

# Electronic Supplementary Information

## Theoretical Elucidation of the Effect of Linkage and Orientation of Carbazole on the Naphthalenediimide and the TADF and RTP Propensity

*Chetan Saini, Siddan Gouthaman, K. R. Justin Thomas\**

Organic Materials Laboratory, Department of Chemistry, Indian Institute of Technology

Roorkee, Roorkee – 247667, India.

\*Corresponding author. E-mail: krjt@cy.iitr.ac.in

### Supporting Information

Computational Methodology	S3
<b>Figure S1.</b> $S_0$ , $S_1$ and $T_1$ optimized geometries in the gaseous state of the investigated molecules.	S4
<b>Figure S2.</b> Frontier orbital distribution at the optimized $S_0$ geometries for the investigated molecules.	S4
<b>Figure S3.</b> Calculated absorption of the proposed molecules using benchmark functional SOGGA11X/6-31+g(d).	S5
<b>Figure S4.</b> Theoretical absorption spectra are generated using the Molden program with FWHM of 0.25 eV for all twelve molecules.	S5-9
<b>Figure S5 (a-b).</b> Natural transition orbitals (NTOs) of the $S_1$ and $T_1$ states for the investigated molecules at $S_1$ and $T_1$ geometry, respectively.	S10-11
<b>Figure S6 (a).</b> HDI at $S_1$ and $T_1$ state at $S_1$ and $T_1$ geometry of the proposed molecules.	S12
<b>Figure S6 (b).</b> EDI at $S_1$ and $T_1$ state at $S_1$ and $T_1$ geometry of the proposed molecules.	S12
<b>Figure S7.</b> $\Lambda$ and $S_m$ index at $S_1$ and $T_1$ geometry of the proposed molecules.	S13
<b>Figure S8.</b> $S_r$ index at $S_1$ and $T_1$ geometry of the proposed molecules.	S13
<b>Figure S9 (a).</b> %CT at $S_1$ geometry of the proposed molecules.	S14
<b>Figure S9 (b).</b> %LE at $T_1$ geometry of the proposed molecules.	S14
<b>Figure S10.</b> D index at $S_1$ and $T_1$ geometry of the proposed molecules.	S15
<b>Figure S11.</b> t index at $S_1$ and $T_1$ geometry of the proposed molecules.	S15
<b>Figure S12 (a-l).</b> Qualitative analysis of the possibilities of ISC and RISC rates.	S16-21
<b>Figure S13 (a-d).</b> ISC and RISC rates of the investigated molecules vs external reorganization energy range.	S21
<b>Figure S14 (a-b).</b> The rate for the RISC process in the studied emitters as a function	S22

of the external reorganization energy.	
<b>Table S1.</b> Bond length and dihedral angle of TADF emitters at $S_0$ , $S_1$ , and $T_1$ optimized geometries.	S23
<b>Table S2.</b> Dihedral angles of the molecules at $S_0$ , $S_1$ and $T_1$ optimized geometries.	S23-24
<b>Table S3.</b> $S_1$ and $T_1$ states calculated by the TDA-DFT approach at $S_1$ and $T_1$ optimized geometries in gaseous state.	S25
<b>Table S4.</b> Benchmarking for absorption of the reported molecules ( <i>Cz2i</i> , <i>pCz2i</i> ).	S26
<b>Table S5.</b> Absorption data calculated using benchmark function SOGGA11X/6-31+G(d).	S26
<b>Table S6.</b> Charge transfer indices of TADF emitters at Singlet ( $S_1$ ) and Triplet ( $T_1$ ) optimized geometries.	S27
<b>Table S7.</b> SOC of the molecules between $S_0$ - $T_1$ state for potential RTP molecules.	S28
<b>Table S8.</b> $k_{ISC}$ and $k_{RISC}$ rate of all the investigated molecules at external reorganization energy ( $\lambda_{ext}$ ) value variation.	S28-31
Optimized XYZ coordinates of all molecules in $S_0$ , $S_1$ and $T_1$ geometries.	S32

## Computational Methodology

The ground state ( $S_0$ ) geometries optimizations of all compounds were performed by DFT using B3LYP<sup>1-2</sup> functional with the 6-31 G(d,p) basis set and D3ZERO (dispersion interaction) in ORCA 5.0.3 software<sup>3</sup>. The Tamm-Dancoff approximation (TDA) is applied on the optimized ground state ( $S_0$ ) geometry for TDA-DFT calculations to avoid the instability of the triplet state in TD-DFT.<sup>4</sup> All the optimized structures were characterized by frequency analysis, and all the frequencies were positive. The geometries of the lowest excited singlet ( $S_1$ ) and triplet ( $T_1$ ) states were optimized by Time dependent TD-DFT with B3LYP/6-31G(d,p) D3ZERO (dispersion interaction) level. All the dihedral angles were calculated using Mercury software. Natural transition orbitals (NTO) and all the charge transfer indices were calculated using a multi-wave functional analyzer program<sup>5</sup>.

The ionization potential (IP) and electron affinity (EA) for the molecules are calculated using the equations give below.

$$IP = E_{M^+} - E_M \quad (S1)$$

$$EA = E_M - E_{M^-} \quad (S2)$$

Where  $E_M$  represents the electronic energy of the molecule,  $E_{M^-}$  and  $E_{M^+}$  represent the energy of the anionic and cationic species by using the optimized geometry of the natural molecule.

To predict the emission properties of the designed TADF molecules, the radiative rates ( $k_r$ ) of the  $S_1$  states were evaluated using the Einstein spontaneous emission rate formula.<sup>6</sup>

$$k_r = \frac{f \Delta E^2}{1.499 \text{ cm}^{-2} \text{ s}} \quad (S3)$$

where  $f$  is the transition oscillator strength, and  $\Delta E$  is the vertical emission energy of the  $S_1$  state in the unit of wavenumbers ( $\text{cm}^{-1}$ ).

The  $k_{ISC}$  and  $k_{RISC}$  can be calculated in the framework of Fermi's golden-rule:<sup>7-9</sup>

$$k_{ISC}^{RISC} = \frac{2\pi}{\hbar} \left| \langle 1_{\Psi_I^0} | H_{SO} | 3_{\Psi_F^0} \rangle \right|^2_{FCWD} \quad (S4)$$

Where FCWD is the Franck-Condon weighted density of states.  $\langle 1_{\Psi_I^0} | H_{SO} | 3_{\Psi_F^0} \rangle$  is the SOC,  $\hbar$  is the reduced Dirac constant.<sup>10-12</sup>

$$FCWD = \frac{1}{\sqrt{4\pi\lambda RT}} \exp\left[-\frac{(\Delta E + \lambda)^2}{4\pi RT}\right] \quad (\text{S5})$$

Where  $\lambda$  is the total reorganization energy and  $\Delta E$  is the difference between the initial and final states and  $T$  is the temperature.

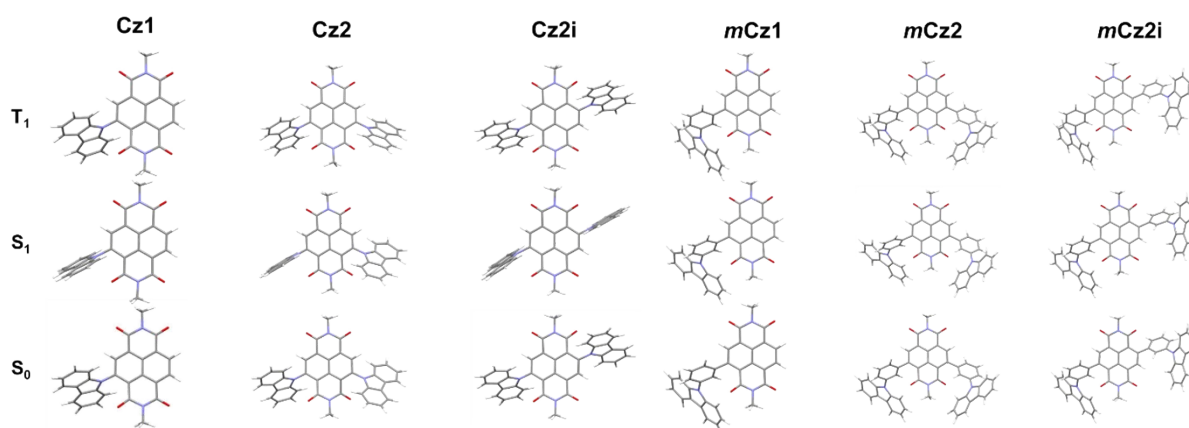
$\lambda$  is the total reorganization energy which is the sum of the inner and outer reorganization energy.  $\lambda = \lambda_{\text{ext}} + \lambda_{\text{in}}$

$$\lambda_{\text{in}}^{\text{ISC}} = E_S^T - E_T^T \quad (\text{S6})$$

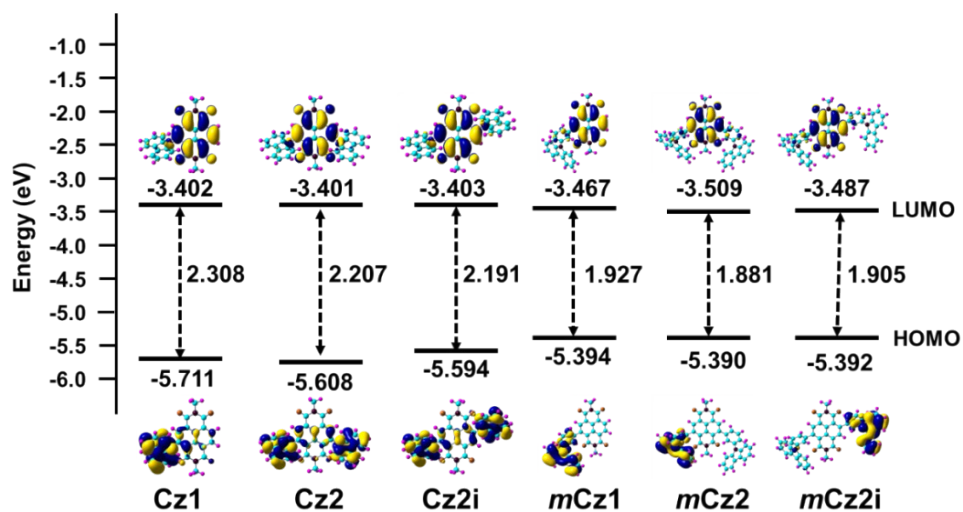
$$\lambda_{\text{in}}^{\text{RISC}} = E_T^S - E_S^S \quad (\text{S7})$$

Where  $E_S^T$  is the energy of triplet state at singlet state geometry,  $E_T^T$  is energy of triplet state at triplet state geometry,  $E_T^S$  is energy of singlet state at triplet state geometry and  $E_S^S$  is the energy of singlet state at singlet state geometry.<sup>13-14</sup>

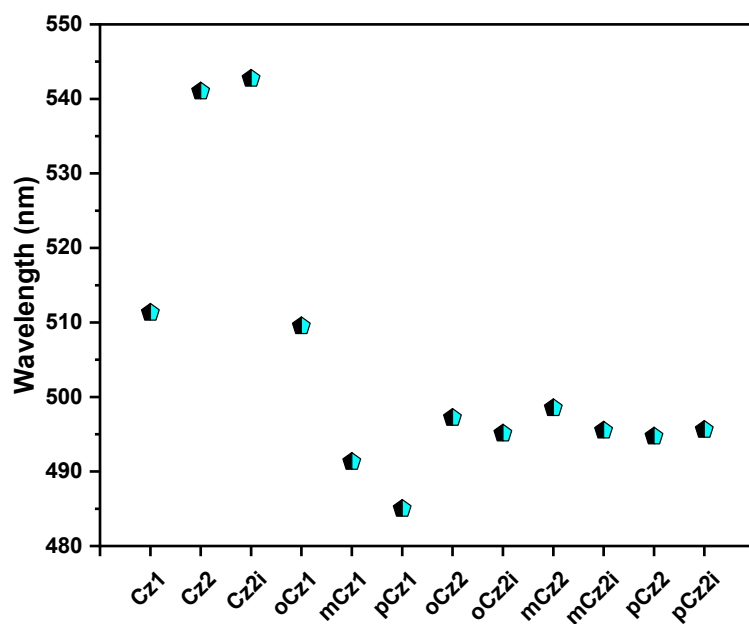
As the golden-rule expression states, ISC,  $\Delta E_{\text{ST}}$ , and SOC matrix elements are vital factors that determine  $k_{\text{ISC}}$  and  $k_{\text{RISC}}$ . SOC values were computed using the ORCA software.



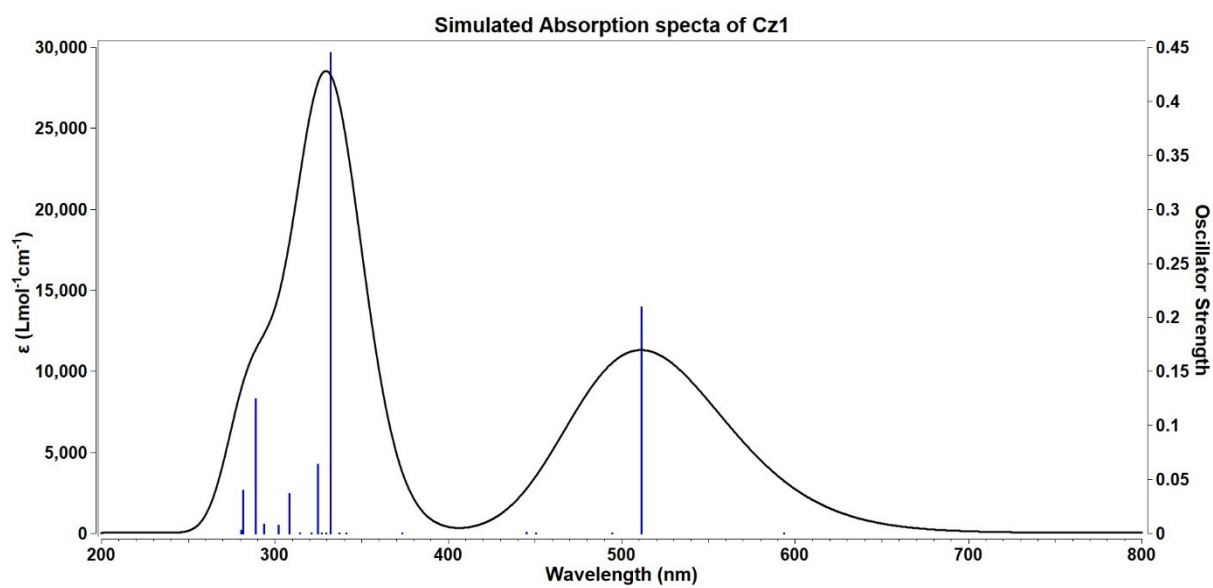
**Figure S1.**  $S_0$ ,  $S_1$  and  $T_1$  optimized geometries in the gaseous state of the investigated molecules.

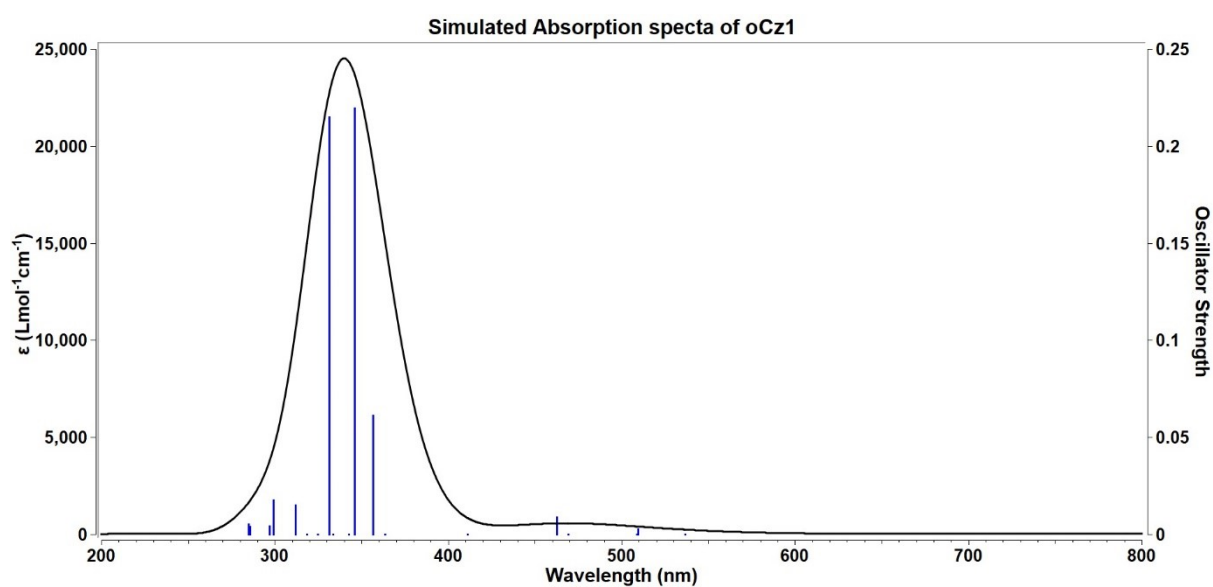
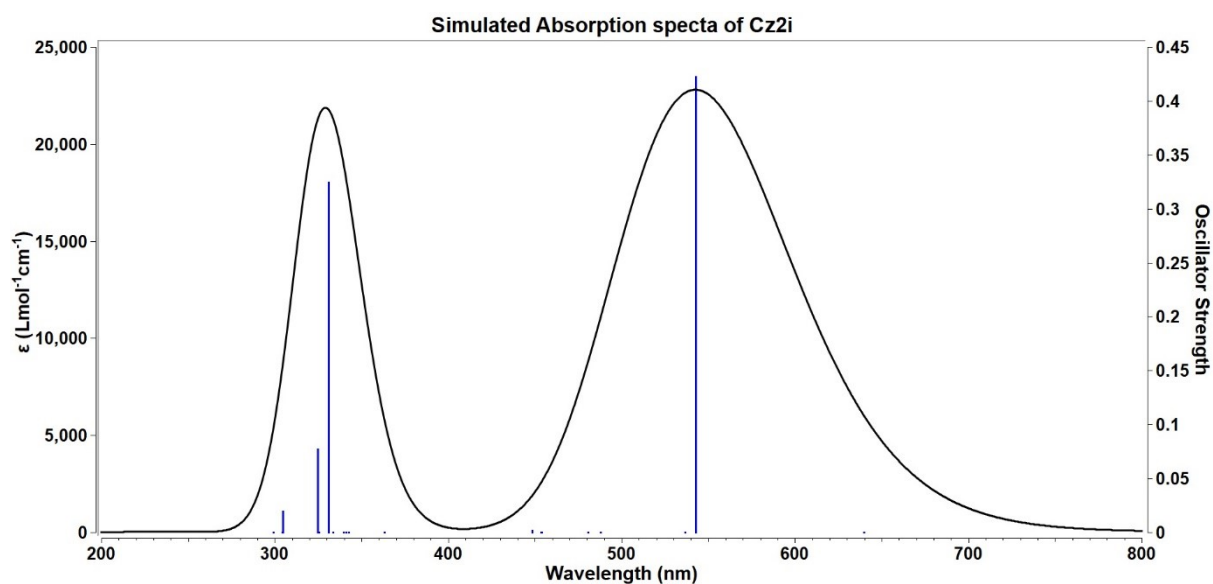
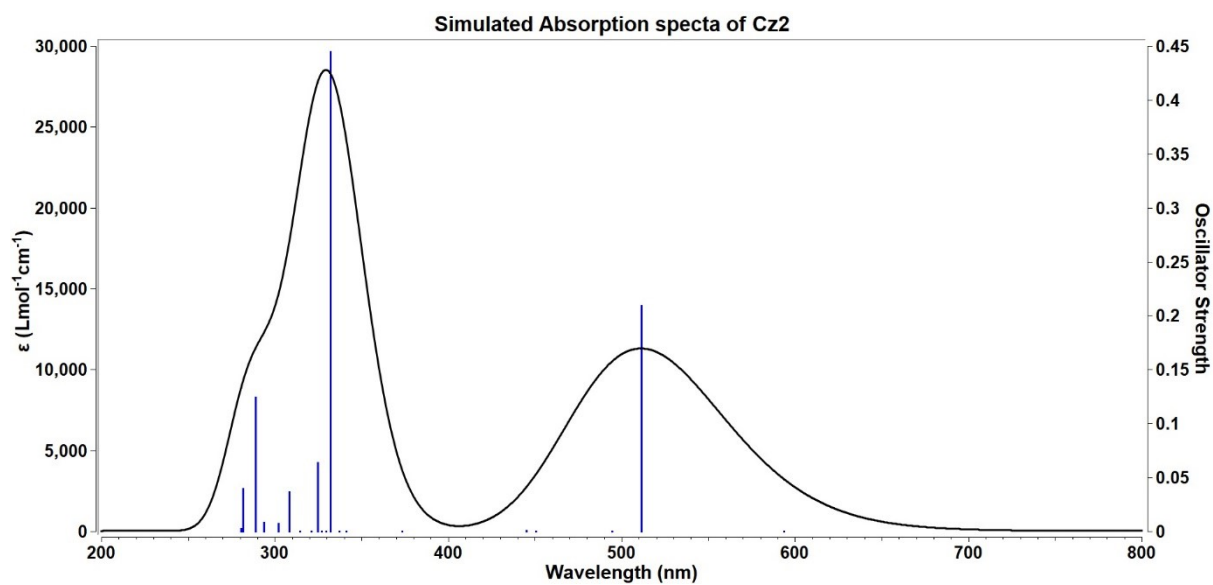


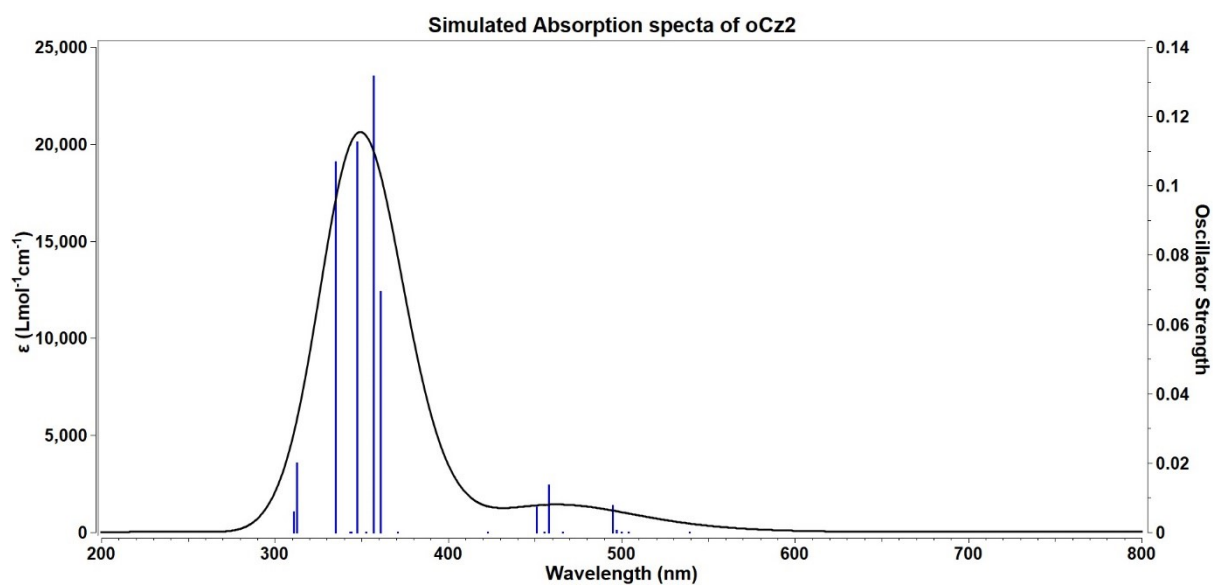
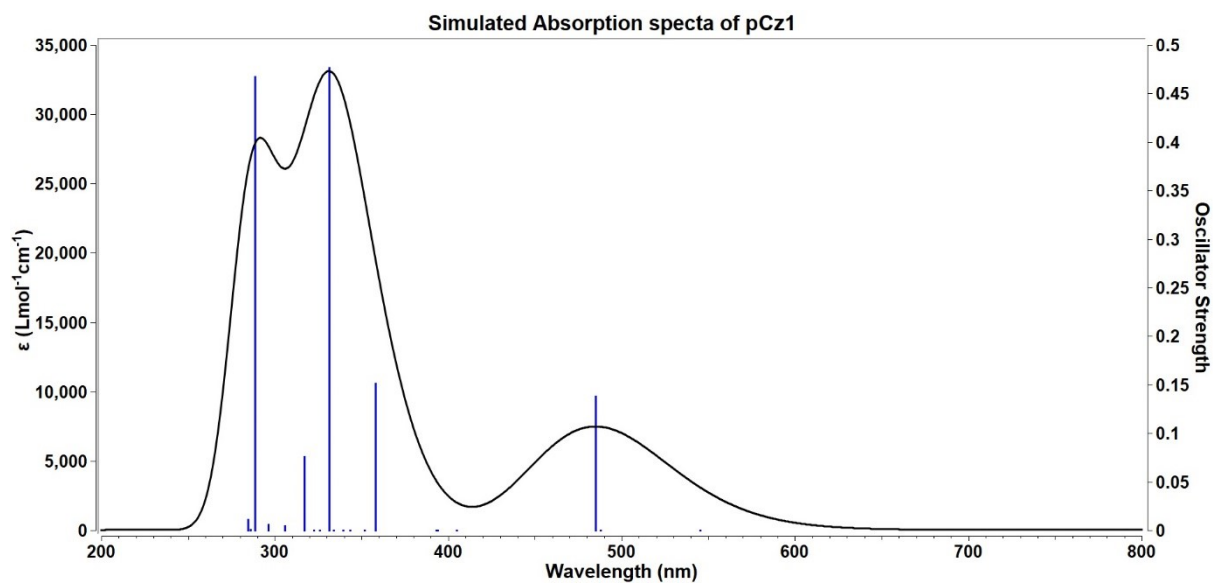
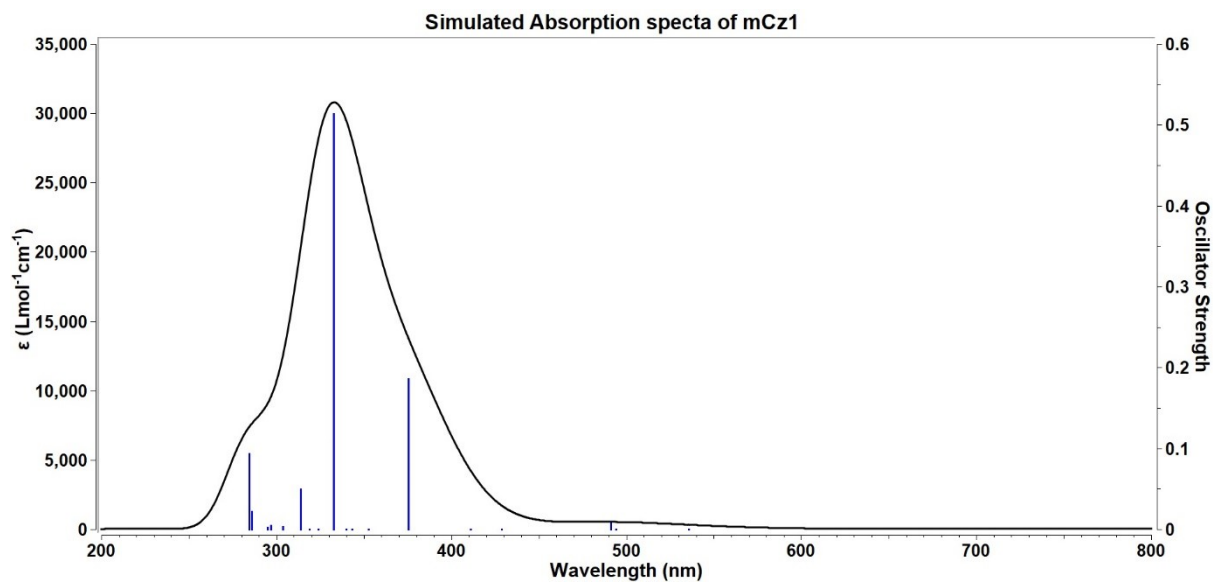
**Figure S2.** Frontier orbital distribution at the optimized  $S_0$  geometries for the investigated molecules.



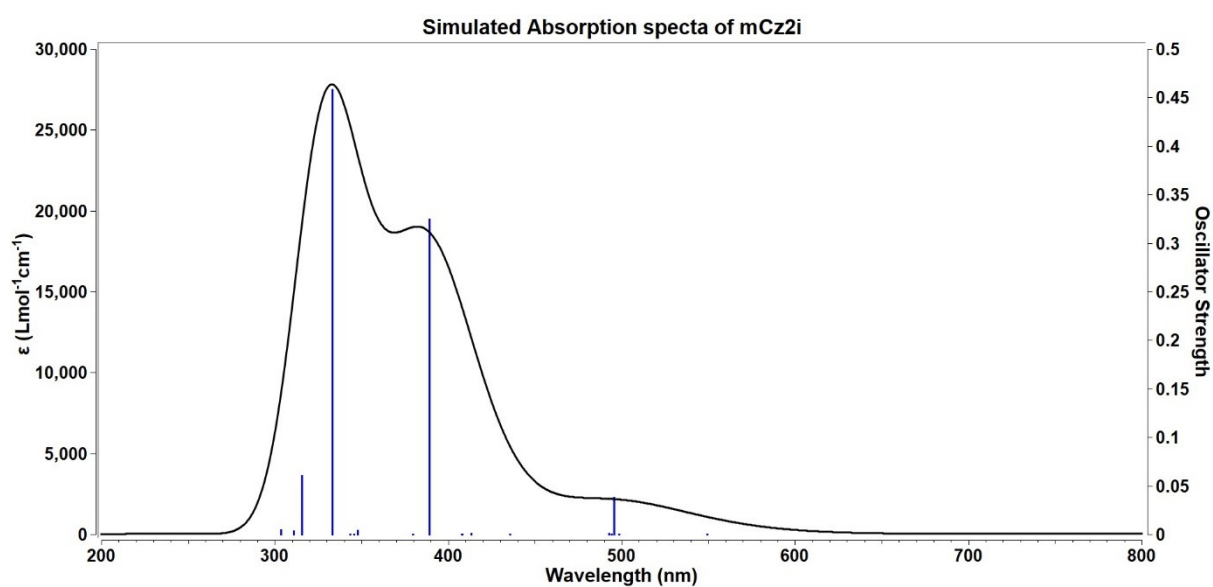
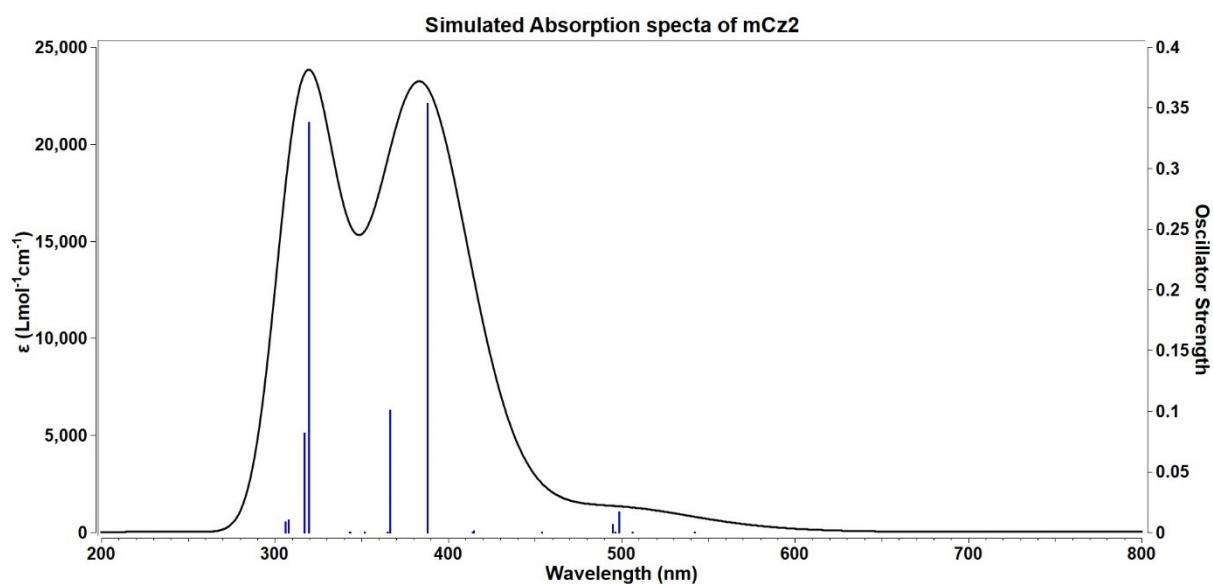
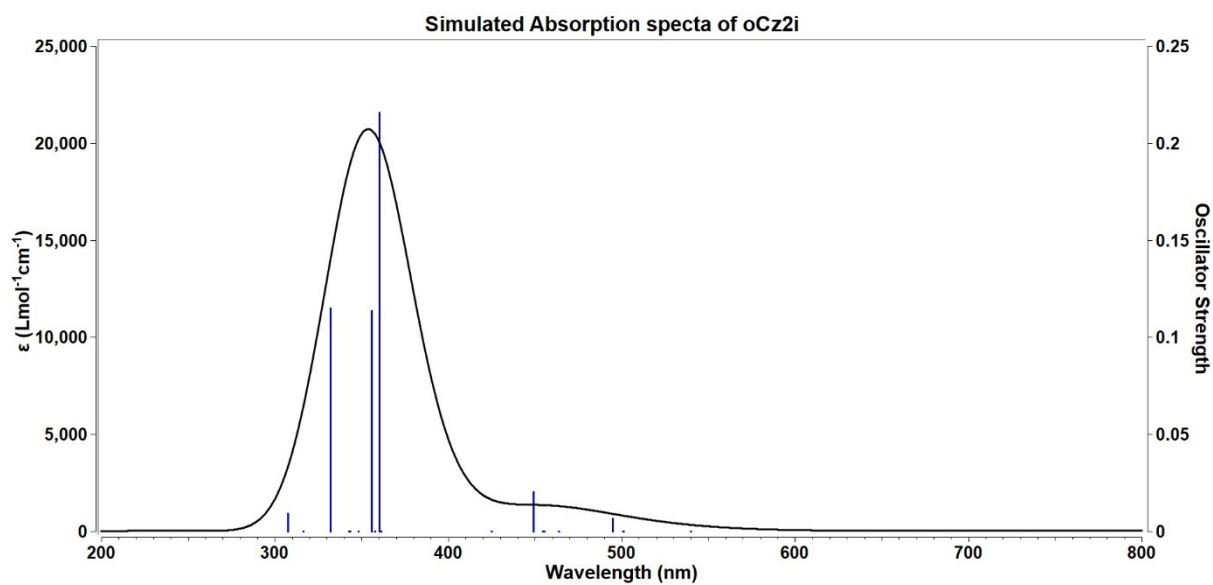
**Figure S3.** Calculated absorption of the proposed molecules using benchmark functional **SOGGA11X/6-31+g(d)**.

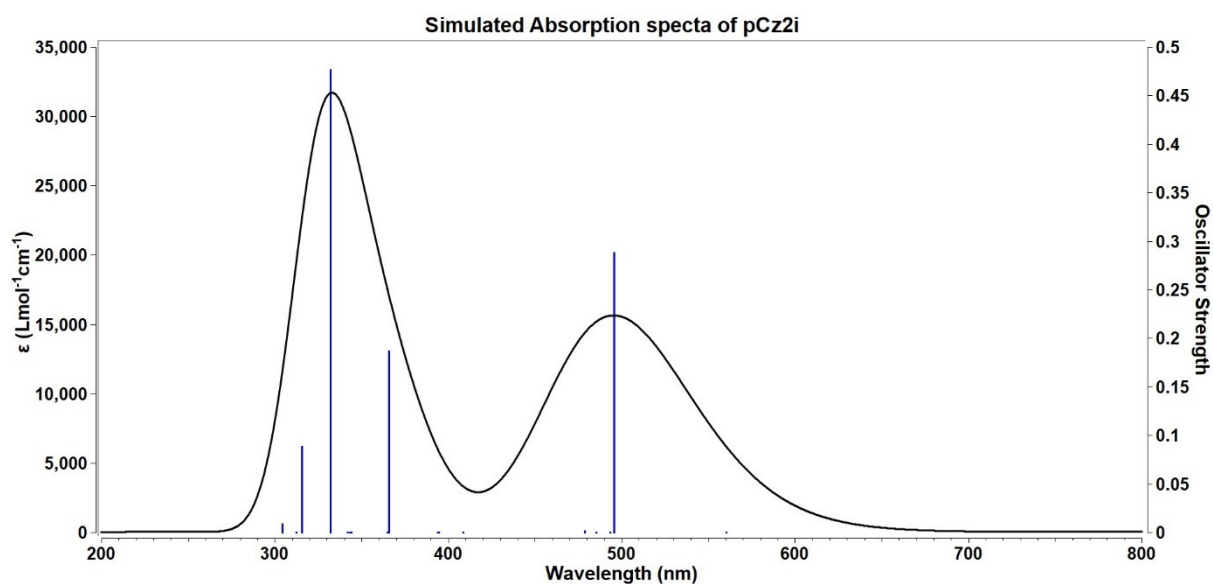
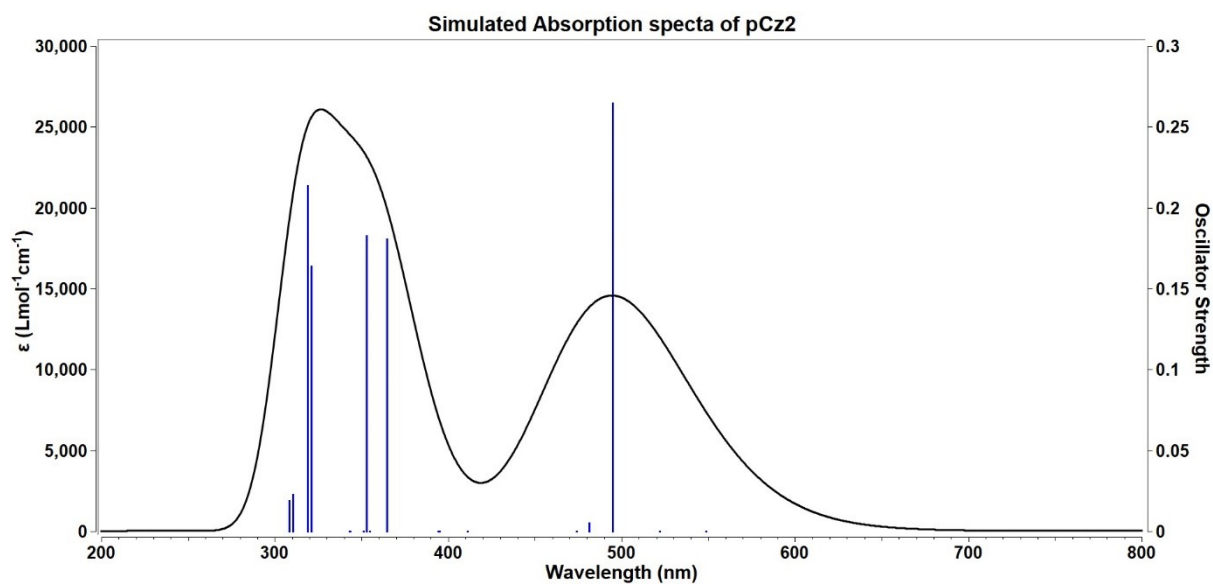




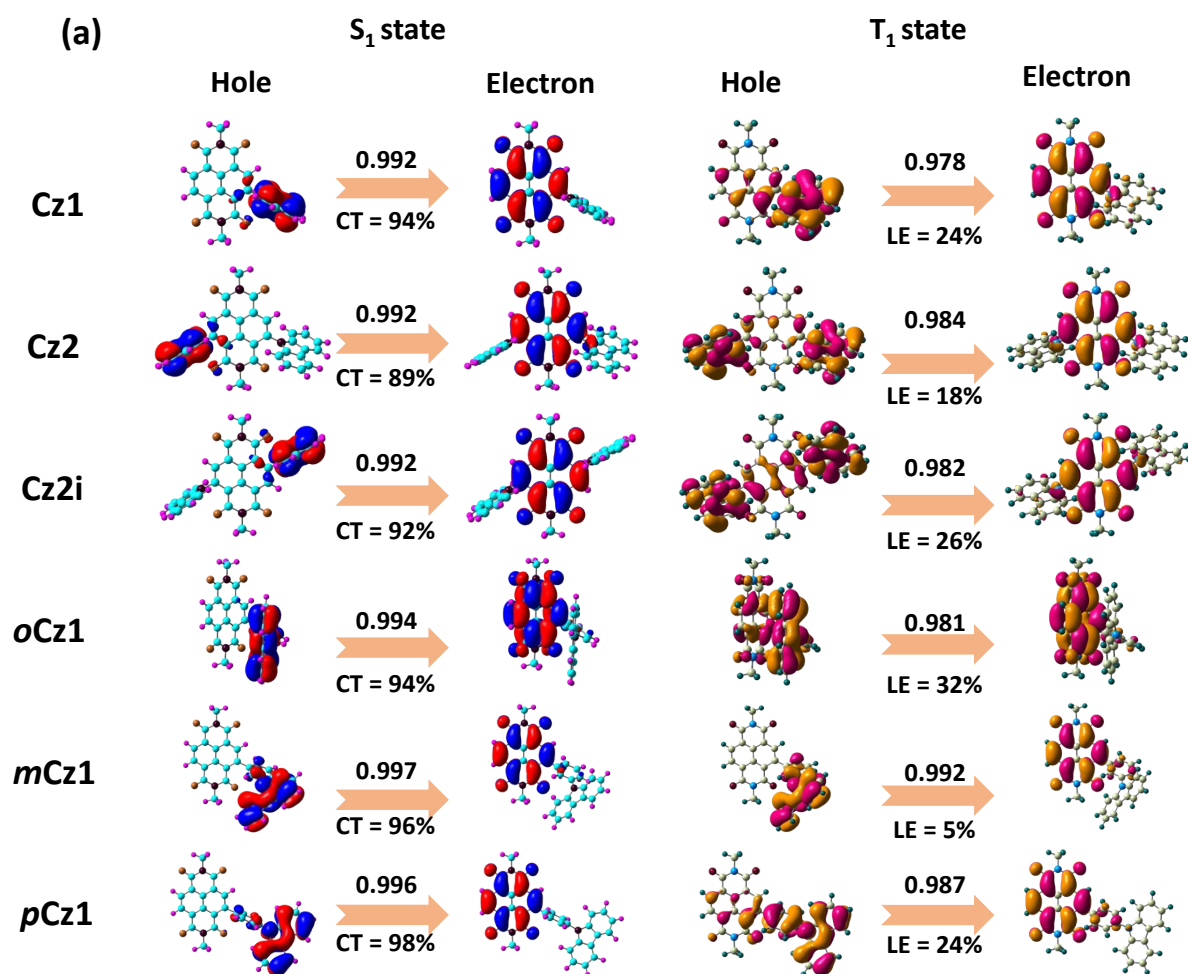








**Figure S4.** Theoretical absorption spectra are generated using the Molden program with FWHM of 0.25 eV for all twelve molecules.



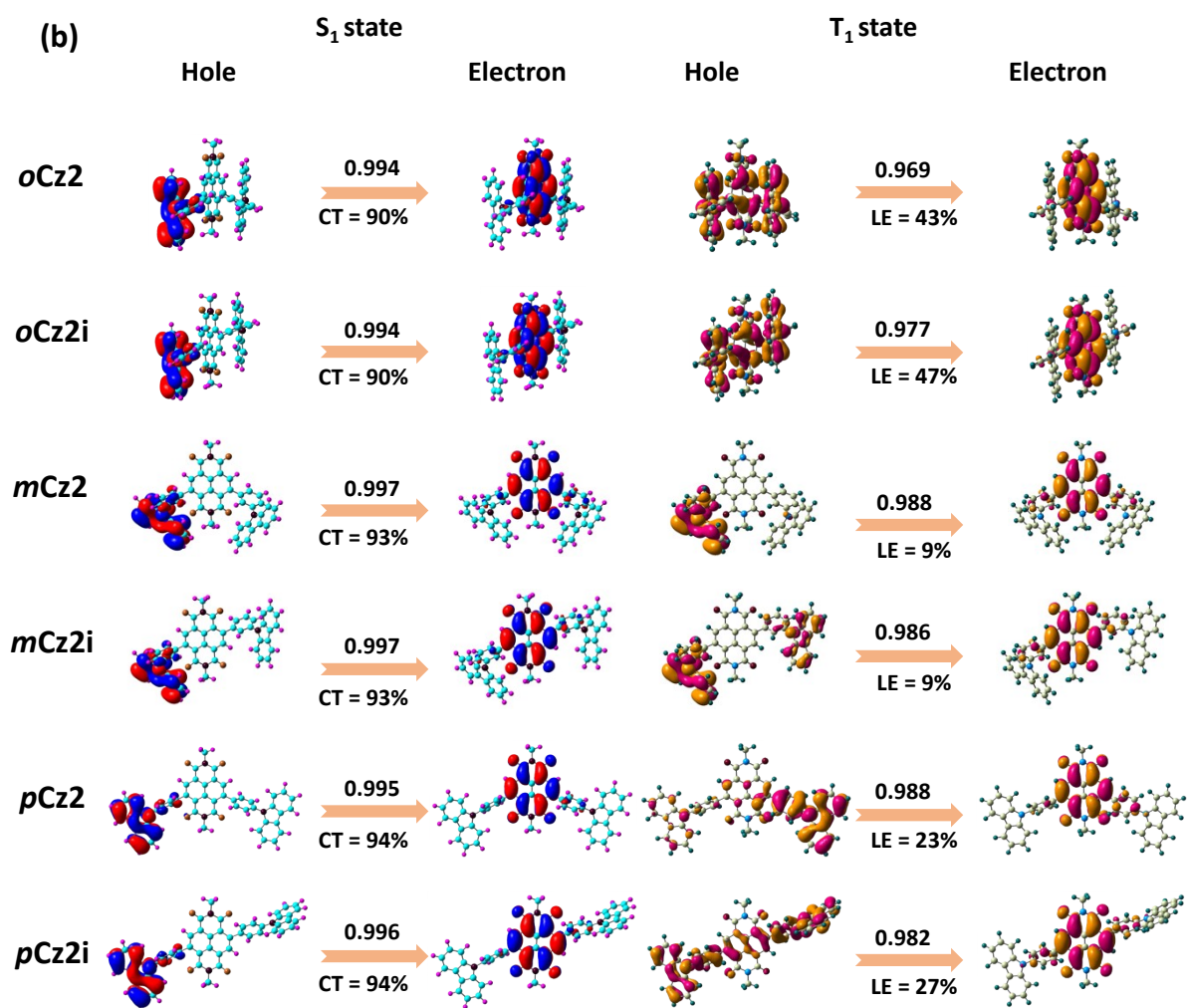


Figure S5 (a-b). Natural transition orbitals (NTOs) of the S<sub>1</sub> and T<sub>1</sub> states for the investigated molecules at S<sub>1</sub> and T<sub>1</sub> geometry, respectively.

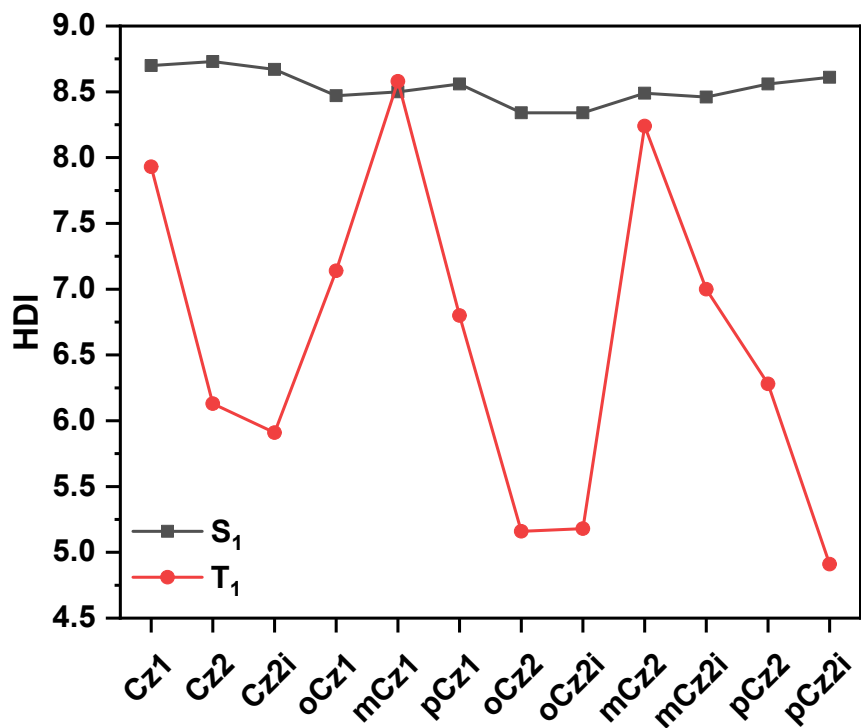


Figure S6 (a). HDI at S<sub>1</sub> and T<sub>1</sub> state at S<sub>1</sub> and T<sub>1</sub> geometry of the proposed molecules

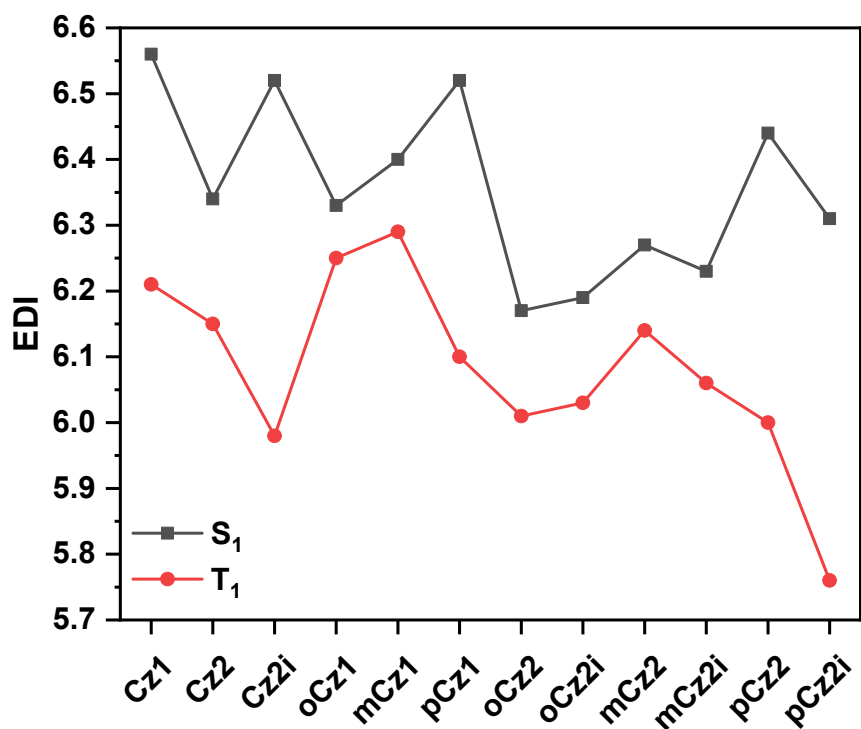


Figure S6 (b). EDI at S<sub>1</sub> and T<sub>1</sub> state at S<sub>1</sub> and T<sub>1</sub> geometry of the proposed molecules

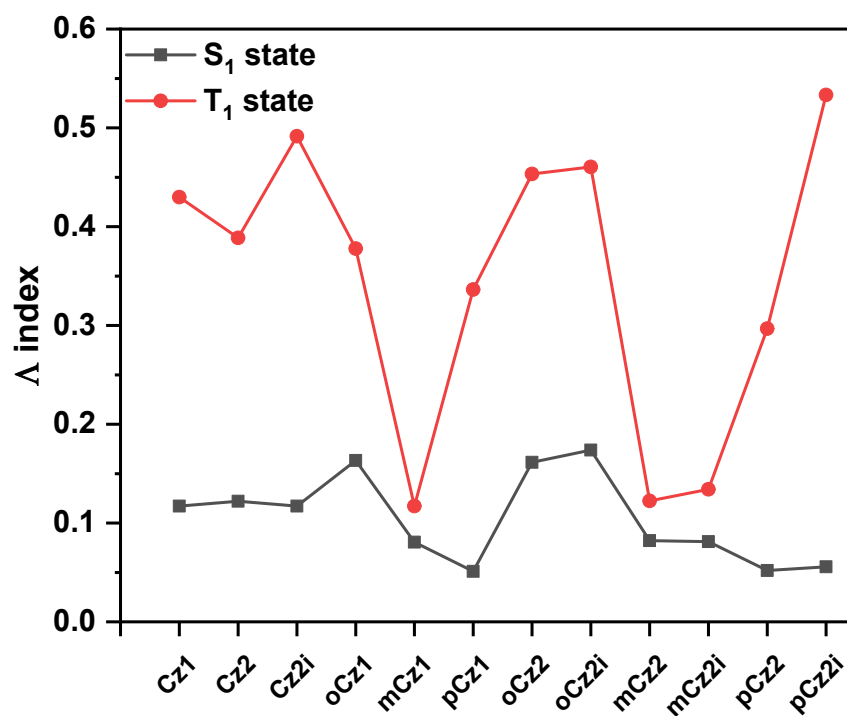


Figure S7.  $\Delta$  index at  $S_1$  and  $T_1$  geometry of the proposed molecules

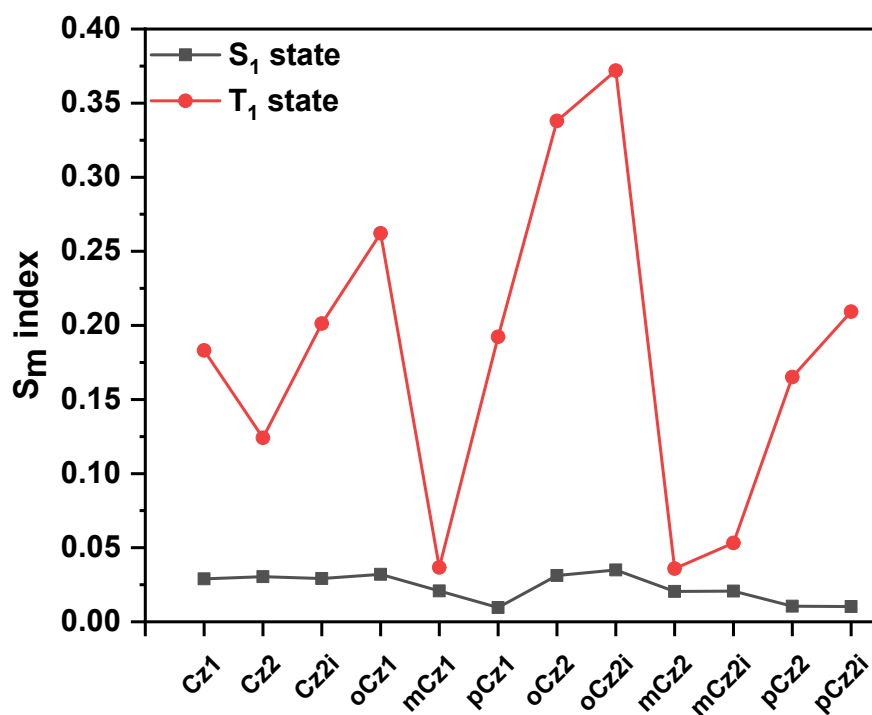


Figure S8.  $S_m$  index at  $S_1$  and  $T_1$  geometry of the proposed molecules

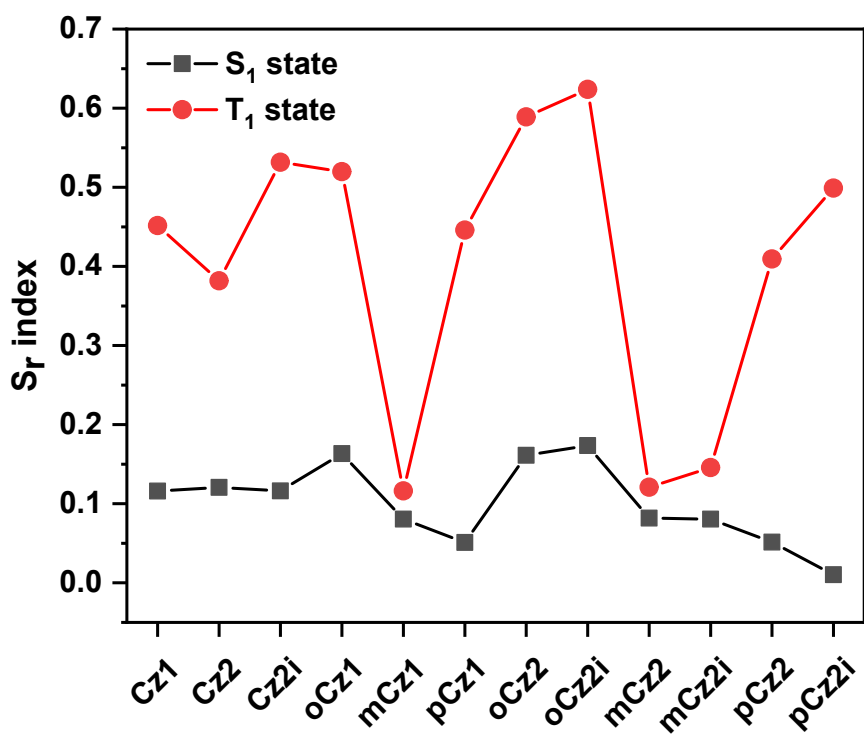


Figure S9.  $S_r$  index at  $S_1$  and  $T_1$  geometry of the proposed molecules

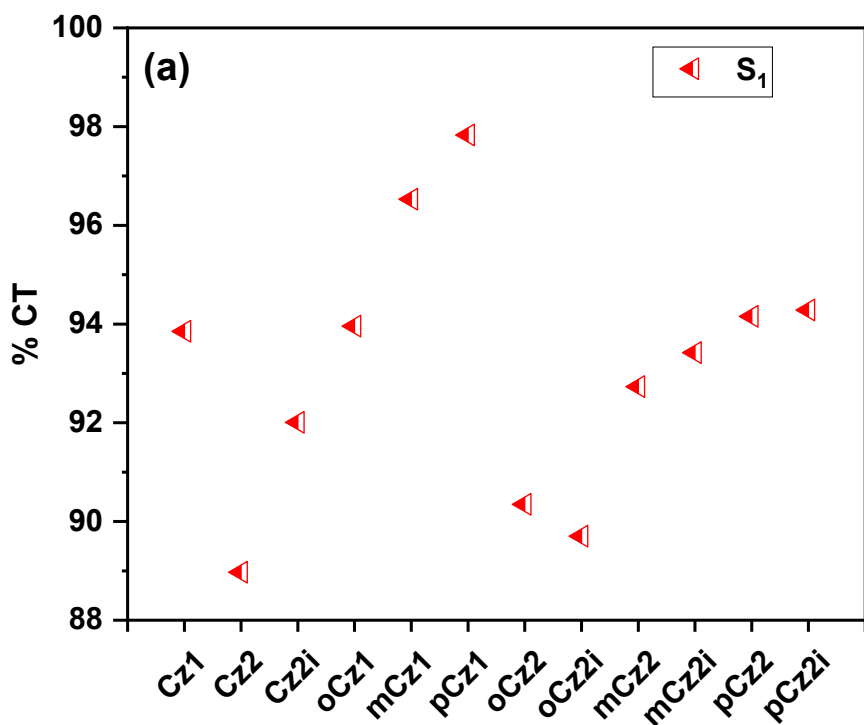


Figure S10 (a). % CT at  $S_1$  geometry of the proposed molecules

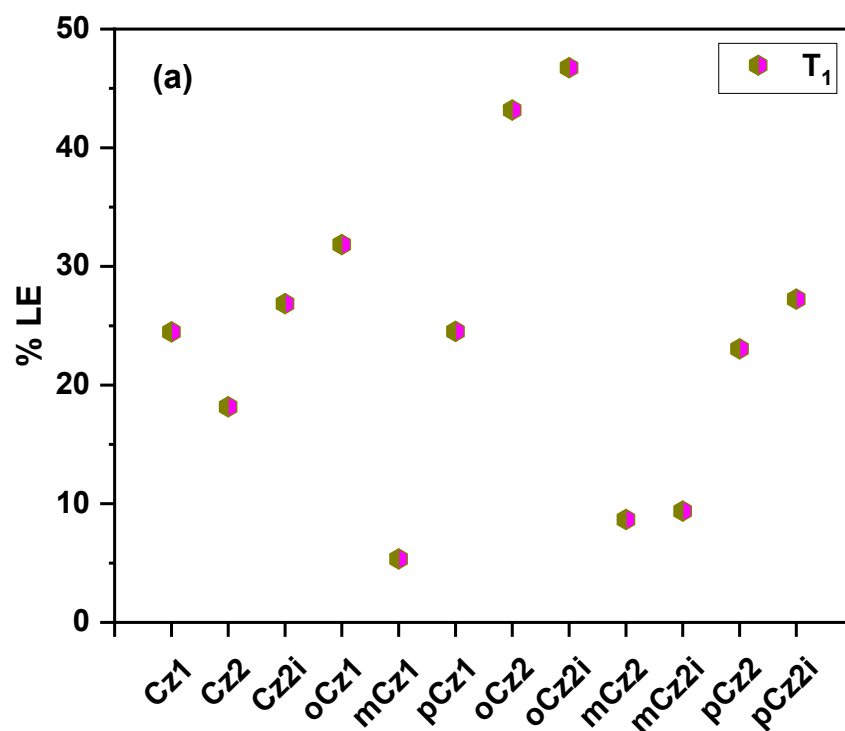


Figure S10 (b). % LE at T<sub>1</sub> geometry of the proposed molecules

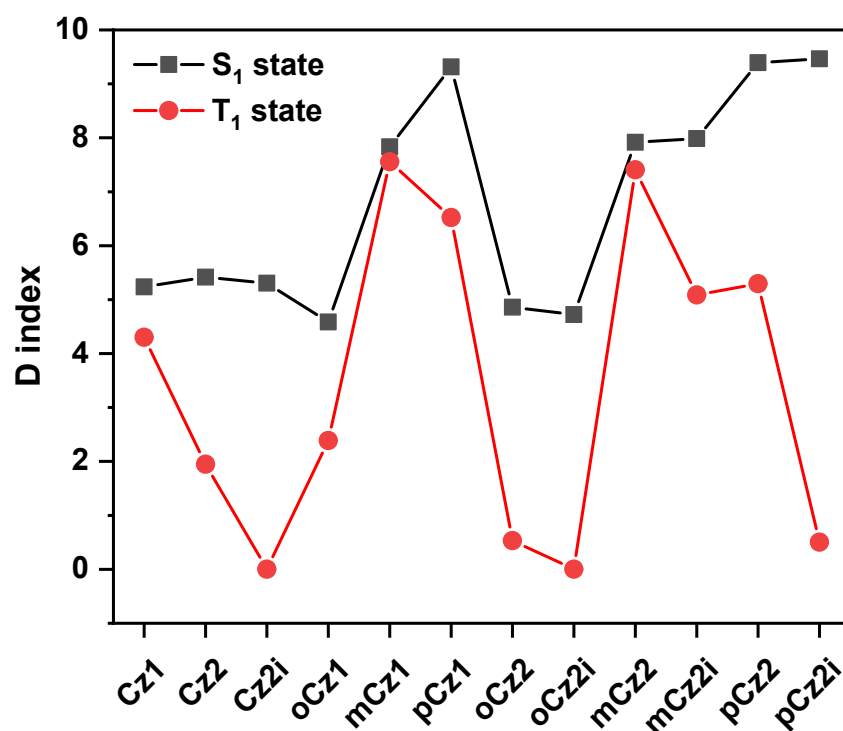


Figure S11. D index at S<sub>1</sub> and T<sub>1</sub> geometry of the proposed molecules



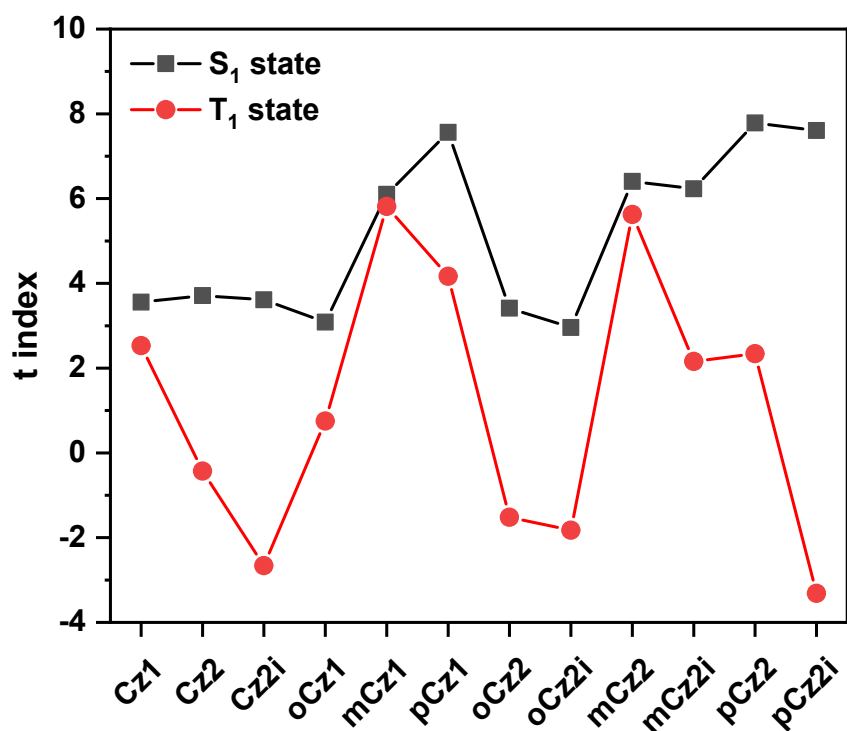
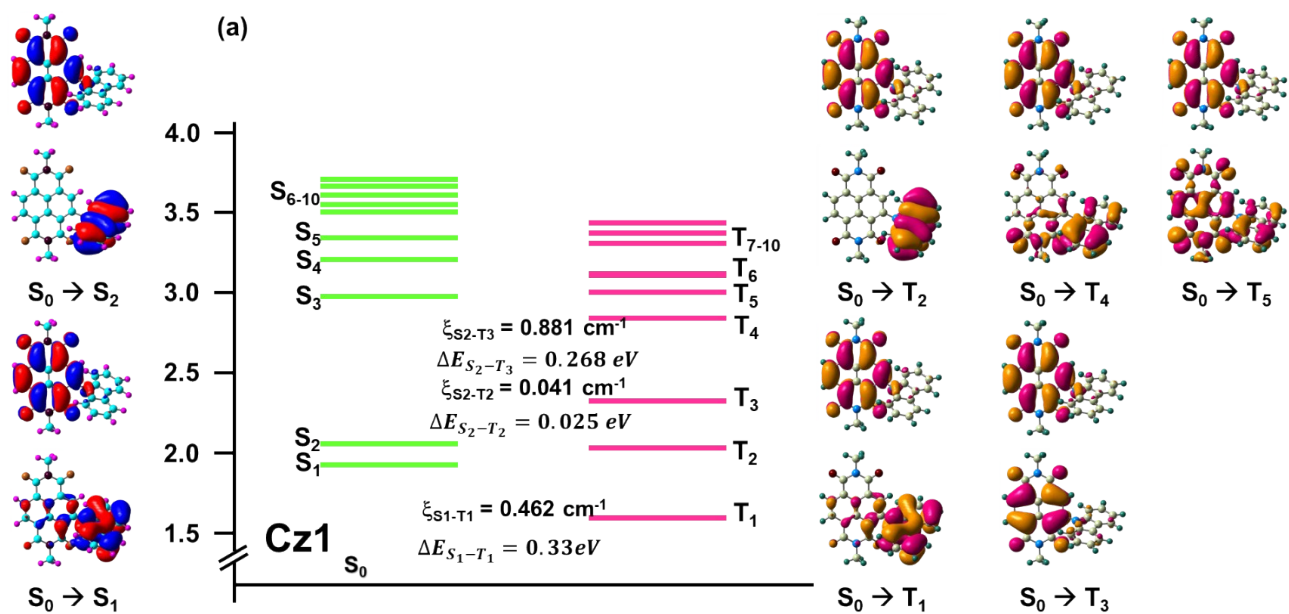
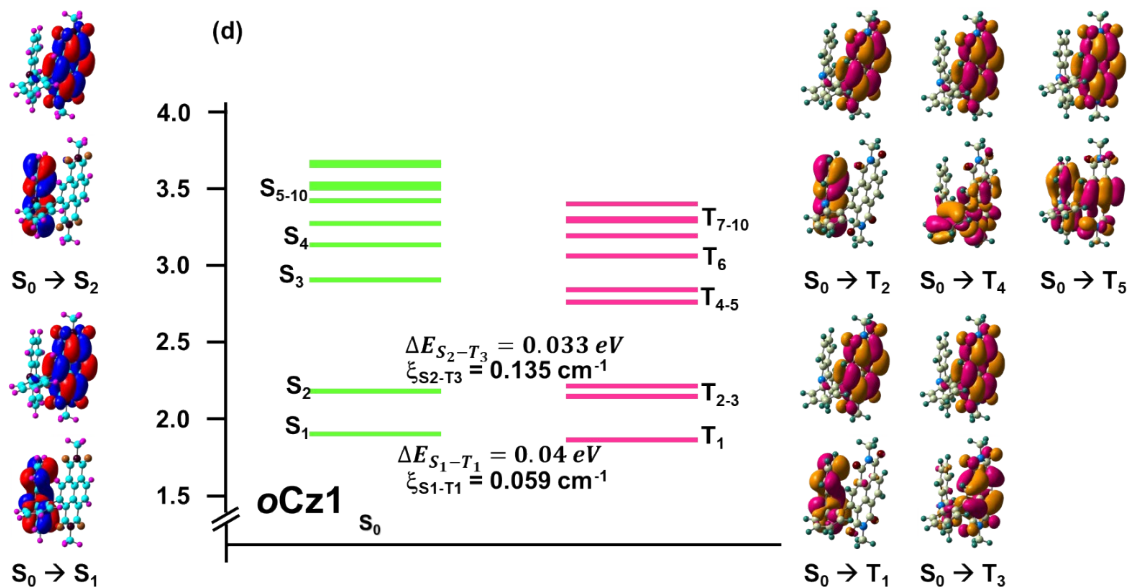
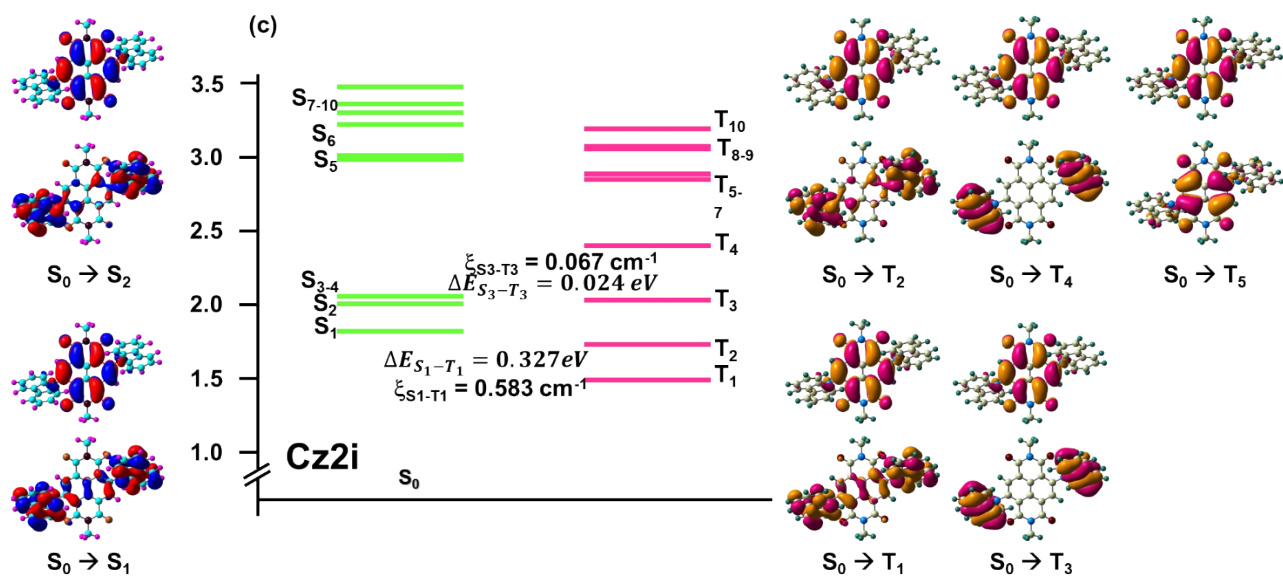
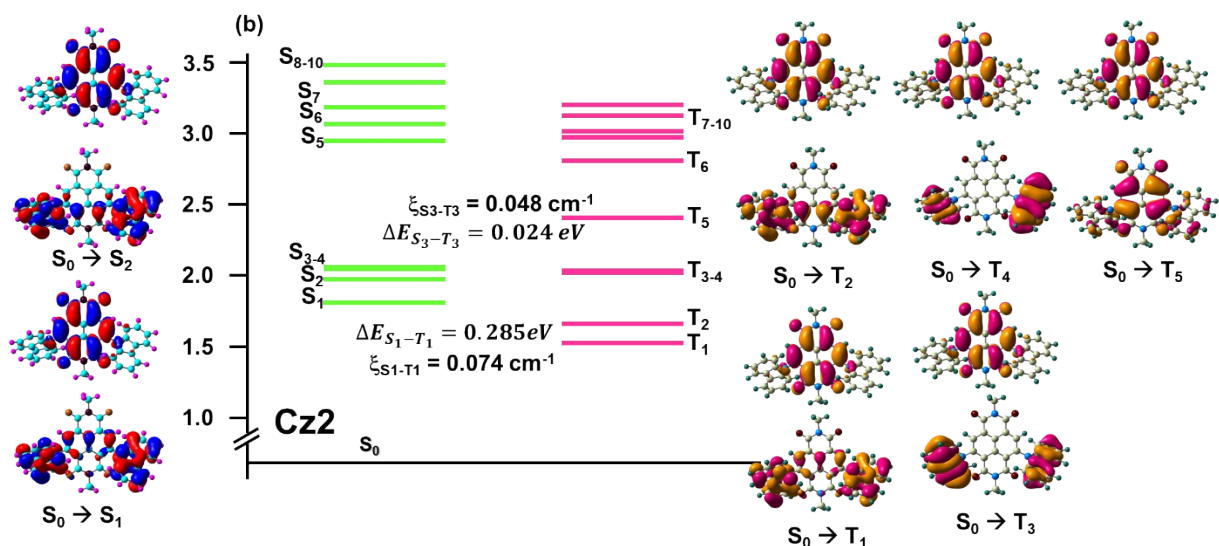
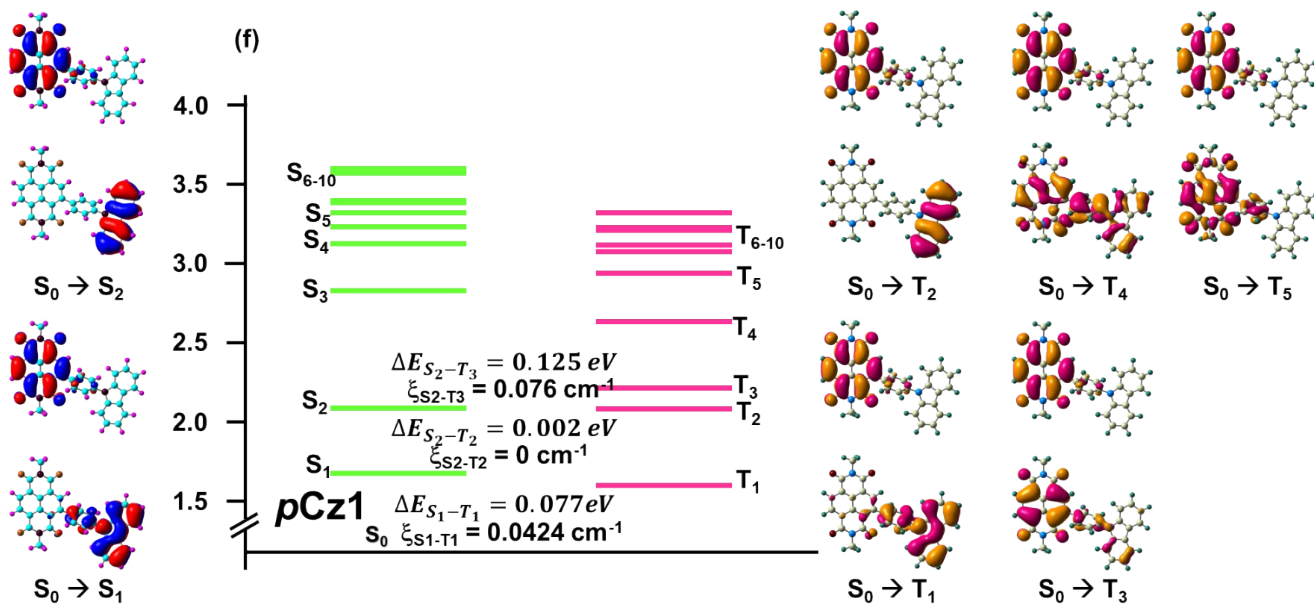
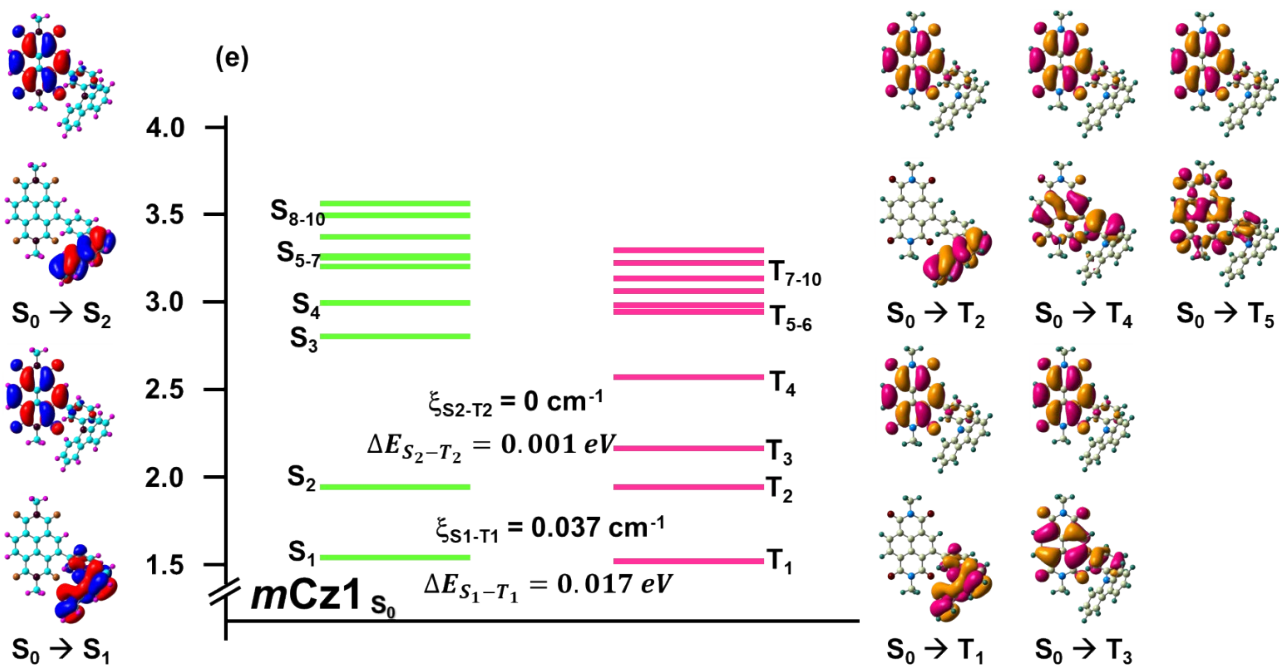
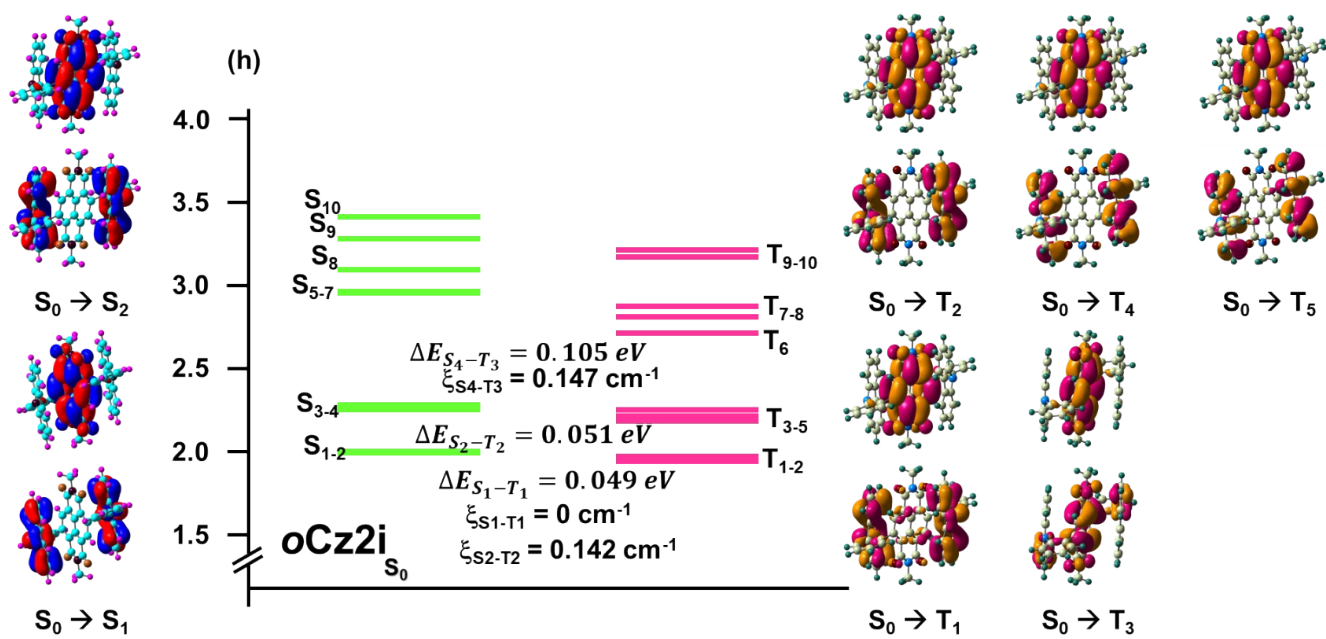
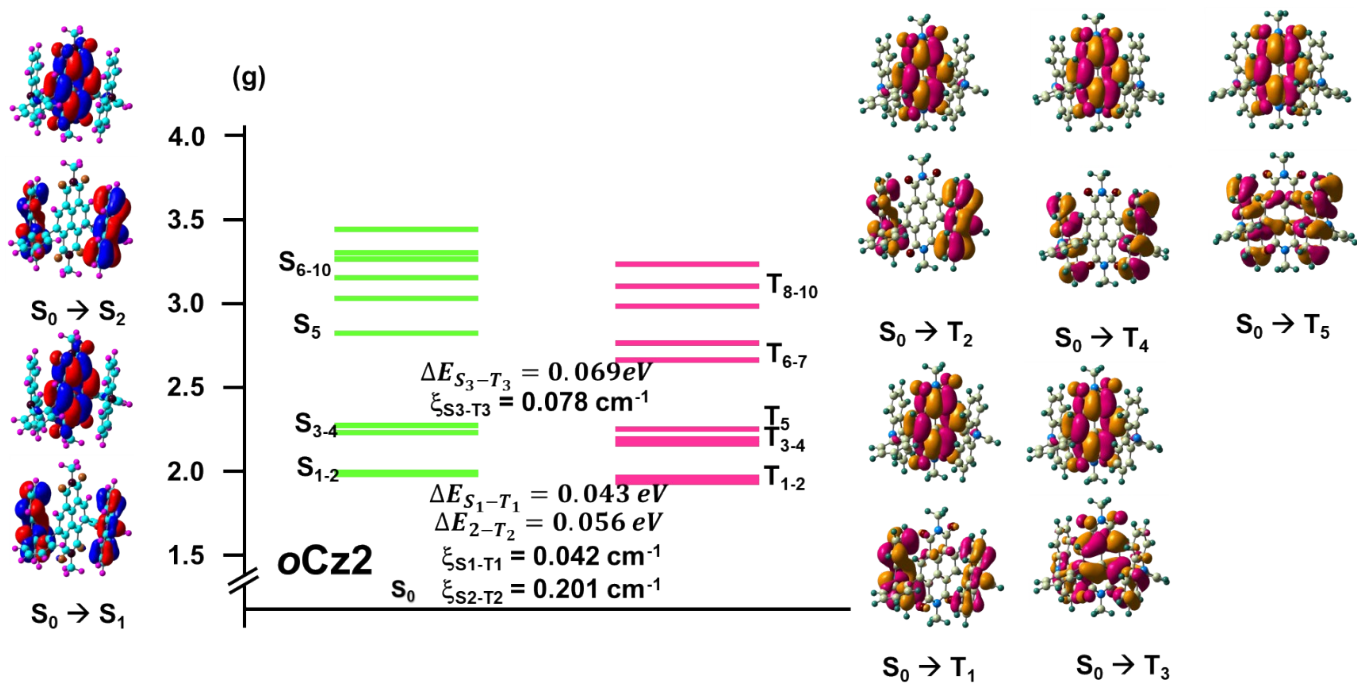


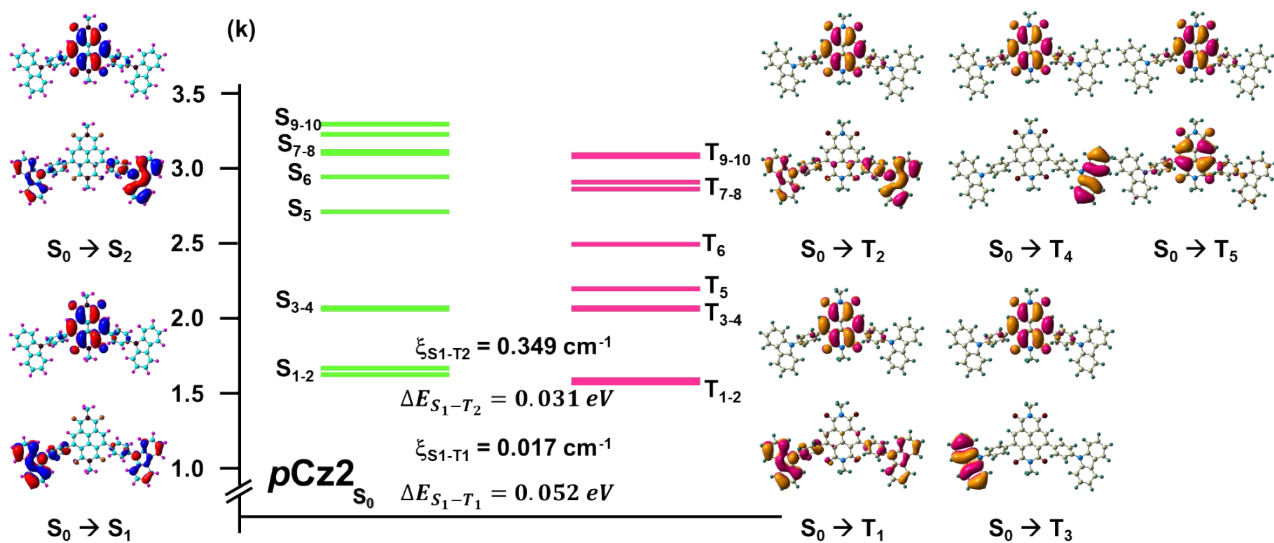
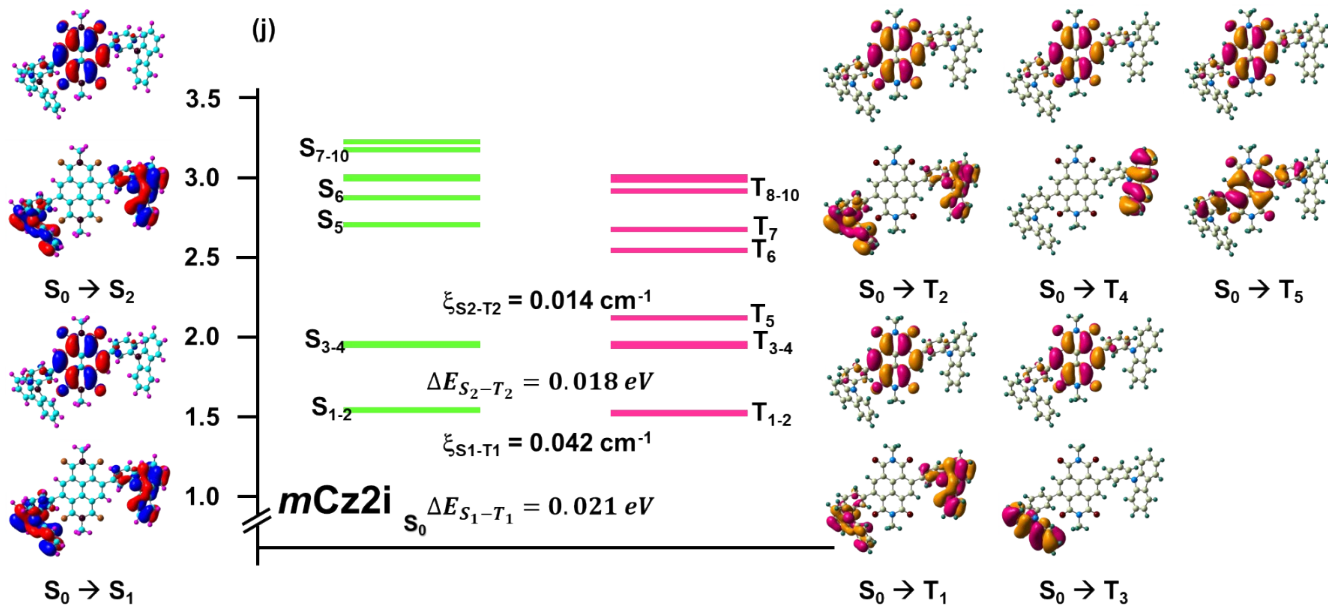
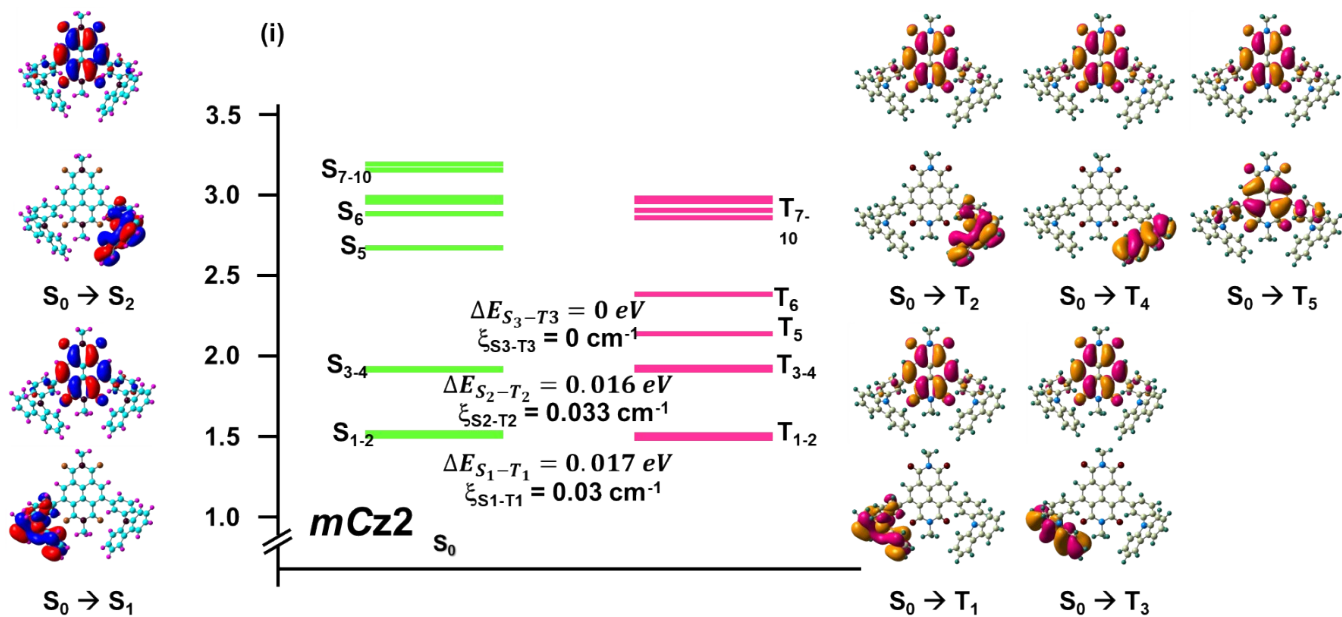
Figure S12. t index at S<sub>1</sub> and T<sub>1</sub> geometry of the proposed molecules













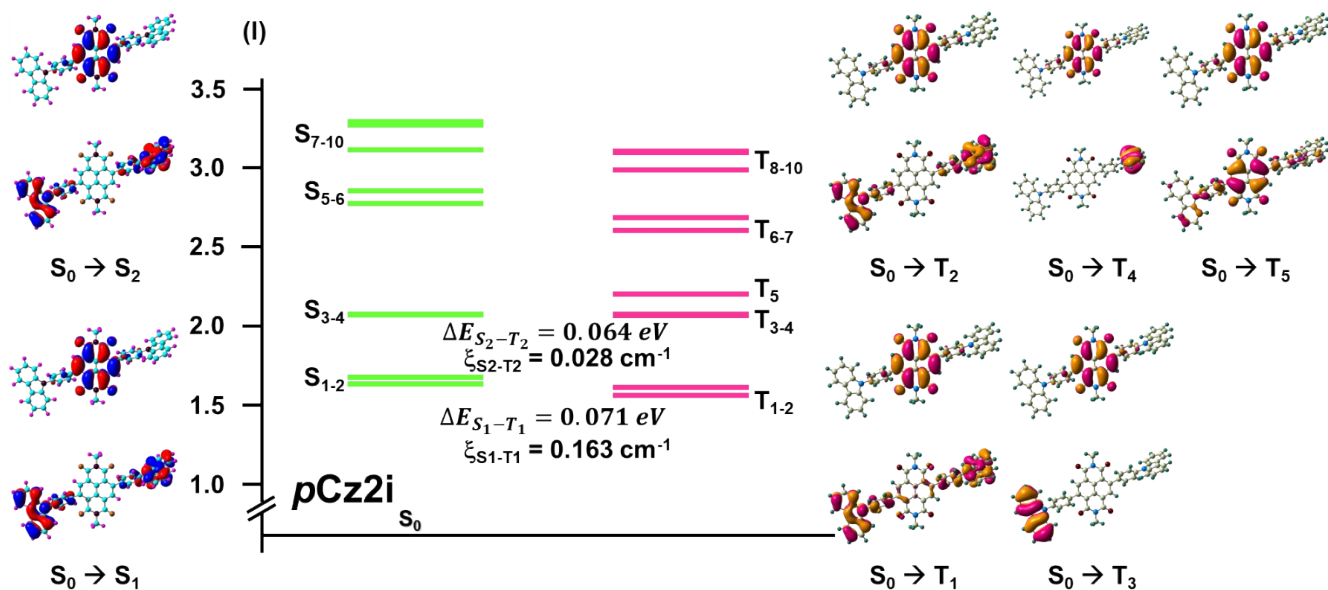


Figure S13 (a-l). Qualitative analysis of the possibilities of ISC and RISC rates.

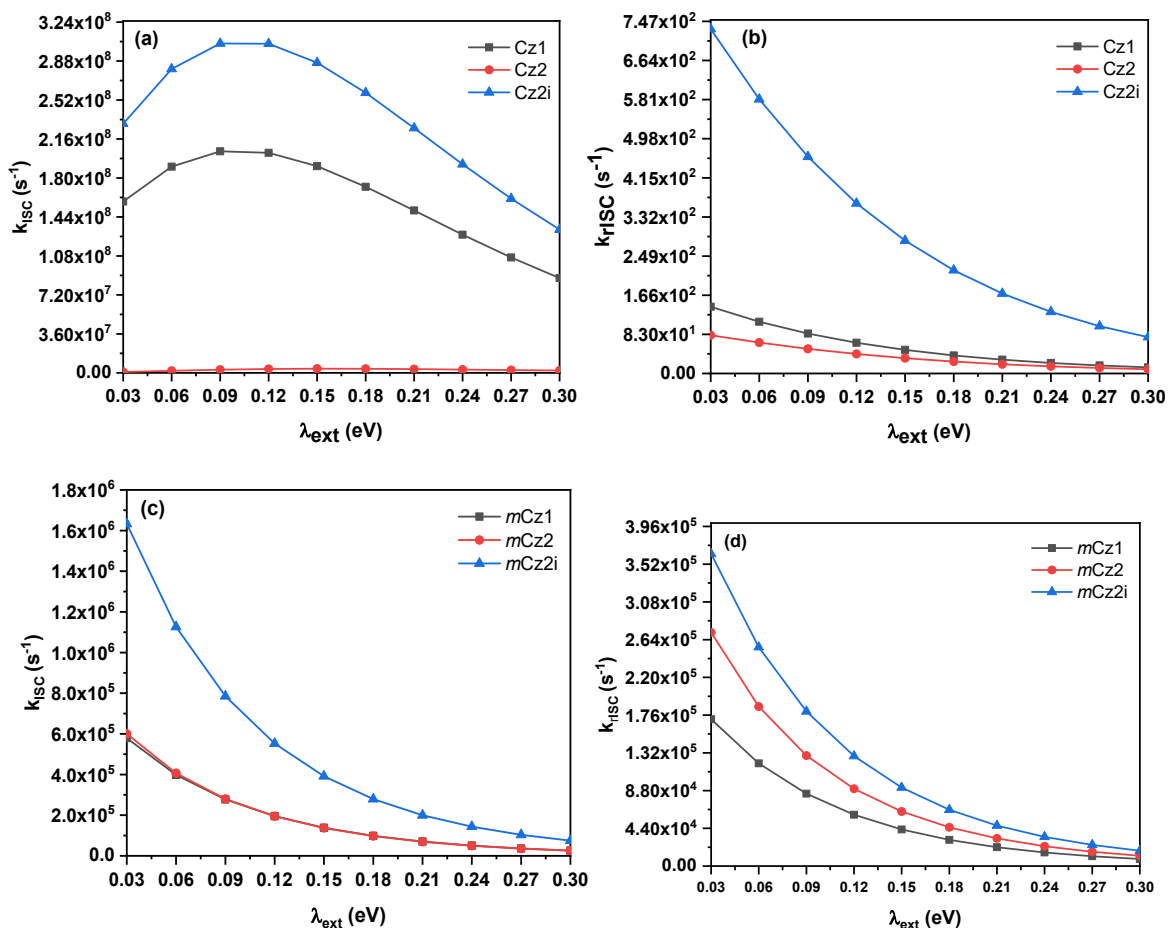
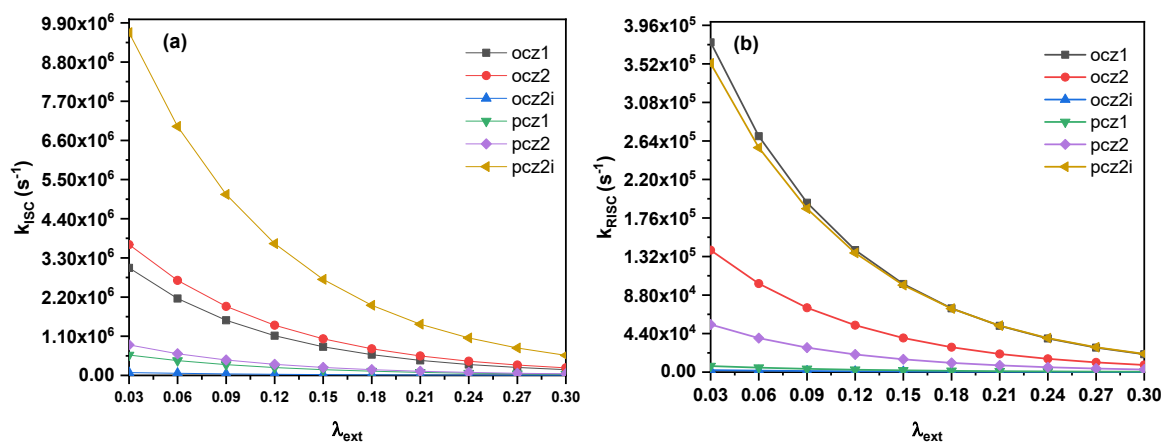


Figure S14 (a-d). ISC and RISC rates of the investigated molecules vs external reorganization energy range.



**Figure S15 (a, b).** The rate for the RISC process in the studied emitters as a function of the external reorganization energy.

**Table S1.** Bond length and dihedral angle of TADF emitters at  $S_0$ ,  $S_1$ , and  $T_1$  optimized geometries.

Molecules/Dihedral angle/length	$S_0$		$S_1$		$T_1$	
	$l_1/l_2$	$\alpha/\beta$	$l_1/l_2$	$\alpha/\beta$	$l_1/l_2$	$\alpha/\beta$
<b>Cz1</b>	1.404	56.94	1.451	89.90	1.406	57.13
<b>Cz2</b>	1.404	54.94/54.13	1.451/1.416	89.39/62.50	1.421/1.422	63.40/65.15
<b>Cz2i</b>	1.404	56.92/56.89	1.450/1.422	89.95/85.97	1.410	58.23/58.22
Molecules/Dihedral angle/length	$l_3/l_4$	$\gamma/\delta$	$l_3/l_4$	$\gamma/\delta$	$l_3/l_4$	$\gamma/\delta$
<b><i>o</i>Cz1</b>	1.495/1.436	80.52/79.25	1.492/1.436	60.84/61.31	1.485/1.435	68.99/67.19
<b><i>m</i>Cz1</b>	1.487/1.416	54.82/49.05	1.495/1.438	58.80/56.55	1.477/1.417	46.53/53.79
<b><i>p</i>Cz1</b>	1.487/1.414	54.81/52.53	1.496/1.438	80.07/63.41	1.463/1.404	44.59/46.85

**Table S2.** Bond length and dihedral angle of TADF emitters at  $S_0$ ,  $S_1$ , and  $T_1$  optimized geometries.

Molecules/Dihedral angle/length	$S_0$				$S_1$				$T_1$			
	$l_3/l_4$	$l_5/l_6$	$\gamma/\delta$	$\gamma'/\delta'$	$l_3/l_4$	$l_5/l_6$	$\gamma/\delta$	$\gamma'/\delta'$	$l_3/l_4$	$l_5/l_6$	$\gamma/\delta$	$\gamma'/\delta'$
<b><i>o</i>Cz2</b>	1.495/1.436	1.495/1.437	83.77/80.67	83.05/80.71	1.494/1.449	1.493/1.436	81.51/78.31	80.20/77.52	1.488/1.433	1.488/1.434	73.40/68.79	72.22/69.12
<b><i>o</i>Cz2i</b>	1.495/1.437	1.495/1.437	81.87/80.15	81.87/80.15	1.490/1.436	1.493/1.435	61.11/61.73	77.66/76.31	1.486/1.433	1.486/1.433	69.34/68.30	69.35/68.31
<b><i>m</i>Cz2</b>	1.487/1.416	1.487/1.416	50.86/52.13	48.04/55.50	1.495/1.437	1.489/1.422	58.65/55.87	50.38/55.64	1.481/1.418	1.488/1.421	48.78/51.82	48.70/53.74



<b><i>mCz2i</i></b>	1.487/1.417	1.490/1.416	47.14/54.97	54.87/53.04	1.494/1.438	1.491/1.422	57.53/56.52	55.35/54.31	1.479/1.418	1.478/1.414	46.01/53.82	47.43/50.34
<b><i>pCz2</i></b>	1.488/1.415	1.486/1.414	57.85/51.49	52.69/52.60	1.496/1.434	1.491/1.423	82.91/60.53	56.86/56.77	1.490/1.418	1.463/1.404	61.14/53.00	43.15/47.45
<b><i>pCz2i</i></b>	1.487/1.414	1.488/1.415	57.35/51.50	57.93/53.24	1.495/1.437	1.491/1.423	79.83/62.55	56.19/56.44	1.470/1.409	1.473/1.411	45.47/49.14	48.26/50.23

**Table S3.** S<sub>1</sub> and T<sub>1</sub> states calculated by the TDA-DFT approach at S<sub>1</sub> and T<sub>1</sub> optimized geometries in gaseous state.

Categories	Molecules	State	<sup>a</sup> Transition	<sup>b</sup> <i>f</i>	Excitation energy (eV)
<b>D-A</b>	<b>Cz1</b>	S <sub>1</sub>	H → L 99.3%	0.00001	0.882
		T <sub>1</sub>	H → L 96.2%		
<b>D-A-D</b>	<b>Cz2</b>	S <sub>1</sub>	H → L 99.2%	0.00004	0.859
		T <sub>1</sub>	H → L 98.5%		
	<b>Cz2i</b>	S <sub>1</sub>	H → L 99.3%	0.00001	0.815
		T <sub>1</sub>	H → L 97.0%		
<b>D-π-A</b>	<b>oCz1</b>	S <sub>1</sub>	H → L 99.4%	0.00564	1.216
		T <sub>1</sub>	H → L 90.3% H-2 → L 7.9%		
	<b>mCz1</b>	S <sub>1</sub>	H → L 99.7%	0.00061	0.97
		T <sub>1</sub>	H → L 99.3%		
	<b>pCz1</b>	S <sub>1</sub>	H → L 99.7%	0.0011	1.111
		T <sub>1</sub>	H → L 90.2% H-2 → L 8.6%		
<b>D-π-A-π-D</b>	<b>oCz2</b>	S <sub>1</sub>	H → L 99.5%	0.00562	1.263
		T <sub>1</sub>	H → L 86.8% H-4 → L 10.1%		
	<b>oCz2i</b>	S <sub>1</sub>	H → L 99.4%	0.00629	1.299
		T <sub>1</sub>	H → L 85.4% H-4 → L 11.0%		
	<b>mCz2</b>	S <sub>1</sub>	H → L 99.7%	0.00143	0.942
		T <sub>1</sub>	H → L 98.8%		
	<b>mCz2i</b>	S <sub>1</sub>	H → L 99.7%	0.00082	0.969
		T <sub>1</sub>	H → L 94.3%		
	<b>pCz2</b>	S <sub>1</sub>	H → L 99.5%	0.00085	1.099
		T <sub>1</sub>	H-1 → L 72.5% H → L 20.5% H-4 → L 5.9%		
	<b>pCz2i</b>	S <sub>1</sub>	H → L 99.6%	0.00239	1.118
		T <sub>1</sub>	H → L 89.5% H-4 → L 8.8%		

<sup>a</sup> Dominant transition with the percentage in the examined states; H and L denotes HOMO and LUMO, respectively. <sup>b</sup> Oscillator strength.

**Table S4.** Benchmarking for absorption of the reported molecules (**Cz2i**, **pCz2i**)

Functional	$\lambda_{\text{abs}}$ , (nm)	
	<b>Cz2i</b>	<b>pCz2i</b>

<b>Experimentally</b>	560	490
<b><math>\omega^*</math>B97XD/6-31+g(d)</b>	567.24	471.91
<b><math>\omega^*</math>B97XD/6-31g(d)</b>	543.96	448.10
<b>LC-<math>\omega^*</math>PBE/6-31+g(d)</b>	612.65	497.30
<b>TPSSH/6-31+g(d)</b>	796.98	890.58
<b>SOGGA11X/6-31+g(d)</b>	<b>550.35</b>	<b>490.97</b>
<b>MPW1K/6-31+g(d)</b>	533.67	471.35
<b>M062X/6-31+g(d)</b>	506.57	429.15

**Cz2i:  $\omega = 0.127$  ( $\omega^*$ B97XD)  $0.162$  (LC- $\omega^*$ PBE)**

***p*Cz2i:  $\omega = 0.132$  ( $\omega^*$ B97XD)  $0.167$  (LC-  $\omega^*$ PBE)**

**(we have used  $\omega^*$ B97XD function with 6-31G(d) basis set.)**

**Table S5.** Absorption data calculated using benchmark function SOGGA11X/6-31+G(d).

<b>Compound</b>	<b><math>\lambda_{\text{abs}}</math>, nm</b>	<b>Oscillator Strength</b>	<b>Assignment</b>
<b>Cz1</b>	511.3	0.20890	H $\rightarrow$ L 96.9%
	332.0	0.44480	H-2 $\rightarrow$ L 92.7%
<b>Cz2</b>	541.0	0.40430	H $\rightarrow$ L 96.6%
	330.5	0.38710	H-5 $\rightarrow$ L 73.7%, H-6 $\rightarrow$ L 16.0%
<b>Cz2i</b>	542.7	0.42210	H $\rightarrow$ L 96.7%
	330.9	0.32470	H-4 $\rightarrow$ L 72.5%, H-6 $\rightarrow$ L 19.0%
<b><i>o</i>Cz1</b>	509.5	0.00260	H $\rightarrow$ L 99.1%
	346.2	0.21960	H-3 $\rightarrow$ L 51.6%, H-2 $\rightarrow$ L 28.7%, H-4 $\rightarrow$ L 11.9%
<b><i>m</i>Cz1</b>	491.3	0.00920	H $\rightarrow$ L 98.4%
	332.5	0.51390	H-4 $\rightarrow$ L 60.9%, H-3 $\rightarrow$ L 24.6%, H-2 $\rightarrow$ L 6.8%
<b><i>p</i>Cz1</b>	485.0	0.13830	H $\rightarrow$ L 94.8%
	331.5	0.47650	H-4 $\rightarrow$ L 75.0%, H-3 $\rightarrow$ L 9.5%, H-2 $\rightarrow$ L 6.7%
<b><i>o</i>Cz2</b>	497.2	0.00050	H $\rightarrow$ L 98.2%
	357.0	0.13150	H-4 $\rightarrow$ L 89.2%, H-7 $\rightarrow$ L 5.5%

<b><i>oCz2i</i></b>	495.1	0.00640	H-1 → L 99.0%
	360.2	0.21560	H-4 → L 85.4%, H-5 → L 6.3%
<b><i>mCz2</i></b>	498.5	0.01670	H → L 98.1%
	319.7	0.33790	H-10 → L 55.6%, H-9 → L 15.4%, H-6 → L 8.7%, H-8 → L 5.7%
<b><i>mCz2i</i></b>	495.5	0.03770	H → L 81.9%, H-1 → L 15.8%
	333.2	0.45790	H-8 → L 70.6%, H-7 → L 8.7%, H-6 → L 6.0%
<b><i>pCz2</i></b>	494.7	0.26480	H → L 91.4%
	318.8	0.21380	H-9 → L 64.0%, H-10 → L 10.1%, H-7 → L 8.0%
<b><i>pCz2i</i></b>	495.6	0.28830	H → L 93.4%
	331.9	0.47640	H-8 → L 79.4%, H-6 → L 7.4%

**Table S6.** Charge transfer indices of the molecules at S<sub>1</sub> and T<sub>1</sub> geometries.

Mol.	State	$\Delta r(\text{\AA})$	$S_m(\text{a.u.})$	$S_r(\text{a.u.})$	$D(\text{\AA})$	$t(\text{\AA})$	HDI	EDI	$\Lambda$	%CT	%LE
<b>Cz1</b>	S <sub>1</sub>	5.23	0.0289	0.1160	5.23	3.55	8.70	6.56	0.117	93.85	6.14
	T <sub>1</sub>	4.45	0.1830	0.4517	4.30	2.52	7.93	6.21	0.429	75.51	24.48
<b>Cz2</b>	S <sub>1</sub>	5.41	0.0304	0.1207	5.41	3.71	8.73	6.34	0.122	88.97	11.02
	T <sub>1</sub>	1.94	0.1241	0.3817	1.95	-0.428	6.13	6.15	0.388	81.82	18.17
<b>Cz2i</b>	S <sub>1</sub>	5.30	0.0291	0.1162	5.30	3.61	8.67	6.52	0.117	92.00	7.99
	T <sub>1</sub>	0.0018	0.2011	0.5317	0.003	-2.66	5.91	5.98	0.491	73.13	26.86
<b>oCz1</b>	S <sub>1</sub>	4.58	0.0320	0.1632	4.58	3.08	8.47	6.33	0.163	93.95	6.04
	T <sub>1</sub>	2.92	0.2621	0.5197	2.38	0.752	7.14	6.25	0.377	68.15	31.84
<b>mCz1</b>	S <sub>1</sub>	7.83	0.0208	0.0804	7.83	6.10	8.50	6.40	0.080	96.53	3.47
	T <sub>1</sub>	7.55	0.0366	0.1162	7.55	5.81	8.58	6.29	0.117	94.64	5.35
<b>pCz1</b>	S <sub>1</sub>	9.31	0.0096	0.0510	9.31	7.56	8.56	6.52	0.051	97.82	2.17
	T <sub>1</sub>	7.59	0.1923	0.4458	6.52	4.16	6.80	6.10	0.336	75.47	24.52
<b>oCz2</b>	S <sub>1</sub>	4.86	0.0312	0.1612	4.86	3.41	8.34	6.17	0.161	90.34	9.65
	T <sub>1</sub>	1.02	0.3379	0.5890	0.532	-1.52	5.16	6.01	0.453	56.81	43.18
<b>oCz2i</b>	S <sub>1</sub>	4.72	0.0349	0.1736	4.72	2.96	8.34	6.19	0.173	89.70	10.29
	T <sub>1</sub>	0.0023	0.3719	0.6236	0.002	-1.82	5.18	6.03	0.460	53.25	46.74
<b>mCz2</b>	S <sub>1</sub>	7.91	0.0204	0.0817	7.91	6.40	8.49	6.27	0.082	92.73	7.26
	T <sub>1</sub>	7.40	0.0359	0.1208	7.40	5.62	8.24	6.14	0.122	91.32	8.67
<b>mCz2i</b>	S <sub>1</sub>	7.98	0.0207	0.0806	7.98	6.23	8.46	6.23	0.081	93.42	6.57
	T <sub>1</sub>	6.93	0.0532	0.1457	5.08	2.15	7.00	6.06	0.134	90.61	9.38
<b>pCz2</b>	S <sub>1</sub>	9.39	0.0105	0.0514	9.39	7.78	8.56	6.44	0.051	94.15	5.84
	T <sub>1</sub>	7.86	0.1651	0.4093	5.29	2.34	6.28	6.00	0.296	76.94	23.06
<b>pCz2i</b>	S <sub>1</sub>	9.46	0.0102	0.0102	9.46	7.60	8.61	6.31	0.055	94.28	5.71
	T <sub>1</sub>	0.533	0.2092	0.4989	0.504	-3.31	4.91	5.76	0.533	72.75	27.24

**Table S7.** SOC of the molecules between  $S_0$ - $T_1$  state for potential RTP molecule

Molecule	$H_{SO}(S_0-T_1)$ ( $\text{cm}^{-1}$ )
<b>Cz1</b>	1.87
<b>Cz2</b>	2.68
<b>Cz2i</b>	0

**Table S8**  $k_{ISC}$  and  $k_{RISC}$  rate of all the investigated molecules at external reorganization energy ( $\lambda_{ext}$ ) value variation.

Mol.	$k_{ISC}$ ( $\text{s}^{-1}$ )	$\lambda_{ext}$ (eV)	$k_{RISC}$
<b>Cz1</b>	$1.5 \times 10^8$	0.03	$1.4 \times 10^2$
	$1.9 \times 10^8$	0.06	$1.0 \times 10^2$
	$2.0 \times 10^8$	0.09	$8.4 \times 10^1$
	$2.0 \times 10^8$	0.12	$6.5 \times 10^1$
	$1.9 \times 10^8$	0.15	$5.0 \times 10^1$
	$1.7 \times 10^8$	0.18	$3.8 \times 10^1$
	$1.5 \times 10^8$	0.21	$2.9 \times 10^1$
	$1.2 \times 10^8$	0.24	$2.2 \times 10^1$
	$1.0 \times 10^8$	0.27	$1.6 \times 10^1$
	$8.7 \times 10^7$	0.3	$1.2 \times 10^1$
<b>Cz2</b>	$8.0 \times 10^5$	0.03	$8.1 \times 10^1$
	$1.9 \times 10^6$	0.06	$6.5 \times 10^1$
	$2.9 \times 10^6$	0.09	$5.2 \times 10^1$
	$3.6 \times 10^6$	0.12	$4.1 \times 10^1$
	$3.8 \times 10^6$	0.15	$3.2 \times 10^1$
	$3.7 \times 10^6$	0.18	$2.5 \times 10^1$
	$3.4 \times 10^6$	0.21	$1.9 \times 10^1$
	$3.0 \times 10^6$	0.24	$1.5 \times 10^1$
	$2.6 \times 10^6$	0.27	$1.1 \times 10^1$
	$2.1 \times 10^6$	0.3	$0.8 \times 10^1$
<b>Cz2i</b>	$2.3 \times 10^8$	0.03	$7.3 \times 10^2$
	$2.8 \times 10^8$	0.06	$5.8 \times 10^2$
	$3.0 \times 10^8$	0.09	$4.5 \times 10^2$
	$3.0 \times 10^8$	0.12	$3.6 \times 10^2$
	$2.8 \times 10^8$	0.15	$2.8 \times 10^2$
	$2.5 \times 10^8$	0.18	$2.1 \times 10^2$
	$2.2 \times 10^8$	0.21	$1.6 \times 10^2$
	$1.9 \times 10^8$	0.24	$1.3 \times 10^2$
	$1.6 \times 10^8$	0.27	$1.0 \times 10^2$
	$1.3 \times 10^8$	0.3	$7.7 \times 10^1$
<b>oCz1</b>	$3.0 \times 10^6$	0.03	$3.7 \times 10^5$
	$2.1 \times 10^6$	0.06	$2.6 \times 10^5$
	$1.5 \times 10^6$	0.09	$1.9 \times 10^5$
	$1.1 \times 10^6$	0.12	$1.3 \times 10^5$
	$8.0 \times 10^5$	0.15	$1.0 \times 10^5$
	$5.8 \times 10^5$	0.18	$7.2 \times 10^4$

	$4.2 \times 10^5$	0.21	$5.2 \times 10^4$
	$3.0 \times 10^5$	0.24	$3.8 \times 10^4$
	$2.2 \times 10^5$	0.27	$2.7 \times 10^4$
	$1.6 \times 10^5$	0.3	$2.0 \times 10^4$
<i>mCz1</i>	$5.7 \times 10^5$	0.03	$1.7 \times 10^5$
	$3.9 \times 10^5$	0.06	$1.1 \times 10^5$
	$2.7 \times 10^5$	0.09	$8.4 \times 10^4$
	$1.9 \times 10^5$	0.12	$5.9 \times 10^4$
	$1.3 \times 10^5$	0.15	$4.2 \times 10^4$
	$9.8 \times 10^4$	0.18	$3.0 \times 10^4$
	$7.0 \times 10^4$	0.21	$2.1 \times 10^4$
	$5.0 \times 10^4$	0.24	$1.5 \times 10^4$
	$3.6 \times 10^4$	0.27	$1.1 \times 10^4$
	$2.6 \times 10^4$	0.3	$8.3 \times 10^3$
<i>pCz1</i>	$5.7 \times 10^5$	0.03	$6.9 \times 10^3$
	$4.1 \times 10^5$	0.06	$5.0 \times 10^3$
	$3.0 \times 10^5$	0.09	$3.7 \times 10^3$
	$2.2 \times 10^5$	0.12	$2.7 \times 10^3$
	$1.6 \times 10^5$	0.15	$1.9 \times 10^3$
	$1.1 \times 10^5$	0.18	$1.4 \times 10^3$
	$8.5 \times 10^4$	0.21	$1.0 \times 10^3$
	$6.2 \times 10^4$	0.24	$7.8 \times 10^2$
	$4.6 \times 10^4$	0.27	$5.7 \times 10^2$
	$3.3 \times 10^4$	0.3	$4.2 \times 10^2$
<i>oCz2</i>	$3.6 \times 10^6$	0.03	$1.3 \times 10^5$
	$2.6 \times 10^6$	0.06	$1.0 \times 10^5$
	$1.9 \times 10^6$	0.09	$7.3 \times 10^4$
	$1.4 \times 10^6$	0.12	$5.3 \times 10^4$
	$1.0 \times 10^6$	0.15	$3.8 \times 10^4$
	$7.4 \times 10^5$	0.18	$2.8 \times 10^4$
	$5.4 \times 10^5$	0.21	$2.0 \times 10^4$
	$3.9 \times 10^5$	0.24	$1.5 \times 10^4$
	$2.9 \times 10^5$	0.27	$1.1 \times 10^4$
	$2.1 \times 10^5$	0.3	$8.1 \times 10^3$
<i>oCz2i</i>	$8.0 \times 10^4$	0.03	$2.2 \times 10^3$
	$5.9 \times 10^4$	0.06	$1.6 \times 10^3$
	$4.3 \times 10^4$	0.09	$1.2 \times 10^3$
	$3.1 \times 10^4$	0.12	$8.9 \times 10^2$
	$2.3 \times 10^4$	0.15	$6.5 \times 10^2$
	$1.7 \times 10^4$	0.18	$4.7 \times 10^2$
	$1.2 \times 10^4$	0.21	$3.5 \times 10^2$
	$9.1 \times 10^3$	0.24	$2.5 \times 10^2$
	$6.7 \times 10^3$	0.27	$1.8 \times 10^2$
	$4.9 \times 10^3$	0.3	$1.3 \times 10^2$
<i>mCz2</i>	$6.0 \times 10^5$	0.03	$2.7 \times 10^5$
	$4.0 \times 10^5$	0.06	$1.8 \times 10^5$
	$2.7 \times 10^5$	0.09	$1.2 \times 10^5$
	$1.9 \times 10^5$	0.12	$9.0 \times 10^4$

	$1.3 \times 10^5$	0.15	$6.3 \times 10^4$
	$9.7 \times 10^4$	0.18	$4.5 \times 10^4$
	$6.9 \times 10^4$	0.21	$3.2 \times 10^4$
	$4.9 \times 10^4$	0.24	$2.3 \times 10^4$
	$3.5 \times 10^4$	0.27	$1.6 \times 10^4$
	$2.5 \times 10^4$	0.3	$1.1 \times 10^4$
<i>mCz2i</i>	$1.6 \times 10^6$	0.03	$3.6 \times 10^5$
	$1.1 \times 10^6$	0.06	$2.5 \times 10^5$
	$7.8 \times 10^5$	0.09	$1.8 \times 10^5$
	$5.5 \times 10^5$	0.12	$1.2 \times 10^5$
	$3.9 \times 10^5$	0.15	$9.1 \times 10^4$
	$2.7 \times 10^5$	0.18	$6.5 \times 10^4$
	$1.9 \times 10^5$	0.21	$4.7 \times 10^4$
	$1.4 \times 10^5$	0.24	$3.4 \times 10^4$
	$1.0 \times 10^5$	0.27	$2.4 \times 10^4$
	$7.4 \times 10^4$	0.3	$1.7 \times 10^4$
<i>pCz2</i>	$8.5 \times 10^5$	0.03	$5.4 \times 10^4$
	$6.0 \times 10^5$	0.06	$3.8 \times 10^4$
	$4.3 \times 10^5$	0.09	$2.7 \times 10^4$
	$3.1 \times 10^5$	0.12	$2.0 \times 10^4$
	$2.2 \times 10^5$	0.15	$1.4 \times 10^4$
	$1.6 \times 10^5$	0.18	$1.0 \times 10^4$
	$1.1 \times 10^5$	0.21	$7.6 \times 10^3$
	$8.3 \times 10^4$	0.24	$5.5 \times 10^3$
	$6.0 \times 10^4$	0.27	$4.0 \times 10^3$
	$4.4 \times 10^4$	0.3	$2.9 \times 10^3$
<i>pCz2i</i>	$9.6 \times 10^6$	0.03	$3.5 \times 10^5$
	$6.9 \times 10^6$	0.06	$2.5 \times 10^5$
	$5.0 \times 10^6$	0.09	$1.8 \times 10^5$
	$3.7 \times 10^6$	0.12	$1.3 \times 10^5$
	$2.6 \times 10^6$	0.15	$9.9 \times 10^4$
	$1.9 \times 10^6$	0.18	$7.2 \times 10^4$
	$1.4 \times 10^6$	0.21	$5.3 \times 10^4$
	$1.0 \times 10^6$	0.24	$3.8 \times 10^4$
	$7.6 \times 10^5$	0.27	$2.8 \times 10^4$
	$5.6 \times 10^5$	0.3	$2.0 \times 10^4$



### XYZ Coordinates of Cz1 in S<sub>0</sub> optimized geometry

N	-0.907113	4.526048	2.075728
C	-2.118384	3.888510	2.401430
C	-3.252154	4.057167	1.451033
C	-3.124416	5.015036	0.403566
C	-1.898537	5.686105	0.165859
C	-0.709507	5.412570	1.012044
C	-4.472912	3.383420	1.611630
C	-1.789779	6.615205	-0.859726
O	-2.188411	3.240506	3.433923
O	0.374353	5.940716	0.804470
H	-0.832681	7.102531	-1.009021
C	-4.234678	5.324758	-0.428981
C	-4.104264	6.277356	-1.464903
C	-5.265521	6.606637	-2.336022
N	-6.463241	5.918458	-2.074754
C	-6.646567	4.970856	-1.060566
C	-5.469119	4.668627	-0.203768
C	-5.577844	3.719750	0.786878
H	-6.518846	3.197109	0.914349
O	-7.731651	4.430694	-0.903772
O	-5.187479	7.431224	-3.234418
C	-2.890773	6.914118	-1.677483
H	-2.816200	7.639445	-2.479857
C	0.207516	4.278394	3.000156
H	0.342662	3.202548	3.121311
H	1.098345	4.739283	2.581423
H	-0.019154	4.706206	3.979384
C	-7.637654	6.201626	-2.910185

H	-7.983056	5.277794	-3.378150
H	-8.445358	6.592965	-2.288133
H	-7.347265	6.929834	-3.662825
N	-4.664819	2.335204	2.525564
C	-5.717098	2.260932	3.452799
C	-3.933511	1.138146	2.585985
C	-5.652209	1.011516	4.115260
C	-6.680083	3.217419	3.776557
C	-4.522777	0.294739	3.556651
C	-2.839859	0.728651	1.824833
C	-6.588654	0.709106	5.107314
C	-7.608072	2.890138	4.765538
H	-6.704784	4.184101	3.285556
C	-3.989840	-0.978493	3.779920
C	-2.327030	-0.545498	2.060942
H	-2.402282	1.376072	1.073097
H	-6.547745	-0.244145	5.626041
C	-7.567226	1.650064	5.423587
H	-8.371434	3.614149	5.033798
C	-2.889539	-1.390997	3.032009
H	-4.434797	-1.635015	4.521871
H	-1.473338	-0.887418	1.483515
H	-8.301526	1.427096	6.191402
H	-2.463259	-2.375791	3.196157

**XYZ Coordinates of Cz1 in S<sub>1</sub> optimized geometry**

N	-1.28861635499383	4.76817313514933	2.49170007082686
C	-2.37504569100190	3.89137604208783	2.51961503789996
C	-3.39714696945524	4.07838569207335	1.49579527884364
C	-3.25599442612966	5.11302564026762	0.53097620517443

C	-2.13254318815609	5.97398212050452	0.54646447882113
C	-1.08994617495675	5.81548596520456	1.56047386362386
C	-4.55276708265347	3.25699494848136	1.41583805428864
C	-2.01039760913394	6.99349472370980	-0.41776444615820
O	-2.42659881802760	3.01009859664129	3.39239634806094
O	-0.09104393252574	6.53046096267063	1.62724614352910
H	-1.13494697776301	7.63099444896422	-0.37103899323230
C	-4.25937988255052	5.29700850891950	-0.47705318205765
C	-4.10982481041554	6.32943432661999	-1.43227136415992
C	-5.12844682089160	6.53116717629905	-2.47047198199318
N	-6.22879025350421	5.64672073838847	-2.44558162666940
C	-6.42391648408356	4.61028658186587	-1.52283382109527
C	-5.38866668826974	4.44337757965403	-0.50467715257132
C	-5.52376531706543	3.42293405808194	0.45282108102922
H	-6.39928670253560	2.78532106600819	0.40872980433795
O	-7.42735668739104	3.89422803008217	-1.59325636595666
O	-5.04837519833572	7.41426832479106	-3.32370124021600
C	-2.98166799414728	7.16892983747610	-1.39041108050490
H	-2.90044937859882	7.94945346615274	-2.13824255364063
C	-0.27706894685300	4.56186348332151	3.53056930094749
H	0.13665342473509	3.55398704962917	3.45039508956569
H	0.49969974554070	5.30927156219582	3.39024830225809
H	-0.73503944295446	4.65928789917196	4.51755233612934
C	-7.27336753734111	5.80277709890288	-3.45984880759117
H	-7.36866709984411	4.87980036584514	-4.03643686524715
H	-8.23314995564634	5.99595653088816	-2.97502704171070
H	-6.99296086472526	6.63267432462919	-4.10361230153570
N	-4.74454557677453	2.18983498540488	2.38038344507292
C	-5.37406576168043	2.32512520864526	3.59275274002539

C	-4.27684741525268	0.90600853031191	2.24288677824300
C	-5.32868832582373	1.08136744522097	4.28466028271249
C	-5.98297896232147	3.46778697939429	4.12751736703045
C	-4.61484949372388	0.15829185715396	3.40639906755166
C	-3.57576609743612	0.35262301788994	1.16414017147269
C	-5.90500594743946	0.98434969143824	5.53641514273440
C	-6.55864066433693	3.34830527161968	5.39118869891170
H	-5.99486066576324	4.39672770271584	3.57186973274005
C	-4.24060140377949	-1.16909971090761	3.48770637970471
C	-3.20811679867909	-0.98808597001181	1.26605985901651
H	-3.33496586862920	0.95413279442216	0.29693028125117
H	-5.88586094119812	0.05399834238091	6.09429860499580
C	-6.52213056331689	2.13076141658930	6.08514965753924
H	-7.03923604601684	4.20822734518440	5.84365593377671
C	-3.53309908511386	-1.73761712572755	2.40501290306043
H	-4.47768188158190	-1.76833311736007	4.36058949814400
H	-2.66254908441377	-1.45622467930755	0.45466588281710
H	-6.97632694813079	2.06492806960769	7.06806472851021
H	-3.23387834891263	-2.77885633934237	2.46007627369308

**XYZ Coordinates of Cz1 in T<sub>1</sub> optimized geometry**

N	-1.00859782673070	4.48874219461573	2.14002731733257
C	-2.24722256445003	3.90648089881322	2.44433153552104
C	-3.30121488234146	4.03845962218708	1.43219381181007
C	-3.14083336191878	4.97644558149132	0.38631112326045
C	-1.89352906084526	5.61372723106334	0.16748702962912
C	-0.75100993698117	5.33497484463291	1.04786676388600
C	-4.58663280837613	3.36975863725387	1.56966398789117
C	-1.73704593905612	6.52922446361769	-0.89788606624951
O	-2.39465484749936	3.30998874473872	3.51334245183287

O	0.36263745759683	5.82384448767589	0.86698652801794
H	-0.76381146788630	6.98591685906868	-1.03490639921623
C	-4.24651437836750	5.30363206170311	-0.46650935055104
C	-4.07137398725677	6.22478672627431	-1.50583099672056
C	-5.19712731443047	6.57989929730466	-2.38598194894189
N	-6.42586658780761	5.95192092527841	-2.11342854254449
C	-6.65925271349901	5.02960675098966	-1.08150304783863
C	-5.51540934794125	4.70108085675257	-0.22869893800748
C	-5.66268510810262	3.74056130173243	0.78098261424700
H	-6.62007899948592	3.24152727714822	0.87973314762766
O	-7.77929719263255	4.54160523108128	-0.92547775934187
O	-5.07836417853430	7.37899830294441	-3.31266949481898
C	-2.80203884918048	6.82932947596689	-1.72038249794608
H	-2.71013038624429	7.53343105757823	-2.53950467234816
C	0.06045640767955	4.26325970298478	3.11885909962314
H	0.15094988257637	3.19346988691752	3.31452285453045
H	0.98168361596048	4.66567211945223	2.70506578174133
H	-0.18232734032186	4.76127488274235	4.06096180587601
C	-7.58030046621480	6.27064753032267	-2.95913926049965
H	-7.95290984199273	5.35863952770009	-3.43074033415421
H	-8.38259458949502	6.68569094174817	-2.34508923411614
H	-7.25863575342431	6.98860970203720	-3.70922776767168
N	-4.74889102240893	2.31855524891095	2.48930472057063
C	-5.74251761983187	2.23088280920948	3.46718224168422
C	-3.97640579024247	1.15127385784856	2.52760802677282
C	-5.58958169151117	1.00541381898276	4.16556481464335
C	-6.72204045696728	3.16655150745659	3.80948382993210
C	-4.46157013344405	0.31321346287932	3.55821848118674
C	-2.93568945779964	0.76824123269205	1.68190181234536

C	-6.44715927659255	0.70714310099189	5.21833268566749
C	-7.57467683544116	2.84390850912721	4.86498752092588
H	-6.81062181349658	4.10506120987706	3.27533664585929
C	-3.85920517544332	-0.92150799042905	3.77589296317145
C	-2.33684527899301	-0.46854204324147	1.92351239650689
H	-2.60572072967522	1.40828501125055	0.87183916920579
H	-6.34260027704839	-0.22105190189666	5.77143452955025
C	-7.44340749190187	1.63145028814627	5.55923274302649
H	-8.34988547959776	3.54604790375689	5.15381343180238
C	-2.78760220144821	-1.30197672632697	2.95746234167792
H	-4.21694051501788	-1.58213007406450	4.55955756053826
H	-1.51592051935723	-0.79325777202379	1.29245981894664
H	-8.12123971199172	1.40877279398983	6.37719311243770
H	-2.30731615458596	-2.26206937095476	3.11733761168808

**XYZ Coordinates of Cz2 in S<sub>0</sub> optimized geometry**

N	1.072155	0.157809	0.099506
C	-0.176169	-0.439343	0.332626
C	-1.133280	-0.406493	-0.807985
C	-0.899811	0.508772	-1.876845
C	0.316266	1.248048	-1.962951
C	1.423137	0.904904	-1.031510
C	-2.309034	-1.176065	-0.804238
C	0.475984	2.200055	-2.983199
O	-0.433439	-0.951986	1.410305
O	2.584147	1.247615	-1.193145
C	-1.896449	0.686464	-2.875760
C	-1.679245	1.600540	-3.932450
C	-2.705615	1.794848	-4.994462

N	-3.882144	1.039238	-4.871925
C	-4.151094	0.125098	-3.844855
C	-3.099431	-0.052614	-2.808011
C	-3.292886	-0.972103	-1.800724
H	-4.198848	-1.566832	-1.793709
O	-5.209089	-0.486086	-3.821774
O	-2.534564	2.567584	-5.925291
C	-0.524076	2.350450	-3.973014
H	-0.397548	3.084459	-4.760096
C	-4.932230	1.195130	-5.887119
H	-5.111399	0.236790	-6.378743
H	-5.859767	1.512111	-5.406561
H	-4.597436	1.938132	-6.606164
C	2.131120	-0.011746	1.103760
H	2.956551	-0.582098	0.672808
H	2.511172	0.968105	1.399185
H	1.704774	-0.533777	1.956164
N	-2.549343	-2.202795	0.122947
C	-1.718338	-3.305466	0.375674
C	-3.714062	-2.336625	0.895682
C	-0.485556	-3.634546	-0.186688
C	-2.359316	-4.152276	1.310044
C	-4.805925	-1.475097	1.009865
C	-3.625038	-3.532549	1.648254
C	0.110292	-4.829679	0.211894
H	-0.003843	-2.985521	-0.909838
C	-1.742038	-5.345244	1.698215
C	-5.832812	-1.845703	1.878310
H	-4.854560	-0.546025	0.452592

C	-4.664155	-3.880151	2.515560
C	-0.505887	-5.676745	1.148604
H	1.071658	-5.107060	-0.209963
H	-2.226230	-6.003397	2.413673
C	-5.767547	-3.035397	2.622089
H	-6.695902	-1.195330	1.983265
H	-4.606272	-4.793559	3.100202
H	-0.013632	-6.598648	1.442263
H	-6.582279	-3.294095	3.291256
N	1.575528	3.070118	-3.050873
C	2.014344	3.936482	-2.037015
C	2.374112	3.274851	-4.187896
C	1.506104	4.129522	-0.752780
C	3.095345	4.703167	-2.531464
C	2.343985	2.623594	-5.421839
C	3.329987	4.277713	-3.896944
C	2.109954	5.100270	0.044159
H	0.669201	3.547200	-0.382970
C	3.688301	5.670003	-1.713690
C	3.276569	3.016009	-6.382193
H	1.629439	1.834436	-5.628430
C	4.257777	4.650178	-4.873280
C	3.193868	5.861137	-0.425698
H	1.734061	5.267466	1.049110
H	4.518466	6.264321	-2.083933
C	4.222121	4.019760	-6.115752
H	3.271951	2.528279	-7.352262
H	4.997391	5.416452	-4.660711
H	3.645818	6.606184	0.221682



H 4.936073 4.300295 -6.883888

**XYZ Coordinates of Cz2 in S<sub>1</sub> optimized geometry**

N	0.98499840892130	0.11587762596984	0.06896308499027
C	-0.15076291658878	-0.68630847255742	0.14088039728344
C	-1.10782401249532	-0.53686281171976	-0.95243366935203
C	-0.89225834827665	0.42576740416877	-1.97977892730381
C	0.25516627975767	1.26807778270663	-1.96756854867890
C	1.29508552629797	1.04007528105250	-0.95759612025114
C	-2.27427367045122	-1.34502028709898	-1.03014500080594
C	0.39488164716829	2.25330591901815	-2.98660874282965
O	-0.31222213970472	-1.48361486538762	1.07828824836053
O	2.39665540542576	1.58009108132915	-0.93657541077090
C	-1.84654558076103	0.53563168706207	-3.04739537300730
C	-1.63744496817579	1.48284997176640	-4.07566071548876
C	-2.59210175967249	1.61242589738354	-5.18471295885984
N	-3.70391912723755	0.74590518194829	-5.15125987318465
C	-3.96247251589073	-0.20751018134342	-4.15878631482356
C	-2.98549076681492	-0.30279648725319	-3.07368145920958
C	-3.19117423443756	-1.24325699198320	-2.05161075765083
H	-4.07294609414301	-1.87212908254693	-2.09422484080219
O	-4.96886351847463	-0.91881494262459	-4.22470104804650
O	-2.44708161332694	2.42367343559593	-6.09776557590800
C	-0.53246356925127	2.33980266333539	-4.01920426525142
H	-0.41926876044922	3.09649575224718	-4.78649801895047
C	-4.68956225079524	0.82926338878965	-6.23146734335184
H	-4.75783965996074	-0.13326153013864	-6.74364898709501
H	-5.67299649661626	1.05937482581437	-5.81551489789677
H	-4.36856457138414	1.60883575345764	-6.91774946806838
C	2.01442614513270	-0.03271283192057	1.10234410749930

H	2.92925877036844	-0.43453206346072	0.66042585458627
H	2.24964635412168	0.94765571353162	1.52050645724941
H	1.63073831522352	-0.70362975698644	1.86619428956000
N	-2.54073983378165	-2.33519277045218	-0.00417779402988
C	-2.09610313107184	-3.63451828734986	-0.02422274646450
C	-3.24672954816520	-2.10516108293972	1.15148765021682
C	-1.33945755060955	-4.27351916303873	-1.01436253076262
C	-2.52622974752537	-4.29335304437101	1.16226897768878
C	-3.86342313185647	-0.91810624765563	1.56568622576717
C	-3.27452852787181	-3.29883020754318	1.92680565443252
C	-1.01034603840437	-5.61061547781164	-0.79776981902344
H	-1.02842563774626	-3.73820840419713	-1.90240512091152
C	-2.18899071457935	-5.61883480717666	1.35771480977678
C	-4.52300741992544	-0.94007106770143	2.79348308231286
H	-3.81877417479123	-0.02930555375281	0.94930922135585
C	-3.93326207176979	-3.29924644910374	3.14135663017785
C	-1.42589044390612	-6.27352770915585	0.36527416460869
H	-0.42421564489287	-6.14378188447378	-1.53753846101531
H	-2.49615314283529	-6.15171270829225	2.25147694846897
C	-4.55897821796409	-2.10715718274942	3.56904648510621
H	-5.01288093025566	-0.04267415572369	3.15377652262933
H	-3.97141214253078	-4.18925299128439	3.76068293673615
H	-1.15483172703487	-7.31382291433356	0.51008619891498
H	-5.07764070373472	-2.09691415498440	4.52170067867953
N	1.44525402502061	3.20270412438022	-2.97403531886290
C	1.67227797187084	4.15946380396096	-1.98543852056450
C	2.42457411872842	3.33866359945665	-3.95946143320547
C	0.94282847625468	4.41859961821089	-0.82489089163925
C	2.80793884882658	4.92827637231336	-2.34096174268505

C	2.61250711804025	2.59854922624413	-5.12798358074717
C	3.29287850855298	4.40093181263004	-3.59905241709155
C	1.37261807785055	5.46363618294088	-0.01052402419799
H	0.07534447732124	3.82017537737448	-0.56768827022750
C	3.21977035959460	5.97335458523487	-1.50711615913787
C	3.68789947428583	2.94400727233588	-5.94493728505475
H	1.94288887989775	1.78598192167271	-5.38812818935702
C	4.36464090347954	4.72689694666834	-4.43611655754316
C	2.50025328211671	6.23527893630352	-0.34398363182463
H	0.82445007403527	5.68564071144829	0.90070875792655
H	4.08799693080929	6.57187879105453	-1.76839087708045
C	4.55643523202875	3.99669292674966	-5.60689571429571
H	3.85603937805249	2.38609690982265	-6.86157998858336
H	5.03800250542108	5.53745939267838	-4.17172878139971
H	2.80986203595593	7.04282783996838	0.31259682753891
H	5.38414152560021	4.24056885248658	-6.26603003857434

**XYZ Coordinates of Cz2 in T<sub>1</sub> optimized geometry**

N	1.04398903795303	0.16090661861977	0.07168095435577
C	-0.15854749424346	-0.54671394000673	0.24141468922766
C	-1.12314826399394	-0.43767169698352	-0.85346467160672
C	-0.91189950826282	0.50695996803359	-1.89508565663299
C	0.27996380733554	1.27822523716045	-1.95101959019070
C	1.35528273364198	1.01418700157755	-0.99646596394751
C	-2.32768632313450	-1.19907890363330	-0.85843165852733
C	0.43111441201833	2.22878802123473	-3.00141145568624
O	-0.34774296988833	-1.21728908784741	1.26004064328919
O	2.48728685578959	1.50092297469420	-1.06425608761692
C	-1.91788476761164	0.68412526552073	-2.90698385425272
C	-1.70181988606508	1.60079645099187	-3.96183893055101

C	-2.70615014435367	1.78802361556076	-5.01682892610082
N	-3.88392506517400	1.02882367275712	-4.89074082831691
C	-4.15870475007672	0.11439005680432	-3.86170331378701
C	-3.11765797785448	-0.05998022271249	-2.84330949989394
C	-3.30733131380099	-0.99915194417569	-1.82091320172234
H	-4.21275227719239	-1.59559872088186	-1.82301927865531
O	-5.22734862397852	-0.49643567846213	-3.84658221140494
O	-2.54093969373913	2.56206838728437	-5.95951365531687
C	-0.53084868545433	2.36990110146824	-3.99219809573374
H	-0.41175470152306	3.10600508442916	-4.77906662518349
C	-4.92994757968310	1.18284313903150	-5.90534533508866
H	-5.11298546812782	0.22352327546565	-6.39491290624499
H	-5.85991631778646	1.50017794042689	-5.42843394639525
H	-4.59165801998562	1.92395438213368	-6.62513868747528
C	2.09854701359997	-0.00320936434981	1.07788278009637
H	2.97503069159624	-0.46886695690044	0.62092877082970
H	2.39758198245851	0.97643963265815	1.45605501347943
H	1.70438968906808	-0.62521746618744	1.87717758295761
N	-2.54362718883391	-2.24398830081462	0.08201883660668
C	-1.79887536166972	-3.41746636424009	0.17929957516043
C	-3.57147267928214	-2.28305754745781	1.01448281142405
C	-0.69659355521823	-3.81561793435684	-0.57720286340682
C	-2.35645931212998	-4.23292165318335	1.19487101178638
C	-4.54920186116219	-1.31972324484691	1.27847719111542
C	-3.49311703924530	-3.50425338226702	1.73634640722866
C	-0.14142889866094	-5.06292720872786	-0.29252473323287
H	-0.28969024220886	-3.17234287557971	-1.34905888745536
C	-1.78781549834197	-5.47513074326274	1.46142150880822
C	-5.47150272681500	-1.60396876906350	2.28496621507708

H	-4.57958113117560	-0.39143088227651	0.71958050755670
C	-4.42144857492850	-3.76264503240935	2.73921497297711
C	-0.67595208436360	-5.88265488071486	0.71347003551504
H	0.71949263683330	-5.40336344181397	-0.85908201690265
H	-2.20028179677720	-6.11845422346681	2.23276360669528
C	-5.41111765500610	-2.80718421484667	3.00647517150422
H	-6.24597159753023	-0.87976759739200	2.51639841082448
H	-4.37885720059403	-4.68664241622793	3.30775954006300
H	-0.22186691373342	-6.84819170577899	0.91301936932149
H	-6.14086851735329	-2.99863317090072	3.78694204675588
N	1.54233957258700	3.11435408511639	-3.03765002072034
C	1.84275225441890	4.08346347028384	-2.08175130195046
C	2.47239964121090	3.19269473081337	-4.06683076787350
C	1.16130123116672	4.38798604428955	-0.90310770949442
C	2.99158936177288	4.79989308334535	-2.49864583510040
C	2.56677437876430	2.41249761396384	-5.22288600618437
C	3.39987257130376	4.22753837444775	-3.77192873784999
C	1.66167232200188	5.43128394024238	-0.12474640203602
H	0.28228245297255	3.82706916634241	-0.60676464767394
C	3.47432904283598	5.83793415101269	-1.70664992737761
C	3.61240708883107	2.69451438353798	-6.10125827755255
H	1.85243610996159	1.62138040085343	-5.41995247553475
C	4.43742963202343	4.48674949779424	-4.66121108303869
C	2.80385891950245	6.14667084224225	-0.51666527694843
H	1.15818291750313	5.69228636597737	0.80072643709445
H	4.35257816620462	6.40102079936718	-2.00756581846705
C	4.53577456661547	3.71645022927642	-5.82748369472232
H	3.71490514091041	2.11031721792043	-7.01015189973056
H	5.16038065688283	5.26973915534205	-4.45370820221231

H 3.17108325960190 6.95284781417615 0.11060225120003  
H 5.34071351959398 3.91036437957124 -6.52946937515312

**XYZ Coordinates of Cz2i in S<sub>0</sub> optimized geometry**

N 0.179713 -0.164646 -0.668368  
C -1.034940 -0.731673 -0.239664  
C -2.237517 -0.488274 -1.084194  
C -2.158510 0.484105 -2.119535  
C -0.918875 1.086673 -2.454745  
C 0.330493 0.722435 -1.736149  
C -3.469809 -1.109161 -0.824800  
C -0.853513 2.055943 -3.432711  
O -1.051117 -1.385038 0.791228  
O 1.420066 1.181327 -2.050157  
H 0.101191 2.528218 -3.633081  
C -3.314126 0.879388 -2.849893  
C -3.235081 1.851552 -3.885409  
C -4.437693 2.094752 -4.730002  
N -5.652875 1.530338 -4.299354  
C -5.803329 0.642025 -3.232538  
C -4.553832 0.277068 -2.514501  
C -4.619182 -0.692373 -1.536724  
H -5.573945 -1.164482 -1.336233  
O -6.892873 0.182890 -2.918802  
O -4.421029 2.745990 -5.762208  
C -2.002795 2.472346 -4.144938  
C -6.830360 1.861166 -5.113169  
H -7.705198 1.443351 -4.621746  
H -6.912634 2.945383 -5.203701  
H -6.718780 1.442398 -6.115808

C	1.356697	-0.494588	0.146536
H	1.447341	-1.579025	0.227001
H	2.230128	-0.065612	-0.337697
H	1.237654	-0.086575	1.152657
N	-3.627182	-2.175177	0.075204
C	-2.943070	-3.400758	0.038975
C	-4.597657	-2.237779	1.088442
C	-1.935621	-3.829086	-0.824307
C	-3.480164	-4.250533	1.034198
C	-5.490301	-1.256400	1.521240
C	-4.527722	-3.508963	1.707720
C	-1.455266	-5.127806	-0.666908
H	-1.537399	-3.177263	-1.593948
C	-2.980843	-5.548757	1.177119
C	-6.343509	-1.579508	2.576550
H	-5.518029	-0.274772	1.061148
C	-5.388618	-3.807332	2.767236
C	-1.966089	-5.980343	0.326236
H	-0.667978	-5.483716	-1.324665
H	-3.385948	-6.209649	1.937810
C	-6.297933	-2.840630	3.193013
H	-7.051836	-0.836038	2.929282
H	-5.343560	-4.777798	3.252705
H	-1.566399	-6.984594	0.427293
H	-6.973909	-3.060011	4.013607
N	-1.845527	3.538099	-5.045291
C	-0.875248	3.600352	-6.058731
C	-2.530337	4.763291	-5.010015
C	0.017848	2.619112	-6.490836

C	-0.945905	4.871028	-6.678986
C	-3.538045	5.191722	-4.147059
C	-1.993790	5.612570	-6.005968
C	0.870789	2.941839	-7.546491
H	0.046190	1.637829	-6.030052
C	-0.085239	5.169017	-7.738801
C	-4.019186	6.490018	-4.305520
H	-3.935836	4.540283	-3.376865
C	-2.493878	6.910393	-6.149916
C	0.824528	4.202456	-8.163931
H	1.579443	2.198426	-7.898686
H	-0.130856	6.139102	-8.224989
C	-3.508878	7.342049	-5.299372
H	-4.806674	6.846018	-3.648051
H	-2.089205	7.570913	-6.911156
H	1.500332	4.421540	-8.984746
H	-3.909191	8.345971	-5.401242

**XYZ Coordinates of Cz2i in S<sub>1</sub> optimized geometry**

N	-0.31766482076623	0.25376976668364	-0.03048783169925
C	-1.39494366914635	-0.65991229362191	-0.02130100904699
C	-2.43596015184713	-0.47340970026957	-1.04775818503954
C	-2.29065418622031	0.57156968129271	-1.99977560201398
C	-1.17322518887350	1.44318328671034	-1.95686578798590
C	-0.13361872931602	1.30138722981154	-0.93636666773506
C	-3.57945264933301	-1.31426744548894	-1.12748959877251
C	-1.03757888406289	2.47260591643042	-2.90365108556735
O	-1.40180680064954	-1.54508470820977	0.82873629992989
O	0.84430154629358	2.05251571315494	-0.87648403548643
H	-0.16932542969791	3.11797491545942	-2.83724205722827



C	-3.27672446588811	0.76228585522749	-3.02732050558380
C	-3.13395463369282	1.80511765614390	-3.98242340554595
C	-4.14244033057348	1.99018239991720	-5.02335238959510
N	-5.22090218045534	1.10531159709176	-5.02295909892951
C	-5.42286468231036	0.04926394081681	-4.10479016740161
C	-4.39341048680085	-0.10416404835098	-3.07612278006972
C	-4.52709942067564	-1.12501423706502	-2.12285154903344
H	-5.39396046058498	-1.77325916589763	-2.16968072337218
O	-6.41065366526873	-0.67745749037775	-4.19023623912556
O	-4.08149915770994	2.87909669683135	-5.88629917420724
C	-1.99204816329714	2.63992323632528	-3.88105679061666
C	-6.21711520187148	1.31084986806933	-6.07728012294730
H	-6.99236797761998	0.55917202714526	-5.95236537949461
H	-6.63616258768204	2.31648291155946	-5.99895209218605
H	-5.74314390037395	1.21870917958497	-7.05712935279115
C	0.69001062591146	0.04397095779645	1.01288841906705
H	1.13574942532073	-0.94702215067621	0.90160953966023
H	1.44416711352429	0.82006252048930	0.91005463246044
H	0.21490802020426	0.08801619451289	1.99502910096257
N	-3.80187123678229	-2.36938745269439	-0.20009319424743
C	-3.29830674784991	-3.66136478549799	-0.32479900779430
C	-4.29987129182824	-2.20801813138360	1.08965011746522
C	-2.67472495435736	-4.25829671104476	-1.42031636577986
C	-3.52341356458925	-4.36258203896951	0.88734896787411
C	-4.86787387954248	-1.07691483348549	1.67528935441255
C	-4.16481413968779	-3.43216790167772	1.79259985343124
C	-2.27798402290713	-5.58817831512850	-1.29004339970364
H	-2.50754679852895	-3.70191913261533	-2.33691791511140
C	-3.12109861755671	-5.69824833341933	0.98962666852794

C	-5.31161265646027	-1.18704155308115	2.99199869288558
H	-4.95590857925443	-0.14792534640637	1.12125943013532
C	-4.62381108585963	-3.51788689583285	3.11100737679241
C	-2.49952649232090	-6.30434844130587	-0.10015030006178
H	-1.78881967046970	-6.08021692615236	-2.12599162141950
H	-3.28689531041600	-6.25117297351224	1.91010509067232
C	-5.19466635419364	-2.39395050264459	3.70449055609788
H	-5.75717124130943	-0.32253019395317	3.47605631160626
H	-4.52963695163614	-4.44822589767008	3.66425921431169
H	-2.17984335784303	-7.33989153713439	-0.03166254457616
H	-5.55167988049339	-2.44723912566841	4.72866986868038
N	-1.79528566723513	3.71851917741475	-4.83040634119925
C	-1.14185189383330	3.60269829972933	-6.03298800954401
C	-2.27733507453746	4.99620891566138	-4.68646126105527
C	-0.51148346731173	2.47273108777128	-6.56930205616785
C	-1.18704437495968	4.85390339301989	-6.71096417385144
C	-3.00258350289206	5.53101410021855	-3.61394172258518
C	-1.92557516908410	5.76004748218816	-5.83536078735951
C	0.08622080183925	2.61285697244880	-7.82070719181864
H	-0.49901728784908	1.53736115679861	-6.02451027391545
C	-0.58872071975734	4.97156579515405	-7.95057443432457
C	-3.38034003274379	6.86936763637576	-3.70719182556564
H	-3.25317578629952	4.91819250230570	-2.75748672792058
C	-2.31020995863344	7.08482753997679	-5.90833580917037
C	0.05000319478401	3.83788602233500	-8.50105478078721
H	0.58408783982568	1.76322696715188	-8.27386258437693
H	-0.60676759166817	5.90823558855553	-8.49775882600233
C	-3.04196516033916	7.63458507024164	-4.83188873242944
H	-3.94397968880027	7.32363567175062	-2.90034835336413

H	-2.06312740177791	7.69610921317205	-6.76995983043107
H	0.52164465715178	3.91997592808145	-9.47444376617772
H	-3.34940378852831	8.67371419783014	-4.88037502675709

**XYZ Coordinates of Cz2i in T<sub>1</sub> optimized geometry**

N	0.12750809329195	-0.16869724429367	-0.61415539938422
C	-1.09776049847645	-0.72290674971535	-0.20962738779111
C	-2.25551399068371	-0.48645471825996	-1.08643437531157
C	-2.15619495624546	0.48122608469921	-2.10957549609192
C	-0.90426419975165	1.07513107666720	-2.42601094095113
C	0.31014387745053	0.71860927040028	-1.68613280476272
C	-3.53159603641833	-1.10294139192017	-0.84584481824949
C	-0.81692469235623	2.05337950092305	-3.42243995091786
O	-1.14591924082344	-1.37238339651323	0.83483080005794
O	1.42036949138651	1.17227360768897	-1.96383214485192
H	0.14271463201034	2.52772830303418	-3.59142668856333
C	-3.31710835832489	0.88212620664098	-2.86027619695633
C	-3.21777564013943	1.84976694190183	-3.88344762710476
C	-4.37558024699888	2.08629987843092	-4.76017561922441
N	-5.60098342216620	1.53273911112547	-4.35515614191853
C	-5.78348613732551	0.64493235299013	-3.28356354022266
C	-4.56904839687254	0.28824796422762	-2.54382015195593
C	-4.65634808686121	-0.69014468289188	-1.54752876418114
H	-5.61597553717187	-1.16453763278062	-1.37859955232883
O	-6.89368568068042	0.19109610458795	-3.00604167984298
O	-4.32732603714230	2.73539256112240	-5.80486187114456
C	-1.94166303879937	2.46610194896697	-4.12419191828177
C	-6.75373597135381	1.85440471740893	-5.20224106972756
H	-7.64030482753126	1.43816809137012	-4.73042502376973
H	-6.83564029056687	2.93791598075773	-5.30646177040334

H	-6.61559811944330	1.42921042393869	-6.19939006396103
C	1.28005468090447	-0.49001278453364	0.23334847742925
H	1.36526696602793	-1.57366347238006	0.33382750982131
H	2.16602315572106	-0.06954515332381	-0.23582723070371
H	1.13900824877558	-0.06889245075227	1.23177950125314
N	-3.67666403548564	-2.17623036472107	0.05750412627385
C	-2.98272732268280	-3.39013401821530	0.00551423882548
C	-4.60898924184714	-2.23891649935427	1.09579732691056
C	-2.01254263714687	-3.80740089838464	-0.90617884900018
C	-3.46616296167242	-4.23954114071926	1.02895190833028
C	-5.50100539324506	-1.25878514226476	1.53825786710961
C	-4.50261170996771	-3.50212086639905	1.73234743084632
C	-1.49811847027994	-5.09402449530032	-0.75462124001002
H	-1.66995615743439	-3.15189475923040	-1.69833954304984
C	-2.94242493691596	-5.52400668824581	1.16045755776915
C	-6.31338276422744	-1.57330712560006	2.62722634637477
H	-5.55532633477994	-0.29178633562939	1.05217723659515
C	-5.32028319319855	-3.79197042125773	2.82140848564439
C	-1.95198541333088	-5.94326533305368	0.26698170585622
H	-0.73539345252603	-5.44447695274676	-1.44282793246090
H	-3.30299764649911	-6.18986234553675	1.93867681660540
C	-6.22894815656004	-2.82315451817084	3.26086559436822
H	-7.02052400124415	-0.83468931653631	2.99106207487828
H	-5.24992260481942	-4.75164582904953	3.32441556146405
H	-1.53323776612161	-6.94051138108501	0.35886022161383
H	-6.87401903557264	-3.03799786052452	4.10704350624888
N	-1.79657907256304	3.53921025141162	-5.02774768611566
C	-0.86421935271054	3.60170869402160	-6.06602415834923
C	-2.49067534763944	4.75303438808515	-4.97614259427193

C	0.02792416085354	2.62155587053168	-6.50817969434191
C	-0.97069761773537	4.86473344230480	-6.70291340032985
C	-3.46100304440902	5.17041573151494	-4.06465191680483
C	-2.00727479731712	5.60222306597827	-5.99977999562152
C	0.84032192316809	2.93587703771662	-7.59719197630715
H	0.08232805497542	1.65469118681220	-6.02184070248746
C	-0.15300396228481	5.15438165384739	-7.79201310898146
C	-3.97558959164031	6.45692885327435	-4.21660790360414
H	-3.80357966411523	4.51507975126541	-3.27234383339934
C	-2.53117092403247	6.88658493385895	-6.13167653488377
C	0.75578636604300	4.18554729697937	-8.23116826976763
H	1.54756089330205	2.19723799476226	-7.96079552515779
H	-0.22344952273234	6.11391446042514	-8.29528080712275
C	-3.52174357543390	7.30595452295797	-5.23839997151581
H	-4.73842465050741	6.80746423694396	-3.52856498587322
H	-2.17062622323694	7.55227287284573	-6.91005260060186
H	1.40087464720829	4.40023321074843	-9.07737316418339
H	-3.94061920306981	8.30311838622162	-5.33058867143172

**XYZ Coordinates of *o*Cz1 in S<sub>0</sub> optimized geometry**

N	0.413476	-0.777006	-3.949969
C	-0.563163	-0.960780	-2.958027
C	-1.908374	-0.372560	-3.221067
C	-2.094403	0.449705	-4.365289
C	-1.076657	0.585898	-5.340589
C	0.233450	-0.083113	-5.149218
C	-2.983079	-0.612529	-2.360815
C	-1.301800	1.319143	-6.495076
O	-0.298853	-1.553002	-1.921799
O	1.135040	-0.021969	-5.973505

H	-0.501880	1.387077	-7.224104
C	-3.346897	1.078178	-4.596140
C	-3.556043	1.826932	-5.777962
C	-4.876121	2.460121	-6.039557
N	-5.864940	2.277970	-5.058272
C	-5.707191	1.542576	-3.875740
C	-4.380776	0.921185	-3.647039
C	-4.192826	0.095781	-2.557914
H	-5.025062	-0.064963	-1.883047
O	-6.640092	1.424188	-3.093307
O	-5.097517	3.103310	-7.055851
C	-2.541826	1.944349	-6.714946
H	-2.730550	2.515847	-7.616936
C	-7.194848	2.857116	-5.280389
H	-7.937991	2.057896	-5.328041
H	-7.452323	3.513283	-4.446895
H	-7.169395	3.412168	-6.214497
C	1.741604	-1.366196	-3.747982
H	1.737334	-1.888790	-2.795476
H	1.955899	-2.054938	-4.565858
H	2.496850	-0.577264	-3.750525
C	-3.013531	-1.731599	-1.369675
C	-3.251553	-3.037648	-1.853004
C	-2.910682	-1.530943	0.007244
N	-3.401569	-3.252274	-3.264523
C	-3.342233	-4.112277	-0.970890
C	-3.001101	-2.609387	0.889223
H	-2.734894	-0.528463	0.384537
C	-2.313463	-3.427464	-4.134506

C	-4.453244	-2.695992	-4.004215
C	-3.208467	-3.900442	0.402825
H	-3.527980	-5.103052	-1.372806
H	-2.906201	-2.439023	1.957329
C	-2.671488	-2.977716	-5.430887
C	-1.049510	-3.947636	-3.854999
C	-4.036301	-2.498034	-5.344885
C	-5.731755	-2.342190	-3.569130
H	-3.278238	-4.739231	1.088389
C	-1.727429	-3.034417	-6.463041
C	-0.132748	-4.006131	-4.902833
H	-0.787007	-4.257277	-2.849921
C	-4.912212	-1.893291	-6.253432
C	-6.584962	-1.738288	-4.490067
H	-6.033278	-2.505032	-2.539791
C	-0.461387	-3.548628	-6.192212
H	-1.979133	-2.677783	-7.457493
H	0.859287	-4.405830	-4.715603
C	-6.177692	-1.505135	-5.816538
H	-4.602595	-1.716627	-7.279461
H	-7.572725	-1.423071	-4.169920
H	0.282084	-3.593948	-6.981607
H	-6.862271	-1.025126	-6.509228

**XYZ Coordinates of *o*Cz1 in S<sub>1</sub> optimized geometry**

N	0.00335030260052	-0.56816792163487	-4.43725620382003
C	-0.89307025436908	-0.83930101802418	-3.39503813867701
C	-2.18094953041308	-0.15136778806819	-3.43777573769423
C	-2.40690037185682	0.84114320771744	-4.42980663702814
C	-1.45950791842919	1.09207349792993	-5.45447032707082

C	-0.21510132705453	0.33327051050875	-5.50128768833679
C	-3.19189780571098	-0.41760548844077	-2.46580383737766
C	-1.71904276163002	2.06199120797226	-6.44252138635289
O	-0.58302255484508	-1.64047992034601	-2.49808118532090
O	0.63483797072883	0.43900899967030	-6.38738087657496
H	-0.96603212035866	2.21659331524810	-7.20716124833557
C	-3.62206326909608	1.59951966310092	-4.42059089590799
C	-3.85705678856868	2.56976543591122	-5.42310990912764
C	-5.10129877044183	3.34640619246190	-5.42305616104274
N	-6.01054666750593	3.06812051533227	-4.37748571019813
C	-5.83096530586785	2.10903506228024	-3.37145477041933
C	-4.57084281507321	1.36394824302665	-3.39801364432455
C	-4.33474309812556	0.37271436993469	-2.43483265715797
H	-5.11596228568319	0.19027328580702	-1.70396957922173
O	-6.71470808679500	1.92149747803287	-2.52976127574694
O	-5.36544612557623	4.19416771642941	-6.27634259122386
C	-2.89703067051117	2.79091112937232	-6.42826999786860
H	-3.10876745142867	3.54360384031918	-7.17907100079052
C	-7.26848820796111	3.81521210258084	-4.32997958927642
H	-8.11352471939186	3.13397142037481	-4.46004866892580
H	-7.37330836552595	4.29439490126179	-3.35430248201147
H	-7.24882284558177	4.55470716449165	-5.12665268780700
C	1.28802460653616	-1.26928289729681	-4.45161898320899
H	1.41723879739908	-1.75855051161999	-3.48959772937887
H	1.30425632513980	-2.01023831693456	-5.25638734979341
H	2.08767624890453	-0.55246883690711	-4.64134273558400
C	-3.17500730891630	-1.58749221822441	-1.54026585466596
C	-3.13266278842718	-2.92858843944372	-1.97856121750770
C	-3.29333190142181	-1.38830532189474	-0.15883493130683



N	-3.03544759997196	-3.24402945514052	-3.37587948124502
C	-3.15609151908989	-4.00513076144662	-1.08733545590346
C	-3.33475179442209	-2.45359768317532	0.74016731274672
H	-3.33093177911178	-0.36686680937607	0.20421176476695
C	-1.98133681672484	-3.93298465316330	-3.95664945702009
C	-3.95375651848999	-2.90080585123433	-4.36083500628917
C	-3.26045443779183	-3.76936149801632	0.28033526940434
H	-3.12356326289054	-5.01745944031823	-1.47724921670687
H	-3.41830902013720	-2.25400635325256	1.80403879941152
C	-2.20692919018123	-4.02973094667579	-5.35663759151106
C	-0.82242301298626	-4.43221828679055	-3.34545332453202
C	-3.47599545031483	-3.35957442571078	-5.61726120705684
C	-5.19090726400549	-2.25973203193094	-4.22097848195645
H	-3.29503796601513	-4.60300365989436	0.97368579360751
C	-1.26788400626280	-4.65793645887799	-6.15621119095095
C	0.09926343300740	-5.07892765805334	-4.16399160059647
H	-0.64117965301716	-4.26420496848721	-2.29303493673631
C	-4.22630438394107	-3.13166981061614	-6.75790311603255
C	-5.93051141515741	-2.03616372221909	-5.37959364772617
H	-5.54022410486900	-1.92657346489871	-3.25399175904027
C	-0.11622276761400	-5.19314413232465	-5.54566263866945
H	-1.40579115045084	-4.73053434418541	-7.22965650368612
H	1.01019052328535	-5.47531422523900	-3.72998162974289
C	-5.45533416926958	-2.45493640721523	-6.63007922178875
H	-3.88022841318221	-3.46428637956002	-7.73073627741055
H	-6.88100733331270	-1.52022042873765	-5.30986780946690
H	0.62787854395016	-5.68630865151013	-6.16204510928017
H	-6.04522360577494	-2.25610007287886	-7.51822258750263

**XYZ Coordinates of *o*Cz1 in T<sub>1</sub> optimized geometry**

N	0.23683017445173	-0.78819347638495	-4.00232349702349
C	-0.66820736061170	-0.88453833753944	-2.93069492313742
C	-1.98189047370558	-0.27386217413510	-3.12785475706680
C	-2.26141942570114	0.42696181692409	-4.32393926761202
C	-1.35705673365690	0.40637837597831	-5.40637368801836
C	-0.05101350902363	-0.24214678276157	-5.25842396781001
C	-3.02393011816383	-0.41271403745077	-2.13014670615494
C	-1.71339436740023	0.99329837285639	-6.65045951984235
O	-0.35318376099914	-1.46859978908820	-1.88851933671751
O	0.77883789987163	-0.29888755773516	-6.16640263863928
H	-0.99019477256147	0.94357221952056	-7.45648081835672
C	-3.51622074518553	1.09730953166282	-4.47894697465982
C	-3.85683032512706	1.65462173976215	-5.71995057687450
C	-5.17240734834369	2.28158880310301	-5.91711487659056
N	-6.01400633098678	2.33305353960306	-4.79270319578790
C	-5.72835888045692	1.77141105610723	-3.53895977148636
C	-4.41635763092091	1.14070399166861	-3.38443669494853
C	-4.15092332256737	0.37276839108112	-2.22040882319902
H	-4.94868728918057	0.28199668375473	-1.49113666603159
O	-6.57213013952945	1.79842895551119	-2.64148118866999
O	-5.52922253108026	2.73257763601804	-7.00472496528777
C	-2.94114012734469	1.58906759426608	-6.81156657563090
H	-3.24535314405369	2.03059273107060	-7.75353911810384
C	-7.33958490663358	2.94140699767733	-4.93660062181809
H	-8.11502416920787	2.17553891586102	-4.84741084501851
H	-7.49241426143865	3.67062333542959	-4.13940231378072
H	-7.38897058129424	3.41422441891394	-5.91428455280186
C	1.58274978204293	-1.34603548183710	-3.84164601832122
H	1.64621866161243	-1.78839029849266	-2.85101450938029

H	1.75874626497958	-2.09679027779175	-4.61229472890246
H	2.32411645878472	-0.55182422461548	-3.95800468402803
C	-3.07467511371727	-1.61467950313093	-1.25991782774570
C	-3.15617929814822	-2.86987652182592	-1.90365082728325
C	-3.13809714779557	-1.57963764216370	0.13487412482859
N	-3.15919393916884	-2.91175967790191	-3.33764137066858
C	-3.22242045519897	-4.05496613701176	-1.17289841442728
C	-3.21502769607762	-2.76294267092299	0.86985059024929
H	-3.09071073835161	-0.61944382119183	0.63829324833954
C	-2.10150089142228	-3.36693644102951	-4.12856322067964
C	-4.14271403216417	-2.37386696474803	-4.17525034883222
C	-3.24480670475129	-4.00020559070859	0.22111170999634
H	-3.27943200499363	-5.00245265533681	-1.69925574363201
H	-3.24081553206699	-2.72016340223060	1.95442623848707
C	-2.37090479398402	-3.04494859715133	-5.48587062834824
C	-0.91463574788219	-3.98367245583890	-3.72567802019826
C	-3.67222746006545	-2.40053986673291	-5.51333191035805
C	-5.39702421899971	-1.85917898349870	-3.84213537798973
H	-3.30219911348256	-4.91881922701099	0.79617688665367
C	-1.41777861073693	-3.34284997702221	-6.45981306944369
C	0.01028141395842	-4.28752297285226	-4.72143541438981
H	-0.71491275285851	-4.17384090095695	-2.67835758090136
C	-4.44670562832513	-1.83159401285516	-6.52208586723556
C	-6.16196653844833	-1.30431819983216	-4.87252948749793
H	-5.75216968476387	-1.87509669302293	-2.81872661315664
C	-0.23144317124343	-3.96697324872835	-6.06949019326911
H	-1.58953632154865	-3.08163749546586	-7.49908261252614
H	0.94557647944827	-4.76489384700878	-4.44704124704227
C	-5.68746794513881	-1.27032274058289	-6.19045677370289

H	-4.08759468893321	-1.80831201172682	-7.54590956493732
H	-7.12872479886635	-0.87264899153549	-4.63464826822341
H	0.52126838109698	-4.19855427327502	-6.81587963448814
H	-6.28907023193784	-0.80582914563727	-6.96478795987606

**XYZ Coordinates of *mCz1* in  $S_0$  optimized geometry**

N	-0.584446	2.007721	0.527472
C	-1.628212	1.076634	0.636266
C	-2.250786	0.591016	-0.630576
C	-1.995890	1.333234	-1.818305
C	-1.034208	2.375962	-1.848317
C	-0.247253	2.713113	-0.634935
C	-3.134056	-0.499507	-0.662317
C	-0.795141	3.082665	-3.017396
O	-1.985250	0.712497	1.747294
O	0.632616	3.561732	-0.639454
H	-0.043235	3.863823	-2.999678
C	-2.697066	1.028560	-3.016556
C	-2.448065	1.771313	-4.194131
C	-3.194935	1.458202	-5.440576
N	-4.127647	0.412301	-5.381196
C	-4.409919	-0.358238	-4.242587
C	-3.640037	-0.024402	-3.012149
C	-3.830835	-0.771672	-1.868929
H	-4.521134	-1.606696	-1.911341
O	-5.243084	-1.252101	-4.263199
O	-3.022604	2.072189	-6.483084
C	-1.507122	2.787673	-4.192794
H	-1.332914	3.338332	-5.110502
C	-4.851841	0.124653	-6.626374

H	-5.521822	-0.710746	-6.440868
H	-5.414369	1.007806	-6.936006
H	-4.137787	-0.120057	-7.415053
C	0.101786	2.347687	1.781639
H	0.481846	1.433043	2.241044
H	0.916831	3.026085	1.543305
H	-0.598024	2.818646	2.475186
C	-3.345941	-1.452176	0.459948
C	-4.642055	-1.838538	0.829577
C	-2.251293	-2.054869	1.091703
C	-4.833559	-2.786083	1.836402
H	-5.499335	-1.381139	0.345304
C	-2.443027	-2.985814	2.111521
H	-1.240261	-1.794249	0.800949
C	-3.742068	-3.355719	2.487569
H	-5.841114	-3.066951	2.126865
N	-1.318800	-3.541246	2.770209
H	-3.879856	-4.072335	3.290111
C	-0.291600	-2.808030	3.379030
C	-1.037421	-4.903774	2.912796
C	0.660851	-3.712588	3.912425
C	-0.162723	-1.424230	3.529291
C	0.186131	-5.047790	3.616310
C	-1.752068	-6.010768	2.448136
C	1.782306	-3.214072	4.585842
C	0.962222	-0.957118	4.207370
H	-0.909252	-0.739191	3.144493
C	0.686208	-6.328970	3.873825
C	-1.231640	-7.275472	2.717416

H	-2.675671	-5.889036	1.892772
C	1.930331	-1.836824	4.725126
H	2.520822	-3.895768	4.998102
H	1.084586	0.113414	4.348217
C	-0.027994	-7.437466	3.426196
H	1.621128	-6.452553	4.413028
H	-1.768575	-8.152995	2.369237
H	2.794841	-1.436663	5.246086
H	0.348187	-8.437123	3.620952

**XYZ Coordinates of *mCz1* in  $S_1$  optimized geometry**

N	-0.72908851964428	2.21830861597291	0.52893108009959
C	-1.52779753791349	1.07511122543799	0.59482129655250
C	-2.18418557443297	0.63667676557647	-0.63376453016377
C	-2.01274611393285	1.42128395505031	-1.81335950333309
C	-1.19153662077722	2.57786815402178	-1.82788371754395
C	-0.49734696113607	3.00906275418539	-0.62289312150566
C	-3.01886448707442	-0.52374915804179	-0.68932905655812
C	-1.03033464723444	3.33025441602127	-3.00948846302396
O	-1.63125667069227	0.49999794980377	1.69699335586428
O	0.24602205397935	3.99035274342645	-0.56329047763072
H	-0.38909829658293	4.20310689359666	-2.96725010415918
C	-2.68013695509550	1.04966675700019	-3.02777269806722
C	-2.50218480727797	1.82625271250575	-4.19913458066169
C	-3.18210337242375	1.44769388460067	-5.43952297346643
N	-4.00197989729560	0.30508136381316	-5.38888457973333
C	-4.21522543018828	-0.50045598337584	-4.25645610164721
C	-3.51254411558723	-0.09164427556683	-3.03927202173641
C	-3.66439399614814	-0.85561100133246	-1.87033075089117
H	-4.29479860087163	-1.73584845565898	-1.92769107526271

O	-4.95281205115623	-1.49027849613160	-4.30531170920435
O	-3.07076739473655	2.06954745130138	-6.49804173393898
C	-1.67439846080532	2.96175832520177	-4.17733665018375
H	-1.56280555838076	3.52973306010283	-5.09391850435393
C	-4.67630913090771	-0.04922581519625	-6.63798002125982
H	-5.26660937969652	-0.94420690936401	-6.45724933819512
H	-5.31397703884634	0.77708369877262	-6.96118443618100
H	-3.93524270598838	-0.22406446962333	-7.42150943974598
C	-0.08648920893104	2.62708803935071	1.77654761568634
H	0.64241970530536	1.87321665727598	2.09020180260414
H	0.41460966669595	3.57468415226650	1.59460370442956
H	-0.83607328723466	2.72249384283365	2.56438113382430
C	-3.23736867911658	-1.44476509497507	0.46826520785658
C	-4.52764641960977	-1.70968024546443	0.93832844747556
C	-2.16818642221865	-2.12348462702272	1.06234757799553
C	-4.75541933549157	-2.61033755121981	1.98546175801490
H	-5.36436989758678	-1.19274045441789	0.48064421177631
C	-2.40063041668974	-2.99332074339333	2.12012123257606
H	-1.15887458420814	-1.94742844166424	0.71200675969989
C	-3.68986749133341	-3.25810600163777	2.59849921286406
H	-5.76676992299735	-2.78784400864726	2.33655183437123
N	-1.27317872045322	-3.60876542919750	2.76761738957960
H	-3.83838761630367	-3.92215191630016	3.44322299372538
C	-0.21579360664933	-2.92554610574458	3.33109221172042
C	-1.08903490707993	-4.97545744004661	2.94184497434627
C	0.69394307659329	-3.86924322055249	3.89508093410090
C	-0.01516805404406	-1.53300553299364	3.39788066183867
C	0.12715684323307	-5.19021137347787	3.64399706333729
C	-1.89728599862355	-6.02682573948102	2.49663218867931

C	1.83413823799346	-3.41256631042201	4.52775868079941
C	1.14676557632061	-1.10479542231138	4.03619089932354
H	-0.71198821805968	-0.82642888492660	2.95564501328810
C	0.53043448287615	-6.48530462371853	3.92310906055482
C	-1.47421261085972	-7.32419265333736	2.79175156215843
H	-2.80751708704184	-5.83345538131992	1.94297559671219
C	2.05524326932504	-2.01829500850521	4.59023063746216
H	2.54574397651107	-4.10134606880360	4.97046259175934
H	1.34717605099580	-0.04194769384435	4.10251058739579
C	-0.28461828135478	-7.55197465056564	3.49486014788473
H	1.45602751821930	-6.68071544324952	4.45424481762639
H	-2.07388754137353	-8.16622304951523	2.46532932424661
H	2.94897196275918	-1.64943012544684	5.08185743326421
H	0.02141721128031	-8.57031761162450	3.70854558695317

**XYZ Coordinates of *m*Cz1 in T<sub>1</sub> optimized geometry**

N	-0.56984120647764	1.98830970621284	0.50576872845844
C	-1.59618191261781	1.03936160293920	0.60698284258315
C	-2.21212574709978	0.57291828934469	-0.64045952622794
C	-1.94687557548185	1.29805582449466	-1.82958558556893
C	-0.96789757427309	2.32106468609373	-1.86772816422907
C	-0.20268078413518	2.66611957258623	-0.66572687924715
C	-3.17571104972150	-0.52824892849520	-0.66964769868984
C	-0.71038974545591	3.03766579084558	-3.06983088778084
O	-1.93321893489438	0.64452413776979	1.72853859343548
O	0.69256889217931	3.51066881157708	-0.66749511182254
H	0.05483711786089	3.80447299107357	-3.04378816064872
C	-2.68183394337172	1.01548676282170	-3.02667718714250
C	-2.42428355346201	1.74431809998066	-4.19605182181541
C	-3.19062673006635	1.47067129821845	-5.42016915032817



N	-4.16402707198330	0.46456802299576	-5.35050021476961
C	-4.46143382540375	-0.29849096383435	-4.20823622217583
C	-3.67993408176152	0.00851514049675	-3.00408876995807
C	-3.89055055036834	-0.74871112196019	-1.83319611327908
H	-4.59771627477482	-1.56782541699193	-1.89723023235196
O	-5.32992822638602	-1.17095995024463	-4.22568032811126
O	-3.00515981017686	2.08318292152729	-6.47049253549989
C	-1.42120335803078	2.75929524432667	-4.20980380203257
H	-1.25283687437993	3.29219434743085	-5.13848696556898
C	-4.91279084140664	0.20771573708779	-6.58521064187380
H	-5.62420229762803	-0.58979108028049	-6.38644309601609
H	-5.42946325375841	1.11784510637920	-6.89747079187749
H	-4.22176125322829	-0.07971683440419	-7.38057424046851
C	0.09832556917441	2.34695115579057	1.76133895083633
H	0.52901212693918	1.45001397754602	2.21240159979464
H	0.87624469594762	3.06990760639488	1.52928241978095
H	-0.62537362537565	2.76989153605954	2.46124050667810
C	-3.35742601888475	-1.48441454191182	0.44125318407188
C	-4.64894829512299	-1.91210014451028	0.80627708419605
C	-2.25415870564668	-2.06016301208783	1.08790219988666
C	-4.83012592543662	-2.87323167565170	1.80009345804884
H	-5.51136243869614	-1.46382809759181	0.32382310118976
C	-2.43816129251703	-3.00964749385828	2.08897871546924
H	-1.24780383763180	-1.77113889910598	0.81141767447336
C	-3.73076204205608	-3.42414795557253	2.45343358442384
H	-5.83328918216634	-3.17777759255376	2.08090396280708
N	-1.31349612811809	-3.54319581332009	2.76662129528438
H	-3.85577742936511	-4.14192958061337	3.25686782482485
C	-0.30331129551700	-2.79485286942861	3.38227757272477

C	-1.02101632115134	-4.90090909499952	2.91638075127708
C	0.65072889447786	-3.68677787653496	3.93624807987724
C	-0.19752766543387	-1.40707059438112	3.52386898222716
C	0.19222395732710	-5.03144166098492	3.64111870939429
C	-1.71796581896287	-6.01322428959646	2.43517129012270
C	1.75244495747018	-3.17397014692079	4.62172331655193
C	0.91543266115843	-0.92333992577277	4.21250324674322
H	-0.94268243993086	-0.73166617165829	3.11895262349530
C	0.69624333383430	-6.30384482362817	3.91203527958043
C	-1.19506496055365	-7.27374061887953	2.72124838097219
H	-2.62561936992331	-5.89812077924082	1.85365566803686
C	1.88183945690162	-1.78881185572591	4.75079132676357
H	2.49297660137670	-3.84153162637002	5.05219624234476
H	1.02676082020438	0.14903278733624	4.34212377087485
C	-0.00570544130463	-7.42120077439179	3.45404199253095
H	1.62285803487793	-6.42178965235963	4.46585805569367
H	-1.71587721286404	-8.15655297708036	2.36370420652861
H	2.73429688752505	-1.37672878447850	5.28173589694391
H	0.37609291574790	-8.41652553190906	3.65850400855773

**XYZ Coordinates of *p*Cz1 in  $S_0$  optimized geometry**

N	-1.911438	5.851155	3.025816
C	-2.855005	4.808893	3.034469
C	-3.533477	4.481617	1.744346
C	-3.320421	5.350788	0.634926
C	-2.388153	6.418302	0.696346
C	-1.614702	6.677868	1.936484
C	-4.424213	3.402710	1.624995
C	-2.179357	7.238924	-0.402355
O	-3.084936	4.233480	4.087226

O	-0.778781	7.567567	2.011525
H	-1.452392	8.038574	-0.313131
C	-4.038561	5.157162	-0.577266
C	-3.815262	6.008452	-1.684980
C	-4.565846	5.804846	-2.954692
N	-5.498079	4.753544	-2.972230
C	-5.758246	3.886460	-1.903491
C	-4.977248	4.103945	-0.657157
C	-5.152509	3.255756	0.414376
H	-5.850217	2.432535	0.307858
O	-6.591250	2.998648	-2.014557
O	-4.385739	6.513624	-3.933810
C	-2.891819	7.037373	-1.596235
H	-2.735754	7.674796	-2.459286
C	-6.272843	4.515376	-4.197112
H	-6.078766	3.504753	-4.561899
H	-7.338924	4.600978	-3.977626
H	-5.971588	5.254167	-4.935112
C	-1.240619	6.111402	4.306705
H	-0.762495	5.196152	4.660019
H	-0.504667	6.894922	4.146647
H	-1.975821	6.421344	5.052451
C	-4.635740	2.336514	2.639286
C	-5.936181	1.977915	3.021132
C	-3.560080	1.583242	3.135182
C	-6.159373	0.916106	3.894581
H	-6.780968	2.553071	2.653912
C	-3.775782	0.503256	3.979012
H	-2.548575	1.837723	2.838294

C	-5.079792	0.164329	4.370771
H	-7.165325	0.668112	4.215003
H	-2.942956	-0.095739	4.330717
N	-5.299235	-0.937696	5.229775
C	-6.163186	-2.011679	4.978283
C	-4.649703	-1.167699	6.449391
C	-6.067940	-2.936628	6.049005
C	-6.983980	-2.252339	3.873347
C	-5.105846	-2.398031	6.986887
C	-3.730062	-0.365349	7.130007
C	-6.829263	-4.110035	6.018075
C	-7.730917	-3.429245	3.866154
H	-7.032172	-1.553390	3.045916
C	-4.610339	-2.839602	8.218589
C	-3.251691	-0.828312	8.354685
H	-3.407068	0.586947	6.724080
C	-7.661029	-4.348921	4.927157
H	-6.764649	-4.825432	6.832968
H	-8.377562	-3.638819	3.019134
C	-3.680866	-2.053627	8.894695
H	-4.952178	-3.780545	8.640329
H	-2.534847	-0.224530	8.903350
H	-8.257659	-5.255208	4.890459
H	-3.286567	-2.384815	9.850507

**XYZ Coordinates of *p*Cz1 in S<sub>1</sub> optimized geometry**

N	-2.28532424283959	5.58953049533781	3.22215275756415
C	-3.03465688251426	4.43212459303001	2.98897936464069
C	-3.62029384815956	4.27774817902555	1.65958548824545
C	-3.42602897115015	5.30011804608435	0.69068092161094

C	-2.66580784755483	6.46079453098674	0.98226552310335
C	-2.05593000038762	6.63501525353919	2.29453356087324
C	-4.38974529023611	3.13044389812961	1.31677079678224
C	-2.49068492871638	7.46039095509041	0.00247778960430
O	-3.16037507897145	3.60419496447087	3.90780826099611
O	-1.37829587025785	7.61444194279627	2.61470835425049
H	-1.90056249256270	8.32967811118774	0.26909351329311
C	-4.00853043014371	5.16747279818730	-0.61283158064856
C	-3.81837076864002	6.18930646707509	-1.57654804065990
C	-4.41069029046352	6.06788546646197	-2.90888874012624
N	-5.15709182705846	4.89301638986426	-3.15252203891473
C	-5.37569993678724	3.85577137477446	-2.23445069054153
C	-4.76818248230683	4.01515815700303	-0.91576164487514
C	-4.94643737451648	3.01265131899179	0.05484974227499
H	-5.53451556471669	2.14462210588264	-0.22155014050229
O	-6.05284391000821	2.87429289001124	-2.56198201792462
O	-4.28297338132614	6.92469363951151	-3.78721739453306
C	-3.05674230420759	7.32873335463810	-1.25322845840362
H	-2.93165531894912	8.08947716100648	-2.01524702395830
C	-5.76969585969310	4.71789465708303	-4.46883338828520
H	-5.39263888046210	3.80391796948249	-4.93430654506241
H	-6.85257878698800	4.61594501449320	-4.36354724399458
H	-5.52092509559581	5.58844709294763	-5.07084814899596
C	-1.70572152643113	5.71538042695109	4.55823292588443
H	-1.04553345898877	4.86780535121227	4.75859098430603
H	-1.15263359961150	6.65087981332925	4.59214512708702
H	-2.49825143398785	5.70757082563630	5.31081448621822
C	-4.63191278016399	2.02593357738542	2.29584832335927
C	-5.85210942005374	1.94190350250786	2.97648151892316

C	-3.66844606272203	1.02840115630406	2.50490333330965
C	-6.09299340259255	0.92386199213819	3.89609147100654
H	-6.60501703825776	2.70255370930758	2.80362253614599
C	-3.87961795069761	0.01412147029408	3.42841319599997
H	-2.73211147038645	1.07864972224031	1.96129055826330
C	-5.08980956752471	-0.01644405957883	4.12693086021033
H	-7.02060306662763	0.88314278659001	4.45816560240466
H	-3.12698496634931	-0.74645852392259	3.61017907475804
N	-5.27845969900207	-1.01261064838540	5.14635681715924
C	-6.24921395360314	-1.99729679957827	5.15521765089696
C	-4.50437361119553	-1.11796390650488	6.28539947246856
C	-6.10231107549552	-2.78147365661043	6.33415299805337
C	-7.22748294466414	-2.25894052192754	4.18698807398077
C	-4.97205477026943	-2.21369649235617	7.06487112299730
C	-3.44655106061336	-0.28911759971388	6.69025198346859
C	-6.96410860610769	-3.84214566663110	6.55024991791915
C	-8.08809379672184	-3.32910068742089	4.42867180868835
H	-7.29977373201522	-1.65052139494129	3.29398821916269
C	-4.34733523709074	-2.50068292693587	8.26503955951533
C	-2.83092648328496	-0.60157162590238	7.90091015414160
H	-3.14114993180191	0.55767573225041	6.08691022805692
C	-7.96181173323812	-4.10652227139472	5.58841311322193
H	-6.87857222308604	-4.46341803729204	7.43535065506010
H	-8.86140530395618	-3.56523715983615	3.70695571404222
C	-3.26742170577383	-1.68791466992876	8.67299332907048
H	-4.67742564219470	-3.32516987810427	8.88786397819648
H	-2.00900347927998	0.01035233029627	8.25336479706023
H	-8.64293697339172	-4.93484337472325	5.74965346473559
H	-2.77122362760510	-1.90518232184725	9.61247696841452

### XYZ Coordinates of *p*Cz1 in T<sub>1</sub> optimized geometry

N	-1.87594738337934	5.77432156998694	2.99715526495052
C	-2.89566886439412	4.81185097439760	3.01488898066333
C	-3.54100167452215	4.48586640043839	1.73967961330513
C	-3.27985405124899	5.31169925442307	0.61945410990364
C	-2.28311181022909	6.31962046427880	0.66353890120877
C	-1.51004858165014	6.55304364693602	1.88928385379800
C	-4.53986392260362	3.41504911458062	1.63109327981390
C	-2.02290418361193	7.12616965571517	-0.47122877727252
O	-3.19565082055206	4.28032963134539	4.09065189879533
O	-0.61177298454067	7.39023562180514	1.95991024581165
H	-1.24534452206008	7.87666598368809	-0.39005981093719
C	-4.04077166807649	5.15648528920711	-0.58566040437666
C	-3.77608549781373	5.97047275144249	-1.69096546533788
C	-4.55547279906196	5.82391141384923	-2.93267308917730
N	-5.56300633771547	4.84436685674542	-2.92774219436114
C	-5.87491090962745	4.00545975014450	-1.84698127587636
C	-5.07887566346286	4.18288370564886	-0.62820571014092
C	-5.30297518015335	3.34453372559230	0.46922861491970
H	-6.04151950024645	2.56115561745458	0.34225913409513
O	-6.77651271051274	3.17352062523166	-1.94865841653699
O	-4.33967920927504	6.51628608946742	-3.92533440751077
C	-2.74885719836188	6.95579269253544	-1.62745243728059
H	-2.57324617748970	7.56179687977517	-2.50883951427928
C	-6.36821163718973	4.65570629287201	-4.13862013888159
H	-6.25153995492027	3.63219452245184	-4.50166171879181
H	-7.42340534495573	4.81369473307261	-3.90542840319177
H	-6.02689383913342	5.36952779011353	-4.88403447786522
C	-1.20619640735358	6.02320567696413	4.27818764727802

H	-0.83017602383403	5.08140042697430	4.68188266201107
H	-0.39246060031586	6.72129346967842	4.09836174863337
H	-1.91597339364089	6.44097285563902	4.99622586671436
C	-4.71656428813980	2.35785291079846	2.62626862074328
C	-6.00973818311384	1.85488067166791	2.90490466570892
C	-3.61715761562317	1.71938260129501	3.25276149128492
C	-6.19979941326229	0.78224663698480	3.75732514145376
H	-6.87396533689105	2.35424520338477	2.48029710931168
C	-3.79682425036174	0.63223440138139	4.08658109586358
H	-2.61243837565128	2.05638256083948	3.03412483358991
C	-5.09160901099665	0.14988713102579	4.35428025952450
H	-7.20144397350275	0.45028728672497	4.00607265370866
H	-2.93934844882065	0.12133925162803	4.50938148102277
N	-5.27969485034811	-0.94791381719715	5.20897415156202
C	-6.11093033502063	-2.05284333940291	4.95515139177023
C	-4.65418464351898	-1.14060643740957	6.45305481181811
C	-6.01542996143388	-2.95537077696496	6.04306706593192
C	-6.87919874689318	-2.34591850184398	3.82506974247078
C	-5.08987580572803	-2.37429255362951	6.99665382312649
C	-3.79640486053314	-0.29056087502864	7.15652100645187
C	-6.73320728710127	-4.15202952430099	6.01466938786392
C	-7.59133414680520	-3.54529867742663	3.82098474681749
H	-6.91158874981810	-1.67727799921404	2.97318666876579
C	-4.62563947395353	-2.78165636105833	8.24829914428303
C	-3.34328003164058	-0.72015609953059	8.40374112932601
H	-3.50381096875482	0.67396143121732	6.75862378038379
C	-7.52746570204580	-4.43706479197370	4.90345053496971
H	-6.66576257825479	-4.85237108389094	6.84174631229700
H	-8.19996101916463	-3.79426521080826	2.95728258866809



C	-3.74421209624500	-1.95301178308752	8.94329987687093
H	-4.95386552387133	-3.72448402260336	8.67552167047303
H	-2.67241787502818	-0.08102747738980	8.96923295816712
H	-8.09283796407310	-5.36293537959732	4.86846795033393
H	-3.37272863147144	-2.25744185704508	9.91668132535272

**XYZ Coordinates of *o*Cz2 in S<sub>0</sub> optimized geometry**

N	0.302167	0.501238	-1.001684
C	-1.024147	0.449158	-0.559912
C	-2.077959	0.557429	-1.607375
C	-1.706625	0.862579	-2.945943
C	-0.343305	1.008775	-3.319661
C	0.717504	0.741565	-2.312420
C	-3.426092	0.389324	-1.278901
C	-0.010866	1.373222	-4.626719
O	-1.285625	0.323854	0.628281
O	1.910238	0.715929	-2.583604
C	-2.717369	1.033811	-3.928779
C	-2.356835	1.267274	-5.273621
C	-3.396820	1.420233	-6.321287
N	-4.730891	1.361466	-5.887586
C	-5.142051	1.167531	-4.562426
C	-4.075706	0.975250	-3.551905
C	-4.414269	0.667391	-2.251283
H	-5.463046	0.575079	-1.996255
O	-6.333553	1.149980	-4.282915
O	-3.115942	1.595668	-7.499408
C	-1.028026	1.430447	-5.607046
H	-0.776004	1.672427	-6.632391
C	-5.802280	1.521946	-6.875430

H	-6.443045	0.637523	-6.866735
H	-6.414187	2.388711	-6.616708
H	-5.342479	1.654226	-7.851407
C	1.375659	0.297341	-0.025880
H	1.965368	-0.573193	-0.316056
H	2.025956	1.172733	-0.015124
H	0.918632	0.147775	0.948316
C	-3.893655	-0.265920	-0.018569
C	-3.858638	-1.676308	0.041564
C	-4.442847	0.440325	1.052008
N	-3.335927	-2.416061	-1.073077
C	-4.329288	-2.349247	1.167237
C	-4.912277	-0.234999	2.179778
H	-4.476141	1.524346	1.008085
C	-1.963457	-2.629550	-1.275991
C	-3.956154	-2.416725	-2.329422
C	-4.850287	-1.627612	2.243083
H	-4.290413	-3.433679	1.181597
H	-5.324139	0.329189	3.011138
C	-1.708516	-2.767696	-2.664214
C	-0.944362	-2.703215	-0.326236
C	-2.982023	-2.618208	-3.339379
C	-5.305973	-2.228852	-2.632657
H	-5.215153	-2.152466	3.120527
C	-0.394755	-2.964405	-3.105765
C	0.352782	-2.913304	-0.790818
H	-1.157485	-2.563698	0.727382
C	-3.371524	-2.587568	-4.683246
C	-5.669307	-2.197333	-3.977011

H	-6.035509	-2.075344	-1.844551
C	0.630057	-3.034937	-2.164750
H	-0.180261	-3.054977	-4.166663
H	1.166798	-2.974889	-0.075013
C	-4.711896	-2.364520	-4.994303
H	-2.635445	-2.718931	-5.471184
H	-6.705874	-2.016635	-4.242136
H	1.654312	-3.181525	-2.492619
H	-5.024128	-2.324386	-6.033442
C	1.329986	1.914077	-5.008714
C	1.602556	3.266207	-4.704057
C	2.280013	1.178707	-5.717889
N	0.612386	4.047449	-4.015894
C	2.815182	3.844690	-5.073532
C	3.494723	1.759372	-6.086267
H	2.073992	0.140104	-5.956293
C	0.439403	4.016745	-2.622675
C	-0.628550	4.353583	-4.590914
C	3.767578	3.088164	-5.759307
H	2.993045	4.886462	-4.826951
H	4.230070	1.170327	-6.626014
C	-0.913687	4.304374	-2.310236
C	1.384816	3.751568	-1.631279
C	-1.599439	4.507792	-3.569843
C	-0.954720	4.474604	-5.943154
H	4.712891	3.539052	-6.044988
C	-1.329013	4.298613	-0.973714
C	0.948542	3.765664	-0.307316
H	2.408459	3.507562	-1.891836

C	-2.932351	4.750280	-3.920527
C	-2.288486	4.711008	-6.268582
H	-0.197532	4.351218	-6.710272
C	-0.394187	4.025378	0.021934
H	-2.366604	4.497356	-0.721321
H	1.660309	3.562431	0.487048
C	-3.271037	4.838407	-5.269523
H	-3.692690	4.848928	-3.151085
H	-2.576834	4.774363	-7.312786
H	-0.702380	4.007082	1.062342
H	-4.303965	5.012018	-5.555457

**XYZ Coordinates of *o*Cz2 in S<sub>1</sub> optimized geometry**

N	0.21592542843855	0.52679498718716	-1.07638718980667
C	-1.10867760753681	0.46400941976814	-0.63389956228773
C	-2.14194831404360	0.65509255717256	-1.64795752855237
C	-1.77688837692909	0.94247802228825	-2.98942223434688
C	-0.41567990983615	1.03466526142848	-3.38132749733518
C	0.63361239186366	0.76937978805292	-2.39895287802058
C	-3.51891225233806	0.53651179668916	-1.30274045415202
C	-0.09039796510999	1.35338519216367	-4.72764470951420
O	-1.36259044643541	0.20918293101911	0.55301557773082
O	1.83780237927110	0.71068673017491	-2.65623913881455
C	-2.80376116286481	1.11856747354288	-3.97269892630873
C	-2.44973723026226	1.27348378537943	-5.33046132941798
C	-3.48017626900381	1.44412910504988	-6.35505556303419
N	-4.81771425121074	1.40986512219935	-5.90089203956637
C	-5.22100778685526	1.24044486321559	-4.57028246885600
C	-4.15785467844337	1.11657692344152	-3.57404206274824
C	-4.49393412347446	0.84472465090384	-2.24029487579659

H	-5.54622542418200	0.75689726889888	-1.99433432516232
O	-6.42377715036838	1.16006749444703	-4.29821905109074
O	-3.22688455057051	1.59752546808821	-7.55088216569523
C	-1.09862756129438	1.39269652819635	-5.68509153104565
H	-0.86481011846463	1.62882289270277	-6.71667044803378
C	-5.89227255127321	1.56794440595404	-6.88094594971370
H	-6.54844533202972	0.69443553363515	-6.85798043028907
H	-6.49643232559214	2.44311831263411	-6.62974903095373
H	-5.43631086208232	1.68445009590067	-7.86095392966501
C	1.29004039968530	0.32001774195658	-0.10632187503507
H	1.88251937513120	-0.55297331433108	-0.38940174564582
H	1.94854079146212	1.18874067167763	-0.10647565729616
H	0.83566422901824	0.18110076850600	0.87119035798632
C	-3.97272130500907	-0.18706666455715	-0.07654933114368
C	-3.90351356873584	-1.59496455431239	-0.04091957935390
C	-4.57700755881976	0.44407034603578	1.01413868875718
N	-3.27773064148755	-2.28113366365274	-1.15282156318378
C	-4.36852977725867	-2.34262873359561	1.03725694334243
C	-5.06082527579259	-0.28957457466647	2.09731808043538
H	-4.64200304480360	1.52696545926255	1.00613786530142
C	-1.93923919261085	-2.63086594658855	-1.19448123351402
C	-3.81317653241158	-2.37646125018684	-2.43105056117392
C	-4.95550879628968	-1.68161127572626	2.11696509525731
H	-4.28363695274162	-3.42444623640764	1.01841849318841
H	-5.51857449624921	0.22892314106101	2.93427836888038
C	-1.57594211540920	-2.91849242605011	-2.54103236660941
C	-1.02263108898178	-2.66192012597016	-0.13586777415643
C	-2.78797846615871	-2.74849458693291	-3.33925093235834
C	-5.12608121162545	-2.12234799658453	-2.83949908821208

H	-5.33086733928713	-2.25170890860099	2.96042746076911
C	-0.25618687735761	-3.20807812026812	-2.83573144593393
C	0.29549330103681	-2.98986662379823	-0.45278948797498
H	-1.32182864062904	-2.37304197696901	0.86256225208373
C	-3.07614868003166	-2.82240466577681	-4.69228036814222
C	-5.40048865267520	-2.21049083199040	-4.20357933605207
H	-5.88000010911635	-1.82163311348724	-2.12272124057836
C	0.67606915528869	-3.24758710090623	-1.77533700378627
H	0.06990508045845	-3.37250196722011	-3.85732281966649
H	1.04313064097145	-3.00655780493444	0.33163677966093
C	-4.39158236184002	-2.54571072328565	-5.11596233468900
H	-2.30465150223874	-3.05605502508203	-5.41795357757578
H	-6.39396634694070	-1.97112699030835	-4.56352624782217
H	1.71621433905180	-3.45970819154637	-1.99789872880525
H	-4.62135195190312	-2.57503054500373	-6.17558858275491
C	1.24636625292106	1.89786443387755	-5.11051760310943
C	1.55096784198007	3.23390048650487	-4.76560874203742
C	2.17063893637614	1.17825306958927	-5.86980096496700
N	0.60074648317170	4.01136965683094	-4.02011040342948
C	2.76467947990174	3.80558582773739	-5.14324588190601
C	3.38583511353604	1.75061544208393	-6.24854112692247
H	1.93652354977790	0.15201131701919	-6.13723264241264
C	0.53398857679934	4.01627085942512	-2.61888797296366
C	-0.67202844504477	4.33564136293484	-4.50860295015552
C	3.68922451338560	3.06150184842533	-5.87915593604761
H	2.96562422527190	4.83526952135307	-4.86487338166119
H	4.09803961179150	1.17074428566237	-6.82838125331578
C	-0.78631521065204	4.33884599677844	-2.21295716466798
C	1.54797989240886	3.76087267045813	-1.69603690251908

C	-1.55974196582852	4.53268309883239	-3.42209373802258
C	-1.09425986564038	4.44971112045464	-5.83391132760998
H	4.63396846574854	3.50915993132307	-6.17221032044757
C	-1.09725777813005	4.37697894946124	-0.84926074621807
C	1.21715951732338	3.82639515076981	-0.34331382464212
H	2.54086854801834	3.48049959321804	-2.02814828033241
C	-2.90705908982895	4.81392704706796	-3.67687825099349
C	-2.44045342735969	4.72168072343696	-6.06393543759849
H	-0.40121212762016	4.28745756932563	-6.65230840759958
C	-0.09126117717983	4.12126693783748	0.07984072636187
H	-2.11077928518106	4.59255744710704	-0.52310263825177
H	1.98555160752028	3.63366795609581	0.39971536563865
C	-3.34216338776281	4.89461201740465	-4.99762683504168
H	-3.60481357746349	4.94600409220541	-2.85497162071355
H	-2.80364391451066	4.77128143169652	-7.08533489840503
H	-0.31860567762087	4.14247846541516	1.14107087329115
H	-4.38885346118060	5.09076788977424	-5.20904847502186

**XYZ Coordinates of *o*Cz2 in T<sub>1</sub> optimized geometry**

N	0.15312444967770	0.49222444161953	-1.22416745201021
C	-1.16726362180451	0.59120242421604	-0.76445929764633
C	-2.20605372847608	0.72752788424369	-1.79051035479553
C	-1.83786976134069	0.87844725966303	-3.14862386245814
C	-0.48321925947866	0.88101833204163	-3.54648317288482
C	0.56255808826431	0.62757375284287	-2.55464501688825
C	-3.59998003892555	0.71188545122830	-1.43006109808328
C	-0.14382154570351	1.14634884648892	-4.92167283728075
O	-1.42263827550753	0.54136118122392	0.44135201472132
O	1.76022571690514	0.53972678334983	-2.83735924081346
C	-2.85639461852549	1.05018495425793	-4.13993329327813

C	-2.50466466559138	1.05521903305060	-5.50333628347166
C	-3.53210693621633	1.21990999106745	-6.53685690589796
N	-4.85106167701235	1.38629624921131	-6.08004179628158
C	-5.24532585137990	1.41259898821315	-4.73511913295477
C	-4.18968591654715	1.23065412441363	-3.73582085622619
C	-4.54320012905392	1.06419284112670	-2.37122143456359
H	-5.59883792994966	1.06352380470799	-2.12331867590056
O	-6.43183767749769	1.56546705349422	-4.44135296054060
O	-3.26415235146427	1.23505820086458	-7.73899038224216
C	-1.13626601845095	1.11247117388368	-5.87663777296440
H	-0.90846583656347	1.30237909373997	-6.91966392250062
C	-5.91932282700501	1.56595490628179	-7.06572650065130
H	-6.65985902208058	0.76986064648222	-6.95798271140891
H	-6.42364174012171	2.51953066678707	-6.89333315738965
H	-5.47006400099920	1.54110005990623	-8.05539745873463
C	1.22289076336253	0.25076351992927	-0.25197840423145
H	1.75551727483962	-0.65999126102073	-0.52608142183869
H	1.92273016947335	1.08593603030612	-0.26524423587937
H	0.76488336800380	0.15016155401950	0.72804814129405
C	-4.07652344803359	0.02875055534738	-0.19659638282607
C	-3.87353778257809	-1.36602068695085	-0.10413769942577
C	-4.79576224532332	0.66513572998491	0.81659587087874
N	-3.17530391379554	-2.04093108433386	-1.15827912380430
C	-4.32666109102510	-2.08485959881492	1.00049056277839
C	-5.25338787373748	-0.05323936430470	1.92241859646631
H	-4.96671076097106	1.73467169934300	0.74594987491908
C	-1.84829777835318	-2.47543631535761	-1.08671940347601
C	-3.59806891015401	-2.13229906133205	-2.48719523320341
C	-5.01120544567898	-1.42447772183218	2.02231978488426



H	-4.15345421628394	-3.15559130926880	1.04058333856073
H	-5.79418693581177	0.46104344121389	2.71122432525003
C	-1.39649551288042	-2.79674065631035	-2.39384136293554
C	-1.02173390118529	-2.57619461341295	0.03370651494277
C	-2.51130537613896	-2.56260528102389	-3.29125892722137
C	-4.85326927938442	-1.85395878839707	-3.03143764206854
H	-5.36608054914442	-1.98240870275250	2.88318657094515
C	-0.07849931329327	-3.22445137353525	-2.57590601922370
C	0.28057860912893	-3.02427780417049	-0.17412100868176
H	-1.37777216674584	-2.28284935068191	1.01384683216794
C	-2.67594513769255	-2.64794163354616	-4.67568432044869
C	-4.99499896063166	-1.95222237240691	-4.41730730336343
H	-5.67963299032588	-1.55100334713290	-2.39913906772718
C	0.75129221619280	-3.34149790326675	-1.46133452422698
H	0.29171056077195	-3.45915926891103	-3.56925158156196
H	0.95076632656912	-3.11462752373704	0.67525522883015
C	-3.91718881064378	-2.32742004199494	-5.23351945233550
H	-1.84659022753613	-2.94595022555643	-5.30994575922808
H	-5.95355346981026	-1.71123393348962	-4.86590936389815
H	1.77665246045621	-3.67426998092823	-1.58801253004081
H	-4.05094652741045	-2.37445780580282	-6.30951896398280
C	1.15003735656024	1.78912399967131	-5.27702397541231
C	1.39345065696766	3.08024291155913	-4.75590091317536
C	2.08002621420274	1.24468504214895	-6.16480140491538
N	0.42106141761222	3.67849033781136	-3.88738776547693
C	2.56260108645050	3.77163696339224	-5.06767788843986
C	3.24905611111327	1.93777481445011	-6.48270835973686
H	1.89411349306694	0.25913696515905	-6.57959315405420
C	0.54637130374058	3.78691306527956	-2.49902061799129

C	-0.88888479382764	4.01515898203610	-4.23948325671126
C	3.49849479074068	3.19440558663369	-5.92758937593000
H	2.71869269604949	4.76109210957678	-4.64956577535601
H	3.97095192958457	1.49129515907965	-7.15989556818671
C	-0.71573756675345	4.13280138075747	-1.94719750935595
C	1.67458113536976	3.57622289355350	-1.70419508572879
C	-1.63545256183958	4.26957720557776	-3.05976094543619
C	-1.46447225320947	4.09916777579459	-5.50872340979588
H	4.40905658726641	3.73147404065104	-6.17382855442874
C	-0.84911581590576	4.24578005237429	-0.56115574034698
C	1.51809670711464	3.72028008910364	-0.32741347582025
H	2.61775896829175	3.27837127742628	-2.14652134464021
C	-2.99907721286905	4.55039475448863	-3.15929185861515
C	-2.82878214506655	4.38900221847930	-5.58369387124646
H	-0.87346959478925	3.92425048908032	-6.40023955063420
C	0.27188757838722	4.03920249224921	0.24143687997619
H	-1.81183608316064	4.48148396019436	-0.11829778789560
H	2.37469007072409	3.56529670561572	0.32149110534285
C	-3.59278218084878	4.59480941501799	-4.42514793172745
H	-3.59314961800686	4.71699256763410	-2.26598136350903
H	-3.30497648061213	4.43188496737333	-6.55800281157785
H	0.18233621384767	4.11904066952428	1.31988893089537
H	-4.65621895958153	4.79309444402872	-4.51217296721097

**XYZ Coordinates of *o*Cz2i in S<sub>0</sub> optimized geometry**

N	-0.42514344495971	-1.24794683034982	-4.57116316928816
C	-0.99145113608818	-1.00540152037545	-3.31051246230953
C	-2.20212387410358	-0.13705466141346	-3.27098232613731
C	-2.63038847231036	0.50993828774279	-4.45978046265390
C	-2.02185648339976	0.21980763008488	-5.70133645961637

C	-0.88482654025865	-0.72416761807615	-5.78116475334075
C	-2.90221716213757	0.07175152656911	-2.08047466236429
C	-2.43278474858843	0.87410834889907	-6.84449187663293
O	-0.48460079007668	-1.47043114387270	-2.29904850087489
O	-0.33552603316170	-1.01868098894595	-6.83456015847887
H	-1.90540930447493	0.67206992318620	-7.76912981519294
C	-3.72555772052735	1.41335512706509	-4.43810460615066
C	-4.15385094265356	2.06031489508779	-5.62691018680379
C	-5.36454121781714	2.92863745414798	-5.58737486884827
N	-5.93077373074964	3.17128025636711	-4.32670980399535
C	-5.47110067158169	2.64748406427115	-3.11671225018662
C	-4.33408728638415	1.70348865335841	-3.19654832402795
C	-3.92319333729951	1.04914841043257	-2.05340291088331
H	-4.45058083943623	1.25117273613915	-1.12876855411590
O	-6.02042309990545	2.94195852076501	-2.06331725346203
O	-5.87150822899826	3.39351209165531	-6.59885129985271
C	-3.45379208965574	1.85147352586661	-6.81743153846191
C	-7.11004448339668	4.03672601850293	-4.23994896509304
H	-7.95218640821420	3.46898969668433	-3.83710693385096
H	-6.89709229462131	4.86681135480856	-3.56512977835412
H	-7.33687312464184	4.39932334525999	-5.23876850286784
C	0.75411530636297	-2.11340733088556	-4.65793245979941
H	0.98125368159844	-2.47558863390922	-3.65903227229940
H	0.54099055811446	-2.94379517323985	-5.33233214716654
H	1.59609468746098	-1.54580707720920	-5.06129360766300
C	-3.56783928726198	2.74490954315322	-8.01051671078620
C	-4.22749111529726	2.37324360535778	-9.18247387000448
C	-2.89548871864154	3.98678105520836	-7.97114393162391
C	-4.25654206240593	3.23211580657338	-10.28258423159516

H	-4.74015153406613	1.41721635631260	-9.21962701429254
C	-2.92360326186392	4.84172338467787	-9.07092638766237
N	-2.17805543249134	4.36453990497076	-6.78525349528175
C	-3.61288792350115	4.46875712768958	-10.22678041437356
H	-4.78617280947313	2.93439359354974	-11.18253671982993
H	-2.39518770800109	5.78774587538986	-9.01075832286615
C	-2.80163124837302	4.94724215602242	-5.67040667364376
C	-1.06211281426265	3.65277505152224	-6.32410606767772
H	-3.63614877757851	5.13695133517017	-11.08205291660757
C	-2.08200706501310	4.60703325147274	-4.49692091030610
C	-3.95172223425012	5.73587693716962	-5.62988912446825
C	-0.97620903356472	3.76815619701920	-4.91361295070070
C	-0.14712781255804	2.89744648686182	-7.05973732383745
C	-2.54357615847371	5.05449036706380	-3.25348421747207
C	-4.38424457824926	6.17800192197979	-4.38102363798556
H	-4.50494672877049	5.95613254035204	-6.53563774601654
C	0.02716849743651	3.07344409573410	-4.22847572061888
C	0.84039041610847	2.21156480547357	-6.35597070417772
H	-0.22997098915252	2.82147070228345	-8.13876104700608
H	-2.01571495366121	4.78591883225950	-2.34312940866236
C	-3.69476017960868	5.83741344592892	-3.20264884006249
H	-5.27950705194960	6.78913262688741	-4.31765684142696
C	0.92187147190510	2.28814826304341	-4.95347791340339
H	0.09374938325061	3.13232511220822	-3.14588695871343
H	1.54339260746359	1.58883890193595	-6.89969553027074
H	-4.06926360842832	6.18340945909344	-2.24456835929467
H	1.69508228326412	1.73225577762418	-4.43190532917845
C	-2.78824727012793	-0.82174966963185	-0.88743110917714
C	-2.12862029535264	-0.45017594952124	0.28456906961792

C	-3.46065608973076	-2.06358831192680	-0.92689244984919
C	-2.09964844362468	-1.30910768819423	1.38463516140671
H	-1.61591523243532	0.50582468602299	0.32179075969960
C	-3.43262120337204	-2.91858849207533	0.17284689539635
N	-4.17806887396001	-2.44125482501694	-2.11282572355156
C	-2.74335942194053	-2.54571499600563	1.32874451836003
H	-1.57003485031258	-1.01145804216212	2.28462158339321
H	-3.96107903172990	-3.86458313259615	0.11261112322728
C	-5.29397444275702	-1.72942909068787	-2.57396906572583
C	-3.55448510354452	-3.02392849317477	-3.22768325935239
H	-2.72015997325212	-3.21395501219190	2.18398279731488
C	-5.37984376035145	-1.84473998950562	-3.98447041780436
C	-6.20895329353042	-0.97410269108599	-1.83832778281523
C	-4.27406548597786	-2.68363793219925	-4.40117225404531
C	-2.40442289098351	-3.81260497173146	-3.26820811144505
C	-6.38317475249708	-1.14995659018650	-4.66960357748559
C	-7.19642652647710	-0.28815187671109	-2.54209000194720
H	-6.12613765795500	-0.89818009749066	-0.75929816829053
C	-3.81247993776780	-3.13105138927589	-5.64461840411334
C	-1.97188449825984	-4.25468603728865	-4.51708350049913
H	-1.85122815785755	-4.03292327306748	-2.36245695706760
H	-6.44972377600393	-1.20877964026300	-5.75219741598081
C	-7.27786996196639	-0.36466357336840	-3.94458905841027
H	-7.89942277479175	0.33457205183982	-1.99835530904510
C	-2.66132309886689	-3.91401392950940	-5.69546131511739
H	-4.34030717948634	-2.86241476911322	-6.55497365664191
H	-1.07664856960872	-4.86585570467436	-4.58045335908139
H	-8.05104555635128	0.19128154166094	-4.46615755479318
H	-2.28680522975226	-4.25997651947381	-6.65354822555623

**XYZ Coordinates of *o*Cz2i in S<sub>1</sub> optimized geometry**

N	-1.05014150778318	-1.27280198522194	-5.11154282246850
C	-1.46924745905496	-0.99477124784699	-3.80437022533663
C	-2.55596246673926	-0.03053067727228	-3.65119217525074
C	-3.00100520237546	0.69827836510801	-4.78537257660690
C	-2.51759535488723	0.40468891851379	-6.08178942149622
C	-1.52357899754667	-0.64059745189029	-6.27897603223711
C	-3.10321022782044	0.26502894042782	-2.36814728673514
C	-2.86260616417093	1.22882074020707	-7.16351782869654
O	-0.93224209377823	-1.56701597411202	-2.84130649421766
O	-1.06486719243013	-0.97374606049848	-7.37390436629273
H	-2.36585157450103	1.04884923447480	-8.11002111035669
C	-3.94915111020126	1.76152951939532	-4.63854774323760
C	-4.32520895522834	2.54915501723028	-5.75491844491984
C	-5.36084633328764	3.57827112350007	-5.59988634151068
N	-5.85290996345031	3.78802357096040	-4.29411332123945
C	-5.43869692961165	3.10704870190675	-3.14685405852005
C	-4.44131926382304	2.05458752607522	-3.34460010213745
C	-4.00036270252359	1.31821539391101	-2.23772817862342
H	-4.43492659824752	1.56134115612203	-1.27340393752827
O	-5.93206445433076	3.37861352289506	-2.04824047565272
O	-5.81490463480872	4.22706658873054	-6.54350483033636
C	-3.68889516812285	2.33559292422867	-7.00705481182117
C	-6.87935427404799	4.81051525529130	-4.09119354610487
H	-7.80290673206684	4.34676339764747	-3.73392984741129
H	-6.53641093724245	5.51738839332312	-3.33489154862908
H	-7.04585639110156	5.31014533660213	-5.04182407418367
C	0.02991166091284	-2.23808141957409	-5.31400945009063
H	0.35559590833663	-2.58919006470315	-4.33847411542330

H	-0.32560149734918	-3.06928730538941	-5.92790871883208
H	0.85361442746825	-1.75924912572510	-5.84802566420496
C	-3.63267582091840	3.38680180066540	-8.06577201091465
C	-4.25811482752836	3.25313069016997	-9.30684368750693
C	-2.82280185797317	4.52407372824221	-7.84060196818009
C	-4.12608860243510	4.23885118264970	-10.28635305775362
H	-4.87273598913572	2.37736297590432	-9.48976470147696
C	-2.69213063607536	5.50861404936860	-8.81861127052880
N	-2.12924280310117	4.67246493208484	-6.59289892812935
C	-3.35190376684127	5.37310621917704	-10.04154712692801
H	-4.63324347601191	4.12174604817495	-11.23966876031858
H	-2.06090066308979	6.36725060990412	-8.61251005725168
C	-2.68023051146266	5.30887998527329	-5.47153675465793
C	-1.14846729557060	3.78180844002305	-6.14051412920457
H	-3.24919079178759	6.14251651652943	-10.80074704785549
C	-2.05441288735706	4.81611775784614	-4.29809946801784
C	-3.68808449618037	6.27181674880402	-5.42185202783799
C	-1.08234417696309	3.83125968510293	-4.72518496843095
C	-0.32849810001500	2.93255256370142	-6.88488075522611
C	-2.46605776883464	5.29091774784480	-3.04766364464912
C	-4.06970202248515	6.73802949163055	-4.16552576558368
H	-4.18271019462565	6.60240725320550	-6.32759001661703
C	-0.20672053187045	2.97535053688445	-4.04705904014723
C	0.53355104393635	2.08874012583674	-6.18868687724010
H	-0.39597029984701	2.90498646688854	-7.96695704976195
H	-2.01230638044605	4.90610289624130	-2.13897001469658
C	-3.47209190076323	6.25221099620407	-2.98830738550092
H	-4.85817815214960	7.48145110745457	-4.09518672913310
C	0.58846359948990	2.09965431665718	-4.78269210196998

H	-0.16622729694910	2.98164663304674	-2.96158274413343
H	1.15318107939716	1.39176695937165	-6.74440341720398
H	-3.80798268176517	6.62253436300490	-2.02483916210153
H	1.25587408837911	1.41547562775535	-4.26740564719596
C	-2.87445267300550	-0.56454236721990	-1.15150474779323
C	-2.37359105637026	0.02422547011855	0.01653414472835
C	-3.21216936610862	-1.93189709568603	-1.06906014882593
C	-2.18510315754475	-0.70748576200178	1.18862854958579
H	-2.10954011174018	1.07567613212216	-0.01927953214931
C	-3.01253568161667	-2.68159580070663	0.09305073964190
N	-3.75996584254598	-2.61865377267137	-2.20460219541756
C	-2.49732763630074	-2.06746073776095	1.23108414992377
H	-1.78535446124404	-0.21467222046129	2.06954135896500
H	-3.29131368528835	-3.73052052081333	0.10327403684175
C	-4.95356469861351	-2.31233386845351	-2.85050237496887
C	-3.15796931504905	-3.68856364792080	-2.84386820994236
H	-2.35464202908869	-2.64190871625117	2.14021114639241
C	-5.12221556375271	-3.19489124776226	-3.94937515456956
C	-5.90856231715077	-1.34661681451665	-2.51364706338016
C	-3.96765601201475	-4.08618842138062	-3.94382681832653
C	-1.92872401093741	-4.29948713819257	-2.55352798658056
C	-6.24561248538077	-3.08083431042730	-4.75033350461379
C	-7.03077744035004	-1.24304767483792	-3.33368802649972
H	-5.76325675944496	-0.68910362555300	-1.66818944287716
C	-3.55121670770004	-5.12832355966452	-4.75312772073855
C	-1.53828872618741	-5.35753084477184	-3.36835057265072
H	-1.29901745243772	-3.91500555572815	-1.76351003249459
H	-6.39546450335357	-3.73764275219994	-5.60063433911355
C	-7.19584156740531	-2.08819622306525	-4.43869893306793



H	-7.77729840669426	-0.48824855436412	-3.11568643561171
C	-2.33316487988853	-5.76875731908607	-4.44965356733040
H	-4.13933035476005	-5.44245256817880	-5.60867713235151
H	-0.59267169987993	-5.85336709003517	-3.18084639291420
H	-8.07266059514924	-1.97864471776894	-5.06756901251705
H	-1.99498549220168	-6.58527844472591	-5.07869391508696

**XYZ Coordinates of *o*Cz2i in T<sub>1</sub> optimized geometry**

N	-0.64757343318000	-1.45819438905099	-4.74481275860019
C	-1.03141192265243	-1.08318085180331	-3.44663614944330
C	-2.14488944160649	-0.13439808299570	-3.33678261935803
C	-2.68532623162777	0.44476660165794	-4.49974663497328
C	-2.30231583482688	-0.00683242111564	-5.78222213361596
C	-1.24288655043044	-1.00656410767464	-5.92699087205312
C	-2.69330086907416	0.21531189300542	-2.04776033820645
C	-2.79934287988796	0.63818542309542	-6.94112857729566
O	-0.44403961570025	-1.53586577640092	-2.46147836945702
O	-0.84386026241560	-1.40960082493002	-7.02082367778913
H	-2.35772732694749	0.36354551232428	-7.89280003312293
C	-3.67083244946150	1.47866938898119	-4.39817745062774
C	-4.21125580087357	2.05783179269692	-5.56113906141517
C	-5.32472408816302	3.00664242053028	-5.45127833586895
N	-5.70852403243611	3.38169654228661	-4.15310307428350
C	-5.11320460983253	2.93007232541374	-2.97092077393714
C	-4.05381531318822	1.93029978316123	-3.11569239934646
C	-3.55678218982865	1.28527959699518	-1.95679208454754
H	-3.99837559884922	1.55989155916420	-1.00510054849986
O	-5.51217281944512	3.33316459279543	-1.87708832739476
O	-5.91207223922695	3.45935747896502	-6.43642938107360
C	-3.66286220864790	1.70812029222297	-6.85014983966497

C	-6.83862896617249	4.29983844150229	-3.99303797273936
H	-7.68691996571006	3.77114851154453	-3.54860895737227
H	-6.54751893219697	5.11086146706442	-3.32654454092023
H	-7.10480641131067	4.67980291291182	-4.97561666488323
C	0.48260122878008	-2.37624609469902	-4.90490246994579
H	0.74892012570341	-2.75608052900687	-3.92231234169016
H	0.19149597626077	-3.18737038235513	-5.57127465548281
H	1.33077592078833	-1.84751913866278	-5.34950582247330
C	-3.72187089180338	2.65954398760695	-7.99059822954679
C	-4.26306246765319	2.34465498749049	-9.23913341536719
C	-3.10363734872908	3.91902973934089	-7.82315242747280
C	-4.24675735210526	3.27824834696996	-10.27603802251045
H	-4.72720499937555	1.37360682131088	-9.37932205535041
C	-3.09058188168285	4.85471243386715	-8.85615881513478
N	-2.49290032345816	4.23611813460962	-6.56619750268197
C	-3.67274724862164	4.53672095323343	-10.08417649351604
H	-4.69085457228542	3.02520355610471	-11.23406669397872
H	-2.60903654128143	5.81376866815771	-8.69385346395143
C	-3.03286328292331	5.10207218971254	-5.61058288961624
C	-1.41004184798757	3.56223881778797	-5.99023005068487
H	-3.66264077988465	5.26292912087466	-10.89090277655550
C	-2.32645655469671	4.93912716966006	-4.38953806200235
C	-4.11513183679106	5.97569836745094	-5.73464362018678
C	-1.29497573059485	3.94836693920074	-4.63048524048449
C	-0.54172019750922	2.63553839467688	-6.56950167941677
C	-2.72698685279002	5.66576517725240	-3.26520085440989
C	-4.48275605765323	6.69870892357892	-4.60239874812865
H	-4.66411430682945	6.05110535959532	-6.66551819169851
C	-0.32490041097422	3.34559025246158	-3.82656650419199

C	0.42049104623993	2.04741228203003	-5.74666834393630
H	-0.62978543851084	2.36794595338839	-7.61596841624369
H	-2.21482643999398	5.53844449505517	-2.31651628611343
C	-3.80311569138428	6.54491322213054	-3.38024867328224
H	-5.32300079392576	7.38357755755776	-4.66238911068911
C	0.52039102062112	2.38520982149097	-4.38773551247360
H	-0.24029490603555	3.60987459162851	-2.77685132687832
H	1.08747497739720	1.30182625195133	-6.16793760539305
H	-4.12713792183968	7.11241608007161	-2.51377158792584
H	1.26556285821846	1.89714977151139	-3.76769943567160
C	-2.63438366538735	-0.73612270374890	-0.90733351464142
C	-2.09343649002508	-0.42115875289749	0.34129593446260
C	-3.25243270302428	-1.99568471982394	-1.07488562463402
C	-2.10977576309627	-1.35476301029323	1.37818340245945
H	-1.62945974188761	0.54996356470996	0.48152945489382
C	-3.26550045534674	-2.93139152407570	-0.04190007636725
N	-3.86296264306799	-2.31275576342505	-2.33193054643132
C	-2.68357048980845	-2.61332329924075	1.18620620875348
H	-1.66587303160023	-1.10168118367140	2.33629212888373
H	-3.74688271980476	-3.89051693950233	-0.20428030137385
C	-4.94589478011554	-1.63903950482787	-2.90796182070202
C	-3.32300709088749	-3.17886445117853	-3.28739605627272
H	-2.69369718916786	-3.33954275456583	1.99292203985267
C	-5.06093110261249	-2.02534506381029	-4.26765434138245
C	-5.81429939433198	-0.71234204782245	-2.32880937878012
C	-4.02940615090520	-3.01609463075790	-4.50846912727026
C	-2.24069543364801	-4.05242277920461	-3.16322703281532
C	-6.03102788603304	-1.42274047810604	-5.07166901524451
C	-6.77653843528640	-0.12439005648356	-3.15173720767757

H	-5.72630314212191	-0.44462176198950	-1.28237129207642
C	-3.62884380847900	-3.74284262972023	-5.63271744187987
C	-1.87304747006420	-4.77556722944981	-4.29538118522309
H	-1.69170351352754	-4.12769596818241	-2.23234799109489
H	-6.11557846866374	-1.68719835135435	-6.12134420810494
C	-6.87639130325125	-0.46234544827260	-4.51063292822850
H	-7.44360762611383	0.62117886226209	-2.73057183147778
C	-2.55268414582949	-4.62194444746617	-5.51755402368221
H	-4.14102198987901	-3.61562500072062	-6.58140679180145
H	-1.03277396365317	-5.46039307118486	-4.23529147161507
H	-7.62159220668071	0.02559802359275	-5.13072537758160
H	-2.22863867869518	-5.18954818417185	-6.38395668137035

**XYZ Coordinates of *m*Cz2 in S<sub>0</sub> optimized geometry**

N	0.994281	-0.044282	0.518987
C	-0.324887	-0.361658	0.867815
C	-1.312426	-0.387872	-0.250984
C	-0.974111	0.284966	-1.462817
C	0.341835	0.781183	-1.700988
C	1.413747	0.390022	-0.742483
C	-2.587558	-0.952447	-0.086807
C	0.621833	1.526143	-2.857498
O	-0.621791	-0.595929	2.030391
O	2.608761	0.442639	-0.994928
C	-1.973704	0.465517	-2.457448
C	-1.665517	1.172457	-3.640879
C	-2.699909	1.383183	-4.691821
N	-3.966164	0.831295	-4.441898
C	-4.322609	0.119290	-3.288922
C	-3.268876	-0.059984	-2.254423

C	-3.554703	-0.766323	-1.105686
H	-4.543029	-1.198447	-0.994704
O	-5.454548	-0.323493	-3.160933
O	-2.462229	2.001998	-5.718306
C	-0.405209	1.702154	-3.818546
H	-0.210837	2.282614	-4.713362
C	-5.023627	1.001931	-5.446913
H	-5.384774	0.022409	-5.765959
H	-5.860637	1.549793	-5.009119
H	-4.604762	1.550417	-6.286525
C	2.050666	-0.197655	1.529840
H	2.745747	-0.979912	1.218021
H	2.599873	0.741088	1.624658
H	1.578077	-0.455494	2.473690
C	-2.985613	-1.805393	1.064492
C	-4.178396	-1.557409	1.756873
C	-2.216990	-2.923490	1.406553
C	-4.568008	-2.395673	2.802670
H	-4.785224	-0.696517	1.493613
C	-2.595611	-3.748755	2.464950
H	-1.310850	-3.150498	0.856552
C	-3.777552	-3.481981	3.170714
H	-5.483102	-2.187374	3.348351
N	-1.770651	-4.840656	2.827224
H	-4.056058	-4.118241	4.003731
C	-0.391259	-4.768843	3.066100
C	-2.175424	-6.173851	2.958537
C	0.091302	-6.070515	3.352806
C	0.446934	-3.650028	3.085120

C	-1.044562	-6.965505	3.286127
C	-3.439924	-6.740952	2.779398
C	1.449590	-6.255376	3.635570
C	1.794957	-3.864237	3.367508
H	0.062835	-2.652736	2.902353
C	-1.195416	-8.345432	3.460627
C	-3.562655	-8.117961	2.957320
H	-4.294536	-6.132721	2.504587
C	2.297166	-5.150781	3.633990
H	1.832436	-7.247750	3.856281
H	2.470095	-3.013116	3.387073
C	-2.455924	-8.914949	3.299288
H	-0.337250	-8.961273	3.714171
H	-4.535399	-8.582640	2.825308
H	3.353717	-5.280395	3.847950
H	-2.587285	-9.984266	3.433567
C	1.908540	2.223399	-3.122659
C	2.522734	2.130279	-4.379700
C	2.464516	3.069614	-2.156042
C	3.688288	2.849711	-4.648288
H	2.099988	1.479233	-5.138668
C	3.639839	3.772021	-2.417847
H	1.988127	3.182572	-1.189000
C	4.257609	3.663249	-3.671271
H	4.165135	2.760639	-5.619429
N	4.204832	4.585396	-1.405263
H	5.177857	4.205626	-3.860200
C	4.510968	4.163928	-0.105557
C	4.482603	5.952161	-1.507260

C	4.990320	5.274492	0.634100
C	4.436340	2.882005	0.447352
C	4.972297	6.414430	-0.258483
C	4.309248	6.812978	-2.593797
C	5.375728	5.097886	1.968363
C	4.830710	2.736163	1.776677
H	4.093807	2.032983	-0.133614
C	5.310782	7.763989	-0.108850
C	4.653257	8.152122	-2.417755
H	3.915106	6.452137	-3.537557
C	5.288590	3.829187	2.535041
H	5.742597	5.940159	2.547963
H	4.794802	1.750180	2.231804
C	5.152310	8.625748	-1.191256
H	5.687599	8.131258	0.841506
H	4.529794	8.842909	-3.246717
H	5.585281	3.677665	3.568420
H	5.411706	9.675001	-1.088732

**XYZ Coordinates of *mCz2* in  $S_1$  optimized geometry**

N	1.15483672479213	-0.10336896806299	0.45186685344423
C	-0.10819782037897	-0.60215627202195	0.76752586693130
C	-1.13023822577261	-0.49163842877277	-0.27088184976039
C	-0.82963662129501	0.23110583908372	-1.46802654756443
C	0.46323729213600	0.78085586041782	-1.71543711470360
C	1.54051612943153	0.45687633500006	-0.78509907104034
C	-2.43670685515325	-1.04556827429555	-0.09399634064918
C	0.70400040864365	1.55274567226340	-2.89392832049456
O	-0.30039723471820	-1.11566511465084	1.88715050990344
O	2.74414444749434	0.63790846766088	-0.98478595096312

C	-1.85786968924414	0.40366315871675	-2.45444116205630
C	-1.57895652464898	1.12127940619282	-3.64142772896002
C	-2.61130956166261	1.31100066220992	-4.66633014002739
N	-3.86880885347289	0.73611081855504	-4.39360526902075
C	-4.19826893556617	0.01321381757162	-3.23928950205630
C	-3.13994386152857	-0.14470530827990	-2.23983783474788
C	-3.40732629215012	-0.86220169718929	-1.06566573232864
H	-4.39802163928764	-1.28703993100691	-0.94989754368031
O	-5.33332092185438	-0.45339999750991	-3.10618487864852
O	-2.41263461667741	1.93190232616582	-5.71173380246353
C	-0.31668266155365	1.69287539507058	-3.83091944267832
H	-0.16164117514909	2.28999289085451	-4.72219316864494
C	-4.93894729806635	0.89136644643867	-5.37967598803350
H	-5.27812257910105	-0.09162275193822	-5.71494436659245
H	-5.79039315840715	1.40164282573332	-4.92327619591728
H	-4.54471713511680	1.46848046838093	-6.21244122656590
C	2.22829121637189	-0.22769554530725	1.43980564089585
H	2.95858954929685	-0.97508627541714	1.11649818633303
H	2.74623690832289	0.72871564004765	1.52907915533814
H	1.78065940283734	-0.51079982286231	2.38876850924596
C	-2.83847057646489	-1.86048796531148	1.09355011308286
C	-3.92469692308293	-1.48095131626591	1.88847414914736
C	-2.19136706656338	-3.06345214867071	1.39255317842924
C	-4.34669728465801	-2.26217276466170	2.97046830041653
H	-4.43841998110888	-0.55311808426345	1.66058370250912
C	-2.59524456462912	-3.81494032156898	2.48897827981048
H	-1.35696408851614	-3.39066686356450	0.78434883453426
C	-3.67767635500194	-3.43690231984472	3.29273468988266
H	-5.18544467152835	-1.93750162668582	3.57759202784601



N	-1.84292753038678	-4.99127789611337	2.83016858988636
H	-3.95418232040503	-4.02937323038701	4.15815801389164
C	-0.48490304816151	-5.01320182463545	3.07100227166236
C	-2.36374476073583	-6.27076881642285	2.98681810568751
C	-0.09606836260804	-6.34742529577614	3.39346840606931
C	0.42087098063854	-3.93476240107786	3.04807068150185
C	-1.31017037141881	-7.15552743814326	3.34109839682400
C	-3.68142532813049	-6.70337217685743	2.80474358299685
C	1.22914810787390	-6.61276349823991	3.68060906570233
C	1.75100264414343	-4.23633454887953	3.33181205281515
H	0.10698130746323	-2.92301497865795	2.80619501137596
C	-1.58810779020619	-8.49805955468285	3.53714253147286
C	-3.94031980650401	-8.05970767929484	3.01098240887500
H	-4.46000306178153	-6.01035289673301	2.51143565902973
C	2.15262701417234	-5.54384068909985	3.64179772458294
H	1.56007682791770	-7.61461550710098	3.93268311612249
H	2.48527089889426	-3.43964520949639	3.31312738152870
C	-2.91529539828564	-8.94221157545471	3.37420998891937
H	-0.80383611292292	-9.19830632253898	3.80458308498899
H	-4.94946964277258	-8.43394082031742	2.88161945933754
H	3.19586611524809	-5.74239907668800	3.86231036660130
H	-3.14447708735171	-9.99134413305961	3.52606559165205
C	1.96006669005644	2.31036976779615	-3.14938382045795
C	2.59424706970677	2.23856340181828	-4.39742898849832
C	2.47322628815378	3.19050923391360	-2.18798221849368
C	3.72820250737980	3.00792973743936	-4.66543764306037
H	2.20294303963409	1.56500997655467	-5.15346151062883
C	3.61940708674852	3.93836619884590	-2.44603459735884
H	1.98668221386631	3.28416498100293	-1.22422028113657

C	4.25646549011342	3.85101476244148	-3.69099384270867
H	4.21407303128510	2.93329990024025	-5.63380013350748
N	4.14784804229173	4.78098555876298	-1.42959602075266
H	5.15555010109561	4.42990336423331	-3.87380360428956
C	4.49522791362225	4.37179223961607	-0.13897809634231
C	4.39517428805406	6.14916828919074	-1.54292494646111
C	4.96994151409799	5.49498218656255	0.58689914790875
C	4.45304070946740	3.09107527146701	0.42180087446512
C	4.90641735749772	6.62978367870451	-0.30841556484315
C	4.18156555978918	7.00153707050239	-2.63011492776252
C	5.39029288705142	5.33124934152384	1.91235550266256
C	4.88028289644995	2.96021650631328	1.74193400802882
H	4.10035448615299	2.23593179846430	-0.14425218096299
C	5.22276125719480	7.98653101723694	-0.17500337943905
C	4.50430265482845	8.34741977744429	-2.46982674339313
H	3.77437247381318	6.62459883060720	-3.56180762135884
C	5.33958166049753	4.06361958111032	2.48545611107560
H	5.75447799542083	6.18315928691405	2.47998346907485
H	4.86397260714226	1.97631434417518	2.20360112661450
C	5.02300536562410	8.83883017950827	-1.25791157680505
H	5.61531973084170	8.36646113227805	0.76420737947299
H	4.34834494054784	9.03063039577688	-3.29978548450146
H	5.66263304716051	3.92220034336751	3.51271281650362
H	5.26548291276593	9.89344218363392	-1.16770956472138

**XYZ Coordinates of *mCz2* in  $T_1$  optimized geometry**

N	0.94235432173984	-0.04153707085385	0.56239677184207
C	-0.37251381114450	-0.39835142999840	0.89427113654401
C	-1.34216075807117	-0.38502498831473	-0.20450804074156
C	-0.99756568776526	0.28936566353497	-1.40962631539366

C	0.32243116891488	0.77185722251784	-1.64874769924263
C	1.36952000444448	0.42984057727650	-0.68482628164232
C	-2.67161603582580	-0.93847846170681	-0.04000910432506
C	0.61863126217087	1.50884480063974	-2.85029252241800
O	-0.65434921877279	-0.70609065208734	2.05837057169264
O	2.58190102621796	0.55480286643227	-0.89052635495911
C	-2.00410006477475	0.48517698276648	-2.41196439099201
C	-1.67987781731938	1.15612571580736	-3.60447703568673
C	-2.69552718664477	1.38283750263810	-4.64326558091790
N	-3.98118759645880	0.88329933167990	-4.37540472596455
C	-4.35793924206940	0.20232280854247	-3.20840120305234
C	-3.31656625105666	0.00789693568708	-2.19260611910522
C	-3.62139426535595	-0.70609915449465	-1.02147888570173
H	-4.61819182468626	-1.12411595436735	-0.93568140092340
O	-5.51416187925415	-0.19837300272858	-3.07304027830605
O	-2.44419545644644	1.97524871540779	-5.69249547915153
C	-0.37835455253095	1.66394405631680	-3.79892823749092
H	-0.19327048063490	2.22955384366765	-4.70500387121136
C	-5.03485094684716	1.07472459639562	-5.37600110468833
H	-5.42900731106351	0.10388076205852	-5.68422541920141
H	-5.85551565740861	1.64997444641449	-4.94135556650696
H	-4.60196054218396	1.60203934995778	-6.22237919881380
C	1.98723421907117	-0.18238768145643	1.58118180757822
H	2.71853272259850	-0.92835807699015	1.26131263927218
H	2.50402306823126	0.77133222011073	1.70845615578052
H	1.51032260305877	-0.47921598573804	2.51151094665702
C	-3.05016562989856	-1.83727150166055	1.07429279462021
C	-4.26692454284799	-1.65979237402508	1.75600791488418
C	-2.25010399029642	-2.93731005302734	1.40837513077764

C	-4.65829114241731	-2.54468546176795	2.76202827328262
H	-4.89228782035397	-0.80805309509429	1.50867920846559
C	-2.63232493168227	-3.80794627740567	2.42567611077957
H	-1.32371737315272	-3.11467059677530	0.87536778747902
C	-3.84312054308410	-3.61685117273435	3.11307701810963
H	-5.59212141928053	-2.38263572368609	3.29120243161409
N	-1.77495429345984	-4.87754542224555	2.78801505546146
H	-4.11107319054985	-4.28506207761157	3.92417043663292
C	-0.41018273853847	-4.75923721585918	3.07375475499006
C	-2.13841431334245	-6.22277556098204	2.88591599513974
C	0.10969832592557	-6.04760435991794	3.36120271504880
C	0.37933447124340	-3.60543844492570	3.13616116413245
C	-0.99395874976030	-6.98251060844192	3.24423988048960
C	-3.37768863905344	-6.82403824069850	2.64566406791090
C	1.45865813251751	-6.18600228574038	3.68815445738685
C	1.72589819840799	-3.77516180819393	3.45784339969595
H	-0.03457567904592	-2.62056172627315	2.94726218611030
C	-1.10615891285795	-8.36469481551597	3.39403731143010
C	-3.46445566578307	-8.20665872312254	2.80372508294516
H	-4.23548900946011	-6.23717457217305	2.33814611309379
C	2.26401684293668	-5.04437221461105	3.72678295130624
H	1.87404228717412	-7.16420351610169	3.91162597498509
H	2.36794077916265	-2.90081459900479	3.50544502859724
C	-2.34639321430440	-8.97023327494387	3.17789665391127
H	-0.24047389296958	-8.96019004328044	3.66831282409615
H	-4.41460429641588	-8.70082333693802	2.62626386956230
H	3.31649710286483	-5.13853045490375	3.97568495247902
H	-2.44690958966565	-10.04506493798360	3.29156294244399
C	1.91089488226048	2.20037262368335	-3.10488922262548

C	2.53928129152373	2.09809920141181	-4.35374405554739
C	2.47078197066777	3.05346273913102	-2.14324742897888
C	3.70790381417431	2.81338306389149	-4.62614916565254
H	2.11901867048723	1.44017919293997	-5.10765805227606
C	3.64569215901663	3.75463780178934	-2.41271542616388
H	1.98816354842547	3.17903578504849	-1.18162244943354
C	4.27517951243031	3.63875510042374	-3.65971313001394
H	4.19101381428275	2.70761155477980	-5.59266416624428
N	4.20173574743659	4.59083348346385	-1.40768942267139
H	5.20004178519857	4.17304184348892	-3.84821167187281
C	4.50013928472405	4.19914256528767	-0.09976775662660
C	4.53626370314475	5.93822244962730	-1.55941645192699
C	5.03152958973018	5.31317059182494	0.60138412808965
C	4.37315401742266	2.93773406131718	0.49355495406544
C	5.05393889316072	6.42429516073580	-0.33035947911625
C	4.38290513779300	6.76745309039362	-2.67466367926978
C	5.41984258453743	5.16504871435366	1.93375992752779
C	4.77144739735926	2.81972123128615	1.82451029361171
H	3.98033781644288	2.08715488217037	-0.05295917643535
C	5.44282340354440	7.76081016896069	-0.22873521448642
C	4.77929726141538	8.09800507027976	-2.54789006238821
H	3.96448032215308	6.38881901367563	-3.60013342501243
C	5.28224676082934	3.91536539474960	2.54169130939004
H	5.82760556602034	6.00725683196112	2.48496335531962
H	4.69028840742812	1.85337449941681	2.31341532558292
C	5.30730545358320	8.59145079748183	-1.34301639438825
H	5.83961239895038	8.14835605849430	0.70500381234160
H	4.67326655688139	8.76478449759079	-3.39810327411110
H	5.57961654256508	3.78610361200041	3.57779308836628

H 5.60741733426594 9.63260647487007 -1.27741878984545

**XYZ Coordinates of *mCz2i* in  $S_0$  optimized geometry**

N	-0.92443724736618	2.07122688120025	0.27349139082180
C	-1.90915715407825	1.08512226657544	0.43379332407500
C	-2.50531308028618	0.49778437646465	-0.80275254028229
C	-2.32818549451117	1.20673249779342	-2.02321305299807
C	-1.43930707523243	2.30639602377503	-2.10289530416469
C	-0.64465803241594	2.73858354359977	-0.92348046416387
C	-3.29848182782788	-0.65874601027438	-0.77213420369931
C	-1.26105093577598	2.97043738450895	-3.29780343656039
O	-2.24011226718786	0.75501200188731	1.56303124099793
O	0.18999037441608	3.62954827288643	-0.98616021359281
H	-0.54127906902950	3.78080004219364	-3.32615518823941
C	-3.02636752467926	0.82538361678360	-3.20295638239009
C	-2.86440017567837	1.54834054182096	-4.41935606126625
C	-3.73845468712956	1.18808817094466	-5.57685023951673
N	-4.53383584088839	0.03475745178845	-5.45762986204761
C	-4.66253077683622	-0.75089752070433	-4.30879953435679
C	-3.88293800807400	-0.30037699915636	-3.12702938259577
C	-3.98592315855035	-1.02346830996693	-1.95610500702250
H	-4.60546524503159	-1.91333649573525	-1.96276573791102
O	-5.38481821383194	-1.73733656650923	-4.27760964063559
O	-3.80310268932806	1.84286271287352	-6.60531896304918
C	-1.95797154676557	2.61604683764896	-4.48028358987812
C	-5.33758698529875	-0.30905739930784	-6.63821546618161
H	-5.84977194058389	-1.24552925801961	-6.43346661114940
H	-6.05833515151667	0.48623302380585	-6.84013858311390
H	-4.68419089612189	-0.40571844557244	-7.50689622485068
C	-0.24749157069686	2.50789306446480	1.50249805112352

H	0.18754953272685	1.63857756672588	1.99945975609977
H	0.52539831346366	3.21905079814342	1.22271680679649
H	-0.96682559491382	2.97188548796606	2.18062718821886
C	-3.41790537504725	-1.57916144199309	0.38909865785884
C	-4.67268934129301	-2.06220861734538	0.78728773098764
C	-2.27079331692466	-2.05421524603313	1.03667554191472
C	-4.77394572284941	-2.97888888726296	1.83500552885591
H	-5.56996141626405	-1.70328843194790	0.29261194053270
C	-2.37385872157168	-2.95271830545689	2.09753409638828
H	-1.28837260822680	-1.71913618583823	0.72511594571097
C	-3.63273254602374	-3.41995977943444	2.50071828729738
H	-5.75093642423984	-3.33504167738775	2.14653559960708
N	-1.20097272829438	-3.37547472036528	2.77022202486484
H	-3.70208596445993	-4.10971412190857	3.33500284123025
C	-0.23811679287680	-2.52665968887551	3.33180870951256
C	-0.79157150013727	-4.69927675481022	2.95988344645120
C	0.80199444902451	-3.31675806602695	3.88300311320202
C	-0.23731740916615	-1.13194753194231	3.42689045996578
C	0.45060017721942	-4.70096495857336	3.64560920064935
C	-1.40717960211006	-5.88543384769319	2.55237179011376
C	1.88029108768260	-2.68976580789664	4.51860512790182
C	0.84736994893431	-0.53576148245997	4.06864453314399
H	-1.04989398742495	-0.53570562627748	3.02811454035278
C	1.07245351376958	-5.91887846486506	3.94169148400536
C	-0.76678152830544	-7.08464570243661	2.86003190924560
H	-2.34696239697346	-5.87192807213646	2.01116233475690
C	1.90022766120448	-1.30028129399024	4.60349731463949
H	2.68459841291514	-3.28283433681004	4.94457844295504
H	0.87090432554664	0.54607848268660	4.16812113535458

C	0.45845899267976	-7.10578180301423	3.54988756916412
H	2.02304698859536	-5.93401592819856	4.46728880338468
H	-1.22505817544689	-8.02140989859185	2.55663947062969
H	2.72960034352584	-0.80100800326707	5.09518355384524
H	0.92954136834565	-8.05768150525284	3.77502962405046
C	-1.61364638035116	3.40904792384780	-5.69326467971364
C	-1.10704898825874	2.80352462288425	-6.85218596849919
C	-1.69635724515490	4.80389144417231	-5.63136151474301
C	-0.69334039457982	3.58704273136479	-7.92509002700308
H	-1.04159184969868	1.72264586373053	-6.90726829476442
C	-1.27561927310174	5.59119880145969	-6.70933006785870
H	-2.10240549157529	5.28914789351744	-4.75029395809775
C	-0.76614059572402	4.97960978558602	-7.85934410298132
H	-0.29391978333240	3.11287625004249	-8.81624523642419
N	-1.35708906538359	7.00228333845259	-6.62129670547637
H	-0.41969853954391	5.59567838722980	-8.68208624443377
C	-0.85023674949358	7.78485350752623	-5.57621586721065
C	-1.98100281714099	7.84792653748098	-7.54667125093357
C	-1.14962685055242	9.14639035507128	-5.83645074470923
C	-0.12471137120192	7.39807126000302	-4.44592743326922
C	-1.87020391647484	9.18646565931511	-7.09113628119815
C	-2.66115398212973	7.52827542962330	-8.72471685141576
C	-0.73200278060070	10.13006802652013	-4.93315592209298
C	0.27982642431024	8.39665439358868	-3.56198850002502
H	0.12410311752843	6.35834367765248	-4.26511684094826
C	-2.43296906013242	10.22163168790727	-7.84571355877639
C	-3.21369036672067	8.57766779726551	-9.45702201860073
H	-2.76362177280655	6.49971358991500	-9.05229966422355
H	-0.95691651430827	11.17599731397353	-5.12154492368348



C	-0.02275374352299	9.74955926097913	-3.79689867973669
H	0.84213321575731	8.11928104000729	-2.67534920304094
C	-3.09900607021560	9.91200449281845	-9.02864425437620
H	-2.35332126794870	11.25064958515114	-7.50694414827882
H	-3.74696014524609	8.35591653884272	-10.37681727449481
H	0.30448732618407	10.50262893700614	-3.08661987799424
H	-3.53934589135776	10.70552869386562	-9.62457163203604

**XYZ Coordinates of *mCz2i* in S<sub>1</sub> optimized geometry**

N	-0.86862574338815	2.21800422079546	0.29605100401997
C	-1.62774845992339	1.05401103225340	0.42166042749729
C	-2.28683860192173	0.53803883818656	-0.77742445114112
C	-2.16396103049870	1.27391077228824	-1.99338899113398
C	-1.38141349163184	2.45113597939570	-2.06315363408913
C	-0.67887901706305	2.95978656248793	-0.89262722538923
C	-3.08321975265398	-0.64708848397958	-0.76207761989329
C	-1.24540193741110	3.14054105899603	-3.27632263934221
O	-1.69903118926713	0.52456467575884	1.54797640145881
O	0.03535506511880	3.96376394756879	-0.89493879420101
H	-0.59666999673949	4.00880245619197	-3.28494146519922
C	-2.84069801951156	0.84722295319289	-3.18653122666779
C	-2.71615937109147	1.58161898618078	-4.40236860560679
C	-3.52968545922065	1.17091820844662	-5.55761828449177
N	-4.27346480870527	-0.02009135346153	-5.43352790734897
C	-4.38046969300164	-0.80542248129666	-4.28018197467060
C	-3.64120501078761	-0.31743313106135	-3.11657846406847
C	-3.74080926797725	-1.03916212057998	-1.91668154635107
H	-4.34754532019742	-1.93755093523201	-1.93013169846794
O	-5.06685092623392	-1.83221844348356	-4.26001665014529
O	-3.60680143251652	1.79518023026464	-6.61638620646486

C	-1.87723887375426	2.73098984005394	-4.44777545375950
C	-5.03715168020639	-0.41262912426395	-6.61924603757936
H	-5.52244909577206	-1.36121602442459	-6.40338051545698
H	-5.77775757913140	0.35484750789056	-6.85679397468041
H	-4.36529379477954	-0.50259089997649	-7.47546138105209
C	-0.22256481771598	2.70227956356989	1.51495838821716
H	0.53368281869589	1.98589529169416	1.85044932069634
H	0.24573178273369	3.65594307807560	1.28397124951291
H	-0.96465224290849	2.81017326643804	2.30816212099380
C	-3.25630065455470	-1.52580114275587	0.43434297382436
C	-4.53312872362967	-1.81692707605037	0.92598443323421
C	-2.15882865679183	-2.14042891856075	1.04659338599052
C	-4.72069690257007	-2.68037615987501	2.01149631383492
H	-5.39138385313139	-1.34974133591849	0.45492861218131
C	-2.35256791386785	-2.97300664665992	2.14169059955063
H	-1.15886279680696	-1.94386752324265	0.68078258755095
C	-3.62807100169204	-3.26354103068208	2.64148083964244
H	-5.72245824360815	-2.87865469239369	2.37846030462965
N	-1.19973548538770	-3.51936438216344	2.80574753330524
H	-3.74643254559289	-3.89654015340798	3.51430308987473
C	-0.16500171863742	-2.77480730631332	3.33323028941132
C	-0.96704887466552	-4.86963465194627	3.03992701324115
C	0.77892966546647	-3.65992474723069	3.93447068843760
C	-0.01357238928496	-1.37469215891097	3.33796469905777
C	0.25834823435063	-5.00990982860146	3.74487960062806
C	-1.73959067340661	-5.96746639800083	2.64639635865753
C	1.90338593498945	-3.13563283950766	4.54233125138060
C	1.13387475505151	-0.87753362039245	3.95220514119990
H	-0.73650630694307	-0.71351297414882	2.86880707935731

C	0.70775183575751	-6.27625373702447	4.07965641366666
C	-1.27027332301962	-7.23464671874776	2.99717820234916
H	-2.65814763003340	-5.83105980274410	2.08948473706325
C	2.07518700312811	-1.73301899384409	4.54268182968125
H	2.63977623321700	-3.77847788754650	5.01268872881125
H	1.29626681020013	0.19365512924805	3.97113901607491
C	-0.07086287237289	-7.38887592206422	3.70366041162854
H	1.64119952692029	-6.41534887554366	4.61472143056625
H	-1.84119342595689	-8.11091152986475	2.71196173973181
H	2.95605554975820	-1.31166167714454	5.01487730301402
H	0.27147599109422	-8.38521898223456	3.96129686134354
C	-1.56258669656150	3.52038651057348	-5.67289556063004
C	-1.00431738354986	2.92449584664463	-6.81413837994541
C	-1.72148431627962	4.90980265103433	-5.64979475280923
C	-0.60916245139727	3.70407427841493	-7.89609232131570
H	-0.89138706892880	1.84694386513099	-6.84695145198537
C	-1.31535721657448	5.69425267204265	-6.73494787843903
H	-2.17334789564217	5.38891979530886	-4.78801480594138
C	-0.75029274365283	5.09326461171053	-7.86207122397386
H	-0.17367306944065	3.23116529388128	-8.77135432345373
N	-1.47276505738002	7.10633359071613	-6.67971905881152
H	-0.42233596035564	5.71129092143536	-8.69111366917272
C	-0.99240753504950	7.94066515125683	-5.66697119009879
C	-2.12786993087385	7.89421147564082	-7.62854621388562
C	-1.34125925268109	9.28252770567037	-5.97090560774217
C	-0.25628499384633	7.61646715792300	-4.52340491782683
C	-2.06632806139254	9.25291201849954	-7.22227140572911
C	-2.79427710978462	7.50772597591352	-8.79507392434222
C	-0.95750135360696	10.30986396141535	-5.10148569294286

C	0.11281800661266	8.65778208004173	-3.67472460188603
H	0.01831940813159	6.59072490695327	-4.30519211495120
C	-2.66764067663184	10.23814143567547	-8.01357748690833
C	-3.38529105478384	8.50837138544181	-9.56369361756253
H	-2.85334270150549	6.46431130410094	-9.08377114173899
H	-1.22045376504177	11.34040989172678	-5.32380153218952
C	-0.23425283470434	9.99199939963161	-3.95509186337763
H	0.68000988082431	8.42890032026670	-2.77729062799392
C	-3.32177271743341	9.86132598500246	-9.18349261744687
H	-2.62618747038399	11.28129344153675	-7.71254522770345
H	-3.90934841105205	8.23388987444750	-10.47470867789787
H	0.06690388602228	10.77913237967739	-3.27033091437082
H	-3.79182713357446	10.61577390458759	-9.80718973104300

**XYZ Coordinates of *mCz2i* in T<sub>1</sub> optimized geometry**

N	-1.31718641303927	2.16741015945254	0.37839051219012
C	-2.16916659525758	1.05947755415727	0.49476940000171
C	-2.69936853086298	0.47500780773553	-0.74710446867669
C	-2.55901577653100	1.20996622960215	-1.94420686426889
C	-1.76833394443550	2.38916733480540	-1.99238159089516
C	-1.06279624430803	2.87583308730099	-0.80450226235542
C	-3.45525621164103	-0.76153050662502	-0.74981809440976
C	-1.60633434400370	3.08739002872915	-3.19724881583428
O	-2.43264854869249	0.63292440098374	1.62279587508555
O	-0.31128464277590	3.85177843788883	-0.82185149306019
H	-0.92783737089501	3.93242980461252	-3.18541924399445
C	-3.23245165187389	0.80220611441435	-3.14646694434859
C	-3.10183233891311	1.54507280782251	-4.34100150357930
C	-3.95494875578280	1.19327310316170	-5.48574375248366
N	-4.71545546120912	0.01812617673073	-5.39211571381554

C	-4.81478289703946	-0.80161304159972	-4.25859518590083
C	-4.05849596348731	-0.35135328494566	-3.08624002265683
C	-4.13034995148408	-1.11406260093503	-1.90969476421967
H	-4.69801703596130	-2.03652033506897	-1.95551440931839
O	-5.50943262349080	-1.81800363096060	-4.25811504292960
O	-4.03633860117434	1.86976613652607	-6.51494801673152
C	-2.21540267766217	2.69080829474399	-4.37993205731775
C	-5.51096846342964	-0.32417221564778	-6.57525287649619
H	-6.00065102081119	-1.27542346851886	-6.38263377837203
H	-6.25027102315294	0.45726026991819	-6.76592218391610
H	-4.85855615211839	-0.39183339691613	-7.44805893776661
C	-0.71961047950240	2.65018850498444	1.62718789689161
H	-0.11331372023359	1.85741740150251	2.07259284129937
H	-0.10307498427930	3.51307161197290	1.38830632259143
H	-1.50606600598912	2.91840296193522	2.33549164285877
C	-3.46972875725780	-1.72300602068503	0.37341914744638
C	-4.66711596844947	-2.35513739284074	0.75684533992845
C	-2.27963969588644	-2.09926262381546	1.01280978207277
C	-4.67471578025922	-3.31846247664722	1.76547401843774
H	-5.59663640560723	-2.06679533387431	0.27674694287109
C	-2.29143832484537	-3.04967037168780	2.02978401437022
H	-1.33892416131104	-1.65061366736836	0.71854356966080
C	-3.49306751826118	-3.66701100882959	2.41486726208350
H	-5.60981339372686	-3.78386181671025	2.06085740108586
N	-1.08416044891125	-3.37718909795110	2.69815275121077
H	-3.48878502887051	-4.38548494492496	3.22742328296700
C	-0.20369192743547	-2.45980288669723	3.28431764886632
C	-0.56074083276592	-4.66251254006049	2.85473827670767
C	0.89850112823125	-3.16876415400621	3.82719869142973

C	-0.32861247699812	-1.07180472559151	3.40648770927786
C	0.67138931613920	-4.57451102867242	3.55400000245894
C	-1.06535372400760	-5.88502069418742	2.40139641940010
C	1.91156820227095	-2.46716261918077	4.48402174718180
C	0.69906084850862	-0.39795276212675	4.06652233101807
H	-1.18282796080917	-0.53691615355788	3.00664191156290
C	1.39325915649364	-5.73847564241372	3.82423405924696
C	-0.32667881989166	-7.03276165989749	2.68582394790113
H	-1.99267446086319	-5.93561191139322	1.84202069818430
C	1.80830391184579	-1.07962738728712	4.59536838954285
H	2.76204051199919	-2.99533406222908	4.90508881370129
H	0.63091546446086	0.68000769465257	4.18042051440832
C	0.88647348541466	-6.96498817258776	3.39172149981897
H	2.33723904900490	-5.68726992242084	4.35887827443345
H	-0.69561063558368	-7.99653480372333	2.34839138874336
H	2.58876627207502	-0.52130203761643	5.10315664968415
H	1.43803529639067	-7.87737915945681	3.59612493342974
C	-1.85046831768366	3.43362860576763	-5.60453813413579
C	-1.44838820964235	2.77329757839164	-6.78498042501240
C	-1.79349917409756	4.83305884691618	-5.56798841032694
C	-0.99132571388761	3.49730779335857	-7.88203163612335
H	-1.48235464042472	1.69197287667289	-6.82669579232970
C	-1.33511504194111	5.55822036471139	-6.67107663419372
H	-2.13839061928863	5.36585220869732	-4.68946711273140
C	-0.92612448070858	4.88904498588973	-7.83592431927416
H	-0.66968320489702	2.97435697736170	-8.77707308684011
N	-1.26539448249991	6.96928097520406	-6.60679093504320
H	-0.54106612660655	5.45911460444464	-8.67417562557167
C	-0.68226533060094	7.71385005836936	-5.57183850516985

C	-1.77303613025229	7.85752267777495	-7.56244635609992
C	-0.80755182020901	9.09353572082139	-5.87488015704687
C	-0.02233561357459	7.27209982937867	-4.42118921891616
C	-1.50240064183545	9.18539804418650	-7.14415858078427
C	-2.48990026445791	7.58616078137767	-8.73150063580205
C	-0.28467827318020	10.04391403103300	-4.99563708143152
C	0.48917461954979	8.23963129276864	-3.55763408963486
H	0.09456231293593	6.21666944734167	-4.20590179033313
C	-1.92699620204967	10.25639834275960	-7.93258134983604
C	-2.90207241775724	8.67242231927473	-9.50240033014268
H	-2.72929249959296	6.56942879297634	-9.02083567394191
H	-0.37464696102916	11.10351417021849	-5.21613252659441
C	0.35718347075440	9.61045481294201	-3.83508923842158
H	0.99813432224355	7.92095048328389	-2.65340916031458
C	-2.62072385122031	9.99289646832340	-9.11438818462626
H	-1.72628558497038	11.27822293936961	-7.62438610949924
H	-3.45901793208582	8.49057534095709	-10.41642732348330
H	0.76331604106208	10.33875885329429	-3.14016455725942
H	-2.95637820310796	10.81661609215841	-9.73661980578277

**XYZ Coordinates of *pCz2* in  $S_0$  optimized geometry**

N	1.598250	-0.092728	0.119777
C	0.399337	-0.795886	0.287162
C	-0.573036	-0.743888	-0.841419
C	-0.361222	0.218919	-1.874835
C	0.809604	1.035188	-1.915259
C	1.920881	0.735501	-0.964955
C	-1.721946	-1.550693	-0.846882
C	0.945183	2.032417	-2.895504
O	0.211876	-1.414182	1.324270

O	3.054852	1.169555	-1.098226
C	-1.350272	0.376962	-2.885578
C	-1.168717	1.339304	-3.903957
C	-2.185052	1.514122	-4.978752
N	-3.314760	0.683952	-4.911220
C	-3.551808	-0.274697	-3.917326
C	-2.513336	-0.424274	-2.863069
C	-2.685227	-1.363196	-1.869158
H	-3.575834	-1.981582	-1.887333
O	-4.572528	-0.946865	-3.938094
O	-2.046291	2.334725	-5.873747
C	-0.055074	2.150887	-3.892343
H	0.037696	2.912812	-4.658173
C	-4.349640	0.810226	-5.945589
H	-4.467765	-0.143965	-6.463034
H	-5.302997	1.067081	-5.479660
H	-4.038982	1.587210	-6.639088
C	2.597237	-0.279283	1.180981
H	2.862107	-1.336083	1.258062
H	3.472713	0.312304	0.927527
H	2.173558	0.035714	2.136227
C	-2.011867	-2.635344	0.129750
C	-3.217756	-2.624692	0.843016
C	-1.147139	-3.728496	0.287271
C	-3.533647	-3.652204	1.728841
H	-3.898197	-1.785517	0.732867
C	-1.471888	-4.774961	1.139367
H	-0.218110	-3.759494	-0.272280
C	-2.663157	-4.736874	1.880176



H	-4.445879	-3.613882	2.313992
H	-0.813291	-5.631195	1.235701
N	-2.979159	-5.788266	2.772447
C	-4.189808	-6.491429	2.818110
C	-2.135944	-6.292371	3.771635
C	-4.119425	-7.458662	3.852909
C	-5.319329	-6.371552	2.003935
C	-2.811932	-7.331284	4.460495
C	-0.852510	-5.881439	4.141710
C	-5.211960	-8.300652	4.087175
C	-6.394171	-7.221692	2.258331
H	-5.356870	-5.647491	1.197880
C	-2.175016	-7.986044	5.520410
C	-0.240790	-6.549153	5.201377
H	-0.353911	-5.065174	3.630996
C	-6.347346	-8.174498	3.291033
H	-5.169346	-9.044423	4.877757
H	-7.284600	-7.145533	1.641226
C	-0.888989	-7.594482	5.882628
H	-2.682603	-8.784064	6.054873
H	0.757266	-6.249856	5.507684
H	-7.203093	-8.819808	3.464013
H	-0.382499	-8.094738	6.702351
C	2.037527	3.039278	-2.938925
C	2.741050	3.269736	-4.129056
C	2.319470	3.846683	-1.825846
C	3.732084	4.246473	-4.196986
H	2.539219	2.652666	-4.999519
C	3.283519	4.841757	-1.893758

H	1.766300	3.697093	-0.904532
C	4.009676	5.039120	-3.078094
H	4.304237	4.389419	-5.107149
H	3.479677	5.479090	-1.038449
N	5.015625	6.031783	-3.133487
C	5.126071	7.041614	-4.097515
C	6.071510	6.170372	-2.223034
C	6.261675	7.837237	-3.799252
C	4.291445	7.332623	-5.179754
C	6.865061	7.280882	-2.606823
C	6.403488	5.376591	-1.121794
C	6.573851	8.928860	-4.616632
C	4.624433	8.425506	-5.978378
H	3.411461	6.733981	-5.386558
C	7.996752	7.613462	-1.853967
C	7.535797	5.729005	-0.389447
H	5.808263	4.511313	-0.852225
C	5.755270	9.215303	-5.706064
H	7.441269	9.545190	-4.398115
H	3.992276	8.671365	-6.826602
C	8.323869	6.837900	-0.744792
H	8.612430	8.462502	-2.136977
H	7.815038	5.128757	0.471525
H	5.987220	10.058334	-6.349642
H	9.198357	7.085793	-0.151036

**XYZ Coordinates of *pCz2* in  $S_1$  optimized geometry**

N	1.36360253533084	-0.26817796992643	0.05919213537455
C	0.21944689975907	-1.06037921462879	0.06404906662283
C	-0.70636705020526	-0.87870947232564	-1.04887721286845

C	-0.44370464969482	0.12127047668866	-2.02822748152822
C	0.70975205702954	0.95898204140036	-1.95642519140233
C	1.70856545541419	0.70355817079613	-0.91582021414319
C	-1.86794762617170	-1.69292748954916	-1.15804258430978
C	0.90833549347258	1.97363335915616	-2.94387768210129
O	0.05203698997592	-1.87679131680937	0.98638157803154
O	2.80361816100538	1.26245956887401	-0.83788319811491
C	-1.36823078437856	0.27692130937507	-3.11489139257028
C	-1.12224117106379	1.25779560684960	-4.10363373326397
C	-2.04199945820960	1.43700465694596	-5.22875629305949
N	-3.16337713721097	0.58040402481704	-5.25342428277337
C	-3.45783512629016	-0.40426094006822	-4.30101943733741
C	-2.51085044536084	-0.55022416926821	-3.19533549423047
C	-2.74753550348843	-1.52534083623284	-2.21281557003317
H	-3.63519562827010	-2.13977220576538	-2.31278200882317
O	-4.47441164896588	-1.09621633129806	-4.42309326781374
O	-1.87011544962033	2.27742127357764	-6.11449347440249
C	0.00072795516878	2.08799793509553	-3.99373845416450
H	0.13273195500668	2.85862345224178	-4.74455668325843
C	-4.11871889482064	0.71140184557183	-6.35343880217224
H	-4.19097071292239	-0.23462188771808	-6.89546089911071
H	-5.10965137424390	0.94580707991451	-5.95718348495221
H	-3.76724527324405	1.50529377908262	-7.00791072492764
C	2.30461025990110	-0.50540812456033	1.15419275834638
H	2.65715806101056	-1.53973596198803	1.12604456326151
H	3.13659353020176	0.18327742931358	1.03361018976655
H	1.80134535489914	-0.34895355029116	2.11112350633750
C	-2.17848272948709	-2.75112981745777	-0.14743167135254
C	-3.08603307609264	-2.49605809487876	0.88870091723921

C	-1.61662141745889	-4.03172589832937	-0.25799189985221
C	-3.37798134957014	-3.46746498200198	1.84096188369268
H	-3.53499893111646	-1.51236649943728	0.96547341099704
C	-1.87999549779927	-5.01005274366978	0.69008390140852
H	-0.93918687041464	-4.24108111181144	-1.07783062527514
C	-2.74856891061624	-4.70978131883978	1.74406731785116
H	-4.04069975952131	-3.25500360687232	2.67372347194938
H	-1.43115908882143	-5.99565652456294	0.61991628936603
N	-2.95825076072665	-5.68819673726604	2.77150726573628
C	-4.17408489630853	-6.24260524345120	3.13461822329748
C	-1.95611884257787	-6.21695404097006	3.56511773896021
C	-3.96148411945784	-7.17046714537609	4.19211881306337
C	-5.43711118535989	-6.00706475604033	2.57651949010334
C	-2.52766440342495	-7.15623542104453	4.46862699648629
C	-0.59166397765071	-5.88978531423580	3.56890924980226
C	-5.04188464728683	-7.86197061410350	4.71168153787670
C	-6.51184626759571	-6.71010052863007	3.11987270504067
H	-5.56070747266719	-5.30953088918357	1.75742008448973
C	-1.70785564187821	-7.80552391295475	5.37435121524642
C	0.21444550487549	-6.56115341583797	4.48668401645079
H	-0.19745892813397	-5.13810013391296	2.89538515536355
C	-6.32077178703987	-7.61958644481578	4.16936529225852
H	-4.91456154989256	-8.57949163456602	5.51520788754858
H	-7.50714888517684	-6.55487060726762	2.71992637857264
C	-0.32917893707705	-7.50495854842413	5.36985777893195
H	-2.10920601137619	-8.52479876696591	6.08019473272698
H	1.27495616779168	-6.34147799856048	4.52375767078627
H	-7.17403811777982	-8.15533087604224	4.57057040326336
H	0.32187389170650	-8.00889500288759	6.07569781409335

C	2.00411588506425	2.98392551460630	-2.90790322017843
C	2.82675966848359	3.16563946119917	-4.02681034502061
C	2.17144217053165	3.84540793589275	-1.81270204846893
C	3.81159324827292	4.15356632241165	-4.04539937547099
H	2.70900921631424	2.50796417348771	-4.88251764451661
C	3.12994095720088	4.84991495620076	-1.83166504987003
H	1.53825979216395	3.72136151407645	-0.94113285284243
C	3.96482926379391	5.00093573226789	-2.94670360208073
H	4.46771730724217	4.26624852345439	-4.90230369548714
H	3.24275041691290	5.52462981628392	-0.98932128446408
N	4.96668475814106	6.01116175554166	-2.95267214252178
C	5.10659330849445	7.02088523499587	-3.90550078226281
C	5.97868204236194	6.15582556444844	-2.00255449906776
C	6.22267639626290	7.82874317951239	-3.56252454005002
C	4.31937621044920	7.29506800704171	-5.02750382633453
C	6.77982226841153	7.27593029545828	-2.34728672694925
C	6.26016426197473	5.36716356121395	-0.88314016064946
C	6.55797620017471	8.92049475126834	-4.37147242608332
C	4.67483440687723	8.38818836223953	-5.81468779339573
H	3.46199075279632	6.67722723946866	-5.27045156469045
C	7.87176178512710	7.61659086214398	-1.54071888788132
C	7.35344473839976	5.72837095981969	-0.09876755722735
H	5.64971188625567	4.50372943622294	-0.64219500665087
C	5.78363713489502	9.19354605328276	-5.49585613712395
H	7.41029005808149	9.54576463888861	-4.12003021970760
H	4.07990039191698	8.62227314179619	-6.69285286780484
C	8.15148034546436	6.84254996676101	-0.41778068919646
H	8.49230585824602	8.47201979274977	-1.79330999846479
H	7.59432799934407	5.13267110742049	0.77712394903580

H	6.03393964794248	10.03663750755743	-6.13280952708617
H	8.99510434632349	7.09662572341454	0.21707884601040

**XYZ Coordinates of *p*Cz2 in T<sub>1</sub> optimized geometry**

N	1.63915824710486	-0.18602935197083	0.01471732207526
C	0.42486244652101	-0.86140716756143	0.20597180327302
C	-0.55661624751795	-0.76946572343701	-0.88503621603575
C	-0.32325519775172	0.16554956121125	-1.93834218183263
C	0.85965644763901	0.94635891303357	-1.99323678554548
C	1.95183698027582	0.64755196822034	-1.06681587459497
C	-1.75675276482282	-1.54559149784434	-0.86608408471646
C	1.02690849301690	1.94704277909860	-3.04532287879246
O	0.25686193772490	-1.49457018499350	1.24740870004698
O	3.09591066536004	1.10445174721922	-1.19052128676186
C	-1.30308511860841	0.30927805329423	-2.97750306801244
C	-1.06366425572413	1.20429292288286	-4.05931574688523
C	-2.04525927333625	1.35158888664097	-5.14222392498504
N	-3.21160397965891	0.57298957949805	-5.03065740833595
C	-3.49612591141736	-0.31420958015093	-3.98386359739783
C	-2.47985627847313	-0.44275684226175	-2.92809610044419
C	-2.69543747021426	-1.35410840156585	-1.86964457788219
H	-3.61074645202727	-1.93533465857001	-1.88319159944910
O	-4.55257126204564	-0.94391218237729	-3.97582917861790
O	-1.87061524618582	2.10772833160229	-6.09769002132859
C	0.08277922331139	2.00012596010162	-4.06865029159309
H	0.16709652333060	2.73396657867948	-4.86196322459621
C	-4.23251670525961	0.67956892668192	-6.07715102360982
H	-4.39209182402188	-0.29855420537866	-6.53642592786529
H	-5.17775341839683	1.00436247348497	-5.63672002240650
H	-3.88279086519613	1.39826711317435	-6.81390085222440

C	2.65286388131263	-0.40111199173820	1.05304490589930
H	2.89100538321850	-1.46499453868760	1.12311695433625
H	3.53732693032457	0.17013023546223	0.78394706196177
H	2.25703688453288	-0.08128136391005	2.01906083926931
C	-2.04873111485694	-2.61425685808501	0.13051194674545
C	-3.21298150696878	-2.55189043449957	0.90644370076702
C	-1.22521152476276	-3.74478752792939	0.24566082322618
C	-3.53170663275590	-3.56898429256413	1.80437510138066
H	-3.85890666210290	-1.68289549619780	0.82775244509127
C	-1.54650221597061	-4.77521435664965	1.11789829123707
H	-0.32774686510580	-3.81251362276273	-0.36008611872130
C	-2.69806735170381	-4.68591220777317	1.91396019697568
H	-4.41283324322661	-3.49517278343581	2.43276960907184
H	-0.91891066193055	-5.65735780363534	1.18627110749035
N	-3.01132755820960	-5.72517001782588	2.82704256608280
C	-4.23171426214237	-6.40162120679048	2.91181391067696
C	-2.14772851276786	-6.24306444001453	3.79725365428217
C	-4.15079511744050	-7.36855258798311	3.94740667392910
C	-5.38239094575378	-6.25532901123621	2.13140136353295
C	-2.82076370851902	-7.26735649398495	4.51226106001092
C	-0.84300031266917	-5.85647510505876	4.11826605381270
C	-5.25327125652620	-8.18434044452049	4.21622897218927
C	-6.46797226076859	-7.08026289061728	2.42040481763865
H	-5.42503482558613	-5.53017094640419	1.32674073666128
C	-2.16068497596551	-7.93122392243715	5.55007701790368
C	-0.20750656844260	-6.53425995942213	5.15728217944845
H	-0.34894365534194	-5.05260929913232	3.58411180757674
C	-6.41005885169247	-8.03236818901381	3.45298761420766
H	-5.20500429133249	-8.92849540802591	5.00602719746074

H	-7.37506759663915	-6.98530974971139	1.83108083049501
C	-0.85305345241930	-7.56385014562175	5.86416534633858
H	-2.66343608020014	-8.71767075535384	6.10572600911159
H	0.80693535506555	-6.25581103586822	5.42668134759528
H	-7.27410012931704	-8.65844992107403	3.65307470206377
H	-0.32821634963389	-8.07253885020750	6.66694884022360
C	2.07585178707042	2.96696361675119	-3.03253435874225
C	2.68171215962910	3.38552807279112	-4.24117365040559
C	2.45383750931563	3.64230545364770	-1.84385378898496
C	3.62799748505091	4.39465924945536	-4.26387930360879
H	2.44251618940739	2.86311331914421	-5.16110453172379
C	3.38346673650218	4.66343417919251	-1.86042247785567
H	1.97168568440689	3.38210924882089	-0.91053334939483
C	3.99459122104439	5.04530743922081	-3.06912335464315
H	4.13091012787489	4.65393917243514	-5.18874862271977
H	3.62590290348101	5.19725554929464	-0.94858086638496
N	4.97210779272552	6.05338231543712	-3.08146280211954
C	5.04226168190582	7.12383633916459	-3.98837367977202
C	6.05206050849741	6.15805573980074	-2.18775054322602
C	6.17202946721663	7.91831321323384	-3.67130770874942
C	4.16006662524644	7.47820967420730	-5.01263983309062
C	6.81570846631790	7.30244301861847	-2.52629211500044
C	6.44019720066245	5.29317397747338	-1.16073496109278
C	6.44358331096592	9.06380668808972	-4.42089697150225
C	4.45387804862524	8.62482931243385	-5.75044514784493
H	3.27135453871084	6.89423688990525	-5.22010128342189
C	7.96429331078212	7.60810177319170	-1.79439790202579
C	7.59003503034923	5.62038886554080	-0.44244471191019
H	5.88087461915198	4.39249413745370	-0.93720033148372



C	5.58459285252451	9.40699076975857	-5.46566205663255
H	7.30568152885812	9.68150462083781	-4.18767050642262
H	3.78739654923207	8.91948505675070	-6.55503343915031
C	8.34128719721421	6.76690672092073	-0.74698760561460
H	8.55877411455145	8.48198041400078	-2.04362143830754
H	7.91143535397751	4.96771633306176	0.36321909169675
H	5.78480698980279	10.29406021226228	-6.05826387942507
H	9.23103537157085	6.99343305110136	-0.16800138789531

**XYZ Coordinates of *pCz2i* in  $S_0$  optimized geometry**

N	-0.801621	1.972989	0.582795
C	-1.592274	0.812042	0.525568
C	-2.122901	0.400202	-0.809557
C	-1.955998	1.292553	-1.907004
C	-1.197067	2.480982	-1.772959
C	-0.557670	2.843815	-0.482238
C	-2.843596	-0.790812	-0.981688
C	-1.050241	3.340214	-2.841786
O	-1.816015	0.203740	1.560710
O	0.128683	3.847709	-0.351831
H	-0.478869	4.248924	-2.688712
C	-2.535951	1.015480	-3.177649
C	-2.366586	1.906614	-4.275895
C	-2.906653	1.500577	-5.608410
N	-3.697408	0.339664	-5.665593
C	-3.937286	-0.533718	-4.601793
C	-3.294645	-0.173154	-3.311926
C	-3.435131	-1.036331	-2.245221
H	-4.002574	-1.947313	-2.399460
O	-4.623713	-1.537655	-4.732031

O	-2.691637	2.115649	-6.641269
C	-1.638062	3.092890	-4.106980
C	-4.246767	0.006318	-6.986578
H	-4.895035	-0.858360	-6.871117
H	-4.802830	0.861347	-7.374205
H	-3.433904	-0.215419	-7.681620
C	-0.261100	2.312283	1.905822
H	0.292204	1.458925	2.301059
H	0.388265	3.176184	1.790672
H	-1.078542	2.537521	2.594360
C	-3.010428	-1.859394	0.038672
C	-4.292686	-2.324359	0.360636
C	-1.901164	-2.492225	0.619520
C	-4.469433	-3.361868	1.273326
H	-5.162428	-1.845372	-0.079274
C	-2.067036	-3.550895	1.500946
H	-0.901543	-2.155387	0.366817
C	-3.355851	-3.984228	1.847899
H	-5.465946	-3.684817	1.553785
H	-1.205305	-4.055095	1.924300
N	-3.522596	-5.041354	2.772766
C	-4.307894	-6.185712	2.582529
C	-2.926169	-5.118257	4.038702
C	-4.210215	-7.004991	3.736027
C	-5.061020	-6.573404	1.471043
C	-3.331537	-6.324816	4.663389
C	-2.098575	-4.198281	4.688367
C	-4.898945	-8.221936	3.780245
C	-5.738596	-7.789659	1.540727

H	-5.110670	-5.954686	0.582075
C	-2.875598	-6.623295	5.952131
C	-1.658335	-4.519441	5.971269
H	-1.817046	-3.263461	4.216613
C	-5.665141	-8.606208	2.682887
H	-4.830188	-8.856865	4.658884
H	-6.332994	-8.112273	0.690922
C	-2.035172	-5.720400	6.598043
H	-3.180571	-7.544707	6.439933
H	-1.013040	-3.821968	6.497224
H	-6.206748	-9.546889	2.704645
H	-1.671798	-5.939843	7.597331
C	-1.449881	4.157618	-5.129594
C	-2.542367	4.822486	-5.705857
C	-0.155985	4.592537	-5.446551
C	-2.348589	5.879653	-6.585037
H	-3.550047	4.495222	-5.473779
C	0.047562	5.652531	-6.327016
H	0.700529	4.096251	-4.999776
C	-1.049417	6.302353	-6.902689
H	-3.196095	6.378303	-7.042539
H	1.051201	5.990906	-6.560395
N	-0.849734	7.382470	-7.795067
C	-1.429351	8.652817	-7.686247
C	-0.018998	7.369453	-8.922869
C	-0.963776	9.462111	-8.753785
C	-2.294386	9.154802	-6.710399
C	-0.067202	8.643977	-9.542502
C	0.732955	6.321062	-9.459669

C	-1.394089	10.789690	-8.853229
C	-2.707771	10.480372	-6.832102
H	-2.627214	8.538011	-5.883137
C	0.673639	8.874293	-10.706946
C	1.460983	6.576143	-10.620512
H	0.742407	5.341649	-8.994635
C	-2.268825	11.291640	-7.893104
H	-1.044517	11.417904	-9.667566
H	-3.381479	10.893481	-6.087114
C	1.438396	7.839131	-11.238217
H	0.645070	9.846840	-11.189980
H	2.054532	5.778328	-11.057253
H	-2.612631	12.319315	-7.959190
H	2.018695	8.004206	-12.140827

**XYZ Coordinates of *pCz2i* in  $S_1$  optimized geometry**

N	-0.94884485393952	1.64953599104686	0.49192443681561
C	-1.62876168893589	0.44064594009671	0.32157630095923
C	-2.12047222370192	0.13543633086411	-1.02163267212131
C	-1.92709841370065	1.07784817715313	-2.06792212199348
C	-1.24433386610479	2.29464663763900	-1.83386393931972
C	-0.71498419197149	2.61677252266281	-0.51298555375933
C	-2.79594335484709	-1.08327310809307	-1.29830658032113
C	-1.08455558970379	3.22163774202954	-2.87474689957009
O	-1.77705815964451	-0.30754290490086	1.30229124726164
O	-0.10169982950230	3.65381350701381	-0.25274698729573
H	-0.59051716388435	4.15728733456175	-2.63923708612597
C	-2.41460332403415	0.81178439145613	-3.39155769815217
C	-2.22016946905782	1.75739024863669	-4.44101494670985
C	-2.63606567493092	1.38767537928032	-5.80074097386980

N	-3.33765905232217	0.17278305021644	-5.95364031996451
C	-3.59981276308735	-0.76009744555487	-4.94386373668962
C	-3.08493296365738	-0.41434663440853	-3.62084169275947
C	-3.26394834878043	-1.33756901668794	-2.57498800910241
H	-3.77938309891538	-2.261911110760169	-2.81011044882207
O	-4.21618207806263	-1.80635877941848	-5.17586678955394
O	-2.41469293304067	2.05800673401964	-6.81088068192393
C	-1.56494685183477	2.99270564333687	-4.16201217080514
C	-3.77013781748168	-0.13600819645774	-7.31744679295635
H	-4.32865534781729	-1.06823187236831	-7.28601373045677
H	-4.38883805451296	0.67835416485492	-7.70051353048154
H	-2.90053499293426	-0.22823757147396	-7.97276372583804
C	-0.45923392946095	1.92418331967079	1.84208200355402
H	0.23241144214766	1.13762039790438	2.15400646439029
H	0.04021460785615	2.88977596753130	1.82289953749572
H	-1.29508660660620	1.93447545364769	2.54591123113873
C	-3.01519711412835	-2.12298361034886	-0.24644703373403
C	-4.26421793576353	-2.25332506366388	0.37200487236163
C	-1.99206565069883	-3.02027530574747	0.09358073029601
C	-4.48062513506470	-3.21509116116370	1.35602160060456
H	-5.06158603096215	-1.57150017865266	0.09880773918982
C	-2.17969819121538	-3.97479128401504	1.08308007305589
H	-1.03196353004334	-2.93704948497120	-0.40246974820523
C	-3.42375898381391	-4.05076603232693	1.71604657877450
H	-5.43431781302122	-3.28796455431954	1.86895519311064
H	-1.38372243890254	-4.65688178757129	1.36421216138807
N	-3.59561263392891	-4.98143461395209	2.79687295845374
C	-4.49673970173919	-6.03063015284181	2.83457816935137
C	-2.87158070141415	-4.95294254338607	3.97382851250889

C	-4.35332570016278	-6.71867092109962	4.07212317525522
C	-5.40539742883595	-6.43030756452104	1.84599431802927
C	-3.30109293968193	-6.02304769552174	4.80828948837341
C	-1.89425269596658	-4.02530012893449	4.36570369196801
C	-5.14841147194787	-7.82195024960913	4.32716281766650
C	-6.20020449710565	-7.54095909537260	2.12722852580853
H	-5.47611313774798	-5.89372173173233	0.90794566561096
C	-2.71823745589642	-6.18291132463020	6.05242347530822
C	-1.31913405821405	-4.20995421705325	5.62179815137678
H	-1.61733421286909	-3.20137822549811	3.71861276857043
C	-6.07711751043659	-8.22465468371129	3.34486754011816
H	-5.06214193710770	-8.37240567152477	5.25788758361614
H	-6.91874063670868	-7.88251207512627	1.39124271351992
C	-1.71789388698254	-5.26959873853273	6.44926639874159
H	-3.02222169345334	-6.98487078578679	6.71655811469000
H	-0.55920085860846	-3.51828760150432	5.96582174378580
H	-6.70580404950616	-9.08737590362676	3.53583709272072
H	-1.25482749598533	-5.38643098354650	7.42288125312232
C	-1.39288194450954	4.10658745131752	-5.13883041427425
C	-2.49143009352597	4.70151166137301	-5.77824900569768
C	-0.12347018276347	4.65963429276571	-5.35052942217576
C	-2.32651777599509	5.79983924165472	-6.61260034019381
H	-3.47941492086960	4.27909262854323	-5.63436211559894
C	0.05166630050357	5.77088268895475	-6.17532434652785
H	0.73659647042103	4.21489015434323	-4.85947946834166
C	-1.05055035056362	6.34248845390486	-6.81355190227944
H	-3.17742113582501	6.24075406117137	-7.12146222118832
H	1.03694549977491	6.20058745169612	-6.32379307504613
N	-0.87915677217162	7.46903725356912	-7.66617551218929

C	-1.52635638451749	8.69821187447682	-7.53509512747717
C	-0.02896303547685	7.53273862079217	-8.77132382371037
C	-1.08612035862611	9.56562631356768	-8.56946440266237
C	-2.44558034677189	9.11728043547399	-6.56885207916349
C	-0.12978510813672	8.82107399053003	-9.35893880682177
C	0.79891623443075	6.54341064129201	-9.30984721908494
C	-1.59261956477944	10.86833060825823	-8.63966000103528
C	-2.93292198593577	10.41916372874687	-6.66151248289194
H	-2.76235264312123	8.44967555259848	-5.77530400693106
C	0.62898646762700	9.12211267535334	-10.49585791820961
C	1.54214783671424	6.86932393398294	-10.44212324566654
H	0.85218297981696	5.55745542920008	-8.86184330664950
C	-2.51636720150917	11.28846759457562	-7.68640371163920
H	-1.26398809288323	11.54068462228271	-9.42738082677665
H	-3.64904488620184	10.76871770062357	-5.92327703469565
C	1.46457967318631	8.14523533398443	-11.03037043332436
H	0.56113102560246	10.10506088649992	-10.95389743902608
H	2.19349209751984	6.11837423260554	-10.88005012698142
H	-2.91839815576475	12.29624328058030	-7.73049401998331
H	2.05978347473435	8.36600727891661	-11.91139662221670

**XYZ Coordinates of *pCz2i* in T<sub>1</sub> optimized geometry**

N	-0.54490212423495	1.82798984855110	0.48334597533884
C	-1.50078853332827	0.80062712002321	0.48521649591685
C	-2.09145606277685	0.41911330179990	-0.80840499589731
C	-1.87161388436406	1.25794604587014	-1.91963446162613
C	-0.94435225460057	2.33478230637629	-1.85442961022995
C	-0.20842189524995	2.62503140507523	-0.61964964108897
C	-2.98453459704451	-0.72091889281885	-0.93276668673498
C	-0.75245059011549	3.17575066376168	-2.95616875844064

O	-1.79734047670578	0.27182129926599	1.55945540717418
O	0.63431455033582	3.51815919503899	-0.53487758620784
H	-0.08421540630109	4.01813195731898	-2.81923386333346
C	-2.57178549122320	1.04780174400607	-3.15858764676628
C	-2.35406069145514	1.88784050424850	-4.26818042121163
C	-2.95551907215217	1.51536077679959	-5.56057479503964
N	-3.91212382176149	0.48832322050676	-5.55769019329719
C	-4.23885055802619	-0.31677674417439	-4.45777215391734
C	-3.49901249476817	-0.03012809362633	-3.22444476310621
C	-3.68433480512853	-0.87591130734663	-2.12624564132595
H	-4.34619762188389	-1.72237050592809	-2.26831618956355
O	-5.07856390039999	-1.21288610093921	-4.54317098361812
O	-2.66576941922941	2.05098442100874	-6.63208862447193
C	-1.45294426648539	3.01940847308884	-4.14832180297544
C	-4.53680933984706	0.19251649957364	-6.85091572911299
H	-5.31528694083191	-0.54759297040242	-6.68335203476440
H	-4.95219686167798	1.10949848493988	-7.27250202536490
H	-3.78861728967592	-0.19133960809443	-7.54883785459870
C	0.07027746858342	2.13220357992244	1.77907847525164
H	0.48875122713321	1.21940030564816	2.20688571169622
H	0.84573749150433	2.87581741072476	1.61302350880499
H	-0.68439119226357	2.51447222268098	2.47081516145034
C	-3.12496958665245	-1.78081433684177	0.07587558481385
C	-4.38868899154376	-2.35571042398986	0.32962796605408
C	-2.00705578756125	-2.33380013835441	0.74055313787712
C	-4.53792652453322	-3.41130127516633	1.21648219725920
H	-5.26882905323691	-1.93038713352297	-0.14110375745916
C	-2.14340334159080	-3.40089708786120	1.60996915471347
H	-1.02002251407976	-1.93778883533467	0.53901558278921



C	-3.41350443736972	-3.94576546207612	1.86736357565255
H	-5.52303438678084	-3.80390650371942	1.44286647273113
H	-1.27045516069847	-3.83982542460494	2.08002832930537
N	-3.55643531632632	-5.01179937155358	2.77683031049759
C	-4.28036405424121	-6.19241415534788	2.55370270810478
C	-2.99650727426983	-5.07082490358217	4.06249581204956
C	-4.17959534784598	-7.01520542226039	3.70373881683319
C	-4.96217396581904	-6.61267965940914	1.40839426472224
C	-3.36483738374541	-6.29947915713852	4.66548148520763
C	-2.24920109332390	-4.11012220922318	4.74977107209951
C	-4.79911533472268	-8.26682770425596	3.71478428365948
C	-5.57626866332150	-7.86416719228826	1.44511452009450
H	-5.00265081734275	-5.99589164367837	0.51818736837281
C	-2.94715746659982	-6.58323219045078	5.96777156131987
C	-1.84225251717239	-4.41754062615373	6.04750384728983
H	-2.00567939121479	-3.15516230728826	4.29865214092911
C	-5.50276525713954	-8.68240585019836	2.58460887440783
H	-4.72524388928189	-8.90716936884945	4.58874868120643
H	-6.11591631990081	-8.21311831894318	0.57001176171301
C	-2.17887202821669	-5.64092718222610	6.65077483565342
H	-3.22600077941881	-7.52014533126330	6.44090224955723
H	-1.25844703638367	-3.68992133239924	6.60287244966576
H	-5.99084895877331	-9.65199815867676	2.57989792119835
H	-1.84548005442894	-5.84835548761144	7.66282560882893
C	-1.30095632007936	4.07625143964632	-5.16293000539016
C	-2.41707085460215	4.67497531984767	-5.78611834974489
C	-0.02539921129543	4.60147479839619	-5.45043999664480
C	-2.26768203883949	5.74919678345472	-6.64690316832252
H	-3.40832369237912	4.28816458594020	-5.58512990416965

C	0.13599190878711	5.66741154884720	-6.32477747857796
H	0.84918179827289	4.15606379570742	-4.98758044096441
C	-0.98690139910907	6.25452737493636	-6.92856367415331
H	-3.13263071294770	6.18889868302415	-7.13083737929716
H	1.12315810123397	6.06811599603002	-6.52678791059428
N	-0.83056992976938	7.34763029933447	-7.80635225743322
C	-1.54048199116083	8.55616085586466	-7.74628945480472
C	0.07927454001210	7.42127746298962	-8.87106800634059
C	-1.07832119545517	9.41074283998641	-8.77873307209954
C	-2.50908995259616	8.97298863296850	-6.82908852647941
C	-0.04737692125104	8.68727082593104	-9.49608112208391
C	0.95749027375276	6.44817006578700	-9.35606538411152
C	-1.62135155878804	10.69090438510974	-8.91180903671658
C	-3.03658566615518	10.25435358145724	-6.98310491887294
H	-2.83309922258118	8.32931297095809	-6.01977834567352
C	0.74744456865824	8.99392262402704	-10.60319629178420
C	1.74092722008312	6.77822445460584	-10.46105413625615
H	1.01862573995063	5.46753501054580	-8.89879177240327
C	-2.60509176835558	11.10487685636862	-8.01456079562522
H	-1.27524122550592	11.35392508660071	-9.69925498457340
H	-3.79315806979260	10.60056521039375	-6.28555436124376
C	1.64533366934105	8.03772194928582	-11.07629205867051
H	0.66052858440203	9.96065147872397	-11.09041020312665
H	2.43376762981175	6.04123399295095	-10.85554738366062
H	-3.03774422172732	12.09611976109340	-8.10746492430327
H	2.27053650559645	8.26318796055722	-11.93457774596510

## References

1. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652
2. C. T. Lee, W. T. Yang and R. G., *Phys. Rev. B*, 1988, **37**, 785
3. Neese F., *WIREs ComputMol Sci.* 2022, **12**, 1606
4. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580
5. L. Liu, Q. Wei, Y. Cheng, H. Ma, S. Xiong and X. Zhang, *J. Mater. Chem. C* 2020, **8**, 5839–5846.
6. A. Einstein, *Phys. Z., The Quantum Theory of Radiation*, 1917, **18**, 124
7. V. Lawetz, G. Orlandi and W. Siebrand, *J. Chem. Phys.*, 1972, **56**, 4058
8. G. W. Robinson and R. P. Frosch, *J. Chem. Phys.*, 1963, **38**, 1187
9. M. J. Thapa, W. Fang and J. O. Richardson, *J. Chem. Phys.*, 2019, **150**, 104107
10. V. Balzani, A. Juris, M. Venturi, S. Campagna and S. Serroni, *Chem. Rev.*, 1996, **96**, 759
11. D. Beljonne, Z. Shuai, G. Pourtois and J. L. Bre 'das, *J. Phys. Chem. A*, 2001, **105**, 3899
12. A. Velardo, R. Borrelli, A. Peluso and A. Capobianco, *J. Phys. Chem. C*, 2016, **120**, 24605
13. P. K. Samanta, D. Kim, V. Coropceanu and J. L. Bre 'das, *J. Am. Chem. Soc.*, 2017, **139**, 4042
14. K. V. Mikkelsen and M. A. Ratner, *Chem. Rev.*, 1987, **87**, 113.