acetonitrile (silica gel, 1:9, v/v) as eluent). Atropurpureus solid **compound 9 (Mes<sub>2</sub>PyIDBTM)** was obtained in 15% yield (0.1 g, 0.1 mmol). **MALDI-TOF** (m/z): [M]<sup>+</sup> calcd. for C<sub>42</sub>H<sub>33</sub>Cl<sub>4</sub>N<sub>2</sub><sup>+</sup>, 707.14;

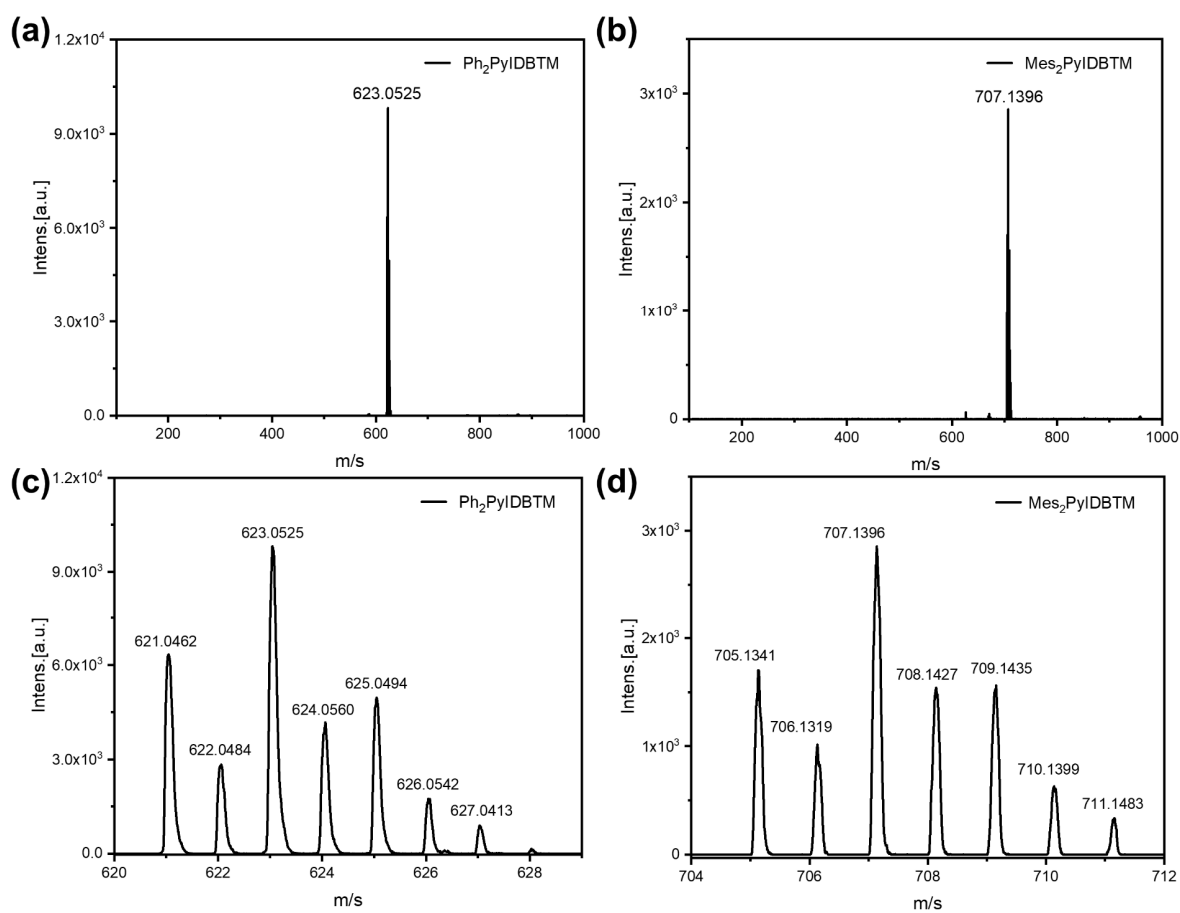
found, 707.14. **Elem. Anal.** calcd. for  $C_{42}H_{33}Cl_4N_2$  (%): C, 71.30; H, 4.70; N, 3.96. Found (%): C, 71.05; H, 4.94; N, 3.87. **IR** (**KBr**) 2921 (m), 2854 (w), 2362 (w), 1618 (m), 1571 (w), 1506 (m), 1458(s), 1429 (s), 1384 (m), 1326 (w), 1269 (w), 1216 (w), 1189 (w), 1033 (w), 852(w), 800(m), 742(m), 609(w).

## 1.2 Structure characterization.

### 1.2.1 MALDI-TOF mass spectra



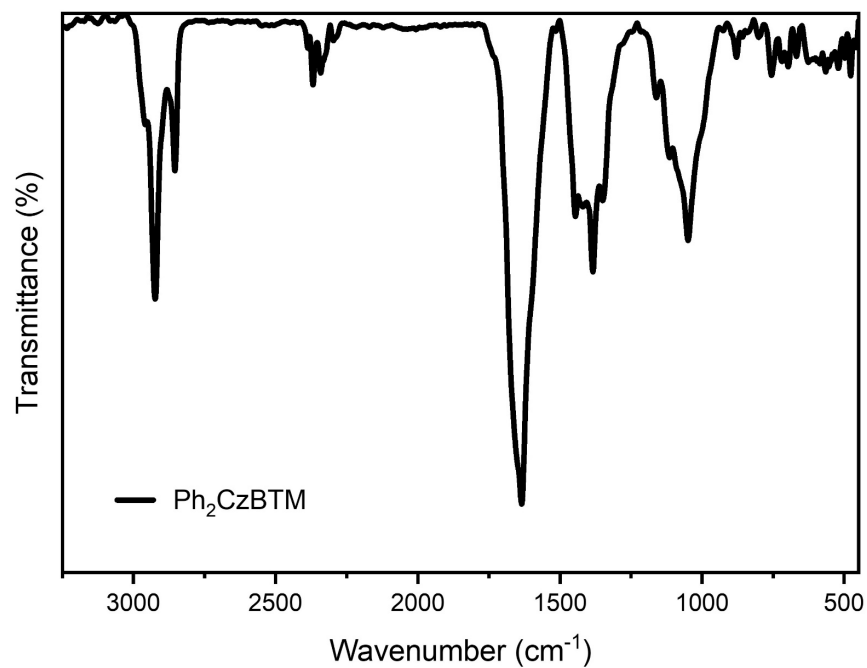
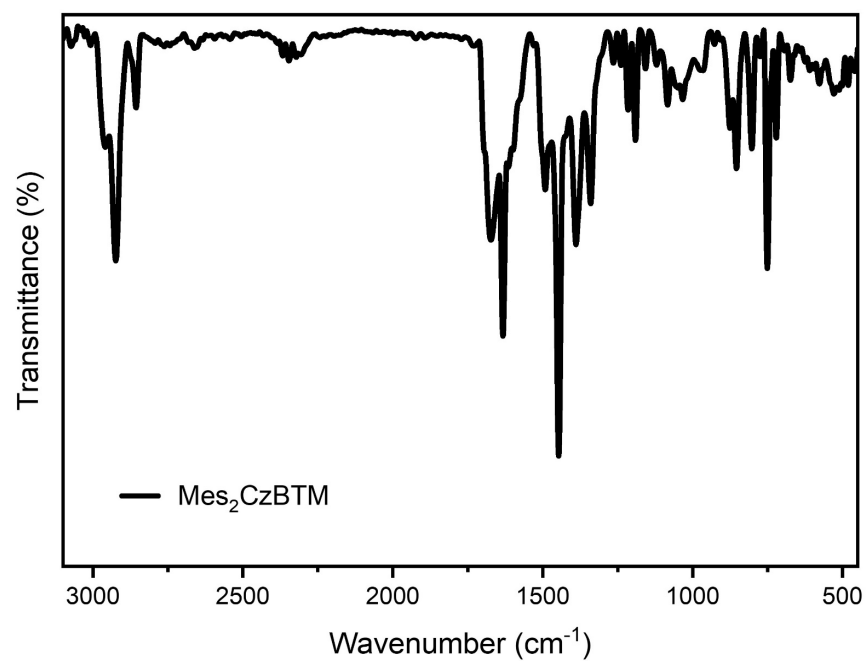
**Figure S2.** MALDI-TOF mass spectra of radicals: (a) (c)  $Ph_2CzBTM$ ; (b) (d)  $Mes_2CzBTM$ .



**Figure S3.** MALDI-TOF mass spectra of radicals: (a) (c)  $\text{Ph}_2\text{PyIDBTM}$ ; (b) (d)  $\text{Mes}_2\text{PyIDBTM}$ .



## 1.2.2 FT-IR spectra

Figure S4. FT-IR spectra of Ph<sub>2</sub>CzBTM.Figure S5. FT-IR spectra of Mes<sub>2</sub>CzBTM.

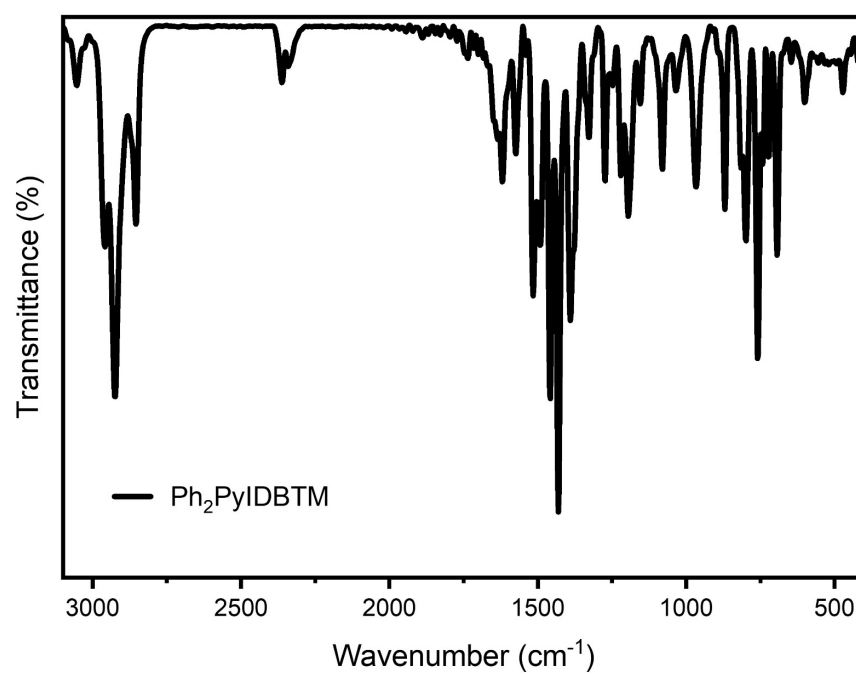


Figure S6. FT-IR spectra of Ph<sub>2</sub>PyIDBTM.

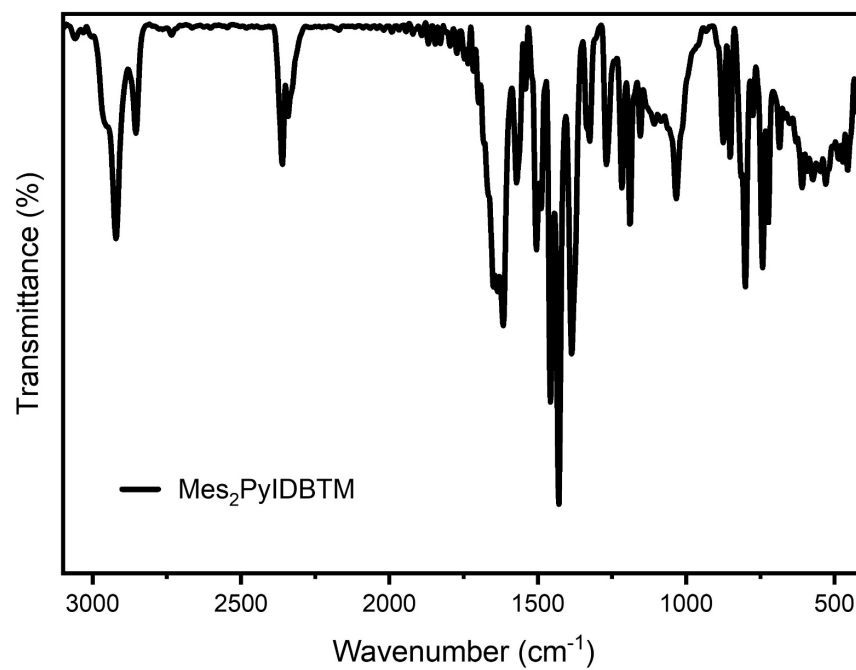
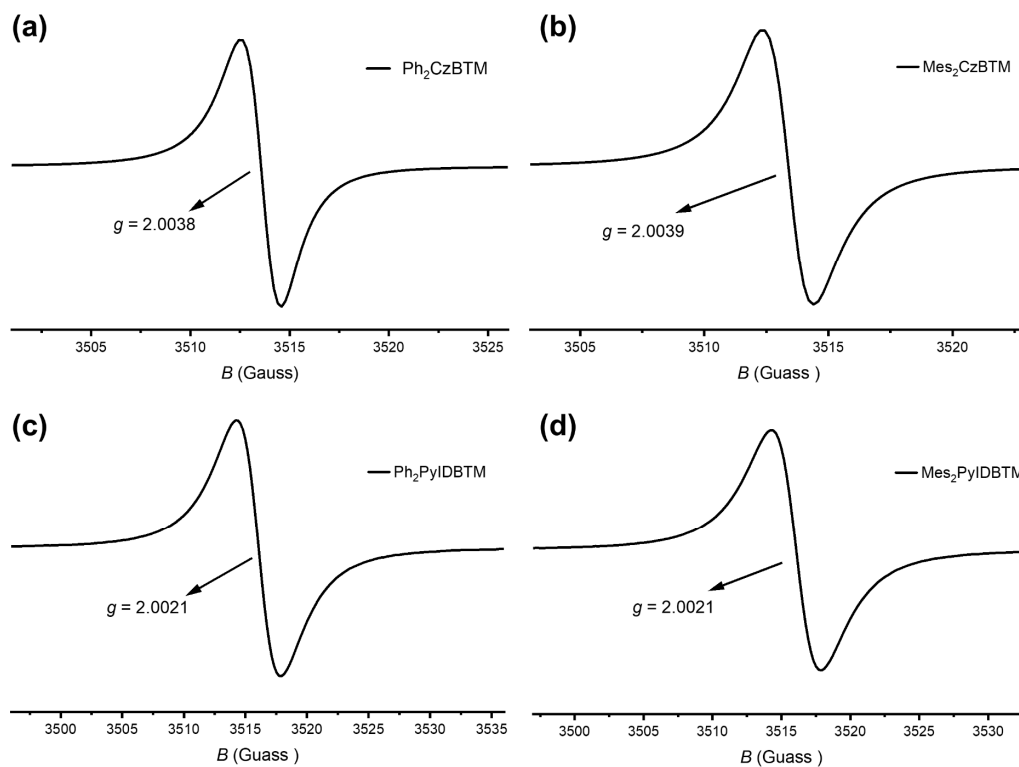


Figure S7. FT-IR spectra of Mes<sub>2</sub>PyIDBTM.

## 1.2.3 EPR spectra



**Figure S8.** EPR spectra of radicals in powder form: (a)  $\text{Ph}_2\text{CzBTM}$ ; (b)  $\text{Mes}_2\text{CzBTM}$ ; (c)  $\text{Ph}_2\text{PyIDBTM}$ ; (d)  $\text{Mes}_2\text{PyIDBTM}$ .

## 2. Crystallographic data.

**Table S1.** X-Ray Crystallographic Data of **Ph<sub>2</sub>CzBTM** and **Mes<sub>2</sub>CzBTM**.

Radicals	Ph <sub>2</sub> CzBTM	Mes <sub>2</sub> CzBTM
CCDC	2341126	2341148
Empirical formula	C <sub>37</sub> H <sub>22</sub> Cl <sub>4</sub> N	C <sub>44</sub> H <sub>36</sub> Cl <sub>6</sub> N
Formula weight	622.35	791.44
Temperature/K	100(2)	100.04(10)
Crystal system	monoclinic	triclinic
Space group	P2 <sub>1</sub> /c	P-1
a/Å	14.0383(4)	8.9349(2)
b/Å	7.8835(2)	12.8888(4)
c/Å	26.2239(8)	17.2990(4)
α/°	90	106.985(2)
β/°	98.265(3)	94.093(2)
γ/°	90	94.636(2)
Volume/Å <sup>3</sup>	2872.08(14)	1889.59(9)
Z	4	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.439	1.391
μ/mm <sup>1</sup>	0.442	0.489
F(000)	1276.0	818.0
Crystal size/mm <sup>3</sup>	0.3 × 0.2 × 0.15	0.26 × 0.25 × 0.2
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.594 to 60.442	4.596 to 61.106
Index ranges	-17 ≤ h ≤ 17, -7 ≤ k ≤ 10, -32 ≤ l ≤ 36	-11 ≤ h ≤ 12, -17 ≤ k ≤ 17, -23 ≤ l ≤ 21
Reflections collected	25690	29171
Independent reflections	6952 [R <sub>int</sub> = 0.0346, R <sub>sigma</sub> = 0.0363]	9495 [R <sub>int</sub> = 0.0291, R <sub>sigma</sub> = 0.0343]
Data/restraints/parameters	6952/0/379	9495/0/466
Goodness-of-fit on F <sup>2</sup>	1.041	1.027
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0383, wR <sub>2</sub> = 0.0898	R <sub>1</sub> = 0.0382, wR <sub>2</sub> = 0.0915
Final R indexes [all data]	R <sub>1</sub> = 0.0525, wR <sub>2</sub> = 0.0977	R <sub>1</sub> = 0.0544, wR <sub>2</sub> = 0.0997
Largest diff. peak/hole / e Å <sup>-3</sup>	0.37/-0.47	0.45/-0.33

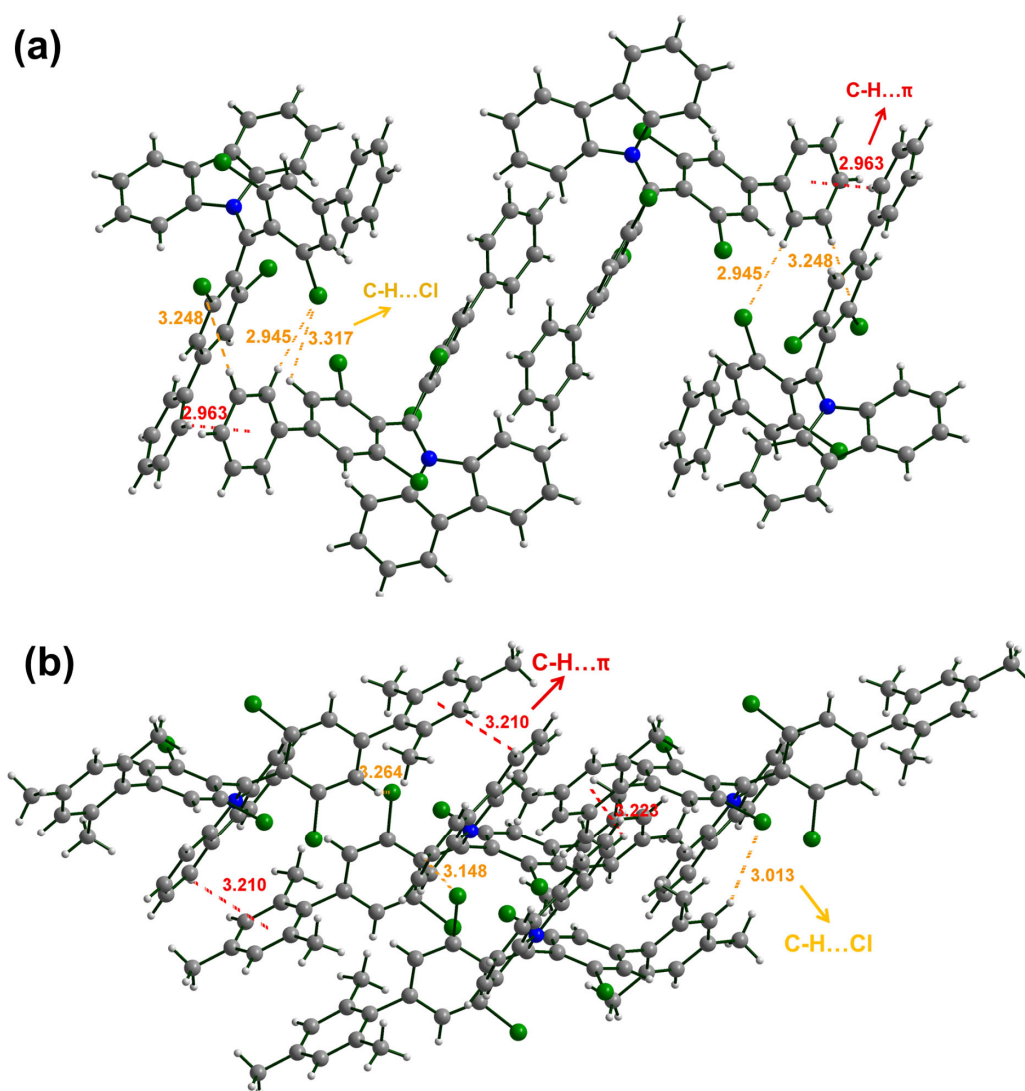


Figure S9. Intermolecular interactions: (a) Ph<sub>2</sub>CzBTM; (b) Mes<sub>2</sub>CzBTM.

### 3. Absorption and fluorescence spectra of radicals in various solutions.

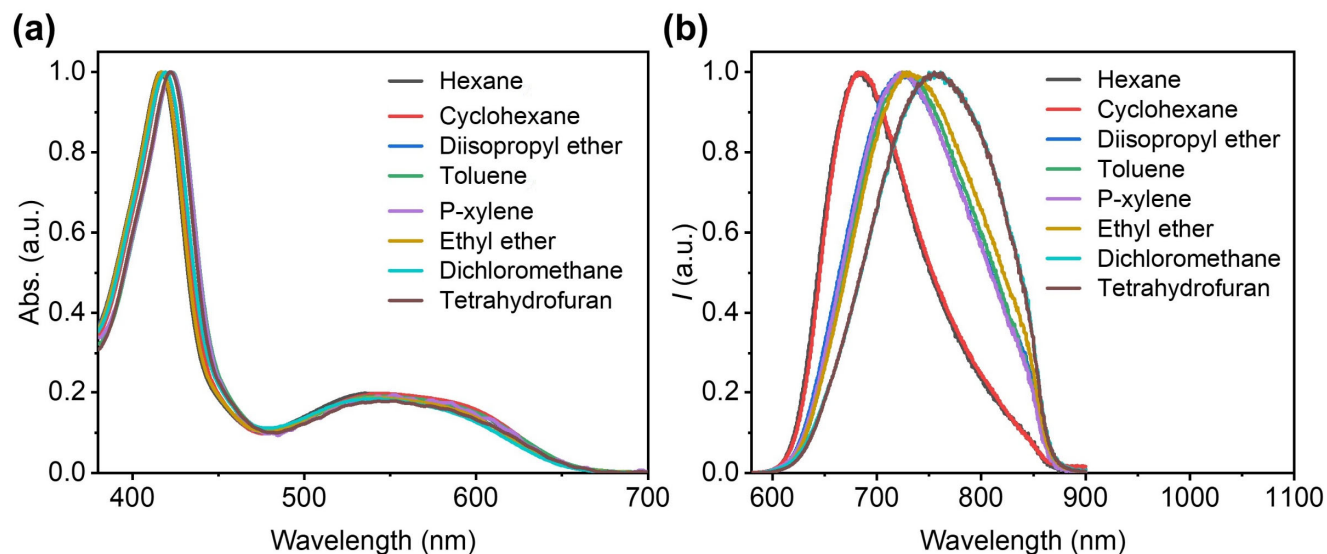


Figure S10. Absorption (a) and fluorescence (b) spectra of **Ph<sub>2</sub>CzBTM** in various solutions at room temperature.

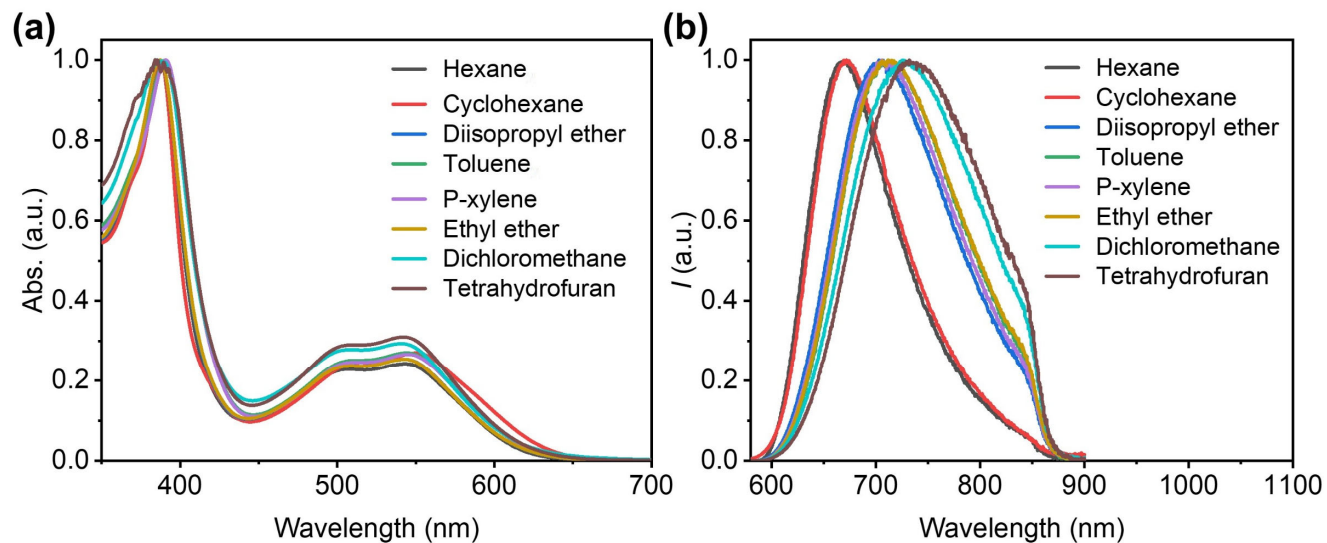
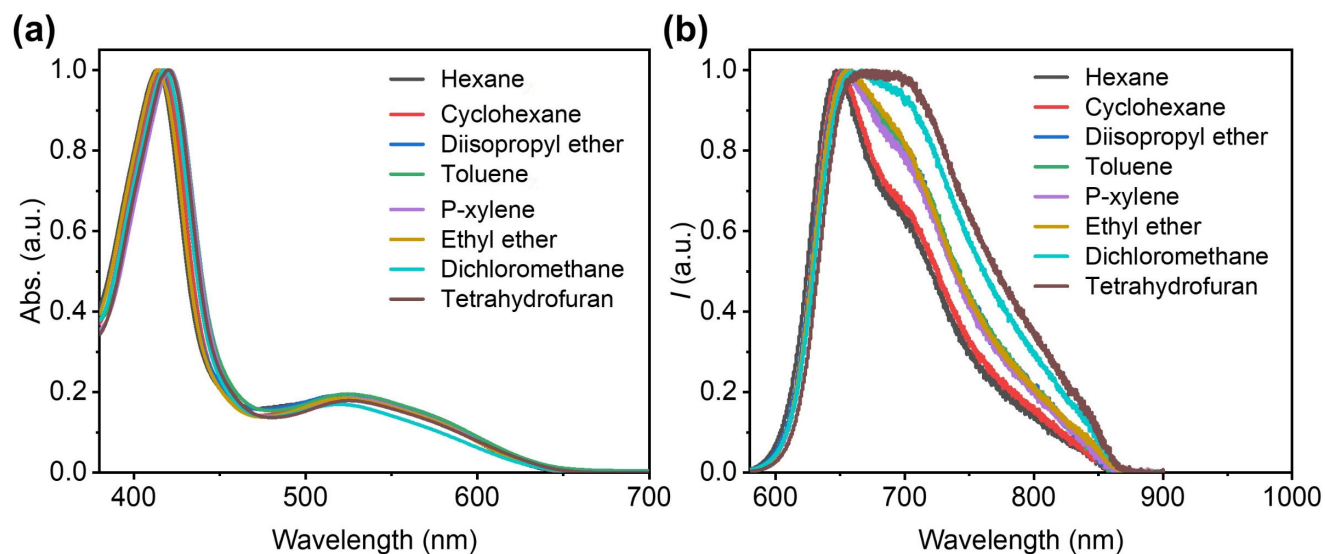
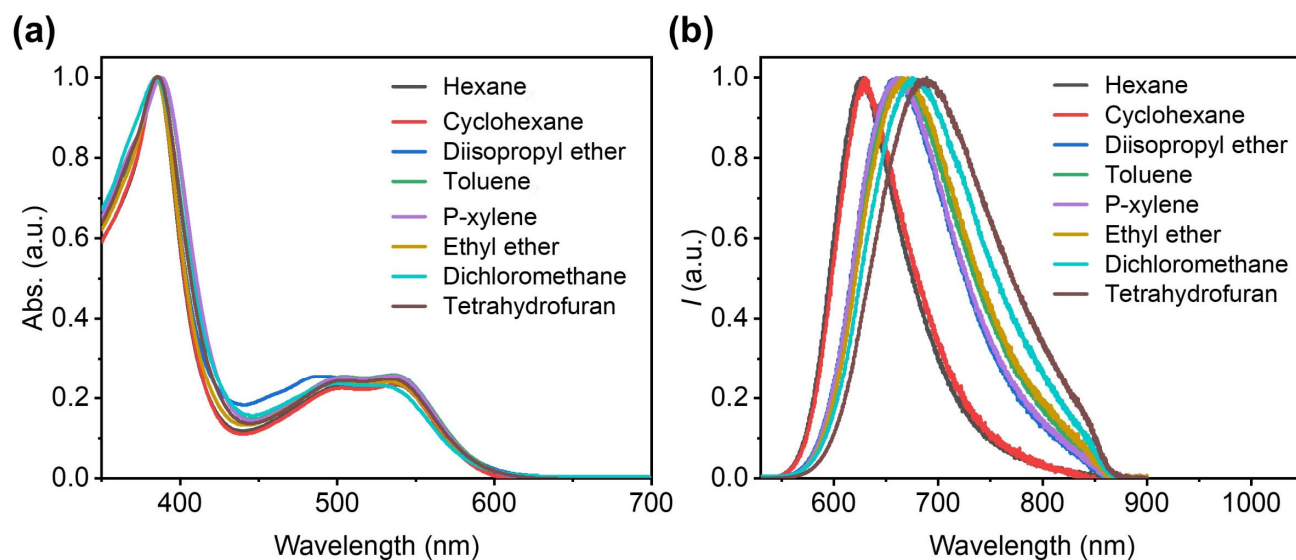


Figure S11. Absorption (a) and fluorescence (b) spectra of **Mes<sub>2</sub>CzBTM** in various solutions at room temperature.

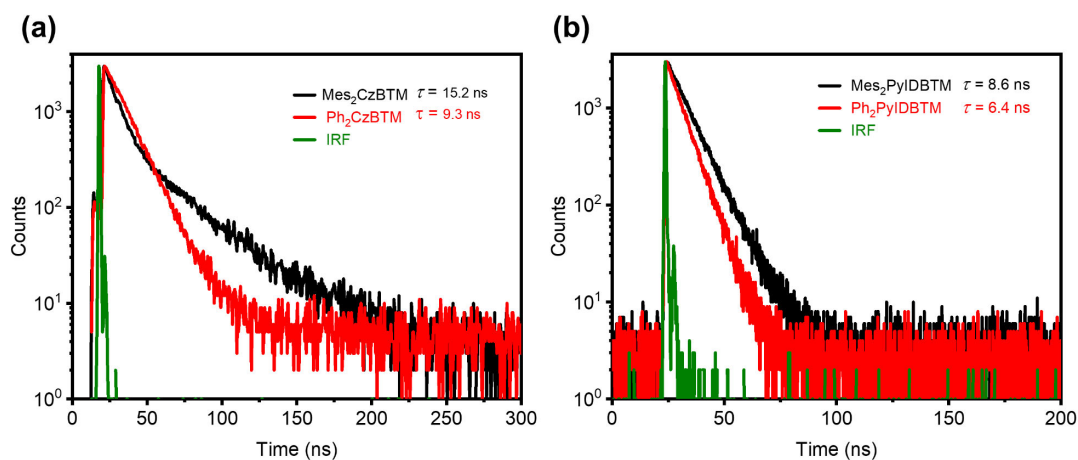


**Figure S12.** Absorption (a) and fluorescence (b) spectra of **Ph<sub>2</sub>PyIDBTM** in various solutions at room temperature.



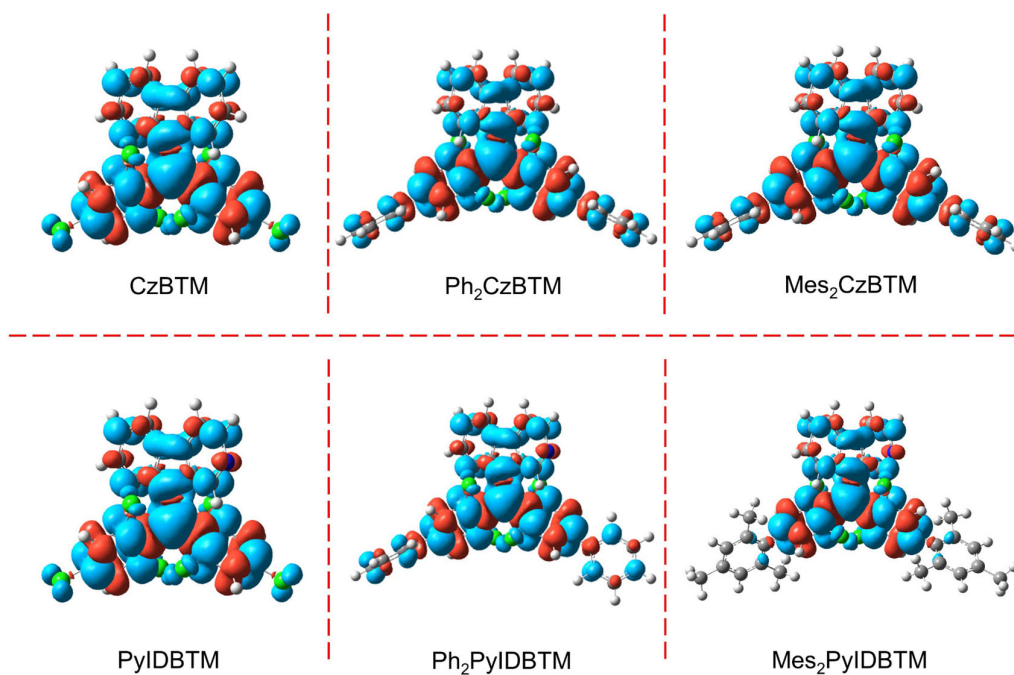
**Figure S13.** Absorption (a) and fluorescence (b) spectra of **Mes<sub>2</sub>PyIDBTM** in various solutions at room temperature.

#### 4. Transient photoluminescence decay spectra.



**Figure S14.** Transient photoluminescence decay spectra of radicals in cyclohexane at room temperature: (a) **Ph<sub>2</sub>CzBTM** (red) and **Mes<sub>2</sub>CzBTM** (black); (b) **Ph<sub>2</sub>PyIDBTM** (red) and **Mes<sub>2</sub>PyIDBTM** (black).

#### 5. Theoretical calculations.



**Figure S15.** Spin density distribution of **CzBTM**, **Ph<sub>2</sub>CzBTM**, **Mes<sub>2</sub>CzBTM**, **PyIDBTM**, **Ph<sub>2</sub>PyIDBTM** and **Mes<sub>2</sub>PyIDBTM** by DFT calculations.



**Table S2.** The values of characteristic torsion angles in radical molecules in crystal structures and theoretical calculations.

Radicals	Angle	Torsion angle (°)		
		Crystal <sup>[b]</sup>	GS <sup>[c]</sup>	OES <sup>[d]</sup>
CzBTM <sup>[a]</sup>	$\alpha$	40.2	43.2	58.0
	$\beta$	49.7	47.0	38.3
	$\gamma$	46.5	47.0	38.3
Ph <sub>2</sub> CzBTM	$\alpha$	47.7	43.9	66.3
	$\beta$	53.6	48.6	41.9
	$\gamma$	37.8	48.6	41.9
	$\theta$	32.9	36.1	33.8
	$\delta$	48.7	36.1	33.8
Mes <sub>2</sub> CzBTM	$\alpha$	35.6	43.9	66.8
	$\beta$	45.9	48.8	42.1
	$\gamma$	51.3	48.8	42.1
	$\theta$	93.5	88.6	93.8
	$\delta$	70.0	88.6	93.8
PyIDBTM	$\alpha$	—	43.6	66.7
	$\beta$		48.8	41.8
	$\gamma$		48.9	42.4
Ph <sub>2</sub> PyIDBTM	$\alpha$	—	43.8	65.7
	$\beta$		48.8	42.2
	$\gamma$		48.2	41.0
	$\theta$		36.1	33.7
	$\delta$		36.0	33.0
Mes <sub>2</sub> PyIDBTM	$\alpha$	—	43.8	65.8
	$\beta$		49.1	42.3
	$\gamma$		49.0	41.7
	$\theta$		88.2	92.9
	$\delta$		87.8	92.0

[a] The data is sourced from the reference literature<sup>Error! Reference source not found.</sup>; [b] Crystallographic data; [c] Ground state; [d] Excited state;  $\alpha$  is the torsion angle of the carbazole ( $\beta$ -carboline) group;  $\beta$  and  $\gamma$  are the torsion angles of the two dichlorobenzene groups;  $\theta$  and  $\delta$  are the torsion angles between the benzene ring (2,4,6-trimethylbenzene) and the dichlorobenzene.

**Table S3.** The bond lengths of radical molecules in crystal structures and theoretical calculations.

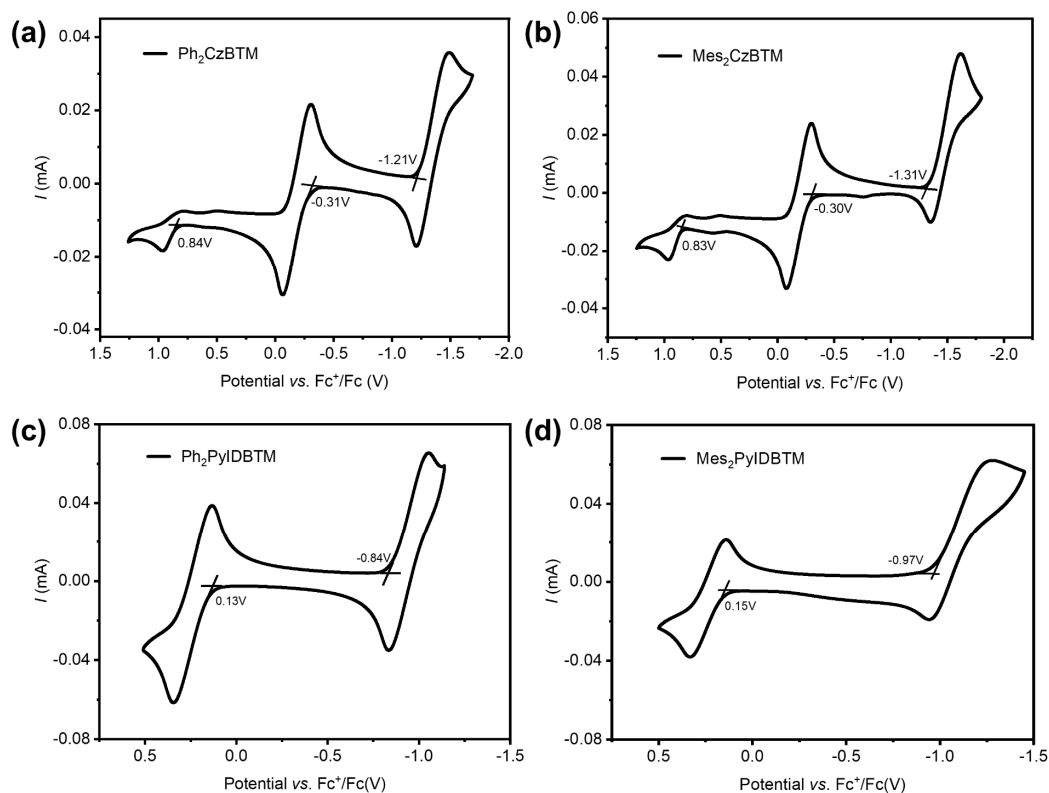
Radicals	Bond	Length (Å)		
		Crystal <sup>[b]</sup>	GS <sup>[c]</sup>	OES <sup>[d]</sup>
CzBTM <sup>[a]</sup>	N1-C13 <sup>[e]</sup>	1.391	1.393	1.439
	C13-C14 <sup>[f]</sup>	1.455	1.468	1.443
	C13-C20 <sup>[f]</sup>	1.446	1.468	1.443
Ph <sub>2</sub> CzBTM	N1-C13 <sup>[e]</sup>	1.399	1.395	1.465
	C13-C14 <sup>[f]</sup>	1.466	1.466	1.442
	C13-C26 <sup>[f]</sup>	1.447	1.466	1.442
	C17-C20 <sup>[g]</sup>	1.396	1.483	1.480
	C29-C32 <sup>[g]</sup>	1.483	1.483	1.480
Mes <sub>2</sub> CzBTM	N1-C13 <sup>[e]</sup>	1.392	1.395	1.464
	C13-C14 <sup>[f]</sup>	1.454	1.468	1.444
	C13-C29 <sup>[f]</sup>	1.460	1.468	1.444
	C17-C20 <sup>[g]</sup>	1.498	1.497	1.497
	C32-C35 <sup>[g]</sup>	1.497	1.497	1.497
PyIDBTM	N2-C12 <sup>[e]</sup>	—	1.395	1.465
	C12-C13 <sup>[f]</sup>		1.467	1.444
	C12-C19 <sup>[f]</sup>		1.468	1.443
Ph <sub>2</sub> PyIDBTM	N2-C12 <sup>[e]</sup>	—	1.397	1.466
	C12-C13 <sup>[f]</sup>		1.466	1.443
	C12-C25 <sup>[f]</sup>		1.465	1.440
	C16-C19 <sup>[g]</sup>		1.483	1.480
	C28-C31 <sup>[g]</sup>		1.482	1.479
Mes <sub>2</sub> PyIDBTM	N2-C12 <sup>[e]</sup>	—	1.397	1.465
	C12-C13 <sup>[f]</sup>		1.467	1.444
	C12-C28 <sup>[f]</sup>		1.468	1.444
	C16-C19 <sup>[g]</sup>		1.497	1.497
	C31-C34 <sup>[g]</sup>		1.497	1.497

[a] Data sourced from the reference literature<sup>Error! Reference source not found.</sup>; [b] Crystallographic data; [c] Ground state; [d] Excited state; [e] Bond length between the carbazole N1 (β-carboline N2) and the central carbon atom; [f] Bond lengths between the central carbon atom and the two carbon atoms connecting to dichlorobenzene; [g] Bond lengths between the two carbon atoms connecting the benzene ring (2,4,6-trimethylbenzene) and the dichlorobenzene.

**Table S4.** The parameters corresponding to the D<sub>1</sub> transition in the TD-DFT calculation results of radicals.

Radicals	Orbital excitation contribution	Transition energy (eV)	<i>f</i>
CzBTM	134 $\beta$ $\rightarrow$ 136 $\beta$ (0.99)	2.19	0.09
Ph <sub>2</sub> CzBTM	159 $\beta$ $\rightarrow$ 160 $\beta$ (0.98)	2.21	0.10
Mes <sub>2</sub> CzBTM	183 $\beta$ $\rightarrow$ 184 $\beta$ (0.99)	2.27	0.09
PyIDBTM	135 $\beta$ $\rightarrow$ 136 $\beta$ (0.99)	2.27	0.09
Ph <sub>2</sub> PyIDBTM	159 $\beta$ $\rightarrow$ 160 $\beta$ (0.98)	2.28	0.10
Mes <sub>2</sub> PyIDBTM	183 $\beta$ $\rightarrow$ 184 $\beta$ (0.99)	2.36	0.09

## 6. Electrochemical properties of radicals.

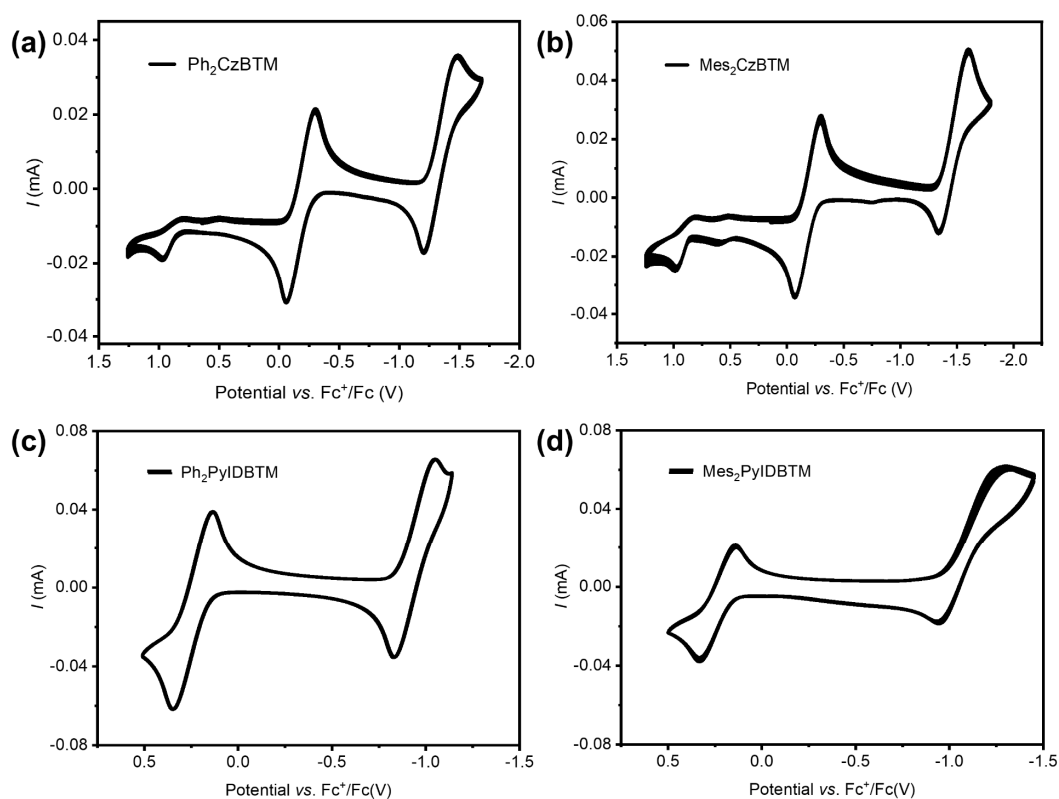
**Figure S16.** Electrochemical properties of radicals: (a) Ph<sub>2</sub>CzBTM; (b) Mes<sub>2</sub>CzBTM; (c) Ph<sub>2</sub>PyIDBTM; (d) Mes<sub>2</sub>PyIDBTM.

**Table S5.** Redox potential of free radicals and their corresponding orbital energy levels.

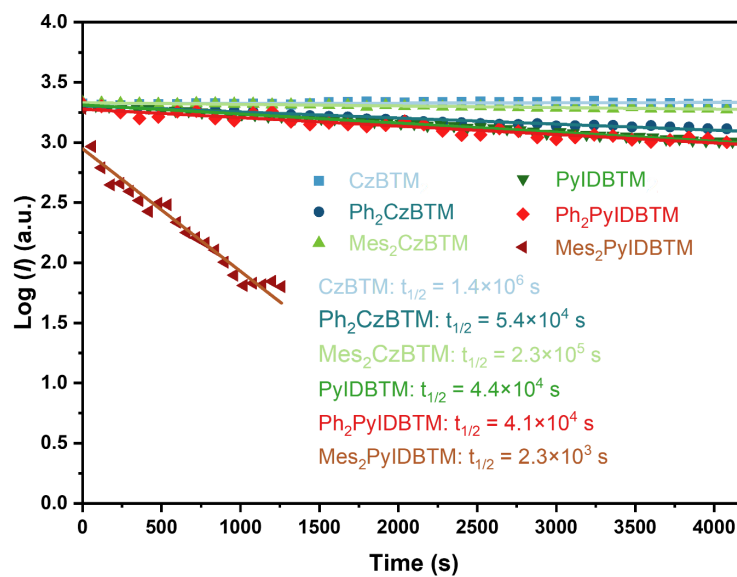
Radicals	$E_{ox}$ (V)	$E_{red}$ (V)	$\alpha$ -SOMO (eV)		$\beta$ -SUMO (eV)	
			Calculated	Experimental	Calculated	Experimental
CzBTM <sup>[a]</sup>	"0.06	"0.92	"4.99	"4.74	"3.01	"3.88
Ph <sub>2</sub> CzBTM	"0.31	"1.21	"4.67	"4.49	"2.74	"3.59
Mes <sub>2</sub> CzBTM	"0.30	"1.31	"4.71	"4.50	"2.67	"3.49
PyIDBTM <sup>[b]</sup>	0.03	"1.03	"5.15	"4.83	"3.13	"3.77
Ph <sub>2</sub> PyIDBTM	0.13	"0.84	"4.82	"4.93	"2.86	"3.96
Mes <sub>2</sub> PyIDBTM	0.15	"0.97	"4.68	"4.95	"2.78	"3.83

[a][b] Data sourced from the reference literature<sup>Error! Reference source not found.[1]</sup>.

## 7. Stability of radicals.



**Figure S17.** Multi-cycle CV measurements (20 cycles) of radicals: (a) Ph<sub>2</sub>CzBTM; (b) Mes<sub>2</sub>CzBTM; (c) Ph<sub>2</sub>PyIDBTM; (d) Mes<sub>2</sub>PyIDBTM.



**Figure S18.** Photostability of radicals under continuous irradiation from xenon lamp in cyclohexane at room temperature.

## Appendix (Calculation data).

CzBTM (UB3LYP/6-31G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.013509	0.167200	0.443877
2	6	0	1.113162	2.219276	-0.468576
3	6	0	-1.243988	2.139438	-0.509676
4	6	0	2.473490	1.978034	-0.492730
5	6	0	0.615448	3.541575	-0.254427
6	6	0	-2.583210	1.806715	-0.580786
7	6	0	-0.844632	3.492127	-0.279904
8	6	0	3.351724	3.055585	-0.303222
9	1	0	2.866841	0.965164	-0.656682
10	6	0	1.489765	4.599292	-0.068244
11	6	0	-3.538373	2.822129	-0.422980
12	1	0	-2.901195	0.769740	-0.757055
13	6	0	-1.794430	4.488090	-0.125506
14	6	0	2.867826	4.343669	-0.094667
15	1	0	4.436694	2.874990	-0.320512
16	1	0	1.114721	5.619016	0.097090
17	6	0	-3.150281	4.139803	-0.199512
18	1	0	-4.607387	2.568522	-0.477513
19	1	0	-1.495273	5.530699	0.051421
20	1	0	3.572598	5.175491	0.051836
21	1	0	-3.914380	4.921866	-0.078597
22	6	0	-1.237677	-0.750669	0.269151
23	6	0	-2.131516	-0.929895	1.325277
24	6	0	-1.452930	-1.402745	-0.944937
25	6	0	-3.239963	-1.761559	1.167481
26	6	0	-2.562203	-2.233922	-1.103266
27	6	0	-3.455612	-2.413526	-0.047283
28	1	0	-3.944199	-1.903370	2.000090
29	1	0	-2.731888	-2.747603	-2.060769
30	6	0	1.275309	-0.665516	0.312980
31	6	0	2.036877	-0.954828	1.445580
32	6	0	1.681227	-1.130596	-0.937812
33	6	0	3.204445	-1.708484	1.327226
34	6	0	2.848601	-1.885330	-1.056233

35	6	0	3.610290	-2.174210	0.075984
36	1	0	3.805108	-1.936032	2.219820
37	1	0	3.168184	-2.252239	-2.042498
38	7	0	-0.031578	1.259240	-0.641813
39	17	0	-1.858790	-0.107844	2.857417
40	17	0	-0.325664	-1.176606	-2.277503
41	17	0	-4.854536	-3.462859	-0.246062
42	17	0	1.524911	-0.366711	3.023430
43	17	0	0.720544	-0.766017	-2.366717
44	17	0	5.083664	-3.125306	-0.072960

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Ph<sub>2</sub>CzBTM (UB3LYP/6-31G(d,p))

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
-----					
1	6	0	0.022262	0.847695	0.497185
2	6	0	1.225778	-0.097742	0.326025
3	6	0	1.109505	-1.238172	-0.468613
4	6	0	2.432652	0.186835	0.965464
5	6	0	2.200024	-2.094432	-0.623719
6	6	0	3.522808	-0.669425	0.810823
7	6	0	3.406301	-1.810607	0.016250
8	1	0	2.107802	-2.993851	-1.249644
9	1	0	4.474033	-0.445815	1.315270
10	6	0	-1.284687	0.042972	0.371071
11	6	0	-1.776179	-0.665576	1.467403
12	6	0	-1.977395	0.023143	-0.839785
13	6	0	-2.960346	-1.394364	1.352995
14	6	0	-3.161033	-0.705833	-0.954377
15	6	0	-3.652442	-1.415090	0.142295
16	1	0	-3.347158	-1.953488	2.217285
17	1	0	-3.706930	-0.722277	-1.908852
18	6	0	-4.959089	-2.220220	0.015649
19	6	0	-4.920314	-3.553035	-0.393799
20	6	0	-6.181664	-1.616504	0.311028
21	6	0	-6.104170	-4.282321	-0.508248
22	1	0	-3.956724	-4.029035	-0.626308
23	6	0	-7.365318	-2.345413	0.196173
24	1	0	-6.211893	-0.565742	0.634233

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25	6	0	-7.326540	-3.678648	-0.213945
26	1	0	-6.073330	-5.332842	-0.831815
27	1	0	-8.329225	-1.869669	0.428222
28	1	0	-8.259764	-4.253230	-0.304737
29	6	0	4.609829	-2.756162	-0.154184
30	6	0	5.432941	-2.642680	-1.274522
31	6	0	4.877121	-3.726013	0.812435
32	6	0	6.523353	-3.499259	-1.428614
33	1	0	5.222528	-1.878076	-2.036264
34	6	0	5.966976	-4.582733	0.658212
35	1	0	4.228201	-3.814986	1.695872
36	6	0	6.790123	-4.469514	-0.462871
37	1	0	7.171636	-3.410040	-2.312362
38	1	0	6.177547	-5.347783	1.419562
39	1	0	7.649212	-5.145127	-0.584571
40	6	0	1.348462	2.713728	-0.538230
41	6	0	-0.988054	2.983161	-0.358451
42	6	0	2.650041	2.274229	-0.686577
43	6	0	1.073397	4.094351	-0.292725
44	6	0	-2.362389	2.852188	-0.300788
45	6	0	-0.373902	4.261251	-0.181383
46	6	0	3.691372	3.209579	-0.591323
47	1	0	2.872666	1.214894	-0.875678
48	6	0	2.107636	5.010675	-0.200203
49	6	0	-3.138386	3.997064	-0.065435
50	1	0	-2.844866	1.874150	-0.435549
51	6	0	-1.147803	5.386108	0.050285
52	6	0	3.424343	4.554340	-0.352309
53	1	0	4.731412	2.870723	-0.707801
54	1	0	1.904177	6.074079	-0.011508
55	6	0	-2.541078	5.242207	0.106781
56	1	0	-4.233452	3.904361	-0.017314
57	1	0	-0.682972	6.372498	0.187397
58	1	0	4.254626	5.272427	-0.281067
59	1	0	-3.166806	6.128186	0.290078
60	7	0	0.063573	1.933926	-0.593685
61	17	0	-0.902683	-0.640208	2.995134
62	17	0	-1.357192	0.917878	-2.222680
63	17	0	2.579095	1.626298	1.967512
64	17	0	-0.412781	-1.597001	-1.275760

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.016290	1.287686	0.505618
2	6	0	1.218911	0.378200	0.368819
3	6	0	1.151537	-0.777455	-0.409301
4	6	0	2.405570	0.710579	1.022864
5	6	0	2.270753	-1.601140	-0.533279
6	6	0	3.524416	-0.113110	0.899346
7	6	0	3.456832	-1.269523	0.121298
8	1	0	2.217085	-2.512571	-1.146185
9	1	0	4.459722	0.148184	1.415315
10	6	0	-1.295132	0.440240	0.371457
11	6	0	-1.782197	-0.266480	1.470940
12	6	0	-1.966819	0.379868	-0.849854
13	6	0	-2.940905	-1.033979	1.349235
14	6	0	-3.124991	-0.387805	-0.971732
15	6	0	-3.611956	-1.095226	0.128103
16	1	0	-3.324211	-1.591642	2.216028
17	1	0	-3.654293	-0.436202	-1.934433
18	6	0	1.299607	3.129749	-0.584421
19	6	0	-1.030878	3.417168	-0.359817
20	6	0	2.594994	2.679570	-0.753495
21	6	0	1.038451	4.515565	-0.353411
22	6	0	-2.404498	3.296115	-0.271547
23	6	0	-0.405113	4.693605	-0.214304
24	6	0	3.643962	3.609308	-0.693688
25	1	0	2.806929	1.616164	-0.931715
26	6	0	2.080152	5.426287	-0.295910
27	6	0	-3.168163	4.449373	-0.036776
28	1	0	-2.895844	2.319435	-0.381900
29	6	0	-1.166886	5.826779	0.017030
30	6	0	3.390478	4.959120	-0.468812
31	1	0	4.679175	3.261946	-0.826909
32	1	0	1.887395	6.493629	-0.118555
33	6	0	-2.559546	5.692909	0.104719
34	1	0	-4.262540	4.364604	0.035562
35	1	0	-0.693080	6.811961	0.129980
36	1	0	4.226577	5.672667	-0.425427
37	1	0	-3.175700	6.585557	0.288091
38	7	0	0.008954	2.357722	-0.601624

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39	17	0	-0.345246	-1.196588	-1.234872
40	17	0	2.490306	2.169235	2.004058
41	17	0	-0.935233	-0.189976	3.011849
42	17	0	-1.352233	1.272305	-2.236735
43	6	0	4.692035	-2.179114	-0.014773
44	6	0	5.463247	-2.139120	-1.176316
45	6	0	5.039941	-3.042831	1.024152
46	6	0	6.582367	-2.963086	-1.299286
47	6	0	6.158506	-3.866971	0.901089
48	6	0	6.929734	-3.827307	-0.261172
49	1	0	7.189725	-2.931875	-2.215465
50	1	0	6.432621	-4.548417	1.719495
51	6	0	-4.890474	-1.943076	-0.006579
52	6	0	-4.815846	-3.243375	-0.505781
53	6	0	-6.123406	-1.410627	0.371295
54	6	0	-5.974213	-4.011386	-0.627500
55	6	0	-7.281600	-2.178229	0.249189
56	6	0	-7.206978	-3.478901	-0.250710
57	1	0	-5.915145	-5.036211	-1.021818
58	1	0	-8.253696	-1.758618	0.546265
59	6	0	-3.454884	-3.831372	-0.922485
60	1	0	-3.077806	-3.293948	-1.767403
61	1	0	-2.765302	-3.746068	-0.108790
62	1	0	-3.575943	-4.862645	-1.180790
63	6	0	-8.485781	-4.326250	-0.385848
64	1	0	-8.641657	-4.575127	-1.414762
65	1	0	-8.380727	-5.224270	0.186361
66	1	0	-9.323477	-3.768097	-0.023040
67	6	0	-6.205296	0.024843	0.922947
68	1	0	-5.581694	0.110536	1.788209
69	1	0	-5.873655	0.713984	0.174617
70	1	0	-7.217437	0.247379	1.189307
71	6	0	5.079575	-1.185423	-2.322988
72	1	0	4.113414	-1.450187	-2.698931
73	1	0	5.057013	-0.179822	-1.958080
74	1	0	5.801721	-1.263625	-3.108666
75	6	0	4.188533	-3.086269	2.306656
76	1	0	4.226902	-2.133786	2.792664
77	1	0	3.174745	-3.317233	2.054093
78	1	0	4.572392	-3.837971	2.964302
79	6	0	8.164510	-4.737491	-0.397165
80	1	0	9.021458	-4.238445	0.004697

81	1	0	7.997474	-5.647795	0.139813
82	1	0	8.332526	-4.958632	-1.430493

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PyIDBTM (UB3LYP/6-31G(d,p))

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.016674	0.166373	0.443695
2	6	0	1.237284	2.144367	-0.510569
3	6	0	-1.120195	2.213068	-0.468243
4	6	0	2.578030	1.818019	-0.582480
5	6	0	0.831647	3.495158	-0.280619
6	6	0	-2.479375	1.965355	-0.491566
7	6	0	-0.628637	3.537719	-0.254419
8	1	0	2.900822	0.782563	-0.758964
9	6	0	1.776824	4.495574	-0.126772
10	6	0	-3.362572	3.038713	-0.301373
11	1	0	-2.868016	0.950620	-0.655191
12	6	0	-1.507828	4.591329	-0.067798
13	6	0	3.134271	4.153759	-0.201559
14	1	0	1.472771	5.536716	0.050437
15	6	0	-2.884675	4.329132	-0.093407
16	1	0	-4.446683	2.852936	-0.317776
17	1	0	-1.137588	5.612872	0.097143
18	1	0	3.894728	4.939436	-0.081094
19	1	0	-3.593294	5.157613	0.053457
20	6	0	1.245102	-0.745672	0.268374
21	6	0	2.140073	-0.920973	1.324200
22	6	0	1.462963	-1.396571	-0.945881
23	6	0	3.252991	-1.746473	1.165497
24	6	0	2.575639	-2.223135	-1.104474
25	6	0	3.470694	-2.398068	-0.049100
26	1	0	3.958799	-1.884201	1.997460
27	1	0	2.746934	-2.736537	-2.061840
28	6	0	-1.268237	-0.672466	0.313487
29	6	0	-2.028086	-0.964967	1.446423
30	6	0	-1.672453	-1.139716	-0.937046
31	6	0	-3.191512	-1.725124	1.328855
32	6	0	-2.836738	-1.899286	-1.054962

33	6	0	-3.596201	-2.192157	0.077726
34	1	0	-3.790148	-1.956247	2.221891
35	1	0	-3.155420	-2.267211	-2.041140
36	17	0	-1.516951	-0.376191	3.024297
37	17	0	-0.714244	-0.770633	-2.366456
38	17	0	-5.064448	-3.151298	-0.070254
39	17	0	1.865390	-0.098470	2.855747
40	17	0	0.333961	-1.175832	-2.277883
41	17	0	4.875157	-3.439769	-0.248963
42	7	0	0.028994	1.258446	-0.642043
43	7	0	3.528479	2.837979	-0.425474

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Ph<sub>2</sub>PyIDBTM (UB3LYP/6-31G(d,p))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.009743	0.851912	0.484763
2	6	0	1.191673	2.843453	-0.489802
3	6	0	-1.167121	2.853477	-0.475335
4	6	0	2.540906	2.549792	-0.540875
5	6	0	0.749742	4.187325	-0.287917
6	6	0	-2.519321	2.571254	-0.509726
7	6	0	-0.711356	4.193540	-0.278974
8	1	0	2.891517	1.519933	-0.695711
9	6	0	1.667759	5.213704	-0.140768
10	6	0	-3.431230	3.625117	-0.348178
11	1	0	-2.880540	1.544410	-0.660109
12	6	0	-1.618726	5.227706	-0.120610
13	6	0	3.034107	4.904956	-0.194261
14	1	0	1.335730	6.249731	0.014906
15	6	0	-2.988197	4.930521	-0.157236
16	1	0	-4.510095	3.411847	-0.373615
17	1	0	-1.276086	6.260913	0.030763
18	1	0	3.773230	5.711474	-0.078849
19	1	0	-3.718969	5.743279	-0.032786
20	7	0	0.007521	1.925271	-0.619544
21	7	0	3.463667	3.595893	-0.390847
22	6	0	1.262547	-0.031769	0.339189
23	6	0	2.150360	-0.164623	1.407182
24	6	0	1.509642	-0.699413	-0.860287
25	6	0	3.285339	-0.964424	1.275413

26	6	0	2.644406	-1.500281	-0.991929
27	6	0	3.532298	-1.632773	0.075606
28	1	0	3.985496	-1.068689	2.116962
29	1	0	2.838756	-2.026897	-1.937644
30	6	0	-1.252193	-0.021114	0.354607
31	6	0	-2.022232	-0.306602	1.482441
32	6	0	-1.625417	-0.526344	-0.890783
33	6	0	-3.164846	-1.097706	1.364932
34	6	0	-2.768898	-1.316890	-1.008665
35	6	0	-3.538538	-1.602743	0.118935
36	1	0	-3.771501	-1.323292	2.253964
37	1	0	-3.063152	-1.714764	-1.990798
38	6	0	4.785559	-2.515877	-0.069534
39	6	0	4.828656	-3.770971	0.538210
40	6	0	5.877537	-2.061063	-0.808638
41	6	0	5.963780	-4.570721	0.407389
42	1	0	3.967898	-4.128928	1.121480
43	6	0	7.012698	-2.861346	-0.940418
44	1	0	5.843669	-1.071953	-1.287850
45	6	0	7.056042	-4.115952	-0.332452
46	1	0	5.998069	-5.559750	0.886914
47	1	0	7.873364	-2.502654	-1.523572
48	1	0	7.950915	-4.746727	-0.435510
49	6	0	-4.800281	-2.476158	-0.010485
50	6	0	-4.790575	-3.789701	0.459602
51	6	0	-5.952808	-1.954056	-0.597546
52	6	0	-5.932971	-4.581108	0.342003
53	1	0	-3.881545	-4.201267	0.921683
54	6	0	-7.095946	-2.745256	-0.714365
55	1	0	-5.960688	-0.918742	-0.967940
56	6	0	-7.086167	-4.058645	-0.244842
57	1	0	-5.925198	-5.616667	0.711940
58	1	0	-8.004647	-2.333201	-1.176909
59	1	0	-7.986803	-4.682811	-0.337403
60	17	0	-1.550184	0.330121	3.053859
61	17	0	-0.654352	-0.166122	-2.313763
62	17	0	1.838764	0.679003	2.920062
63	17	0	0.389681	-0.532222	-2.207631

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Mes2PyIDBTM (UB3LYP/6-31G(d,p))  
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Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	-0.001790	1.272337	0.531438
2	6	0	1.175604	3.290403	-0.392750
3	6	0	-1.183236	3.284502	-0.400462
4	6	0	2.527225	3.006752	-0.436757
5	6	0	0.722657	4.627097	-0.168831
6	6	0	-2.533100	2.994049	-0.453187
7	6	0	-0.738469	4.623448	-0.173625
8	1	0	2.886279	1.982476	-0.608365
9	6	0	1.632242	5.656456	0.007058
10	6	0	-3.453641	4.038472	-0.279722
11	1	0	-2.885892	1.967980	-0.627037
12	6	0	-1.654307	5.648271	-0.003685
13	6	0	3.001103	5.357882	-0.039500
14	1	0	1.291719	6.687006	0.179801
15	6	0	-3.021319	5.342788	-0.059101
16	1	0	-4.530742	3.818593	-0.319554
17	1	0	-1.320146	6.680559	0.171102
18	1	0	3.733601	6.166864	0.098662
19	1	0	-3.758744	6.148086	0.074279
20	6	0	-1.256474	0.393682	0.372273
21	6	0	-1.509333	-0.248294	-0.839947
22	6	0	-2.139989	0.239406	1.440922
23	6	0	-2.645954	-1.044445	-0.983852
24	6	0	-3.276605	-0.556157	1.296975
25	6	0	-3.529814	-1.197985	0.084061
26	1	0	-2.845422	-1.549814	-1.939914
27	1	0	-3.973610	-0.677413	2.138864
28	6	0	1.258314	0.400009	0.380506
29	6	0	1.631863	-0.074341	-0.876873
30	6	0	2.026584	0.084650	1.501541
31	6	0	2.773616	-0.864422	-1.013415
32	6	0	3.167812	-0.705630	1.365179
33	6	0	3.541211	-1.180593	0.107324
34	1	0	3.067417	-1.238873	-2.004732
35	1	0	3.773222	-0.955001	2.248688
36	6	0	-4.784924	-2.076059	-0.074956
37	6	0	-5.887570	-1.595497	-0.781199
38	6	0	-4.818789	-3.352553	0.487028
39	6	0	-7.024446	-2.391243	-0.925331
40	6	0	-5.955536	-4.147981	0.343376

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41	6	0	-7.058834	-3.666990	-0.362739
42	1	0	-7.893877	-2.011790	-1.481521
43	1	0	-5.982860	-5.153917	0.786822
44	6	0	4.801025	-2.053419	-0.043154
45	6	0	5.959550	-1.515440	-0.603462
46	6	0	4.783621	-3.382236	0.381527
47	6	0	7.100833	-2.306290	-0.739485
48	6	0	5.924445	-4.173092	0.245134
49	6	0	7.083294	-3.635003	-0.315887
50	1	0	8.013795	-1.882083	-1.181966
51	1	0	5.910872	-5.220744	0.579107
52	6	0	5.979015	-0.048526	-1.071846
53	1	0	5.279568	0.079916	-1.871332
54	1	0	5.709816	0.589846	-0.256424
55	1	0	6.961184	0.203878	-1.413219
56	6	0	3.504496	-3.975661	1.000627
57	1	0	3.269429	-3.452303	1.903811
58	1	0	2.694043	-3.875658	0.309205
59	1	0	3.661272	-5.011337	1.219021
60	6	0	8.342734	-4.508296	-0.466792
61	1	0	8.365879	-4.934316	-1.448052
62	1	0	9.214437	-3.905655	-0.318949
63	1	0	8.322951	-5.291684	0.261776
64	6	0	-3.600954	-3.882983	1.266209
65	1	0	-2.739104	-3.871082	0.632194
66	1	0	-3.424895	-3.261356	2.119135
67	1	0	-3.792704	-4.885054	1.588674
68	6	0	-5.850120	-0.186655	-1.401973
69	1	0	-5.661689	0.535890	-0.635603
70	1	0	-5.071918	-0.140412	-2.134887
71	1	0	-6.790733	0.023429	-1.866745
72	6	0	-8.314018	-4.545088	-0.521026
73	1	0	-9.186211	-3.925318	-0.512959
74	1	0	-8.262791	-5.076697	-1.448209
75	1	0	-8.365161	-5.243358	0.288112
76	17	0	-0.394556	-0.054177	-2.187979
77	17	0	-1.820173	1.049119	2.970524
78	17	0	1.555216	0.683958	3.087808
79	17	0	0.663050	0.323863	-2.291241
80	7	0	-0.000999	2.367112	-0.551644
81	7	0	3.441393	4.055803	-0.257560

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**Excited states calculated by TD-DFT calculations**

CzBTM (UB3LYP/6-31G(d))

Excited State 1: 2.055-A 2.1924 eV 565.52 nm f=0.0891 <S\*\*2>=0.806  
134B ->136B 0.98719

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

Total Energy, E(TD-HF/TD-DFT) = -3775.72772659

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

Excited State 2: 2.071-A 2.2585 eV 548.98 nm f=0.0000 <S\*\*2>=0.823  
135B ->136B 0.98767

Excited State 3: 2.187-A 2.5895 eV 478.80 nm f=0.0467 <S\*\*2>=0.945  
134A ->137A 0.14559  
136A ->137A 0.90060  
130B ->136B 0.26309  
133B ->136B 0.15720

Excited State 4: 2.100-A 2.9800 eV 416.06 nm f=0.0015 <S\*\*2>=0.853  
134A ->138A 0.11091  
136A ->138A 0.92880  
131B ->136B 0.30741

Excited State 5: 2.143-A 3.0387 eV 408.02 nm f=0.0000 <S\*\*2>=0.899  
136A ->139A 0.91626  
132B ->136B 0.32992

Excited State 6: 2.664-A 3.1134 eV 398.23 nm f=0.0210 <S\*\*2>=1.524  
134A ->144A -0.14389  
135A ->139A -0.17837  
135A ->140A 0.26707  
136A ->137A -0.19480  
136A ->144A 0.18167  
133B ->136B 0.73886  
134B ->144B 0.16013  
135B ->136B -0.12034  
135B ->139B 0.24483  
135B ->140B -0.26328

Excited State 7: 2.461-A 3.2086 eV 386.41 nm f=0.0181 <S\*\*2>=1.264  
130A ->137A -0.21696  
131A ->139A 0.12340



132A ->138A	0.13650
133A ->137A	-0.10621
134A ->141A	0.14139
136A ->139A	0.10182
136A ->141A	0.46857
136A ->143A	-0.22585
129B ->136B	0.59017
130B ->137B	0.18811
131B ->138B	0.14654
132B ->136B	-0.32651
132B ->139B	0.11194

Excited State 8: 2.361-A 3.2301 eV 383.84 nm f=0.0027 <S\*\*2>=1.144

134A ->139A	0.12887
136A ->139A	-0.22005
136A ->140A	0.80644
129B ->136B	0.13121
132B ->136B	0.41926
134B ->139B	-0.14993
134B ->140B	0.13422

Excited State 9: 2.815-A 3.2415 eV 382.49 nm f=0.0706 <S\*\*2>=1.731

134A ->137A	0.12435
134A ->144A	0.10572
135A ->139A	0.23115
135A ->140A	-0.34068
136A ->137A	-0.28693
136A ->138A	-0.14117
136A ->144A	-0.12819
130B ->136B	0.44331
131B ->136B	0.31295
133B ->136B	0.33668
134B ->144B	-0.12353
135B ->139B	-0.27469
135B ->140B	0.29115

Excited State 10: 2.210-A 3.3224 eV 373.18 nm f=0.0127 <S\*\*2>=0.971

135A ->139A	-0.10545
135A ->140A	0.14987
136A ->138A	-0.29159
130B ->136B	-0.17877
131B ->136B	0.86180

133B ->136B -0.22052

135B ->140B -0.10060

Excited State 11: 2.184-A 3.3561 eV 369.43 nm f=0.0038 <S\*\*2>=0.943

136A ->139A -0.25161

136A ->140A -0.47778

136A ->141A 0.21571

129B ->136B 0.18300

132B ->136B 0.75179

134B ->139B 0.10151

Excited State 12: 2.463-A 3.3763 eV 367.22 nm f=0.0583 <S\*\*2>=1.266

134A ->137A 0.14916

135A ->139A -0.19101

135A ->140A 0.26694

136A ->137A -0.19346

130B ->136B 0.70422

133B ->136B -0.46222

135B ->139B 0.15989

135B ->140B -0.16382

Excited State 13: 2.428-A 3.6753 eV 337.34 nm f=0.0692 <S\*\*2>=1.224

130A ->137A 0.12843

132A ->138A -0.11043

133A ->144A 0.10282

136A ->140A 0.10997

136A ->141A 0.79535

136A ->143A 0.17146

136A ->145A 0.13162

129B ->136B -0.32222

131B ->138B -0.12509

132B ->139B -0.10323

Excited State 14: 3.083-A 3.7489 eV 330.72 nm f=0.0172 <S\*\*2>=2.126

131A ->138A -0.28664

132A ->139A -0.23130

132A ->140A -0.12408

134A ->137A -0.33760

136A ->137A 0.11039

136A ->142A -0.36823

129B ->137B -0.14534

130B ->136B 0.36899

131B ->136B	0.10519
131B ->139B	-0.19820
131B ->140B	-0.14908
132B ->138B	-0.26598
133B ->136B	0.11080
134B ->137B	0.41270

Excited State 15: 2.309-A 3.7610 eV 329.66 nm f=0.0014 <S\*\*2>=1.083

131A ->138A	-0.11611
134A ->137A	-0.19003
136A ->142A	0.90851
130B ->136B	0.12277
132B ->138B	-0.11215
134B ->137B	0.16057

Excited State 16: 3.038-A 3.8410 eV 322.80 nm f=0.0133 <S\*\*2>=2.058

130A ->137A	0.17029
130A ->138A	-0.13331
131A ->139A	-0.31573
131A ->140A	-0.16589
132A ->138A	-0.34940
136A ->145A	-0.10555
129B ->136B	0.54895
130B ->137B	-0.20192
131B ->138B	-0.32160
132B ->139B	-0.25664
132B ->140B	-0.18970
133B ->137B	-0.10971
134B ->139B	-0.11769

Excited State 17: 2.626-A 3.9034 eV 317.63 nm f=0.0121 <S\*\*2>=1.474

133A ->144A	-0.15032
134A ->139A	0.12583
134A ->140A	-0.14509
134A ->141A	0.13280
136A ->140A	-0.14495
136A ->141A	0.13516
136A ->143A	0.74071
136A ->145A	-0.11334
128B ->136B	-0.12270
131B ->138B	0.11369
133B ->144B	0.13696

134B ->139B	-0.27466
134B ->140B	0.20493
134B ->141B	-0.11552

Excited State 18: 2.447-A 3.9703 eV 312.28 nm f=0.0205 <S\*\*2>=1.247

134A ->139A	-0.10775
134A ->140A	0.13190
136A ->140A	0.10085
136A ->141A	-0.14398
136A ->143A	0.48243
128B ->136B	0.58608
129B ->136B	0.27837
134B ->139B	0.34361
134B ->140B	-0.25783

Excited State 19: 2.742-A 3.9955 eV 310.31 nm f=0.0067 <S\*\*2>=1.630

134A ->144A	-0.18746
136A ->144A	0.78536
133B ->136B	-0.12234
133B ->139B	-0.11048
133B ->140B	0.11558
134B ->144B	0.26340
135B ->139B	-0.30094
135B ->140B	0.24870

Excited State 20: 2.876-A 4.0042 eV 309.63 nm f=0.0001 <S\*\*2>=1.817

134A ->140A	0.10922
135A ->137A	0.89101
135A ->144A	-0.10116
136A ->140A	0.10076
136A ->143A	0.13105
128B ->136B	-0.27338
134B ->139B	0.17632
134B ->140B	-0.13259

Excited State 21: 2.451-A 4.0255 eV 308.00 nm f=0.0019 <S\*\*2>=1.252

134A ->139A	0.16815
134A ->140A	-0.20980
135A ->137A	0.44120
135A ->144A	0.14587
136A ->140A	-0.18820
136A ->141A	0.10131

136A ->143A	-0.21675
128B ->136B	0.67382
134B ->139B	-0.24910
134B ->140B	0.19153
135B ->137B	0.12310

Excited State 22: 3.167-A 4.0621 eV 305.22 nm f=0.0139 <S\*\*2>=2.257

131A ->138A	0.30477
132A ->139A	0.24602
132A ->140A	0.12476
134A ->137A	-0.10201
131B ->139B	0.20521
131B ->140B	0.14805
132B ->138B	0.27716
134B ->137B	0.79102

Excited State 23: 2.814-A 4.1491 eV 298.82 nm f=0.0002 <S\*\*2>=1.730

128B ->136B	-0.15117
135B ->137B	0.98412

Excited State 24: 2.473-A 4.1827 eV 296.42 nm f=0.0825 <S\*\*2>=1.279

131A ->138A	-0.15705
132A ->139A	-0.11964
134A ->137A	0.82128
126B ->136B	0.10380
131B ->139B	-0.14758
131B ->140B	-0.10145
132B ->138B	-0.19833
134B ->137B	0.37449
134B ->138B	-0.11591

Excited State 25: 3.336-A 4.2475 eV 291.90 nm f=0.0023 <S\*\*2>=2.533

131A ->137A	-0.13938
133A ->139A	0.10679
134A ->137A	0.10617
134A ->138A	-0.38721
136A ->138A	0.10816
129B ->138B	-0.14301
133B ->139B	-0.11954
134B ->138B	0.82098

Excited State 26: 3.103-A 4.2628 eV 290.85 nm f=0.0090 <S\*\*2>=2.157

128A ->140A	0.10241
133A ->144A	-0.18374
134A ->141A	0.15153
134A ->145A	0.14628
135A ->138A	0.27849
135A ->144A	-0.22038
135A ->146A	-0.17838
136A ->141A	0.10897
136A ->143A	-0.12739
136A ->145A	-0.27002
127B ->136B	-0.13582
128B ->136B	0.14058
128B ->139B	-0.11612
128B ->140B	0.13206
129B ->136B	-0.17153
133B ->144B	0.20889
134B ->139B	0.43014
134B ->140B	-0.14962
134B ->141B	-0.25119
134B ->143B	0.21671
134B ->145B	0.17070
135B ->138B	-0.12804
135B ->144B	0.10401
135B ->146B	-0.16128

Excited State 27: 3.376-A 4.3471 eV 285.21 nm f=0.0011 <S\*\*2>=2.599

130A ->138A	0.17638
132A ->137A	-0.23690
133A ->138A	0.12360
134A ->139A	-0.31176
134A ->140A	-0.26990
135A ->144A	0.13378
136A ->139A	0.11157
129B ->136B	0.10489
129B ->139B	-0.12985
130B ->138B	-0.19805
131B ->137B	-0.18123
133B ->138B	-0.13707
134B ->139B	0.37055
134B ->140B	0.58318

Excited State 28: 2.821-A 4.3618 eV 284.25 nm f=0.0018 <S\*\*2>=1.740

135A ->138A	0.95140
136A ->145A	0.10401
134B ->139B	-0.13903

Excited State 29: 2.582-A 4.4221 eV 280.37 nm f=0.0208 <S\*\*2>=1.416

133A ->139A	0.18450
133A ->140A	-0.14750
134A ->138A	-0.34965
135A ->139A	0.73346
135A ->140A	0.10832
136A ->144A	-0.18578
133B ->139B	-0.11670
134B ->138B	-0.25263
134B ->144B	0.21634
135B ->139B	0.18814

Excited State 30: 2.854-A 4.4263 eV 280.11 nm f=0.0000 <S\*\*2>=1.786

130A ->137A	-0.12633
130B ->137B	0.11822
134B ->139B	0.13212
135B ->138B	0.92399

Ph<sub>2</sub>CzBTM (UB3LYP/6-31G(d))

Excited State 1: 2.068-A 2.2051 eV 562.25 nm f=0.1018 <S\*\*2>=0.819

159B ->160B	0.98442
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This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -3318.67193087

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

Excited State 2: 2.082-A 2.3228 eV 533.78 nm f=0.0004 <S\*\*2>=0.833

160A ->161A	0.10857
158B ->160B	0.97849

Excited State 3: 2.202-A 2.3914 eV 518.46 nm f=0.0894 <S\*\*2>=0.963

158A ->161A	0.12418
160A ->161A	0.89582
157B ->160B	0.29498
158B ->160B	-0.12382

Excited State 4: 2.461-A 2.8988 eV 427.70 nm f=0.0224 <S\*\*2>=1.264

157A ->161A	-0.23948
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158A ->162A	0.15615
160A ->162A	0.61029
160A ->163A	-0.10742
148B ->160B	0.16988
156B ->160B	0.58576
157B ->161B	0.22478

Excited State 5: 2.264-A 2.9591 eV 419.00 nm f=0.2970 <S\*\*2>=1.031

158A ->161A	0.15832
160A ->161A	-0.36971
160A ->164A	0.12174
150B ->160B	0.15700
155B ->160B	-0.10170
156B ->161B	0.12108
157B ->160B	0.83866

Excited State 6: 2.142-A 3.0367 eV 408.29 nm f=0.0137 <S\*\*2>=0.897

160A ->164A	0.74524
155B ->160B	-0.60444
157B ->160B	-0.12412

Excited State 7: 2.191-A 3.0504 eV 406.45 nm f=0.0008 <S\*\*2>=0.950

158A ->165A	-0.10006
160A ->162A	0.19481
160A ->163A	0.74814
160A ->165A	-0.21368
154B ->160B	0.53509
156B ->160B	-0.11469

Excited State 8: 2.273-A 3.1445 eV 394.29 nm f=0.0000 <S\*\*2>=1.041

158A ->163A	0.13298
160A ->163A	-0.56900
160A ->165A	-0.42951
154B ->160B	0.63015
156B ->160B	-0.13830
159B ->162B	0.14330

Excited State 9: 3.132-A 3.1717 eV 390.91 nm f=0.0162 <S\*\*2>=2.202

149A ->174A	-0.11879
154A ->163A	-0.10508
158A ->168A	0.11172
158A ->169A	-0.14321



159A ->163A	0.42677
159A ->165A	0.24297
160A ->168A	-0.12913
160A ->169A	0.18068
149B ->173B	0.12233
153B ->160B	-0.46239
153B ->162B	-0.11488
158B ->160B	0.13472
158B ->162B	0.47059
158B ->165B	0.20045
159B ->168B	-0.12866
159B ->169B	0.15392

Excited State 10: 2.113-A 3.2416 eV 382.47 nm f=0.0126 <S\*\*2>=0.866

160A ->164A	0.62356
153B ->160B	-0.10663
155B ->160B	0.75264

Excited State 11: 2.175-A 3.3258 eV 372.80 nm f=0.0104 <S\*\*2>=0.932

158A ->163A	-0.10042
160A ->163A	-0.12643
160A ->165A	0.82083
154B ->160B	0.48678
159B ->162B	-0.13019

Excited State 12: 2.568-A 3.3750 eV 367.36 nm f=0.0121 <S\*\*2>=1.399

158A ->161A	-0.10354
159A ->163A	0.34632
159A ->165A	0.19258
153B ->160B	0.81436
155B ->160B	0.12086
158B ->162B	0.27020
158B ->165B	0.11256

Excited State 13: 2.264-A 3.4037 eV 364.26 nm f=0.1217 <S\*\*2>=1.032

157A ->161A	0.19613
158A ->162A	-0.11180
160A ->162A	0.71642
160A ->163A	-0.16547
160A ->170A	0.13549
154B ->160B	-0.14374
156B ->160B	-0.53613

Excited State 14: 3.206-A 3.5078 eV 353.46 nm f=0.0328 <S\*\*2>=2.320

151A ->167A	-0.13845
152A ->166A	-0.13994
153A ->161A	-0.19870
155A ->164A	-0.13235
156A ->165A	-0.10323
157A ->162A	-0.24912
158A ->161A	0.42959
150B ->160B	-0.17657
151B ->167B	0.13674
152B ->166B	-0.13966
153B ->160B	0.20838
154B ->163B	0.11941
155B ->165B	-0.10068
156B ->161B	0.25676
157B ->160B	-0.32369
157B ->164B	0.23357
159B ->161B	-0.42800

Excited State 15: 3.056-A 3.5800 eV 346.32 nm f=0.0079 <S\*\*2>=2.086

151A ->166A	0.14779
152A ->167A	0.14646
153A ->162A	0.19669
155A ->165A	-0.14470
156A ->164A	-0.18790
157A ->161A	0.37342
158A ->162A	-0.14788
148B ->160B	0.13448
151B ->166B	-0.14289
152B ->167B	0.14022
154B ->160B	0.11855
154B ->165B	-0.12452
155B ->163B	0.16178
156B ->160B	0.49412
156B ->164B	-0.22481
157B ->161B	-0.39857
159B ->164B	0.12833

Excited State 16: 3.113-A 3.6664 eV 338.17 nm f=0.0004 <S\*\*2>=2.172

148A ->161A	-0.11106
150A ->162A	-0.11959

151A ->167A	0.15827
152A ->166A	0.16059
153A ->161A	0.16246
155A ->164A	-0.21768
156A ->163A	0.11929
156A ->165A	-0.16813
157A ->162A	0.10897
158A ->161A	0.20772
160A ->161A	-0.10380
160A ->168A	-0.21759
160A ->169A	-0.12384
148B ->161B	0.16332
150B ->160B	0.47103
151B ->167B	-0.15848
152B ->166B	0.16284
154B ->163B	0.20826
155B ->162B	0.10291
155B ->165B	-0.17073
156B ->161B	-0.12144
157B ->160B	-0.16432
157B ->164B	-0.11670
159B ->161B	-0.24300

Excited State 17: 3.207-A 3.7353 eV 331.93 nm f=0.0014 <S\*\*2>=2.321

150A ->161A	-0.20888
151A ->166A	0.17564
152A ->167A	0.17340
153A ->162A	0.14804
155A ->163A	-0.15796
155A ->165A	0.21899
156A ->164A	0.28607
157A ->168A	0.12977
160A ->170A	0.17470
160A ->172A	-0.10066
148B ->160B	0.40393
150B ->161B	0.21400
151B ->166B	-0.17698
152B ->167B	0.17251
154B ->162B	-0.13339
154B ->165B	0.22658
155B ->163B	-0.28162
156B ->160B	-0.11437

156B ->164B -0.13845

157B ->168B -0.11230

Excited State 18: 2.248-A 3.7845 eV 327.61 nm f=0.0002 <S\*\*2>=1.014

160A ->166A 0.14810

160A ->167A -0.22514

151B ->160B 0.48078

151B ->161B -0.14423

152B ->160B 0.78383

Excited State 19: 2.248-A 3.7846 eV 327.60 nm f=0.0004 <S\*\*2>=1.013

160A ->166A 0.23603

160A ->167A 0.14120

151B ->160B 0.78115

152B ->160B -0.48252

152B ->161B -0.14434

Excited State 20: 2.874-A 3.8511 eV 321.94 nm f=0.0005 <S\*\*2>=1.815

159A ->161A 0.99449

Excited State 21: 2.396-A 3.8702 eV 320.36 nm f=0.1561 <S\*\*2>=1.185

155A ->164A -0.13993

156A ->165A -0.10634

158A ->161A 0.39943

150B ->160B 0.10326

154B ->163B 0.10894

156B ->161B 0.10345

157B ->160B -0.10296

159B ->161B 0.84275

Excited State 22: 3.145-A 3.8741 eV 320.04 nm f=0.0034 <S\*\*2>=2.222

149A ->163A 0.13587

154A ->168A -0.12780

154A ->169A 0.16730

158A ->162A 0.11485

158A ->163A 0.32958

158A ->165A 0.16336

159A ->174A -0.11443

160A ->162A 0.12392

160A ->163A 0.16387

160A ->165A 0.19674

160A ->170A -0.20010

160A ->173A	0.10703
149B ->160B	-0.12417
149B ->162B	0.14269
153B ->168B	0.11995
153B ->169B	-0.14949
156B ->160B	-0.10469
158B ->161B	-0.11560
158B ->173B	0.13086
159B ->162B	0.57500
159B ->164B	-0.11324
159B ->165B	0.20621
159B ->170B	-0.10442

Excited State 23: 2.144-A 3.9342 eV 315.15 nm f=0.0031  $\langle S^2 \rangle = 0.899$

160A ->166A	0.88714
160A ->168A	0.18140
160A ->171A	0.22055
151B ->160B	-0.29811

Excited State 24: 2.794-A 3.9413 eV 314.58 nm f=0.0025  $\langle S^2 \rangle = 1.701$

149B ->160B	0.13790
158B ->161B	0.97335

Excited State 25: 2.167-A 3.9436 eV 314.39 nm f=0.0002  $\langle S^2 \rangle = 0.924$

160A ->165A	0.12402
160A ->167A	0.90623
160A ->170A	0.14616
152B ->160B	0.29266

Excited State 26: 2.658-A 3.9488 eV 313.98 nm f=0.0056  $\langle S^2 \rangle = 1.516$

158A ->168A	0.12245
158A ->169A	-0.14079
159A ->163A	-0.10800
160A ->166A	0.10692
160A ->168A	-0.50427
160A ->169A	0.62149
153B ->160B	0.15119
153B ->162B	-0.13106
158B ->162B	-0.35638
158B ->165B	-0.12662
159B ->168B	-0.15174
159B ->169B	0.18156

Excited State 27: 3.134-A 4.0142 eV 308.86 nm f=0.0628  $\langle S^2 \rangle = 2.206$

153A ->161A	0.14004
155A ->164A	0.28723
156A ->163A	-0.15405
156A ->165A	0.21307
158A ->161A	0.69447
160A ->168A	-0.10330
150B ->160B	-0.14252
154B ->163B	-0.29675
155B ->162B	-0.14829
155B ->165B	0.23285
156B ->161B	-0.12088

Excited State 28: 2.293-A 4.0655 eV 304.97 nm f=0.0055  $\langle S^2 \rangle = 1.064$

158A ->163A	0.17572
159A ->169A	-0.11933
160A ->170A	0.13161
149B ->160B	0.89294
158B ->161B	-0.16606
158B ->169B	0.10826
159B ->162B	0.10844

Excited State 29: 2.254-A 4.0830 eV 303.66 nm f=0.0148  $\langle S^2 \rangle = 1.020$

155A ->164A	0.13186
160A ->166A	-0.21346
160A ->168A	0.42673
160A ->169A	0.38978
160A ->171A	0.49028
150B ->160B	0.49436
154B ->163B	-0.12753
155B ->165B	0.10448
157B ->160B	-0.10331

Excited State 30: 2.395-A 4.1056 eV 301.99 nm f=0.0028  $\langle S^2 \rangle = 1.184$

160A ->167A	-0.16109
160A ->170A	0.76192
160A ->173A	-0.12443
148B ->160B	-0.21068
149B ->160B	-0.26206
159B ->162B	0.34842
159B ->164B	0.12970

Mes<sub>2</sub>CzBTM (UB3LYP/6-31G(d))

Excited State 1: 2.057-A 2.2726 eV 545.55 nm f=0.0900 <S\*\*2>=0.808  
183B ->184B 0.98663

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

Total Energy, E(TD-HF/TD-DFT) = -3554.58004198

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

Excited State 2: 2.082-A 2.3830 eV 520.29 nm f=0.0000 <S\*\*2>=0.834  
182B ->184B 0.98492

Excited State 3: 2.209-A 2.6831 eV 462.10 nm f=0.0619 <S\*\*2>=0.970  
182A ->185A 0.15030  
184A ->185A 0.88892  
173B ->185B -0.10648  
174B ->184B -0.28626  
175B ->184B -0.17165

Excited State 4: 2.121-A 3.0639 eV 404.66 nm f=0.0003 <S\*\*2>=0.875  
182A ->187A 0.10565  
184A ->187A 0.75213  
176B ->184B -0.60965  
178B ->184B -0.11190

Excited State 5: 2.220-A 3.0748 eV 403.23 nm f=0.0016 <S\*\*2>=0.982  
182A ->188A -0.10600  
184A ->186A 0.80716  
184A ->188A -0.18395  
177B ->184B -0.49725  
183B ->186B 0.10868

Excited State 6: 2.266-A 3.1602 eV 392.33 nm f=0.0002 <S\*\*2>=1.033  
182A ->186A -0.12796  
184A ->186A 0.51085  
184A ->188A 0.44349  
177B ->184B 0.66660  
179B ->184B -0.16093  
183B ->186B 0.14548

Excited State 7: 3.010-A 3.1633 eV 391.95 nm f=0.0169 <S\*\*2>=2.015  
175A ->186A -0.10574  
182A ->194A 0.16484  
183A ->186A -0.40308

183A ->188A	-0.21345
184A ->185A	0.14842
184A ->194A	-0.20991
172B ->198B	0.11445
175B ->184B	0.53832
175B ->186B	0.11223
182B ->184B	-0.14561
182B ->186B	-0.43875
182B ->188B	-0.17261
183B ->194B	0.19612

Excited State 8: 2.074-A 3.2190 eV 385.16 nm f=0.0000 <S\*\*2>=0.826  
 180B ->184B 0.96419  
 181B ->184B 0.22008

Excited State 9: 2.092-A 3.2191 eV 385.15 nm f=0.0007 <S\*\*2>=0.844  
 180B ->184B -0.22064  
 181B ->184B 0.96130

Excited State 10: 2.147-A 3.2724 eV 378.88 nm f=0.0175 <S\*\*2>=0.902  
 184A ->187A 0.61213  
 174B ->184B 0.13459  
 175B ->184B 0.10031  
 176B ->184B 0.66486  
 178B ->184B 0.30233  
 182B ->186B 0.11079

Excited State 11: 2.488-A 3.2762 eV 378.44 nm f=0.0224 <S\*\*2>=1.298  
 174A ->185A -0.20476  
 175A ->185A -0.10506  
 176A ->187A 0.15988  
 177A ->188A 0.13036  
 182A ->189A 0.15320  
 184A ->188A -0.37075  
 184A ->189A 0.45879  
 173B ->184B 0.58154  
 174B ->185B 0.17702  
 176B ->187B 0.16808  
 177B ->184B 0.13827  
 177B ->188B -0.13704

Excited State 12: 2.530-A 3.2917 eV 376.66 nm f=0.1256 <S\*\*2>=1.350



182A ->185A	-0.11706
183A ->186A	0.27682
183A ->188A	0.14493
184A ->185A	0.33572
184A ->187A	-0.10109
174B ->184B	0.48577
175B ->184B	0.53987
176B ->184B	-0.19056
178B ->184B	-0.16786
182B ->186B	0.26497
182B ->188B	0.10331

Excited State 13: 2.092-A 3.3379 eV 371.44 nm f=0.0002 <S\*\*2>=0.844

184A ->188A	0.32040
184A ->189A	0.10199
173B ->184B	0.10156
179B ->184B	0.92348

Excited State 14: 2.067-A 3.3471 eV 370.42 nm f=0.0014 <S\*\*2>=0.818

184A ->187A	-0.12654
176B ->184B	-0.32780
178B ->184B	0.92796

Excited State 15: 2.194-A 3.3752 eV 367.34 nm f=0.0022 <S\*\*2>=0.953

184A ->186A	-0.12979
184A ->188A	0.67405
184A ->189A	0.22379
173B ->184B	0.20940
177B ->184B	-0.50522
179B ->184B	-0.32258
183B ->186B	0.10638

Excited State 16: 2.366-A 3.4640 eV 357.92 nm f=0.0636 <S\*\*2>=1.149

182A ->185A	-0.11303
183A ->186A	-0.26695
183A ->188A	-0.13005
184A ->185A	0.17795
174B ->184B	0.68037
175B ->184B	-0.55843
182B ->186B	-0.17573

Excited State 17: 3.469-A 3.6302 eV 341.54 nm f=0.0002 <S\*\*2>=2.758

178A ->193A	-0.30352
179A ->192A	-0.29385
180A ->191A	0.39013
181A ->190A	-0.39164
178B ->193B	0.30282
179B ->192B	0.30235
180B ->190B	-0.38974
181B ->189B	0.39034

Excited State 18: 3.468-A 3.6305 eV 341.51 nm f=0.0000 <S\*\*2>=2.757

178A ->192A	-0.29432
179A ->193A	-0.30372
180A ->190A	0.38973
181A ->191A	-0.39086
178B ->192B	0.30241
179B ->193B	0.30254
180B ->189B	-0.38951
181B ->190B	0.39053

Excited State 19: 2.688-A 3.7685 eV 329.00 nm f=0.0926 <S\*\*2>=1.556

174A ->185A	0.10922
175A ->194A	0.15956
176A ->187A	-0.11732
182A ->186A	-0.17395
182A ->189A	-0.11296
182A ->197A	-0.10530
184A ->188A	-0.12634
184A ->189A	0.69899
184A ->197A	0.16780
172B ->186B	0.10619
173B ->184B	-0.29223
175B ->194B	0.14658
176B ->187B	-0.14024
177B ->188B	0.11845
182B ->198B	-0.10126
183B ->186B	0.24132
183B ->191B	-0.13353

Excited State 20: 3.241-A 3.8159 eV 324.91 nm f=0.0136 <S\*\*2>=2.377

176A ->186A	0.19389
176A ->188A	-0.29021
177A ->187A	-0.36086

182A ->185A	0.31361
184A ->185A	-0.13501
173B ->185B	-0.15323
174B ->184B	0.38631
175B ->184B	0.12394
176B ->186B	0.15511
176B ->188B	-0.29585
177B ->187B	0.34540
183B ->185B	-0.31704

Excited State 21: 3.105-A 3.8824 eV 319.35 nm f=0.0044 <S\*\*2>=2.160

174A ->185A	0.13863
176A ->187A	-0.38050
177A ->186A	0.19993
177A ->188A	-0.30223
182A ->186A	0.13393
184A ->189A	0.10736
184A ->197A	-0.10681
173B ->184B	0.48733
174B ->185B	-0.15954
176B ->187B	-0.35702
177B ->186B	-0.15764
177B ->188B	0.30003
183B ->186B	-0.20612

Excited State 22: 2.670-A 3.9559 eV 313.42 nm f=0.0077 <S\*\*2>=1.532

182A ->194A	-0.16423
183A ->186A	-0.10917
184A ->192A	-0.20570
184A ->194A	0.77566
174B ->184B	-0.11873
175B ->184B	0.14109
175B ->186B	-0.13383
182B ->186B	-0.36479
182B ->188B	-0.11249
183B ->194B	-0.24013

Excited State 23: 2.848-A 3.9599 eV 313.10 nm f=0.0106 <S\*\*2>=1.778

173A ->186A	-0.10968
175A ->194A	0.11068
182A ->186A	-0.30184
182A ->188A	-0.15665

183A ->194A	0.10368
184A ->186A	-0.18415
184A ->188A	-0.13712
184A ->189A	-0.38933
173B ->184B	0.37913
183B ->186B	0.60830
183B ->188B	0.16887

Excited State 24: 2.089-A 4.1054 eV 302.00 nm f=0.0054 <S\*\*2>=0.841

184A ->191A	-0.17041
184A ->192A	-0.15010
184A ->195A	0.95398

Excited State 25: 2.273-A 4.1165 eV 301.19 nm f=0.0089 <S\*\*2>=1.042

182A ->186A	-0.15324
183A ->185A	-0.12212
183A ->194A	0.16300
172B ->184B	0.91219
182B ->185B	-0.10366
182B ->194B	-0.15765

Excited State 26: 2.098-A 4.1431 eV 299.25 nm f=0.0002 <S\*\*2>=0.850

184A ->190A	0.99218
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Excited State 27: 2.117-A 4.1455 eV 299.08 nm f=0.0003 <S\*\*2>=0.871

184A ->191A	0.97174
184A ->195A	0.16384

Excited State 28: 3.332-A 4.1702 eV 297.31 nm f=0.0028 <S\*\*2>=2.525

176A ->186A	0.14583
176A ->188A	-0.21085
177A ->187A	-0.27125
182A ->185A	-0.33129
184A ->191A	-0.10378
176B ->186B	0.11668
176B ->188B	-0.21345
177B ->187B	0.25773
183B ->185B	0.75652

Excited State 29: 2.815-A 4.2036 eV 294.95 nm f=0.0007 <S\*\*2>=1.731

183A ->185A	0.95437
184A ->196A	0.17212

172B ->184B 0.14551

Excited State 30: 2.317-A 4.2363 eV 292.67 nm f=0.0006 <S\*\*2>=1.092

183A ->185A -0.23834

183A ->194A -0.10256

184A ->196A 0.86143

184A ->197A 0.16032

171B ->184B -0.13257

183B ->186B -0.14452

183B ->191B -0.10359

PyIDBTM (UB3LYP/6-31G(d))

Excited State 1: 2.059-A 2.2747 eV 545.05 nm f=0.0874 <S\*\*2>=0.810

135B ->136B 0.98590

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

Total Energy, E(TD-HF/TD-DFT) = -3791.75747652

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

Excited State 2: 2.147-A 2.6082 eV 475.37 nm f=0.0090 <S\*\*2>=0.902

136A ->137A 0.47033

132B ->136B -0.21165

134B ->136B 0.81478

Excited State 3: 2.182-A 2.6389 eV 469.83 nm f=0.0314 <S\*\*2>=0.940

135A ->137A 0.11589

136A ->137A 0.74494

129B ->136B -0.23895

132B ->136B -0.15991

134B ->136B -0.53013

Excited State 4: 2.338-A 2.9417 eV 421.47 nm f=0.0046 <S\*\*2>=1.117

135A ->138A -0.11919

136A ->138A 0.95373

135B ->138B 0.18902

Excited State 5: 2.113-A 3.0313 eV 409.01 nm f=0.0022 <S\*\*2>=0.866

135A ->139A 0.10204

136A ->139A 0.87001

130B ->136B -0.31888

131B ->136B -0.24600

132B ->136B -0.14750

Excited State 6: 2.128-A 3.1112 eV 398.52 nm f=0.0143 <S\*\*2>=0.882

136A ->137A	-0.15311
136A ->139A	-0.14464
136A ->140A	-0.24146
136A ->141A	-0.13049
128B ->136B	0.18315
132B ->136B	-0.19375
133B ->136B	0.85595

Excited State 7: 2.170-A 3.1344 eV 395.56 nm f=0.0007 <S\*\*2>=0.928

135A ->138A	0.10026
136A ->140A	0.66181
130B ->136B	-0.32902
131B ->136B	0.54754
133B ->136B	0.27021

Excited State 8: 2.431-A 3.2033 eV 387.06 nm f=0.0563 <S\*\*2>=1.227

134A ->138A	0.18153
135A ->144A	-0.10171
136A ->137A	0.26566
136A ->140A	-0.16265
136A ->141A	-0.20466
136A ->144A	0.13389
128B ->136B	0.28913
129B ->136B	0.10195
132B ->136B	0.69289
133B ->136B	0.10252
134B ->136B	0.13584
134B ->138B	0.19731
135B ->144B	-0.11793

Excited State 9: 2.391-A 3.2303 eV 383.81 nm f=0.0222 <S\*\*2>=1.179

129A ->137A	0.14861
132A ->137A	0.12693
135A ->141A	-0.11456
136A ->140A	-0.18955
136A ->141A	-0.37214
136A ->143A	-0.15804
128B ->136B	0.51674
129B ->137B	-0.12927
130B ->136B	-0.14550
131B ->136B	0.19102

131B ->140B	0.10644
132B ->136B	-0.29540
132B ->137B	-0.11016
133B ->136B	-0.38784

Excited State 10: 2.682-A 3.2833 eV 377.62 nm f=0.0383 <S\*\*2>=1.549

134A ->138A	-0.31680
134A ->140A	0.10462
135A ->144A	0.13524
136A ->137A	0.17985
136A ->139A	0.30895
136A ->140A	-0.10680
136A ->144A	-0.18345
129B ->136B	0.32961
130B ->136B	0.39367
131B ->136B	0.34996
132B ->136B	0.19683
134B ->136B	-0.13191
134B ->138B	-0.34890
135B ->144B	0.14762

Excited State 11: 2.420-A 3.3119 eV 374.36 nm f=0.0413 <S\*\*2>=1.214

134A ->138A	0.23718
136A ->137A	-0.18431
136A ->139A	0.28191
136A ->140A	-0.16545
136A ->144A	0.10856
129B ->136B	-0.42491
130B ->136B	0.48614
131B ->136B	0.46290
134B ->138B	0.23105

Excited State 12: 2.157-A 3.3458 eV 370.56 nm f=0.0043 <S\*\*2>=0.913

136A ->140A	0.58369
136A ->141A	-0.20536
128B ->136B	0.20541
130B ->136B	0.55414
131B ->136B	-0.43493

Excited State 13: 2.531-A 3.4555 eV 358.80 nm f=0.0312 <S\*\*2>=1.351

134A ->138A	0.36568
134A ->140A	-0.10927

136A ->137A	0.11795
129B ->136B	0.68565
130B ->136B	0.12420
131B ->136B	0.14157
132B ->136B	-0.42931
134B ->138B	0.27252

Excited State 14: 2.582-A 3.6942 eV 335.62 nm f=0.0820 <S\*\*2>=1.416

132A ->144A	-0.10812
135A ->138A	-0.20693
136A ->138A	-0.10975
136A ->140A	0.11562
136A ->141A	0.71761
136A ->145A	-0.14545
128B ->136B	0.33244
135B ->138B	0.29477

Excited State 15: 3.247-A 3.7721 eV 328.69 nm f=0.0110 <S\*\*2>=2.386

128A ->137A	0.11722
130A ->139A	0.23238
130A ->140A	0.15420
131A ->139A	-0.23666
131A ->140A	0.26186
135A ->137A	-0.34584
136A ->137A	0.13882
136A ->142A	-0.13380
128B ->137B	-0.16092
129B ->136B	-0.31701
130B ->139B	-0.21268
130B ->140B	-0.15893
131B ->139B	0.22916
131B ->140B	-0.24891
132B ->136B	-0.19487
135B ->137B	0.34816

Excited State 16: 3.041-A 3.8125 eV 325.21 nm f=0.0018 <S\*\*2>=2.062

129A ->137A	-0.12205
130A ->139A	-0.23573
130A ->140A	-0.15305
131A ->139A	-0.11042
131A ->140A	0.15150
132A ->137A	-0.11509



135A ->138A	-0.28377
136A ->138A	-0.14968
136A ->140A	0.10549
136A ->141A	-0.32882
136A ->142A	-0.24145
136A ->143A	0.15057
128B ->136B	0.22615
129B ->137B	0.12108
130B ->139B	0.22908
130B ->140B	0.14439
131B ->139B	0.10095
131B ->140B	-0.15145
132B ->137B	0.10432
135B ->138B	0.48885

Excited State 17: 2.302-A 3.8333 eV 323.44 nm f=0.0037 <S\*\*2>=1.075

131A ->139A	-0.10381
131A ->140A	0.13297
136A ->142A	0.90175
128B ->136B	0.17071
131B ->140B	-0.12993

Excited State 18: 2.852-A 3.8460 eV 322.37 nm f=0.0070 <S\*\*2>=1.783

130A ->139A	-0.20967
130A ->140A	-0.12940
131A ->139A	-0.11922
131A ->140A	0.16170
135A ->138A	0.24109
135A ->140A	-0.10140
136A ->138A	0.15020
136A ->141A	0.26927
136A ->142A	-0.26508
136A ->143A	-0.11389
128B ->136B	0.48035
129B ->137B	0.11192
130B ->139B	0.18425
130B ->140B	0.10890
131B ->140B	-0.13921
135B ->138B	-0.44291

Excited State 19: 3.274-A 3.9584 eV 313.22 nm f=0.0025 <S\*\*2>=2.429

133A ->138A	0.54171
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133A ->140A	-0.15711
133A ->145A	0.10125
133A ->146A	0.16155
134A ->138A	-0.11639
136A ->144A	0.41227
133B ->138B	-0.51851
133B ->140B	0.12437
133B ->145B	-0.15693
134B ->138B	-0.23590
135B ->144B	-0.13006

Excited State 20: 2.959-A 3.9837 eV 311.23 nm f=0.0063 <S\*\*2>=1.939

132A ->138A	-0.10566
133A ->138A	-0.35378
133A ->140A	0.10441
133A ->146A	-0.10830
134A ->138A	-0.12755
135A ->144A	-0.13353
136A ->144A	0.65723
132B ->138B	0.14708
133B ->138B	0.32608
133B ->145B	0.11457
134B ->138B	-0.32734
135B ->144B	-0.18763

Excited State 21: 2.266-A 3.9924 eV 310.55 nm f=0.0171 <S\*\*2>=1.033

136A ->143A	0.90553
136A ->145A	-0.10908
128B ->136B	0.15411
135B ->138B	-0.16612

Excited State 22: 3.347-A 4.1354 eV 299.81 nm f=0.0022 <S\*\*2>=2.550

130A ->139A	-0.22888
130A ->140A	-0.14623
131A ->139A	0.18801
131A ->140A	-0.19717
135A ->137A	-0.31674
130B ->139B	0.21098
130B ->140B	0.14865
131B ->139B	-0.18205
131B ->140B	0.18423
135B ->137B	0.73280

Excited State 23: 3.054-A 4.2525 eV 291.56 nm f=0.0188 <S\*\*2>=2.082

127A ->138A	0.15039
129A ->144A	-0.13634
132A ->144A	0.16697
134A ->144A	0.13993
134A ->146A	-0.16518
135A ->141A	0.18732
135A ->145A	-0.17819
136A ->141A	0.14475
136A ->143A	0.17264
136A ->145A	0.34566
127B ->138B	-0.17466
128B ->136B	0.23559
129B ->144B	-0.14545
132B ->138B	0.10126
132B ->144B	0.20091
134B ->145B	-0.10785
135B ->138B	0.30901
135B ->141B	-0.30192
135B ->143B	-0.22441
135B ->145B	0.16438
135B ->146B	-0.10292

Excited State 24: 2.232-A 4.2667 eV 290.59 nm f=0.0845 <S\*\*2>=0.995

135A ->137A	0.77041
126B ->136B	-0.11097
135B ->137B	0.54436

Excited State 25: 3.333-A 4.3313 eV 286.25 nm f=0.0029 <S\*\*2>=2.528

129A ->138A	-0.10553
129A ->140A	0.13342
130A ->137A	0.12890
131A ->137A	-0.10723
132A ->138A	0.25958
134A ->138A	0.10630
135A ->139A	-0.36973
136A ->144A	0.18868
136A ->146A	-0.13023
128B ->139B	-0.14349
129B ->140B	-0.13420
132B ->138B	-0.26516

135B ->138B 0.12610

135B ->139B 0.61079

Excited State 26: 2.178-A 4.3441 eV 285.41 nm f=0.0036 <S\*\*2>=0.936

135A ->138A -0.43465

127B ->136B 0.80038

134B ->144B -0.16886

135B ->138B -0.23590

Excited State 27: 3.192-A 4.3766 eV 283.29 nm f=0.0013 <S\*\*2>=2.297

129A ->138A 0.26810

130A ->137A 0.10103

130A ->138A 0.10015

131A ->138A 0.12545

132A ->138A -0.29307

132A ->140A 0.16745

134A ->138A -0.22356

135A ->138A -0.10580

135A ->139A -0.21035

135A ->144A -0.11761

135A ->146A -0.10746

136A ->144A -0.35828

136A ->146A 0.14808

129B ->138B -0.24378

131B ->138B -0.10792

132B ->138B 0.29121

132B ->140B -0.16050

135B ->139B 0.40338

135B ->144B -0.17057

Excited State 28: 3.236-A 4.4032 eV 281.58 nm f=0.0004 <S\*\*2>=2.368

129A ->137A 0.10407

129A ->139A 0.11654

130A ->137A 0.13864

131A ->137A 0.15585

132A ->137A 0.27654

134A ->137A 0.62402

135A ->140A -0.22660

127B ->136B 0.10146

129B ->137B -0.13023

129B ->139B -0.13646

130B ->137B -0.11954

131B ->137B	-0.12788
132B ->137B	-0.21299
132B ->139B	-0.10367
135B ->140B	0.31744

Excited State 29: 3.200-A 4.4179 eV 280.64 nm f=0.0005 <S\*\*2>=2.310

129A ->139A	-0.11390
130A ->137A	-0.13624
131A ->137A	-0.20423
132A ->139A	-0.16822
134A ->137A	0.62904
135A ->138A	0.17152
135A ->140A	0.30145
128B ->140B	0.13206
129B ->139B	0.12900
130B ->137B	0.10787
131B ->137B	0.15058
132B ->139B	0.17059
135B ->140B	-0.42764

Excited State 30: 3.006-A 4.4544 eV 278.34 nm f=0.0006 <S\*\*2>=2.009

129A ->137A	-0.29765
130A ->139A	0.14801
131A ->139A	0.10755
131A ->140A	-0.13271
132A ->137A	-0.29571
134A ->137A	0.33507
135A ->138A	0.24845
135A ->140A	-0.12914
136A ->143A	-0.14491
136A ->145A	-0.10040
125B ->136B	0.26986
127B ->136B	0.12363
129B ->137B	0.24153
130B ->139B	-0.13149
131B ->140B	0.11478
132B ->137B	0.25262
134B ->137B	-0.17003
134B ->144B	0.10547
135B ->138B	0.13841
135B ->140B	0.23009

Ph<sub>2</sub>PyIDBTM (UB3LYP/6-31G(d))

Excited State 1: 2.076-A 2.2795 eV 543.91 nm f=0.0983 <S\*\*2>=0.828

159B ->160B 0.98220

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

Total Energy, E(TD-HF/TD-DFT) = -3334.70280711

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

Excited State 2: 2.236-A 2.4288 eV 510.47 nm f=0.0663 <S\*\*2>=1.000

157A ->163A -0.10618

159A ->161A 0.12720

160A ->161A 0.86880

149B ->160B -0.11804

157B ->160B 0.35485

Excited State 3: 2.129-A 2.6764 eV 463.25 nm f=0.0078 <S\*\*2>=0.884

158A ->162A 0.10967

152B ->160B -0.10939

158B ->160B 0.96358

158B ->162B -0.10720

Excited State 4: 2.346-A 2.8754 eV 431.18 nm f=0.0220 <S\*\*2>=1.125

157A ->161A -0.10868

159A ->162A -0.12566

160A ->162A 0.85929

160A ->163A 0.21070

155B ->160B -0.15876

156B ->160B 0.20911

157B ->160B -0.16176

159B ->162B 0.16801

Excited State 5: 2.384-A 2.8958 eV 428.16 nm f=0.0518 <S\*\*2>=1.171

157A ->161A -0.18976

159A ->163A 0.11677

160A ->161A 0.17258

160A ->162A -0.41696

160A ->163A 0.44146

148B ->160B -0.14330

154B ->160B 0.13036

155B ->160B -0.25756

156B ->160B 0.39008

157B ->160B -0.40736

157B ->161B 0.18068

Excited State 6: 2.239-A 2.9453 eV 420.96 nm f=0.2873 <S\*\*2>=1.004

157A ->161A -0.10445

159A ->161A 0.10741

160A ->161A -0.37870

160A ->163A 0.25139

149B ->160B -0.12922

155B ->160B -0.25718

156B ->160B 0.26971

157B ->160B 0.71356

Excited State 7: 2.141-A 3.0412 eV 407.68 nm f=0.0278 <S\*\*2>=0.896

160A ->164A -0.48328

160A ->165A 0.15987

153B ->160B 0.31009

154B ->160B 0.71212

155B ->160B 0.22971

157B ->160B 0.14417

Excited State 8: 2.143-A 3.0711 eV 403.71 nm f=0.0007 <S\*\*2>=0.898

160A ->163A -0.11198

160A ->164A -0.30107

160A ->165A -0.32271

153B ->160B 0.73860

154B ->160B -0.39005

155B ->160B -0.20343

Excited State 9: 2.098-A 3.2189 eV 385.18 nm f=0.0097 <S\*\*2>=0.851

160A ->163A -0.11716

154B ->160B -0.20734

155B ->160B 0.64071

156B ->160B 0.69617

Excited State 10: 2.199-A 3.2619 eV 380.10 nm f=0.0112 <S\*\*2>=0.959

158A ->162A 0.13768

160A ->164A 0.74187

152B ->160B -0.12125

153B ->160B 0.47935

154B ->160B 0.31866

158B ->162B -0.12431

Excited State 11: 3.052-A 3.2725 eV 378.86 nm f=0.0048 <S\*\*2>=2.078



151A ->162A	-0.13620
158A ->162A	-0.44942
159A ->168A	0.18855
160A ->164A	0.25340
160A ->168A	-0.25409
152B ->160B	0.39814
152B ->162B	0.13228
153B ->160B	0.10105
158B ->160B	0.21204
158B ->162B	0.45840
159B ->168B	0.20887

Excited State 12: 2.141-A 3.3584 eV 369.18 nm f=0.0234 <S\*\*2>=0.896

160A ->163A	0.22932
160A ->165A	0.85034
153B ->160B	0.25886
154B ->160B	-0.31248

Excited State 13: 2.163-A 3.4252 eV 361.98 nm f=0.1156 <S\*\*2>=0.920

160A ->163A	0.69121
160A ->165A	-0.24850
160A ->170A	0.12774
152B ->160B	-0.10049
154B ->160B	-0.14271
155B ->160B	0.44616
156B ->160B	-0.33762
159B ->162B	-0.11450

Excited State 14: 2.655-A 3.4703 eV 357.27 nm f=0.0046 <S\*\*2>=1.513

153A ->161A	0.11173
157A ->163A	0.13418
158A ->162A	0.33398
159A ->161A	-0.18153
152B ->160B	0.77180
155B ->161B	0.10028
156B ->161B	-0.10846
157B ->160B	0.10130
157B ->164B	-0.11617
158B ->162B	-0.24093
159B ->161B	0.11392

Excited State 15: 3.120-A 3.5253 eV 351.70 nm f=0.0253 <S\*\*2>=2.183

150A ->166A	0.10921
152A ->167A	0.17350
153A ->161A	-0.18429
155A ->165A	0.12722
157A ->163A	-0.24774
158A ->162A	0.15568
159A ->161A	0.37104
149B ->160B	0.18089
150B ->166B	-0.10833
151B ->167B	0.17336
152B ->160B	0.37044
154B ->165B	-0.11349
155B ->161B	-0.16643
156B ->161B	0.16332

157B ->160B -0.25135

157B ->161B -0.11661

157B ->164B 0.21625

158B ->162B -0.11554

159B ->161B -0.33124

Excited State 16: 3.144-A 3.5628 eV 347.99 nm f=0.0024 <S\*\*2>=2.220

150A ->166A -0.18167

152A ->167A 0.11523

153A ->163A 0.19453

154A ->164A -0.16947

154A ->165A -0.10239

155A ->165A 0.11348

157A ->161A 0.39635

159A ->163A -0.16618

160A ->163A 0.18549

148B ->160B -0.11926

150B ->166B 0.17753

151B ->167B 0.11181

153B ->163B -0.15864

154B ->160B 0.12199

154B ->164B -0.10159

155B ->160B -0.27334

155B ->164B 0.12197

156B ->160B 0.25619

156B ->161B -0.10923

156B ->164B -0.15165

157B ->161B -0.38822

159B ->164B 0.12127

Excited State 17: 2.832-A 3.6761 eV 337.27 nm f=0.0016  $\langle S^2 \rangle = 1.755$

150A ->166A -0.11540

152A ->167A -0.10004

153A ->161A 0.10843

154A ->164A 0.19170

154A ->165A 0.10133

155A ->165A 0.15956

159A ->161A 0.19652

160A ->161A -0.10452

160A ->169A -0.14469

148B ->161B -0.13482

149B ->160B -0.43347

150B ->166B 0.11839

151B ->160B 0.52484

151B ->167B -0.10484

153B ->163B 0.18680

154B ->165B -0.14810

157B ->160B -0.15773

159B ->161B -0.17202

Excited State 18: 2.485-A 3.6798 eV 336.93 nm f=0.0002  $\langle S^2 \rangle = 1.293$

154A ->164A -0.11342

155A ->165A -0.10888

159A ->161A -0.11837

149B ->160B 0.28729

151B ->160B 0.80947

151B ->161B -0.13139

153B ->163B -0.11067

154B ->165B 0.10014

159B ->161B 0.10790

Excited State 19: 2.739-A 3.7349 eV 331.96 nm f=0.0006 <S\*\*2>=1.626

149A ->161A 0.12063

150A ->166A -0.10411

154A ->164A 0.13489

155A ->165A -0.12246

159A ->162A -0.16880

160A ->166A -0.11315

148B ->160B -0.27105

149B ->161B -0.12505

150B ->160B 0.68033

150B ->161B 0.11512

150B ->166B 0.10591

153B ->163B 0.12747

154B ->165B 0.11652

159B ->162B 0.26198

Excited State 20: 2.771-A 3.7364 eV 331.82 nm f=0.0007 <S\*\*2>=1.670

149A ->161A -0.10702

154A ->164A -0.11678

155A ->165A 0.11079

159A ->162A 0.22404

160A ->162A 0.12486

160A ->166A -0.10288

148B ->160B	0.24148
149B ->161B	0.11236
150B ->160B	0.66297
150B ->161B	0.11314
153B ->163B	-0.11081
154B ->165B	-0.10533
159B ->162B	-0.34246

Excited State 21: 3.180-A 3.7395 eV 331.55 nm f=0.0022 <S\*\*2>=2.278

149A ->161A	-0.13078
152A ->167A	-0.11635
153A ->162A	-0.10539
154A ->164A	-0.13443
155A ->164A	-0.11040
155A ->165A	0.14542
159A ->162A	-0.37111
160A ->162A	-0.18580
160A ->163A	0.17917
160A ->165A	-0.13674
160A ->170A	-0.10974
148B ->160B	0.25134
149B ->161B	0.12210
151B ->167B	-0.11592
153B ->163B	-0.13763
154B ->163B	-0.10150
154B ->165B	-0.14062
159B ->162B	0.54695

Excited State 22: 2.684-A 3.9237 eV 315.99 nm f=0.0098 <S\*\*2>=1.551

156A ->162A -0.11243

158A ->162A -0.17196

159A ->168A -0.15911

160A ->168A 0.78086

152B ->160B 0.17200

152B ->162B -0.13697

158B ->162B 0.40027

159B ->168B -0.19712

Excited State 23: 2.576-A 3.9761 eV 311.82 nm f=0.1152 <S\*\*2>=1.409

154A ->164A 0.11415

159A ->161A 0.25308

149B ->160B -0.17749

159B ->161B 0.87824

Excited State 24: 3.437-A 3.9823 eV 311.34 nm f=0.0005 <S\*\*2>=2.704

156A ->162A 0.64985

156A ->173A 0.20326

160A ->168A 0.15468

154B ->162B 0.12730

155B ->162B -0.40623

155B ->173B -0.13820

156B ->162B -0.44368

156B ->173B -0.14525

Excited State 25: 2.173-A 4.0025 eV 309.77 nm f=0.0017 <S\*\*2>=0.931

157A ->166A -0.10046

160A ->166A 0.88873

160A ->167A -0.17307

160A ->170A -0.22891

160A ->171A -0.15837

150B ->160B 0.17341

Excited State 26: 2.234-A 4.0290 eV 307.73 nm f=0.0002 <S\*\*2>=0.998

159A ->161A -0.10774

160A ->166A 0.18711

160A ->167A 0.81368

160A ->169A 0.30450

160A ->170A -0.12042

160A ->171A 0.22930

149B ->160B -0.10827

151B ->160B 0.11268

159B ->162B -0.10202

Excited State 27: 2.837-A 4.0688 eV 304.72 nm f=0.0915 <S\*\*2>=1.762

150A ->166A -0.13095

152A ->167A -0.14199

153A ->161A 0.13687

154A ->164A -0.16339

155A ->165A -0.10816

159A ->161A 0.72587

160A ->166A -0.10337

160A ->167A 0.12685

160A ->170A -0.15656

149B ->160B 0.30051



150B ->166B 0.12973

151B ->167B -0.13631

153B ->163B -0.18055

154B ->165B 0.11612

Excited State 28: 2.817-A 4.0774 eV 304.08 nm f=0.0064 <S\*\*2>=1.734

150A ->166A -0.10124

152A ->167A -0.12135

154A ->164A 0.23440

154A ->165A 0.11458

155A ->164A -0.16481

155A ->165A 0.25432

159A ->161A -0.18497

149B ->160B 0.68331

151B ->167B -0.10654

153B ->163B 0.23621

153B ->165B -0.10783

154B ->163B -0.11582

154B ->164B -0.10810

154B ->165B -0.23901

157B ->160B 0.13198

159B ->161B 0.11077

Excited State 29: 2.728-A 4.0928 eV 302.93 nm f=0.0042 <S\*\*2>=1.610

151A ->168A -0.15761

155A ->165A -0.11386

159A ->161A 0.14484

159A ->163A -0.11685

159A ->172A	-0.10809
160A ->166A	0.18167
160A ->167A	0.29324
160A ->169A	-0.20347
160A ->170A	0.43273
160A ->172A	0.15623
160A ->173A	0.10884
160A ->174A	-0.12675
148B ->160B	0.34638
152B ->168B	-0.17386
154B ->165B	0.11012
159B ->162B	0.26433
159B ->164B	0.17753
159B ->170B	0.12071
159B ->172B	-0.12673

Excited State 30: 2.305-A 4.1699 eV 297.33 nm f=0.0067 <S\*\*2>=1.078

160A ->166A	0.18268
160A ->167A	-0.17832
160A ->169A	0.25986
160A ->170A	0.61761
160A ->171A	0.42964
160A ->172A	-0.13888
148B ->160B	-0.33124

Mes<sub>2</sub>PyIDBTM (UB3LYP/6-31G(d))

Excited State 1: 2.063-A 2.3605 eV 525.24 nm f=0.0879 <S\*\*2>=0.814

183B ->184B	0.98511
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This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -3570.61025951

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

Excited State 2: 2.214-A 2.7126 eV 457.07 nm f=0.0332 <S\*\*2>=0.976

183A ->186A	0.12910
184A ->186A	0.73569
173B ->184B	-0.18851
174B ->184B	-0.27829
182B ->184B	0.49092

Excited State 3: 2.174-A 2.7470 eV 451.35 nm f=0.0198 <S\*\*2>=0.931

182A ->185A	-0.11572
184A ->186A	-0.45641
173B ->184B	0.18299
182B ->184B	0.82642
182B ->185B	-0.10371

Excited State 4: 2.350-A 2.8869 eV 429.48 nm f=0.0060 <S\*\*2>=1.131

183A ->185A	-0.13453
184A ->185A	0.95639
183B ->185B	0.20145

Excited State 5: 2.120-A 3.0682 eV 404.09 nm f=0.0024 <S\*\*2>=0.873

184A ->187A	-0.50887
184A ->188A	0.13043
175B ->184B	0.41560
176B ->184B	0.60021
177B ->184B	0.30719
180B ->184B	-0.17971
181B ->184B	0.10135

Excited State 6: 2.069-A 3.0960 eV 400.47 nm f=0.0010 <S\*\*2>=0.820

181B ->184B	0.98764
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Excited State 7: 2.131-A 3.1005 eV 399.89 nm f=0.0013 <S\*\*2>=0.885

184A ->187A	-0.26495
184A ->188A	-0.34283
175B ->184B	0.65464
176B ->184B	-0.51897
177B ->184B	-0.12146
178B ->184B	-0.15818
180B ->184B	0.16427

Excited State 8: 2.071-A 3.1604 eV 392.31 nm f=0.0004 <S\*\*2>=0.822  
179B ->184B 0.99106

Excited State 9: 2.063-A 3.2112 eV 386.10 nm f=0.0006 <S\*\*2>=0.814  
184A ->188A 0.10170  
176B ->184B 0.16452  
177B ->184B 0.10259  
180B ->184B 0.96378

Excited State 10: 2.295-A 3.2271 eV 384.20 nm f=0.0555 <S\*\*2>=1.066  
182A ->185A 0.12834  
184A ->186A 0.23597  
184A ->187A 0.19112  
184A ->189A 0.20489  
172B ->184B -0.27364  
173B ->184B 0.12750  
174B ->184B 0.35686  
176B ->184B -0.24530  
177B ->184B 0.64010  
182B ->184B 0.11587  
182B ->185B 0.13764

Excited State 11: 2.741-A 3.2697 eV 379.19 nm f=0.0292 <S\*\*2>=1.629  
173A ->186A 0.10742  
182A ->185A 0.31350  
183A ->192A 0.13194  
184A ->186A 0.14879  
184A ->188A -0.15426  
184A ->189A -0.28063  
184A ->192A -0.18102  
172B ->184B 0.37039  
174B ->184B 0.44798  
175B ->187B -0.11170  
177B ->184B -0.17079  
182B ->184B 0.17948  
182B ->185B 0.31243  
183B ->192B -0.15726

Excited State 12: 2.070-A 3.2759 eV 378.47 nm f=0.0054 <S\*\*2>=0.821  
184A ->187A -0.37562  
176B ->184B -0.16251

178B ->184B 0.88983

Excited State 13: 2.086-A 3.3073 eV 374.88 nm f=0.0114 <S\*\*2>=0.837

184A ->187A 0.65272

175B ->184B 0.53154

176B ->184B 0.28697

178B ->184B 0.40352

Excited State 14: 2.744-A 3.3156 eV 373.94 nm f=0.0480 <S\*\*2>=1.632

182A ->185A -0.33802

183A ->192A -0.11201

184A ->186A 0.18587

184A ->187A 0.12778

184A ->188A -0.23078

184A ->189A -0.24434

184A ->192A 0.16641

172B ->184B 0.35454

173B ->184B 0.27156

174B ->184B 0.12561

175B ->187B -0.11063

177B ->184B 0.36744

182B ->184B -0.12886

182B ->185B -0.33290

183B ->192B 0.13271

Excited State 15: 2.318-A 3.3457 eV 370.58 nm f=0.0885 <S\*\*2>=1.093

182A ->185A 0.17172

184A ->186A -0.25833

184A ->188A -0.19893

184A ->189A -0.15212

172B ->184B 0.19365

173B ->184B -0.35444

174B ->184B -0.48743

176B ->184B -0.12670

177B ->184B 0.52820

182B ->185B 0.17987

Excited State 16: 2.185-A 3.4011 eV 364.54 nm f=0.0030 <S\*\*2>=0.943

184A ->188A 0.81549

184A ->189A -0.21100

172B ->184B 0.19975

175B ->184B 0.23169

176B ->184B -0.33250

183B ->185B -0.10626

Excited State 17: 2.367-A 3.5547 eV 348.79 nm f=0.0333 <S\*\*2>=1.150

182A ->185A 0.30618

184A ->186A 0.11541

173B ->184B 0.74089

174B ->184B -0.48907

182B ->185B 0.20567

Excited State 18: 3.469-A 3.6305 eV 341.51 nm f=0.0002 <S\*\*2>=2.758

178A ->193A -0.40710

179A ->190A 0.43918

180A ->190A -0.28050

180A ->194A 0.11093

181A ->191A -0.16862

178B ->193B 0.40709

179B ->189B -0.52392

180B ->194B -0.13406

181B ->190B 0.17034

Excited State 19: 3.469-A 3.6310 eV 341.46 nm f=0.0000 <S\*\*2>=2.758

178A ->193A -0.13416

179A ->190A 0.14421

179A ->194A -0.21564

180A ->194A -0.33671

181A ->191A 0.51029

178B ->193B 0.13389

179B ->189B -0.17282

180B ->194B 0.40727

181B ->190B -0.51916

Excited State 20: 3.034-A 3.7216 eV 333.15 nm f=0.0610 <S\*\*2>=2.052

172A ->185A -0.10167

173A ->192A -0.11502

174A ->192A 0.14229

183A ->185A -0.38582

184A ->185A -0.20527

184A ->188A 0.14152

184A ->189A 0.39922

184A ->197A -0.12445

171B ->185B -0.10842

172B ->184B	0.22784
173B ->192B	0.10035
174B ->192B	-0.12306
183B ->185B	0.58816
183B ->191B	-0.12331

Excited State 21: 3.267-A 3.8290 eV 323.81 nm f=0.0086 <S\*\*2>=2.419

172A ->186A	-0.11415
175A ->187A	-0.29432
175A ->188A	-0.19052
176A ->187A	0.22932
176A ->188A	-0.30503
183A ->186A	0.27812
184A ->186A	-0.15039
184A ->192A	0.10568
172B ->186B	0.15249
173B ->184B	0.30086
174B ->184B	0.20351
175B ->187B	0.27272
175B ->188B	0.20000
176B ->187B	-0.23063
176B ->188B	0.26968
177B ->188B	0.10731
183B ->186B	-0.25386

Excited State 22: 2.852-A 3.8525 eV 321.83 nm f=0.0257 <S\*\*2>=1.784

173A ->186A	0.10666
174A ->186A	0.12102
175A ->187A	0.19489
175A ->188A	0.12081
176A ->187A	0.13085
176A ->188A	-0.17895
183A ->185A	0.20899
184A ->185A	0.12091
184A ->189A	0.65580
175B ->187B	-0.21052
175B ->188B	-0.12302
176B ->187B	-0.12438
176B ->188B	0.18964
183B ->185B	-0.40895

Excited State 23: 2.840-A 3.8857 eV 319.08 nm f=0.0194 <S\*\*2>=1.766

175A ->187A	-0.28191
175A ->188A	-0.17417
176A ->187A	-0.16895
176A ->188A	0.23071
183A ->185A	0.11182
184A ->189A	0.24690
184A ->197A	-0.12843
172B ->184B	0.61722
173B ->186B	0.11266
174B ->186B	0.11831
175B ->187B	0.25249
175B ->188B	0.14739
176B ->187B	0.12767
176B ->188B	-0.20140
183B ->185B	-0.22545

Excited State 24: 2.693-A 3.9315 eV 315.36 nm f=0.0103 <S\*\*2>=1.563

177A ->185A	0.11820
182A ->185A	0.16063
183A ->192A	-0.13662
184A ->191A	-0.11710
184A ->192A	0.76091
173B ->184B	-0.18022
174B ->184B	0.11613
177B ->185B	-0.11707
182B ->185B	0.39787
183B ->192B	0.19753

Excited State 25: 3.435-A 3.9901 eV 310.73 nm f=0.0005 <S\*\*2>=2.699

176A ->185A	-0.11102
177A ->185A	0.64689
177A ->197A	0.13822
177A ->198A	0.17933
184A ->192A	-0.15546
174B ->185B	0.10174
176B ->185B	0.18806
177B ->185B	-0.58268
177B ->197B	-0.19960

Excited State 26: 2.093-A 4.1665 eV 297.57 nm f=0.0048 <S\*\*2>=0.845

184A ->193A	0.13117
184A ->194A	0.23821



184A ->195A 0.93719

Excited State 27: 2.111-A 4.2290 eV 293.17 nm f=0.0005 <S\*\*2>=0.864  
184A ->190A 0.98259

Excited State 28: 3.396-A 4.2488 eV 291.81 nm f=0.0004 <S\*\*2>=2.633  
175A ->187A -0.20567  
175A ->188A -0.12763  
176A ->187A 0.14450  
176A ->188A -0.18500  
183A ->186A -0.46779  
172B ->186B -0.10860  
175B ->187B 0.19280  
175B ->188B 0.13473  
176B ->187B -0.14661  
176B ->188B 0.16074  
183B ->186B 0.66455

Excited State 29: 2.872-A 4.2606 eV 291.00 nm f=0.0112 <S\*\*2>=1.812  
171A ->185A 0.13074  
173A ->192A -0.13424  
174A ->185A 0.11738  
174A ->192A 0.16556  
182A ->192A 0.13016  
182A ->198A 0.14182  
183A ->185A -0.12263  
183A ->189A -0.18487  
183A ->197A 0.16515  
184A ->189A -0.20195  
184A ->196A 0.42162  
184A ->197A -0.33189  
171B ->185B -0.15808  
172B ->184B -0.17190  
173B ->192B 0.14838  
174B ->185B -0.11261  
174B ->192B -0.19125  
182B ->197B 0.11754  
183B ->185B -0.28507  
183B ->186B -0.10552  
183B ->191B -0.30826  
183B ->197B -0.11968  
183B ->198B -0.12932

Excited State 30: 2.117-A 4.2971 eV 288.53 nm f=0.0004 <S\*\*2>=0.870  
184A ->191A 0.97571  
184A ->192A 0.10831

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