

# Photophysical Properties of Sulfone-Based TADF Emitters In Relation To Their Structural Properties

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## Contents

### List of Tables

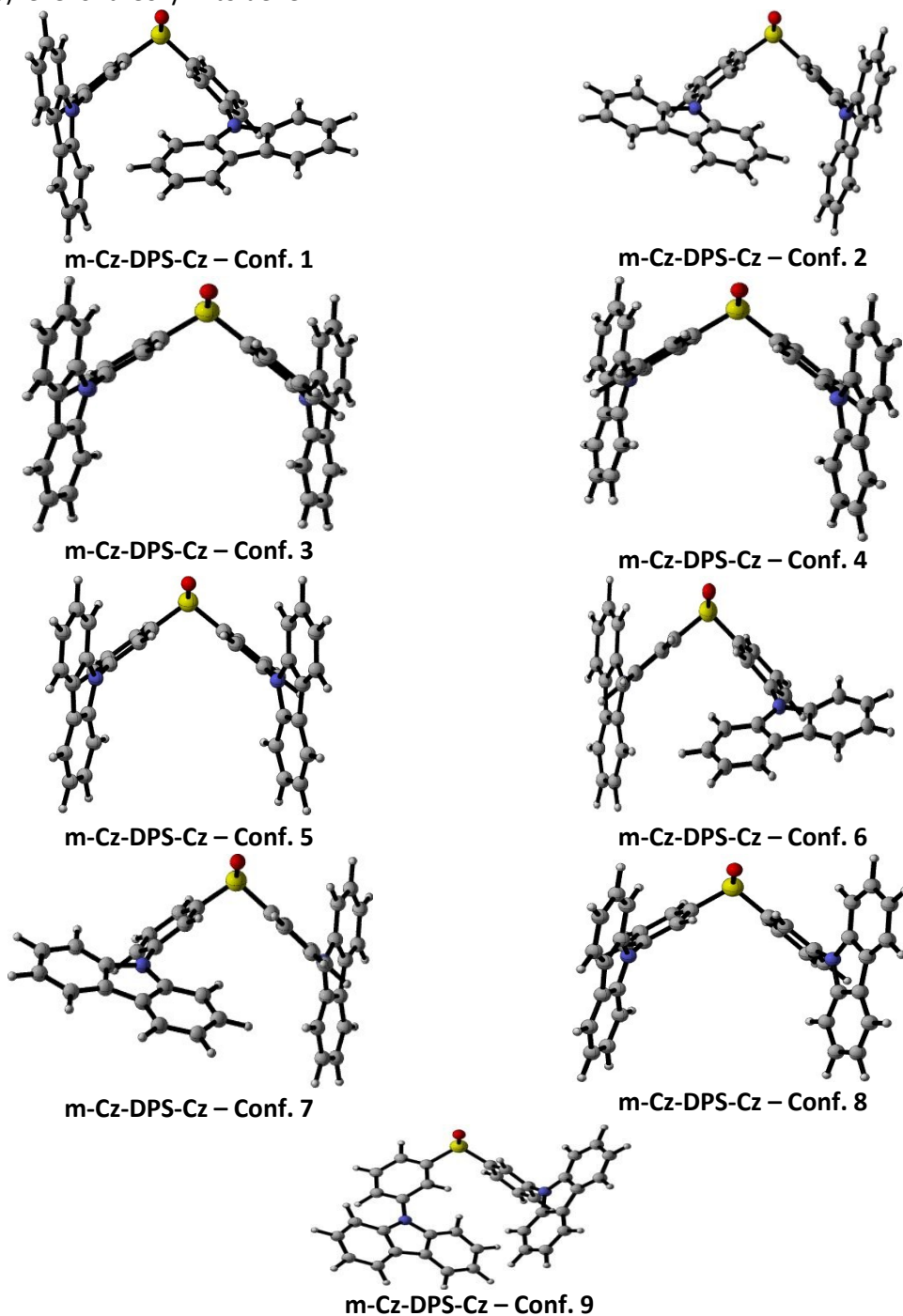
<b>Table S1</b> 3D representations of the ground state structures of all molecules, optimized at M06-2X/6-31+G(d,p) level of theory in toluene.....	3
<b>Table S2</b> Torsion angles of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	21
<b>Table S3</b> Torsion angles of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	22
<b>Table S4</b> Torsion angles of the emitters with TXO2 and DBTO acceptor moieties computed at M06-2X/6-31+G(d,p) level of theory.....	23
<b>Table S5</b> Torsion angles of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	24
<b>Table S6</b> Torsion angles of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	24
<b>Table S7</b> Energies, oscillator strengths and $\Phi_s$ indices of m-Cz-DPS-Cz emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	25
<b>Table S8</b> Energies, oscillator strengths and $\Phi_s$ indices of m-DMAC-DPS-DMAC emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	25
<b>Table S9</b> Energies, oscillator strengths and $\Phi_s$ indices of m-DPA-DPS-DPA emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	25
<b>Table S10</b> Energies, oscillator strengths and $\Phi_s$ indices of m-PTZ-DPS-PTZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	26
<b>Table S11</b> Energies, oscillator strengths and $\Phi_s$ indices of m-PXZ-DPS-PXZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	26
<b>Table S12</b> Energies, oscillator strengths and $\Phi_s$ indices of p-Cz-DPS-Cz emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	26
<b>Table S13</b> Energies, oscillator strengths and $\Phi_s$ indices of p-DMAC-DPS-DMAC emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	27
<b>Table S14</b> Energies, oscillator strengths and $\Phi_s$ indices of p-DPA-DPS-DPA emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	27
<b>Table S15</b> Energies, oscillator strengths and $\Phi_s$ indices of p-PTZ-DPS-PTZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	27
<b>Table S16</b> Energies, oscillator strengths and $\Phi_s$ indices of p-PXZ-DPS-PXZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	28
<b>Table S17</b> Energies, oscillator strengths and $\Phi_s$ indices of DBTO-ACR emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	28
<b>Table S18</b> Energies, oscillator strengths and $\Phi_s$ indices of DBTO-NO emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	28
<b>Table S19</b> Energies, oscillator strengths and $\Phi_s$ indices of DMAC-TTR emitter calculated at wB97XD/6-31+G(d,p) level of theory.....	29
<b>Table S20</b> Energies, oscillator strengths and $\Phi_s$ indices of PXZ-TTR emitter calculated at wB97XD/6-	

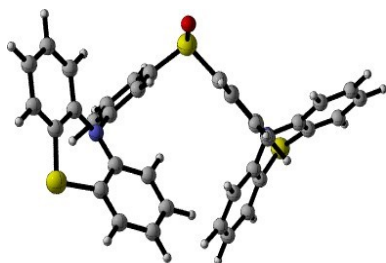
31+G(d,p) level of theory.....	29
<b>Table S21</b> Oscillator strengths for singlet excitations of Group 1 and Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	35
<b>Table S22</b> Experimental and calculated energy gaps and, and root mean square coupling element ( $ \langle S_1   H^{SOC}   T_n \rangle $ ) for $T_n \rightarrow S_1$ transition.....	35
<b>Table S23</b> Natures of $S_1$ , $T_1$ - $T_5$ states of the emitters in Group 1 and Group 2 computed at M062X/6-31+G(d,p) level of theory in toluene.....	36
<b>Table S24</b> Natures of $S_1$ , $T_1$ - $T_5$ states computed at M062X/6-31+G(d,p) level of theory in toluene (TXO2-PXZ, p-PXZ-DPS-PXZ, TXO2-DMAC, p-DMAC-DPS-DMAC, DBTO-DMAC) and in dichloromethane (DBTO-PXZ).....	36
<b>Table S25</b> Natures of $S_1$ , $T_1$ - $T_5$ states computed at M062X/6-31+G(d,p) level of theory in toluene (for Cz-Ph-TTR, DMAC-TTR, DMAC-Ph-TTR, PXZ-TTR, PXZ-Ph-TTR, PTZ-TTR, PTZ-Ph-TTR) and in ethyl ethanoate (Cz-TTR). .....	36
<b>Table S26</b> Reorganization energies (kcal/mol) between the $S_1$ and $T_1$ geometries of selected compounds. ....	37
<b>Table S27</b> Electron and hole orbitals of sulfone based emitters computed from ground state geometries at M062X/6-31+G(d,p) level of theory .....	38
<b>Table S28</b> Experimental absorption wavelengths of the modeled sulfone based TADF emitters.....	40
<b>Table S29</b> Relative energies of the different conformers of the emitters <i>m</i> -Cz-DPS-Cz and <i>m</i> -PTZ-DPS-PTZ computed at M06-2X/6-31+G(d,p) level of theory.....	42
<b>Table S30</b> Relative energies of the different conformers of the emitters <i>m</i> -Cz-DPS-Cz and <i>m</i> -PTZ-DPS-PTZ computed at M06-2X/6-31+G(d,p) level of theory.....	43
<b>Table S31</b> Relative energies of the different conformers of the emitter <i>m</i> -DPA-DPS-DPA computed at M06-2X/6-31+G(d,p) level of theory.....	44
<b>Table S32</b> Relative energies of the different conformers of Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	44
<b>Table S33</b> Relative energies of the different conformers of Group 3 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	45
<b>Table S34</b> Relative energies of the different conformers of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory .....	45
<b>Table S35</b> Relative energies of the different conformers of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory.....	46

## List of Figures

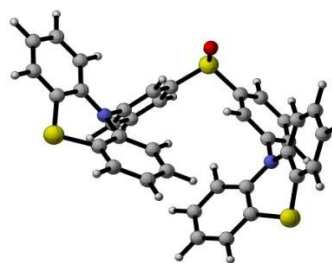
<b>Figure S1</b> Torsion angle coding of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory .....	21
<b>Figure S2</b> Torsion angle coding of the Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory .....	22
<b>Figure S3</b> Torsion angle coding of the emitters with TXO2 and DBTO acceptor moieties computed at M06-2X/6-31+G(d,p) level of theory .....	23
<b>Figure S4</b> Torsion angle coding of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory...24	
<b>Figure S5</b> Torsion angle coding of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory...24	
<b>Figure S6</b> A) Relation between the torsion angle and $\Delta E_{ST}$ , B) Relation between the torsion angle and $E_g$ .29	
<b>Figure S7</b> Absorption Spectra of Sulfone Based TADF Emitters computed at B3LYP/6-31+G(d,p), M06-2X/6-31+G(d,p), PBE0/6-31+G(d,p) and BLYP/6-31+G(d,p) level of theories. ....	36
<b>Cartesian Coordinates</b> .....	47

**Table S1** 3D representations of the ground state structures of all molecules, optimized at M06-2X/6-31+G(d,p) level of theory in toluene.

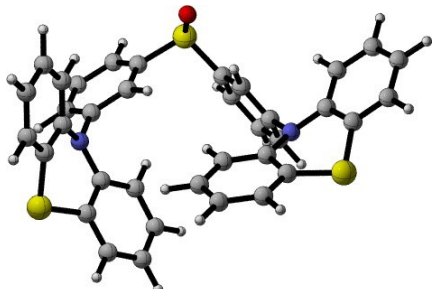




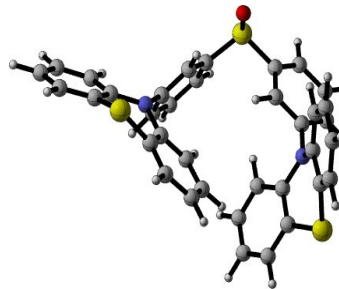
m-PTZ-DPS-PTZ – Conf. 1



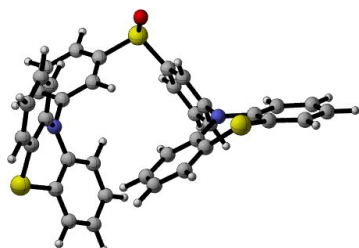
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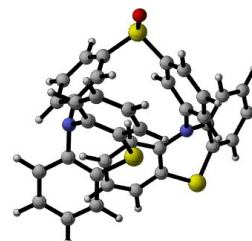
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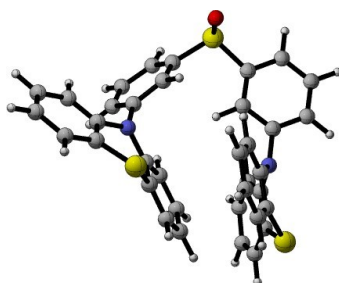
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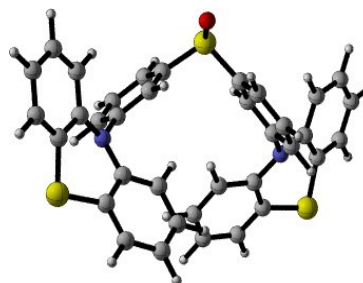
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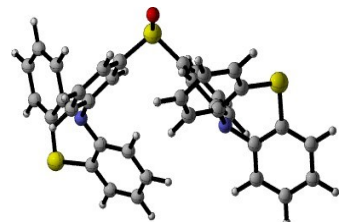
m-PTZ-DPS-PTZ – Conf. 6



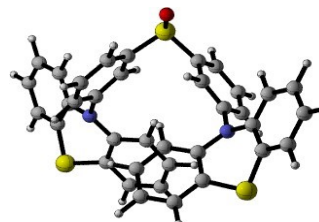
m-PTZ-DPS-PTZ – Conf. 7



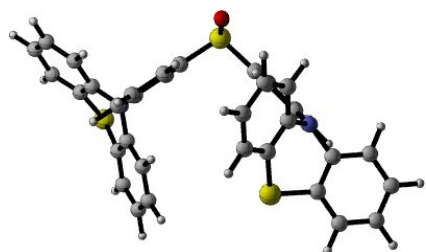
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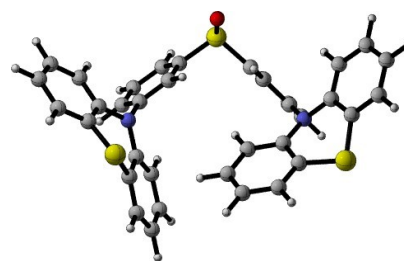
m-PTZ-DPS-PTZ – Conf. 9



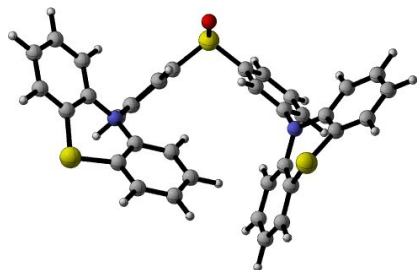
m-PTZ-DPS-PTZ – Conf. 10



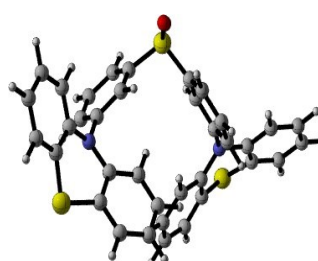
**m-PTZ-DPS-PTZ – Conf. 11**



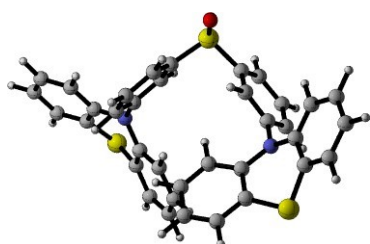
**m-PTZ-DPS-PTZ – Conf. 12**



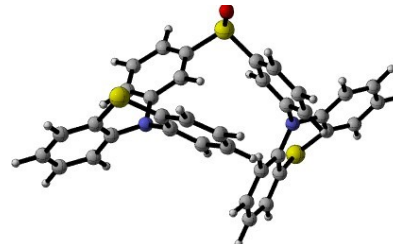
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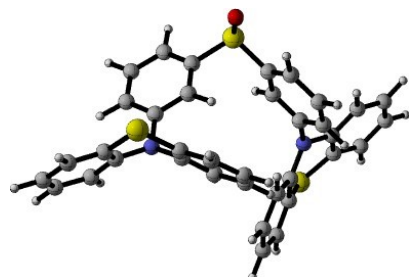
**m-PTZ-DPS-PTZ – Conf. 14**



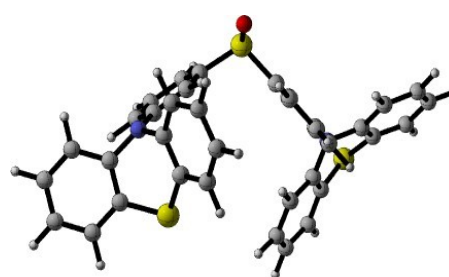
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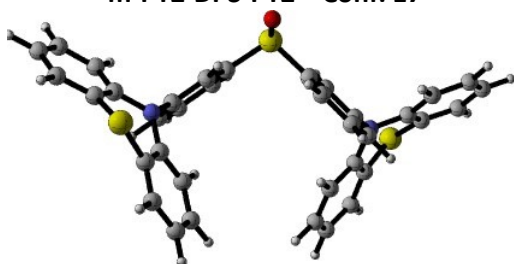
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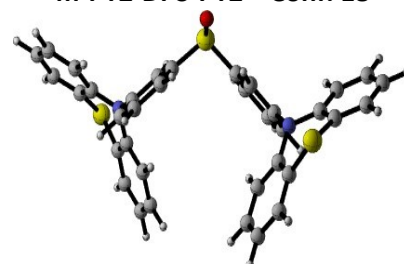
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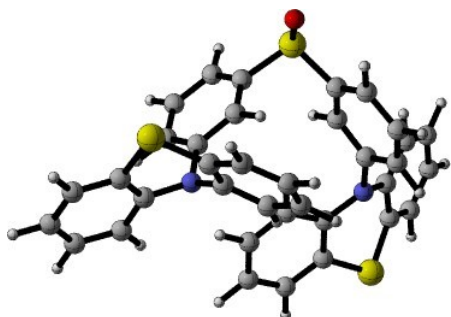
**m-PTZ-DPS-PTZ – Conf. 18**



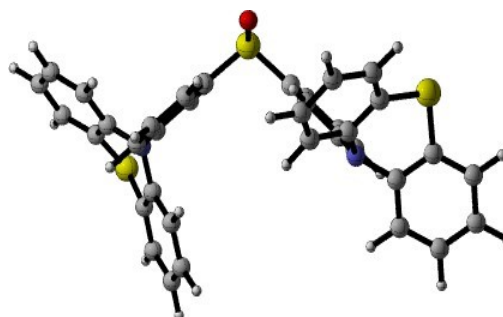
**m-PTZ-DPS-PTZ – Conf. 19**



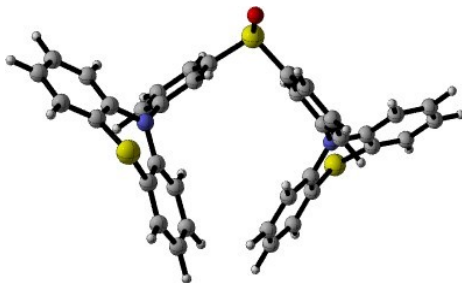
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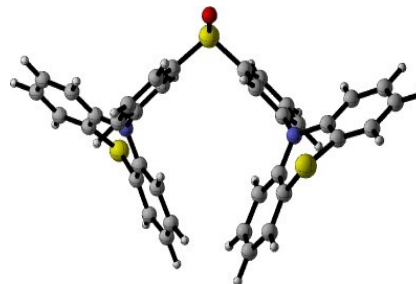
m-PTZ-DPS-PTZ – Conf. 21



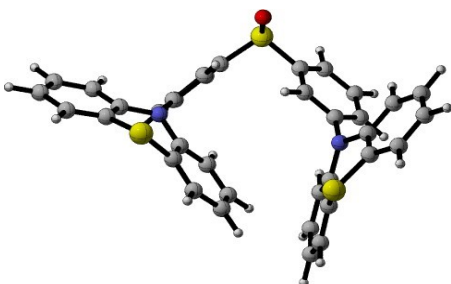
m-PTZ-DPS-PTZ – Conf. 22



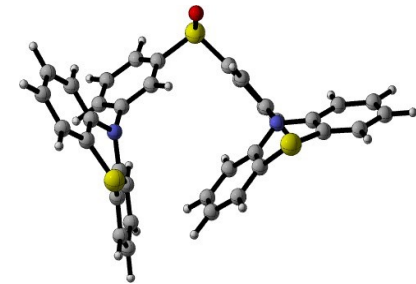
m-PTZ-DPS-PTZ – Conf. 23



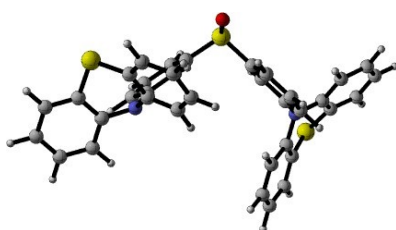
m-PTZ-DPS-PTZ – Conf. 24



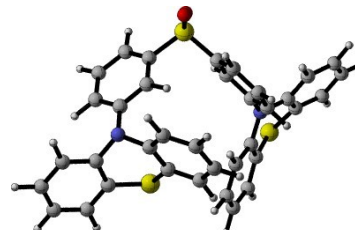
m-PTZ-DPS-PTZ – Conf. 25



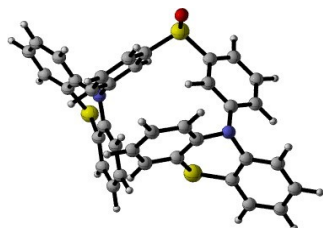
m-PTZ-DPS-PTZ – Conf. 26



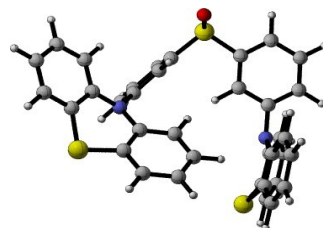
m-PTZ-DPS-PTZ – Conf. 27



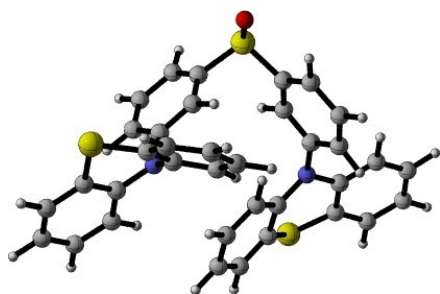
m-PTZ-DPS-PTZ – Conf. 28



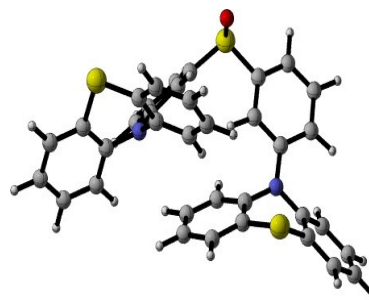
m-PTZ-DPS-PTZ – Conf. 29



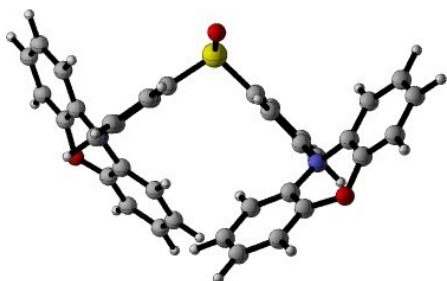
m-PTZ-DPS-PTZ – Conf. 30



**m-PTZ-DPS-PTZ – Conf. 31**

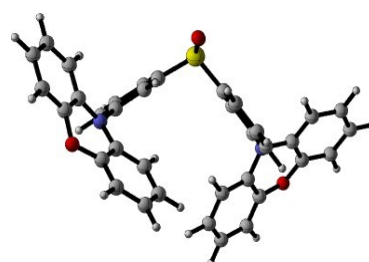


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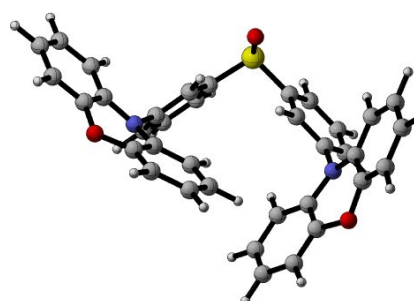


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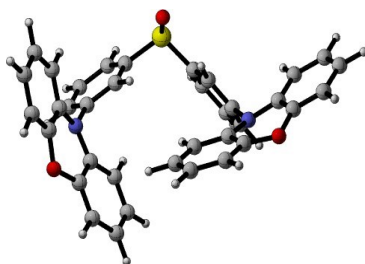
**m-PXZ-DPS-PXZ – Conf. 3**



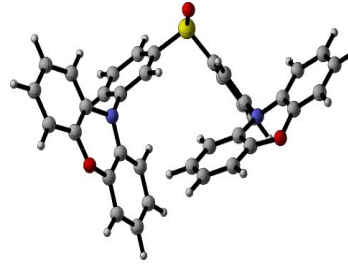
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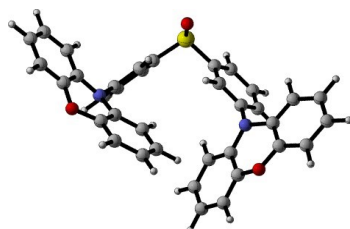
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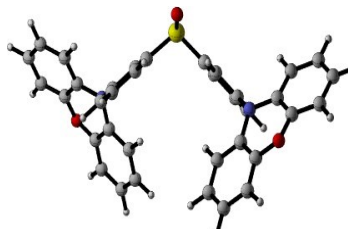
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**m-PXZ-DPS-PXZ – Conf. 6**

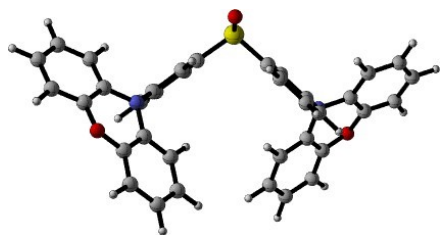


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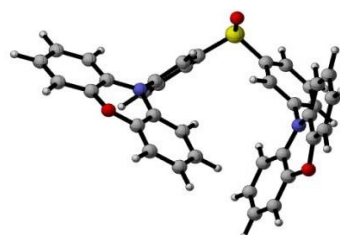


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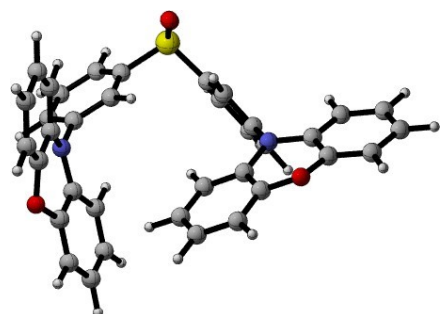




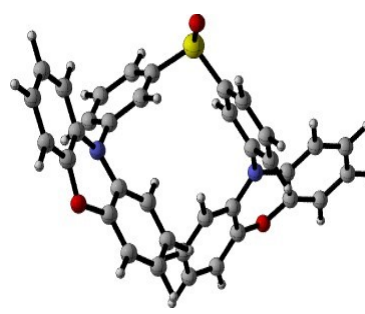
m-PXZ-DPS-PXZ – Conf. 9



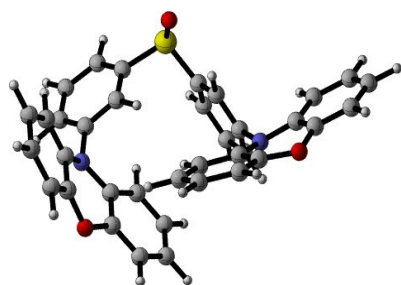
m-PXZ-DPS-PXZ – Conf. 10



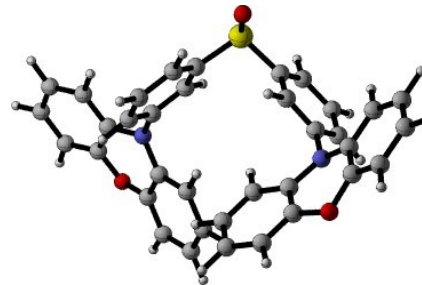
m-PXZ-DPS-PXZ – Conf. 11



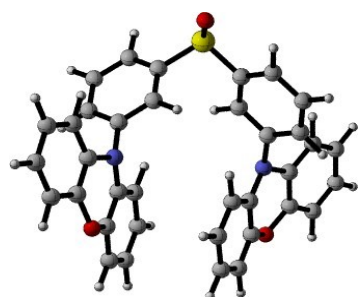
m-PXZ-DPS-PXZ – Conf. 12



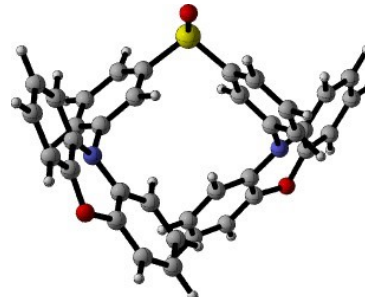
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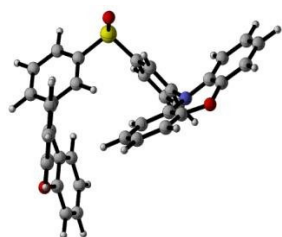
m-PXZ-DPS-PXZ – Conf. 14



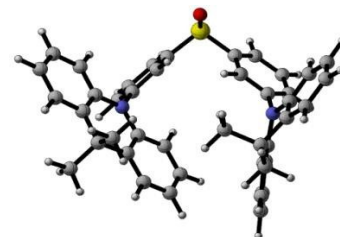
m-PXZ-DPS-PXZ – Conf. 15



m-PXZ-DPS-PXZ – Conf. 16

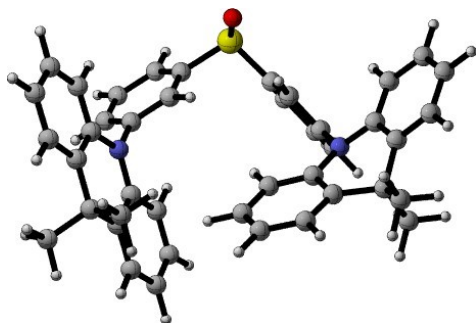


m-PXZ-DPS-PXZ – Conf. 17

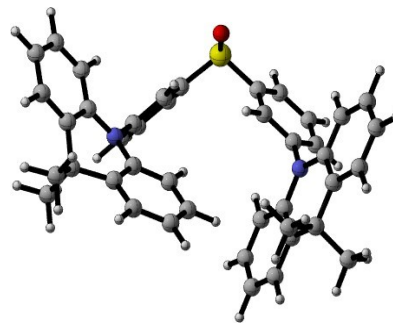


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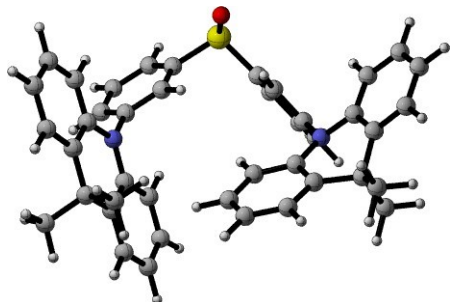




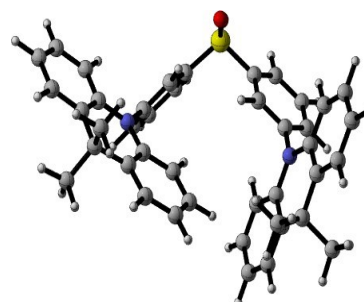
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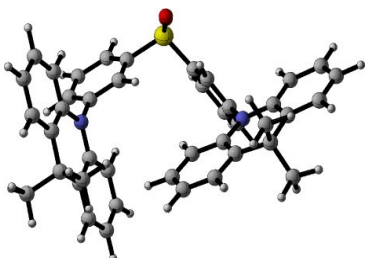
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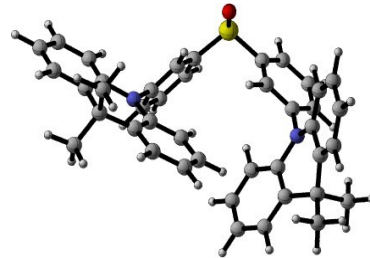
m-DMAC-DPS-DMAC – Conf. 4



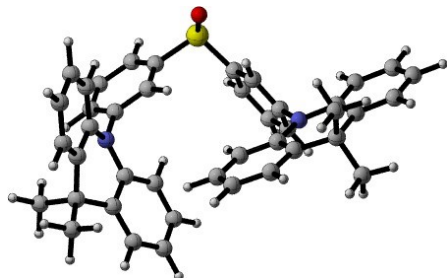
m-DMAC-DPS-DMAC – Conf. 5



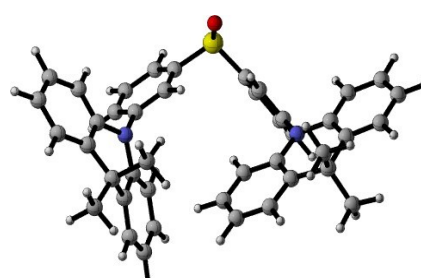
m-DMAC-DPS-DMAC – Conf. 6



m-DMAC-DPS-DMAC – Conf. 7



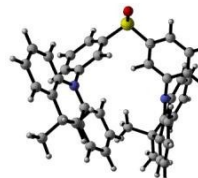
m-DMAC-DPS-DMAC – Conf. 8



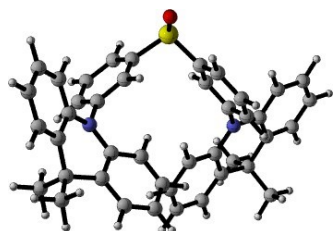
m-DMAC-DPS-DMAC – Conf. 9



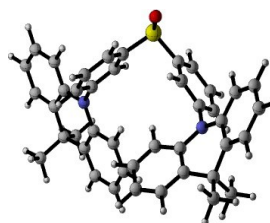
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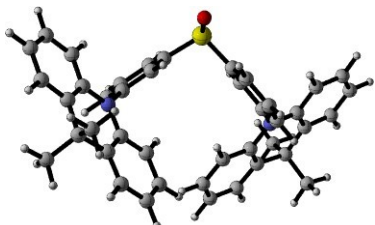
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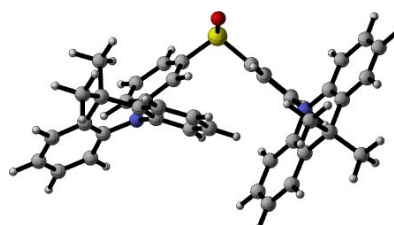
m-DMAC-DPS-DMAC – Conf. 12



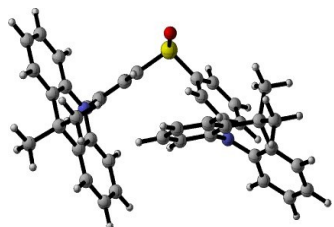
m-DMAC-DPS-DMAC – Conf. 13



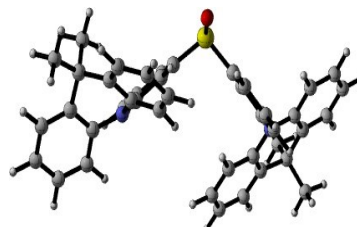
m-DMAC-DPS-DMAC – Conf. 14



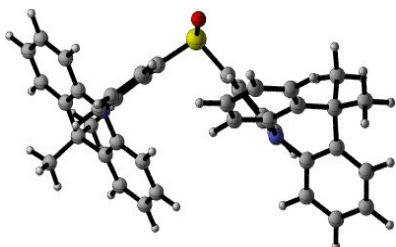
m-DMAC-DPS-DMAC – Conf. 15



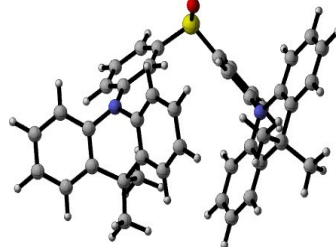
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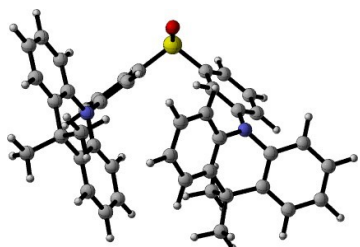
m-DMAC-DPS-DMAC – Conf. 17



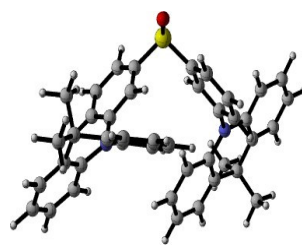
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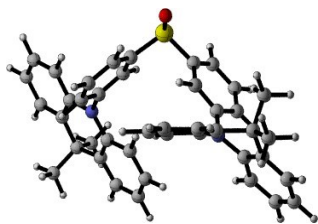
m-DMAC-DPS-DMAC – Conf. 19



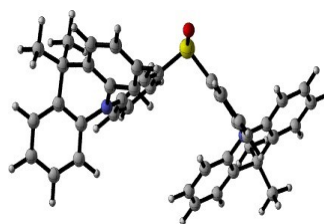
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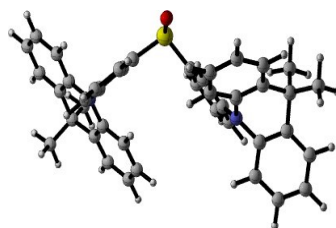
m-DMAC-DPS-DMAC – Conf. 21



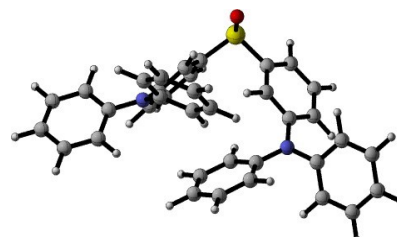
m-DMAC-DPS-DMAC – Conf. 22



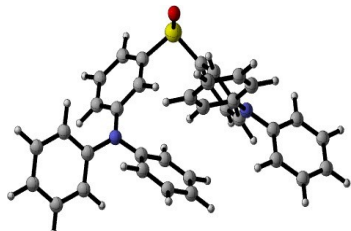
m-DMAC-DPS-DMAC – Conf. 23



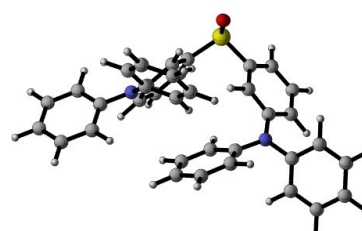
m-DMAC-DPS-DMAC – Conf. 24



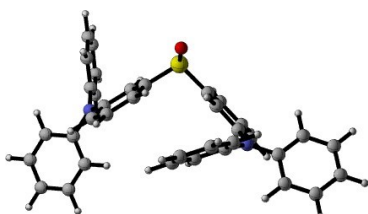
m-DPA-DPS-DPA – Conf. 1



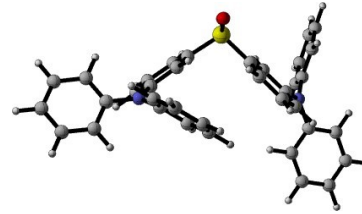
m-DPA-DPS-DPA – Conf. 2



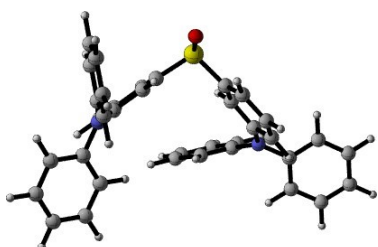
m-DPA-DPS-DPA – Conf. 3



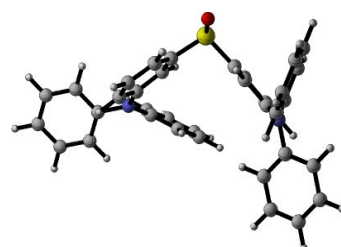
m-DPA-DPS-DPA – Conf. 4



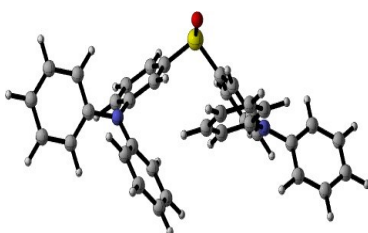
m-DPA-DPS-DPA – Conf. 5



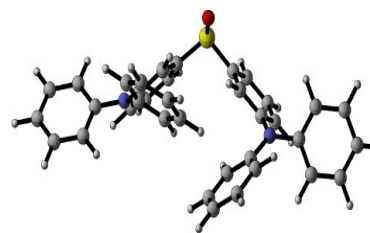
m-DPA-DPS-DPA – Conf. 6



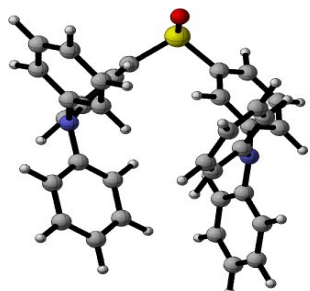
m-DPA-DPS-DPA – Conf. 7



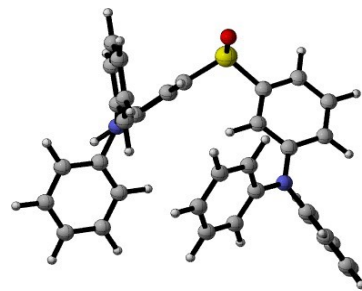
m-DPA-DPS-DPA – Conf. 8



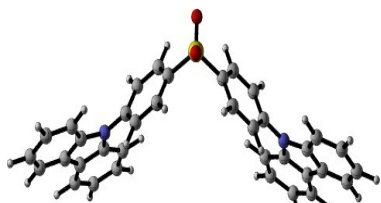
m-DPA-DPS-DPA – Conf. 9



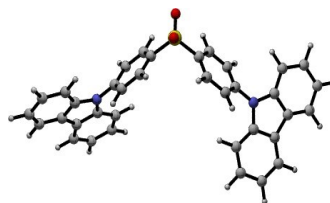
m-DPA-DPS-DPA – Conf. 10



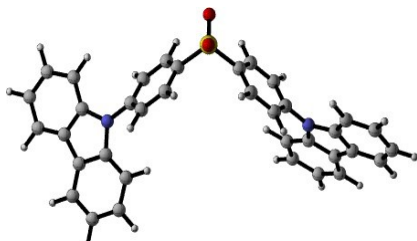
m-DPA-DPS-DPA – Conf. 11



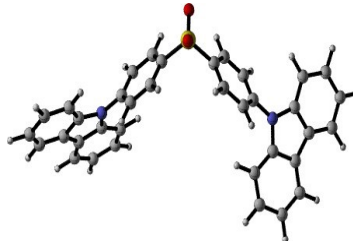
**p-Cz-DPS-Cz – Conf. 1**



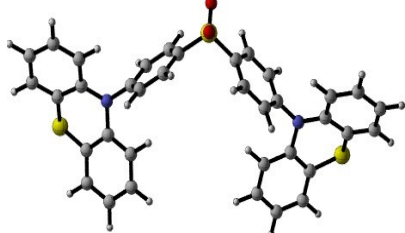
**p-Cz-DPS-Cz – Conf. 2**



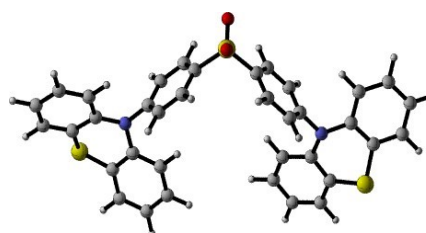
**p-Cz-DPS-Cz – Conf. 3**



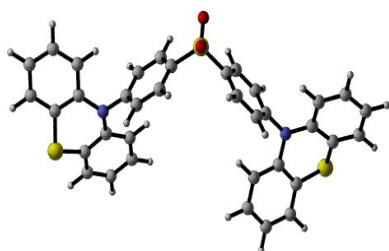
**p-Cz-DPS-Cz – Conf. 4**



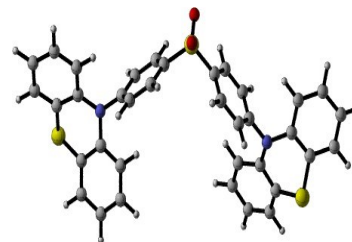
**p-PTZ-DPS-PTZ – Conf. 1**



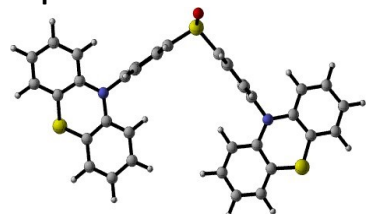
**p-PTZ-DPS-PTZ – Conf. 2**



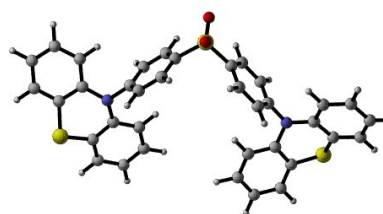
**p-PTZ-DPS-PTZ – Conf. 3**



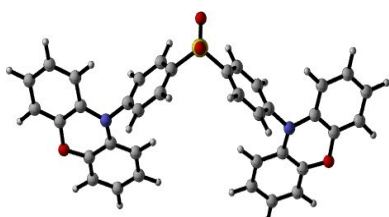
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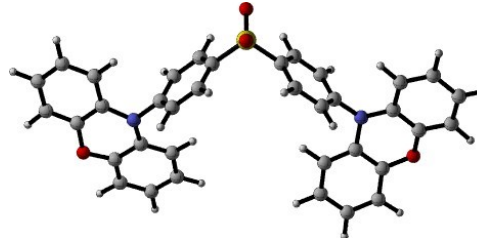
**p-PTZ-DPS-PTZ – Conf. 5**



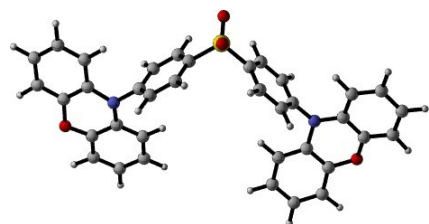
**p-PTZ-DPS-PTZ – Conf. 6**



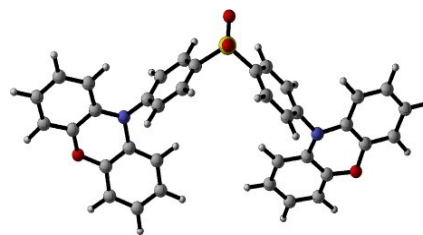
**p-PXZ-DPS-PXZ – Conf. 1**



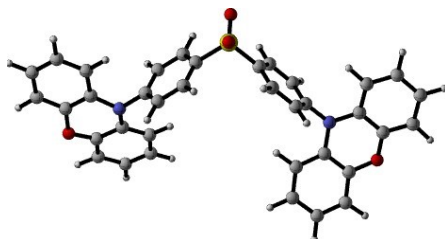
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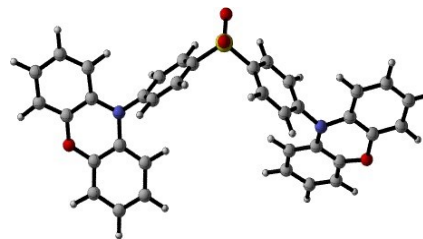
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**p-PXZ-DPS-PXZ – Conf. 4**

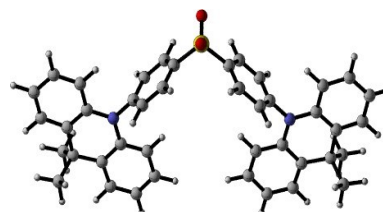


**p-PXZ-DPS-PXZ – Conf. 5**

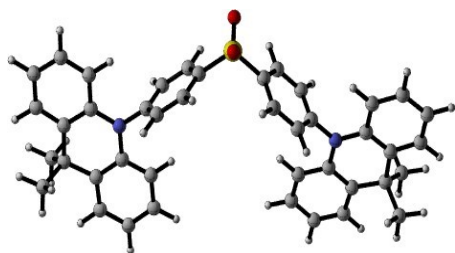


**p-PXZ-DPS-PXZ – Conf. 6**

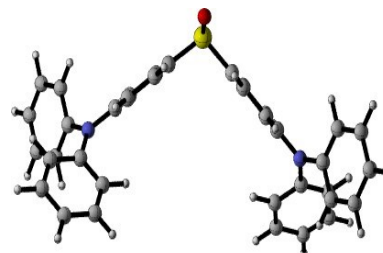
**p-DMAC-DPS-DMAC – Conf. 1**



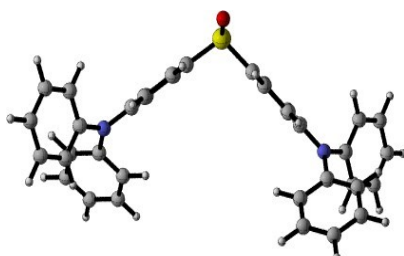
**p-DMAC-DPS-DMAC – Conf. 2**



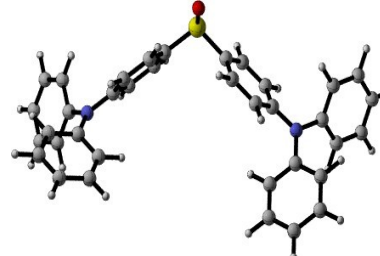
**p-DMAC-DPS-DMAC – Conf. 3**



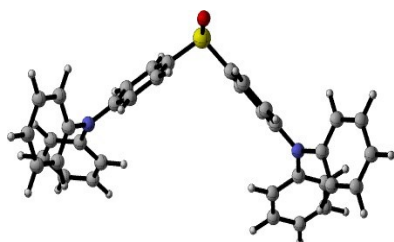
**p-DPA-DPS-DPA – Conf. 1**



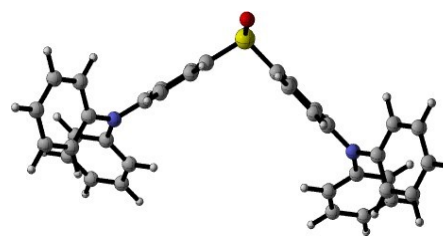
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**p-DPA-DPS-DPA – Conf. 3**



**p-DPA-DPS-DPA – Conf. 4**

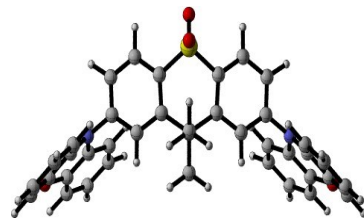


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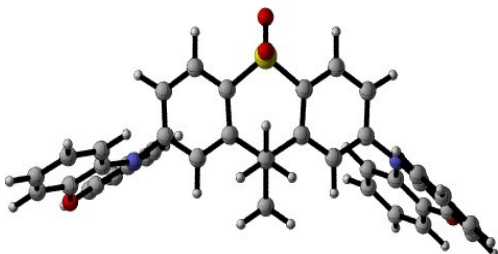




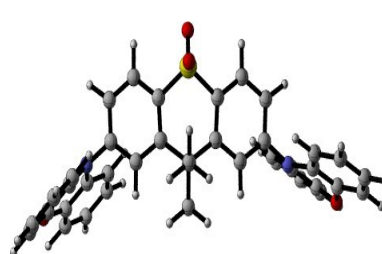
TXO2-NO – Conf. 1



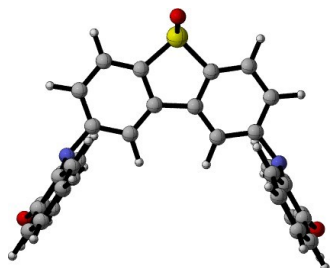
TXO2-NO – Conf. 2



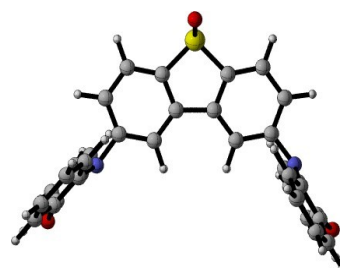
TXO2-NO – Conf. 3



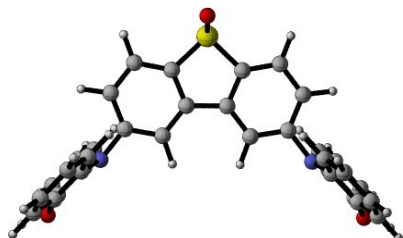
TXO2-NO – Conf. 4



DBTO-NO – Conf. 1

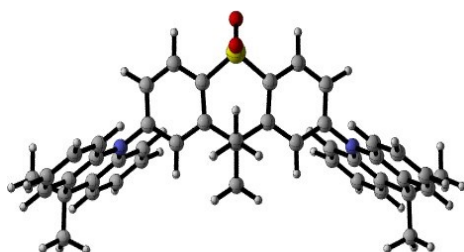


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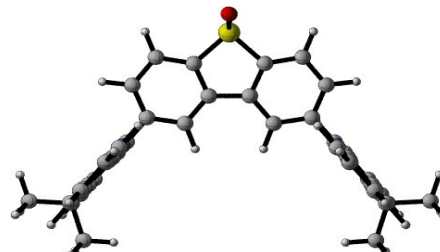


DBTO-NO – Conf. 3

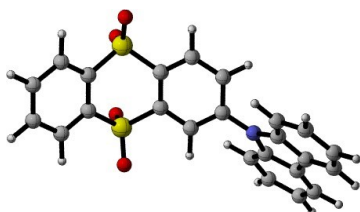
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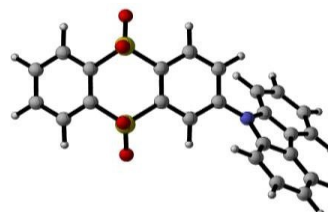
TXO2-ACR – Conf. 1



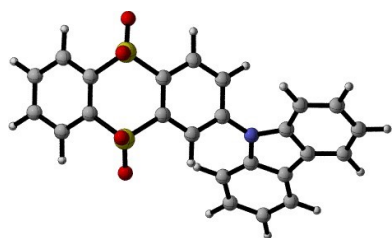
DBTO-ACR – Conf. 1



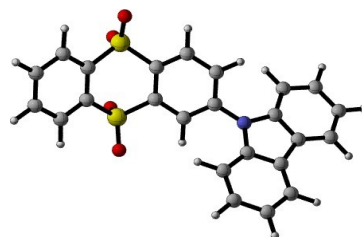
Cz-TTR – Conf. 1



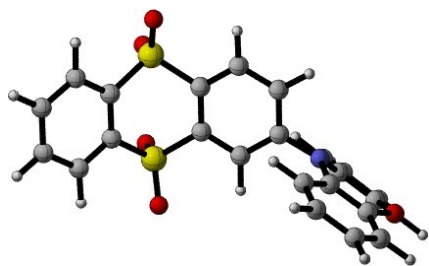
Cz-TTR – Conf. 2



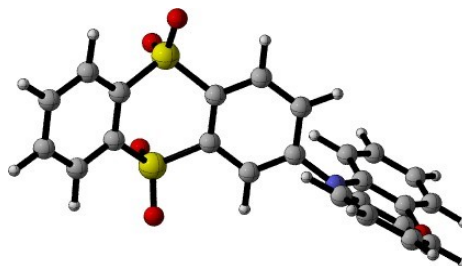
Cz-TTR – Conf. 3



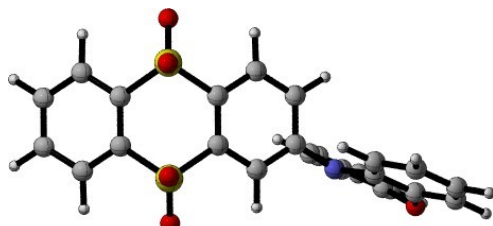
Cz-TTR – Conf. 4



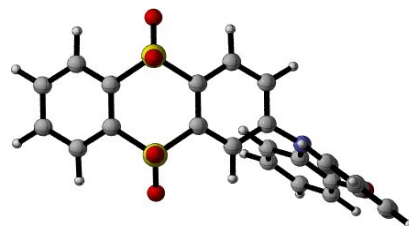
PXZ-TTR – Conf.1



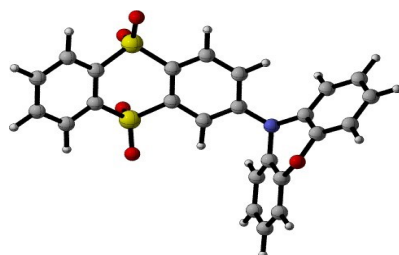
PXZ-TTR – Conf.2



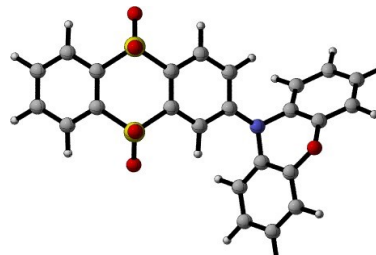
PXZ-TTR – Conf.3



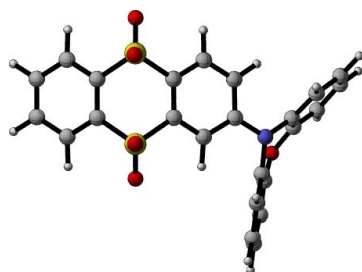
PXZ-TTR – Conf.4



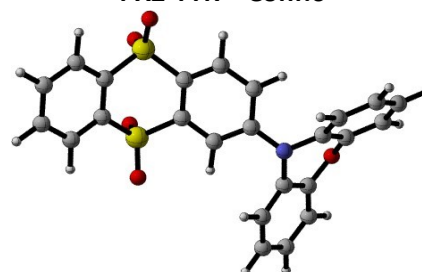
PXZ-TTR – Conf.5



PXZ-TTR – Conf.6

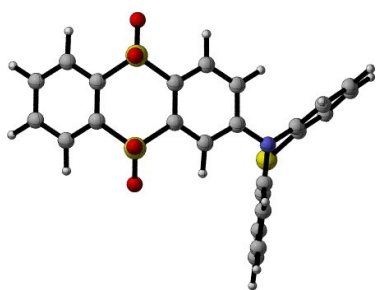


PXZ-TTR – Conf.7

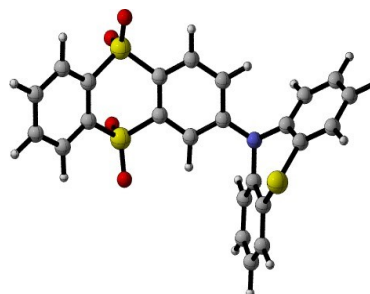


PXZ-TTR – Conf.8

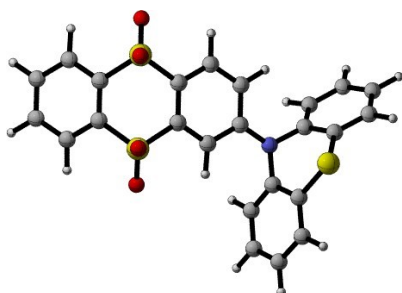




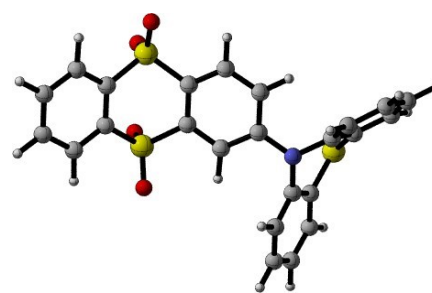
PTZ-TTR – Conf.1



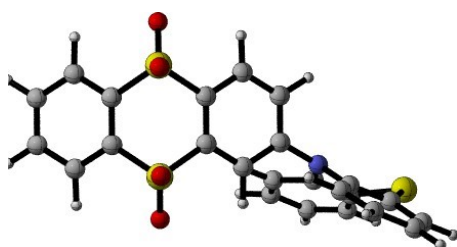
PTZ-TTR – Conf.2



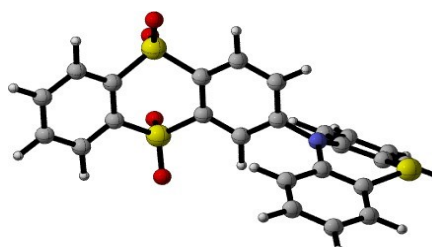
PTZ-TTR – Conf.3



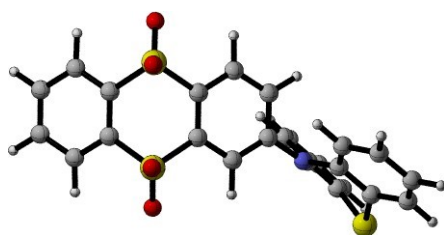
PTZ-TTR – Conf.4



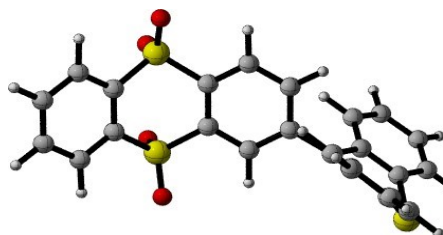
PTZ-TTR – Conf.5



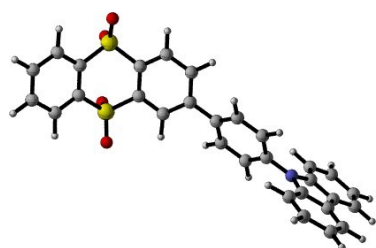
PTZ-TTR – Conf.6



PTZ-TTR – Conf.7



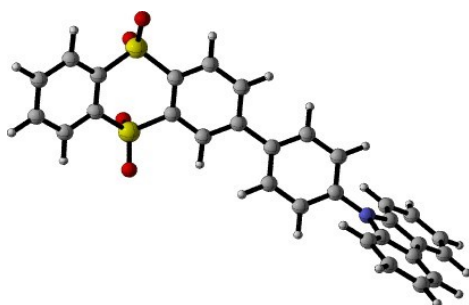
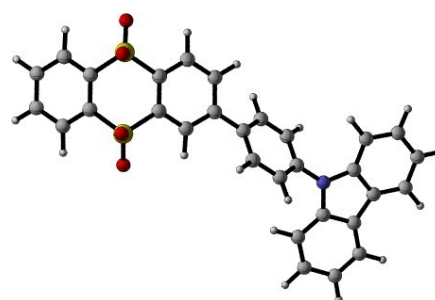
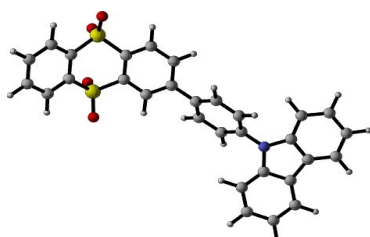
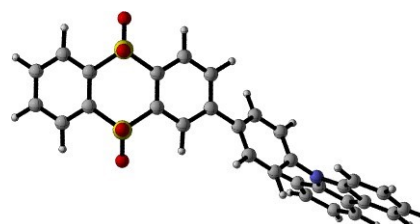
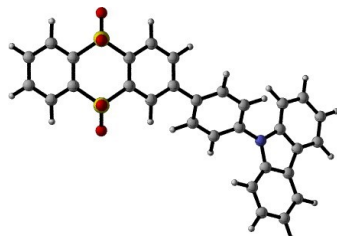
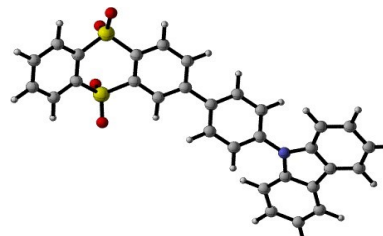
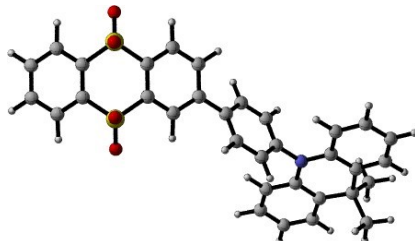
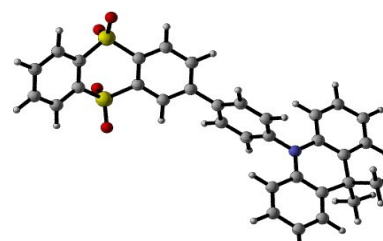
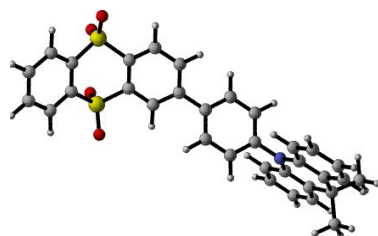
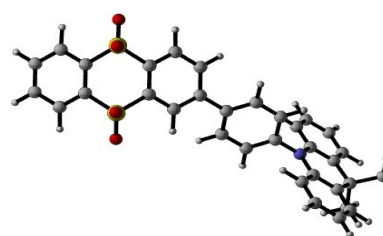
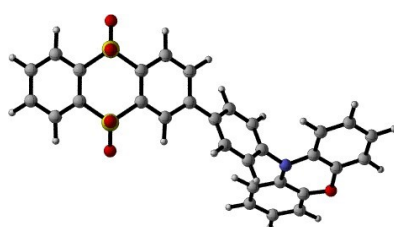
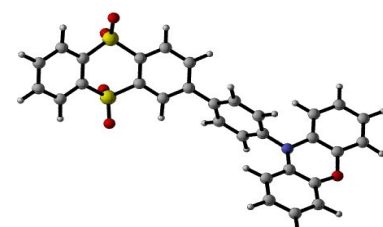
PTZ-TTR – Conf.8

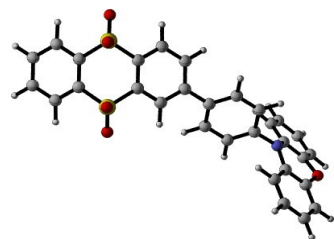
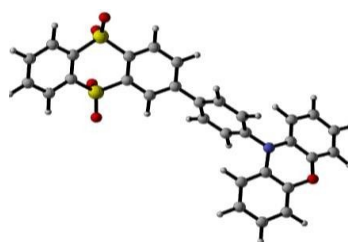
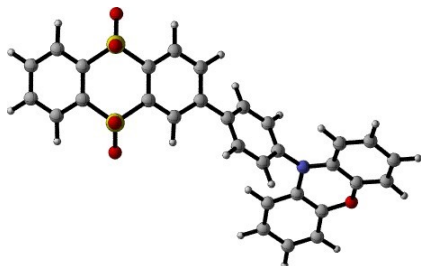
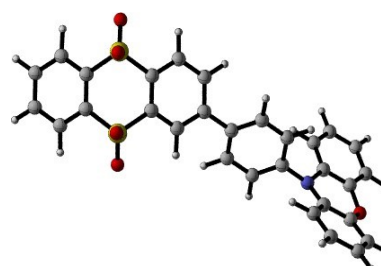
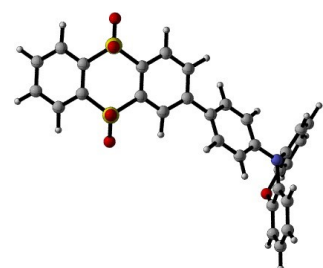
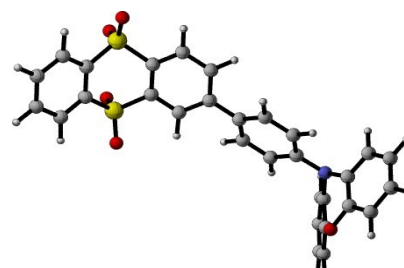
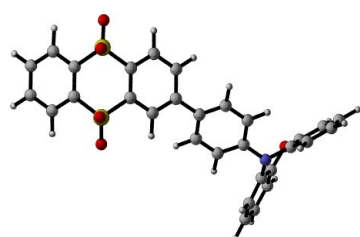
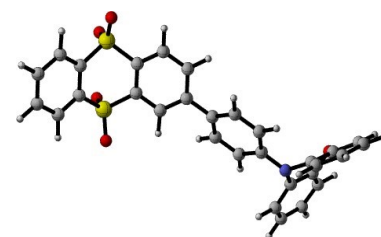
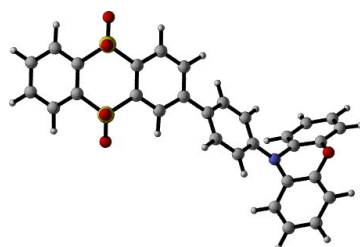
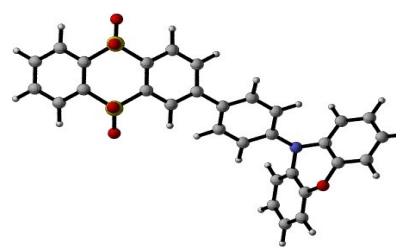


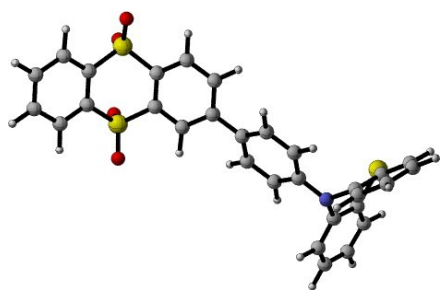
Cz-Ph-TTR – Conf.1



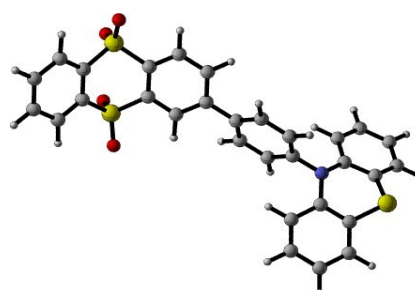
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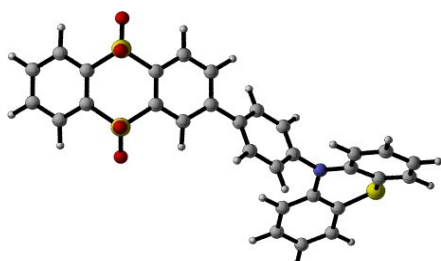
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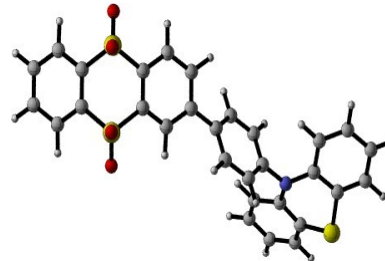
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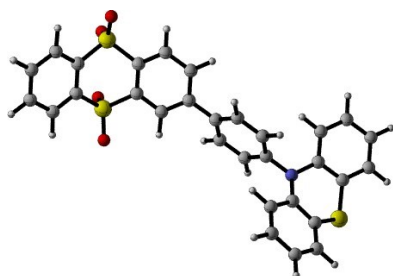
PTZ-Ph-TTR – Conf.2



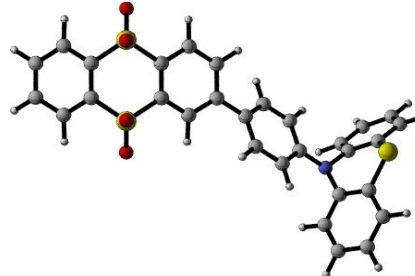
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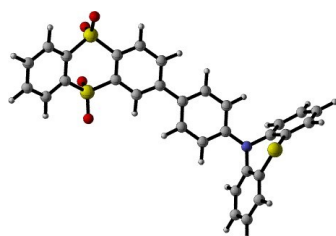
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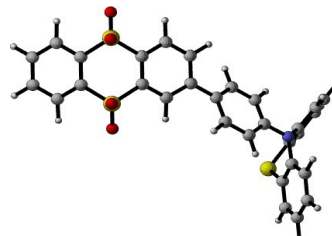
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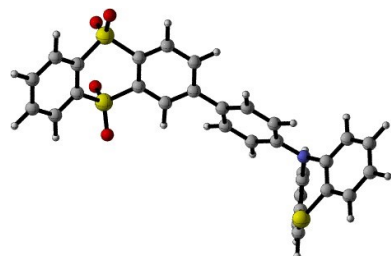
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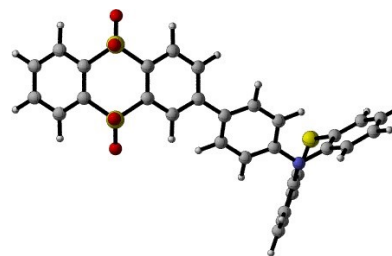
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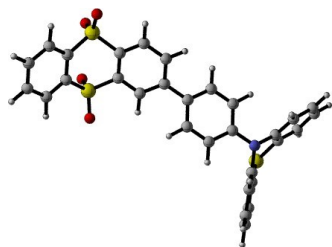
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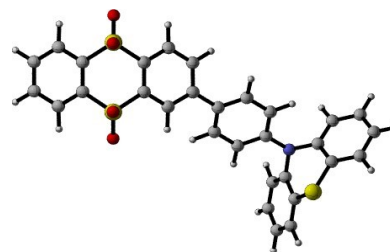
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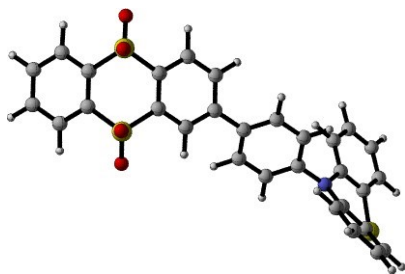
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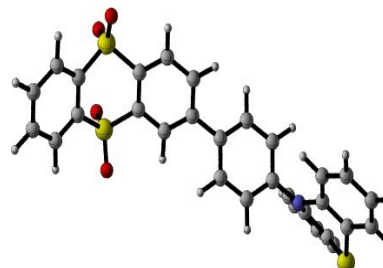
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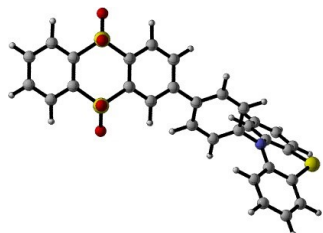
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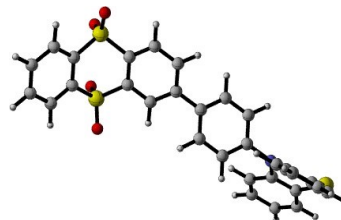
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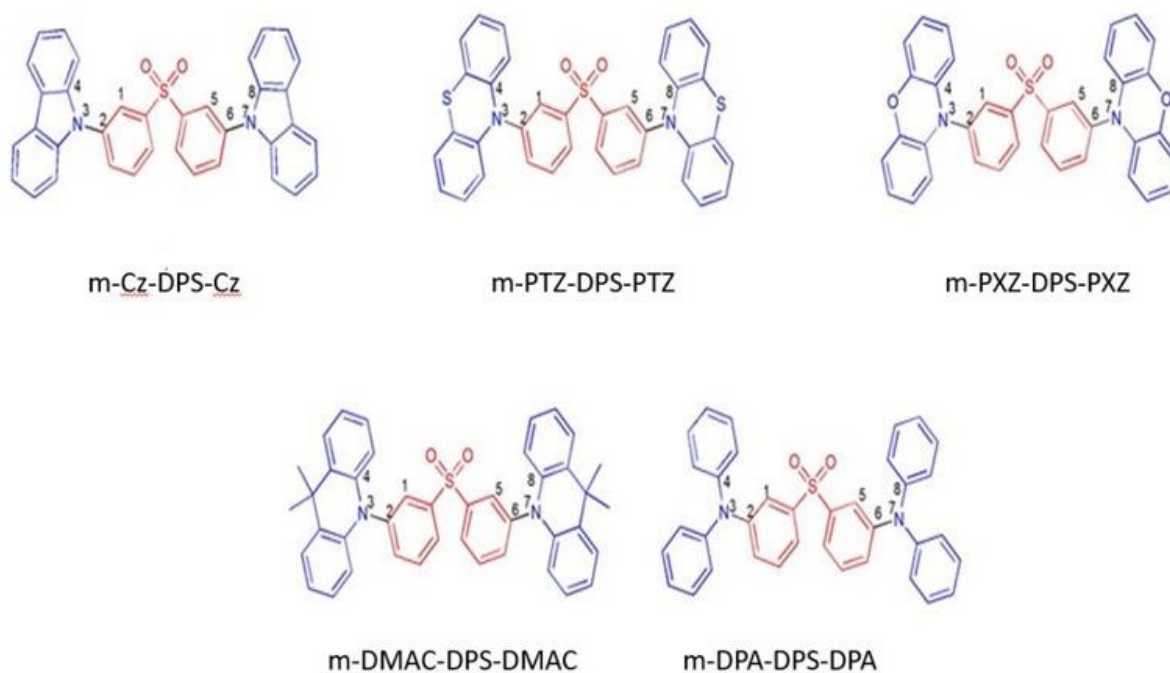
PTZ-Ph-TTR – Conf.14



PTZ-Ph-TTR – Conf.15



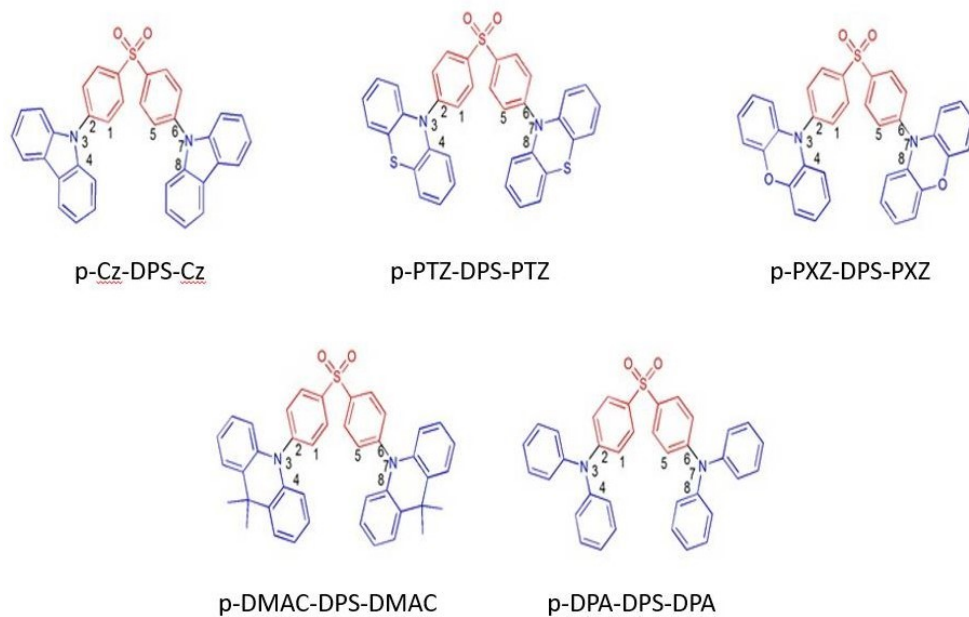
PTZ-Ph-TTR – Conf.16



**Figure S1** Torsion angle coding of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory.

**Table S2** Torsion angles of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compounds	$\Theta(\text{D-A})_1$ $S_0/S_1/T_1$	$\Theta(\text{D-A})_2$ $S_0/S_1/T_1$
m-Cz-DPS-Cz	52.45/59.74/55.72	53.17/60.72/44.73
m-PTZ-DPS-PTZ	-99.76/-88.74/-89.89	-75.03/-77.68/-78.82
m-PXZ-DPS-PXZ	73.63/88.17/84.75	73.63/87.71/84.75
m-DMAC-DPS-DMAC	-92.38/-89.71/-104.21	108.04/106.61/113.13
m-DPA-DPS-DPA	-25.20/-41.88/-22.79	41.79/53.01/53.02

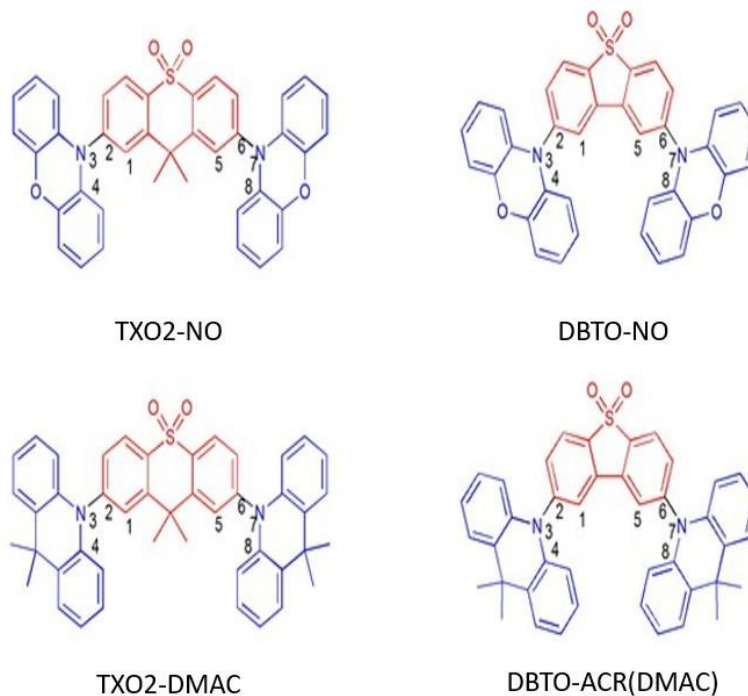


**Figure S2** Torsion angle coding of the Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory.

**Table S3** Torsion angles of the Group 1 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compounds	$\Theta(\text{D-A})_1$ $S_0/S_1/T_1$	$\Theta(\text{D-A})_2$ $S_0/S_1/T_1$
p-Cz-DPS-Cz	-51.39/-53.88/-45.78	51.40/63.11/46.54
p-PTZ-DPS-PTZ	-74.86/-74.47/-71.45	71.11/88.05/96.55
p-PXZ-DPS-PXZ	-104.20/-105.73/-106.21	102.17/89.53/69.12
p-DMAC-DPS-DMAC	-91.08/-92.03/-105.44	89.23/89.55/72.95
p-DPA-DPS-DPA	-30.48/-43.11/-34.82	-30.40/-43.18/-32.57

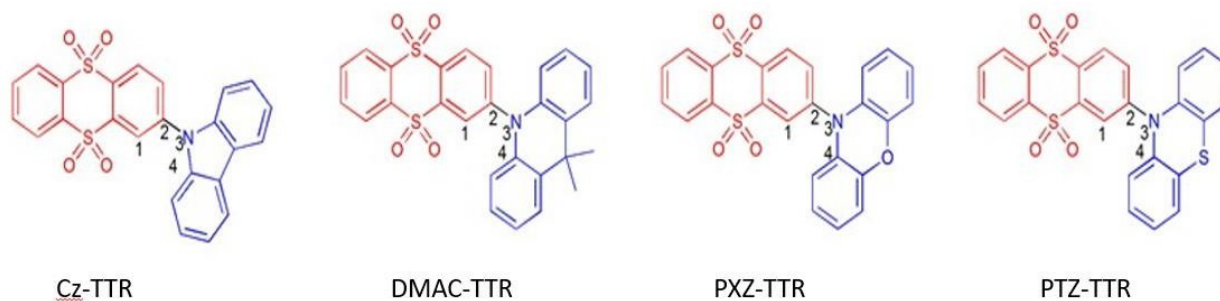




**Figure S3** Torsion angle coding of the emitters with TXO2 and DBTO acceptor moieties computed at M06-2X/6-31+G(d,p) level of theory.

**Table S4** Torsion angles of the emitters with TXO2 and DBTO acceptor moieties computed at M06-2X/6-31+G(d,p) level of theory.

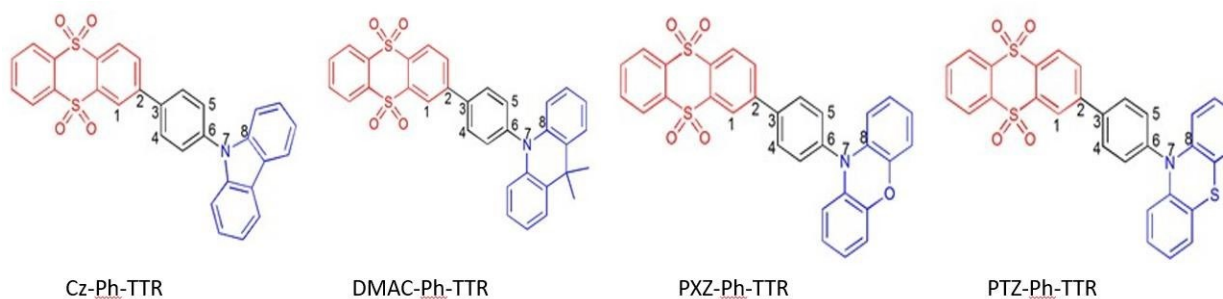
Compounds	$\Theta(\text{D-A})_1$ $S_0/S_1/T_1$	$\Theta(\text{D-A})_2$ $S_0/S_1/T_1$
TXO2-NO	102.26/102.74/105.58	-102.27/-90.17/-105.58
DBTO-NO	75.80/89.64/90.06	-75.83/-78.61/-90.08
TXO2-DMAC	89.07/90.14/101.81	-89.07/-89.30/-101.81
DBTO-ACR(DMAC)	90.15/91.23/90.62	-90.16/-91.50/-90.63



**Figure S4** Torsion angle coding of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory.

**Table S5** Torsion angles of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compounds	$\Theta(\text{D-A})_1$ $S_0/S_1/T_1$
Cz-TTR	49.02/65.43/45.36
DMAC-TTR	-9.57/-90.38/-5.43
PXZ-TTR	-83.98/-92.63/-102.05
PTZ-TTR	15.11/-90.76/5.53



**Figure S5** Torsion angle coding of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory.

**Table S6** Torsion angles of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compounds	$\Theta(\text{D-A})_1$ $S_0/S_1/T_1$	$\Theta(\text{D-A})_2$ $S_0/S_1/T_1$
Cz-Ph-TTR	37.70/13.59/-1.93	53.36/46.33/42.18
DMAC-Ph-TTR	-38.58/-10.41/-8.05	90.40/92.63/62.57
PXZ-Ph-TTR	-39.45/-10.79/-12.91	102.92/92.30/72.00
PTZ-Ph-TTR	36.08/20.08/2.63	17.34/-1.56/2.32

**Benchmark study computed at wB97XD/6-31+G(d,p) level of theory.****Table S7** Energies, oscillator strengths and  $\Phi_S$  indices of m-Cz-DPS-Cz emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	4.3627	3.6082	0.6460	0.9834	0.0224
2	4.4338	3.6163	0.6629	0.9835	0.1097
3	4.4759	3.7125	0.8804	0.8030	0.0288
4	4.4866	3.7221	0.8810	0.8284	0.0853
5	4.6711	3.7704	0.6947	0.9075	0.0660
6	4.7338	3.8778	0.6888	0.8942	0.2629
7	4.8738	4.0334	0.9040	0.7996	0.3816
8	4.9059	4.1083	0.9172	0.7395	0.2699
9	5.2148	4.2588	0.4563	0.9271	0.0080
10	5.3106	4.2662	0.7230	0.9280	0.0162

**Table S8** Energies, oscillator strengths and  $\Phi_S$  indices of m-DMAC-DPS-DMAC emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9098	3.6210	0.4506	0.8858	0.0002
2	4.1019	3.7921	0.4139	0.8983	0.0185
3	4.2113	3.8110	0.4077	0.6652	0.0010
4	4.4175	3.8997	0.4104	0.7644	0.0127
5	4.6311	3.9271	0.8393	0.9031	0.0749
6	4.6943	3.9900	0.8043	0.8315	0.3425
7	4.7857	4.0396	0.8435	0.8816	0.0590
8	4.9269	4.0900	0.8011	0.9314	0.3516
9	4.9807	4.1146	0.8781	0.9144	0.2476
10	5.0804	4.1445	0.8875	0.9396	0.0116

**Table S9** Energies, oscillator strengths and  $\Phi_S$  indices of m-DPA-DPS-DPA emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	4.0298	3.3051	0.7577	0.8661	0.0178
2	4.0815	3.4841	0.7123	0.8528	0.0756
3	4.3273	3.5681	0.7576	0.8586	0.1113
4	4.4110	3.5743	0.7757	0.8294	0.5466
5	4.5339	3.6727	0.7460	0.8694	0.4100
6	4.5966	3.7085	0.7079	0.9015	0.2558
7	4.7982	4.1291	0.8324	0.9736	0.1407
8	4.8383	4.1510	0.8516	0.9391	0.0989
9	5.0660	4.1793	0.8753	0.9050	0.0445
10	5.0505	4.2150	0.8768	0.8123	0.0306

**Table S10** Energies, oscillator strengths and  $\Phi_S$  indices of m-PTZ-DPS-PTZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9630	3.4100	0.6198	0.8614	0.0005
2	4.0578	3.4452	0.7089	0.8675	0.0001
3	4.2121	3.8223	0.6894	0.8505	0.0053
4	4.2499	3.8343	0.5182	0.8681	0.0028
5	4.4369	3.9408	0.5915	0.7563	0.0163
6	4.4885	3.9573	0.3901	0.9463	0.0037
7	4.5790	4.0014	0.8237	0.7664	0.0512
8	4.5964	4.0335	0.8192	0.9112	0.0541
9	4.7584	4.0615	0.8485	0.8625	0.1068
10	4.8468	4.1536	0.8053	0.9841	0.0931

**Table S11** Energies, oscillator strengths and  $\Phi_S$  indices of m-PXZ-DPS-PXZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9245	3.4327	0.4742	0.8763	0.0002
2	3.9370	3.4332	0.4452	0.8772	0.0012
3	4.1812	3.7958	0.4402	0.6622	0.0085
4	4.1852	3.7998	0.4382	0.6635	0.0049
5	4.3860	3.8989	0.7782	0.7940	0.0862
6	4.3879	3.9002	0.7739	0.7877	0.1085
7	4.7204	3.9788	0.8780	0.9636	0.0051
8	4.7221	4.0704	0.8806	0.5375	0.0007
9	4.7790	4.0707	0.8192	0.5580	0.1697
10	4.7839	4.0905	0.8262	0.9763	0.1628

**Table S12** Energies, oscillator strengths and  $\Phi_S$  indices of p-Cz-DPS-Cz emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	4.2332	3.5922	0.7480	0.9051	0.7430
2	4.4194	3.6108	0.7340	0.9852	0.2762
3	4.4898	3.6108	0.8750	0.9852	0.0284
4	4.4983	3.7191	0.8638	0.8434	0.0006
5	4.8393	3.7300	0.8448	0.7813	0.0153
6	4.8931	3.7631	0.9017	0.8711	0.3222
7	4.8977	4.2624	0.9136	0.9208	0.1488
8	4.9207	4.2632	0.8850	0.9193	0.1310
9	5.1617	4.3819	0.7213	0.9617	0.0000
10	5.1626	4.4178	0.7128	0.9740	0.0002

**Table S13** Energies, oscillator strengths and  $\Phi_S$  indices of p-DMAC-DPS-DMAC emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.8130	3.6288	0.1609	0.9121	0.0001
2	3.8138	3.6288	0.1622	0.9114	0.0003
3	4.3926	3.7955	0.7222	0.2746	0.0021
4	4.3934	3.7961	0.7071	0.2105	0.0046
5	4.6324	3.8914	0.8867	0.7474	0.1070

6	4.6359	3.8915	0.8884	0.7442	0.0461
7	4.7113	3.9296	0.8161	0.9584	0.3338
8	4.7241	4.0221	0.8237	0.8014	0.5045
9	5.0615	4.0221	0.8743	0.7986	0.0821
10	5.0667	4.1349	0.8861	0.9826	0.1226

**Table S14** Energies, oscillator strengths and  $\Phi_S$  indices of p-DPA-DPS-DPA emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9767	3.2358	0.7701	0.8662	1.0057
2	4.3075	3.3860	0.7701	0.8726	0.3267
3	4.3256	3.6765	0.7764	0.9092	0.1083
4	4.3668	3.6793	0.7724	0.9110	0.0316
5	4.6096	3.8699	0.7181	0.7658	0.0627
6	4.6115	3.9140	0.7162	0.7504	0.5257
7	4.9253	4.1150	0.8905	0.9774	0.0347
8	4.9902	4.1689	0.8927	0.9820	0.0719
9	5.0624	4.3168	0.8850	0.8011	0.0301
10	5.0657	4.3633	0.8835	0.8069	0.0200

**Table S15** Energies, oscillator strengths and  $\Phi_S$  indices of p-PTZ-DPS-PTZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9572	3.4117	0.5271	0.8505	0.0012
2	3.9587	3.4150	0.5340	0.8528	0.0009
3	4.1178	3.8243	0.6665	0.8475	0.0007
4	4.1244	3.8259	0.6758	0.8543	0.0021
5	4.5684	3.9027	0.7357	0.8543	0.0717
6	4.5756	3.9399	0.7462	0.5983	0.0529
7	4.5771	3.9630	0.8043	0.8711	0.0568
8	4.5798	4.0415	0.7996	0.9067	0.0458
9	4.9267	4.0489	0.6692	0.8917	0.0513
10	4.9311	4.1034	0.6768	0.8183	0.0567

**Table S16** Energies, oscillator strengths and  $\Phi_S$  indices of p-PXZ-DPS-PXZ emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.7805	3.4164	0.2478	0.8701	0.0022
2	3.7817	3.4201	0.2422	0.8729	0.0013
3	4.2340	3.7449	0.7163	0.4022	0.0033
4	4.2379	3.7458	0.7382	0.3776	0.0037
5	4.4499	3.8779	0.7640	0.7749	0.1476
6	4.4566	3.8836	0.7609	0.7806	0.2006
7	4.7071	3.9183	0.8906	0.7385	0.0097
8	4.7138	3.9200	0.8942	0.7088	0.0030
9	4.8806	3.9416	0.8344	0.9580	0.0879
10	4.8852	4.0935	0.8303	0.9776	0.1033

**Table S17** Energies, oscillator strengths and  $\Phi_S$  indices of DBTO-ACR emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.7114	3.3601	0.1750	0.9588	0.0000
2	3.7237	3.6206	0.1750	0.8121	0.0000
3	4.0165	3.6230	0.3573	0.8312	0.0002
4	4.0255	3.6999	0.3747	0.3703	0.0000
5	4.5754	3.7102	0.8276	0.3411	0.1747
6	4.6414	3.9000	0.8676	0.7425	0.0341
7	4.6428	3.9000	0.8706	0.7471	0.0724
8	4.7016	3.9029	0.7726	0.5044	0.0000
9	4.7114	3.9083	0.7787	0.5135	0.6906
10	4.8755	4.1532	0.9162	0.9761	0.1735

**Table S18** Energies, oscillator strengths and  $\Phi_S$  indices of DBTO-NO emitter calculated at wB97XD/6-31+G(d,p) level of theory.

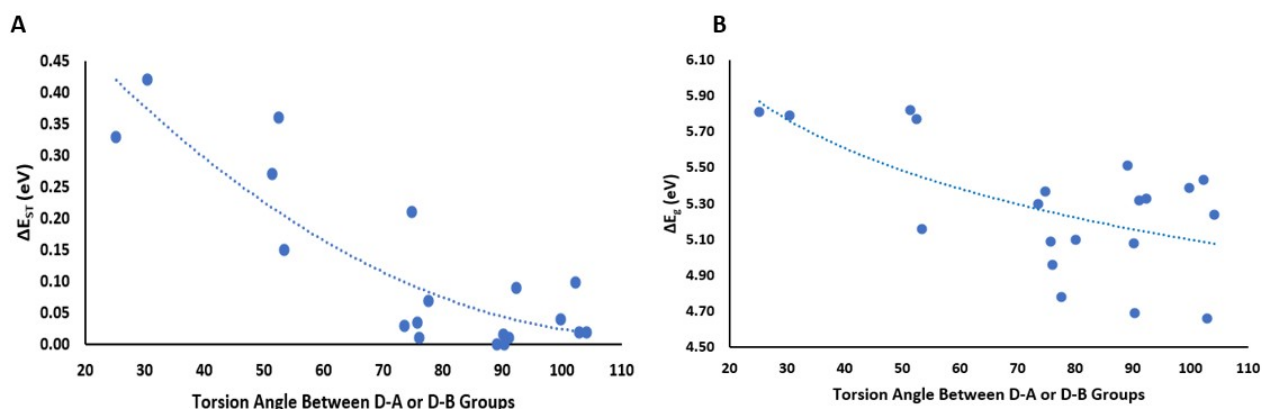
Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.7010	3.3995	0.2073	0.9617	0.0004
2	3.7155	3.4168	0.2125	0.8375	0.0000
3	3.9273	3.4181	0.3502	0.8425	0.0068
4	3.9377	3.7016	0.3677	0.2339	0.0000
5	4.3783	3.7145	0.7573	0.2220	0.0001
6	4.3803	3.7850	0.7583	0.6328	0.1803
7	4.6001	3.7915	0.8147	0.6512	0.1144
8	4.7106	3.8923	0.8781	0.7926	0.0153
9	4.7175	3.8923	0.7491	0.7918	0.0056
10	4.7572	4.0907	0.8128	0.9787	0.0000

**Table S19** Energies, oscillator strengths and  $\Phi_S$  indices of DMAC-TTR emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.9299	3.6269	0.3953	0.9187	0.0002
2	3.9365	3.6270	0.3638	0.9193	0.0001
3	4.4199	3.8855	0.7062	0.7752	0.0015
4	4.4223	3.8857	0.7041	0.7744	0.0098
5	4.6277	3.9146	0.8902	0.4754	0.0841
6	4.6296	3.9200	0.8909	0.4388	0.0493
7	4.7126	3.9783	0.8164	0.9664	0.0899
8	4.7222	4.0228	0.8215	0.7588	0.7607
9	5.0796	4.0231	0.8474	0.7626	0.0198
10	5.0843	4.0477	0.8522	0.9757	0.1699

**Table S20** Energies, oscillator strengths and  $\Phi_S$  indices of PXZ-TTR emitter calculated at wB97XD/6-31+G(d,p) level of theory.

Excited State	$E_S$ (eV)	$E_T$ (eV)	$\Phi_{S_S}$	$\Phi_{S_T}$	$f_S$
1	3.8931	3.4182	0.3085	0.8726	0.0001
2	3.8976	3.4183	0.3029	0.873	0.0040
3	4.2471	3.8263	0.7364	0.5708	0.0012
4	4.2478	3.8282	0.7327	0.5838	0.0127
5	4.4638	3.8836	0.7065	0.7940	0.0369
6	4.4678	3.8837	0.7096	0.7946	0.3221
7	4.7058	3.9443	0.8868	0.6851	0.0121
8	4.7098	3.9463	0.8863	0.6463	0.0015
9	4.9048	3.9866	0.7120	0.9644	0.0194
10	4.9082	4.0546	0.7139	0.9751	0.1484



**Figure S6** A) Relation between the torsion angle and  $\Delta E_{ST}$ , B) Relation between the torsion angle and  $E_g$ .

Figure S6 represents the Torsion Angle -  $\Delta E_{ST}$  (A) and Torsion Angle -  $E_g$  (B) correlations for the molecules under investigation. As represented in A), smallest  $\Delta E_{ST}$  values were obtained around the  $90^\circ$ , which represents the favorable effect of orthogonality. Therefore, angles between  $75^\circ$ - $105^\circ$  represent the acceptable geometry for the energy gap. On the other hand, correlation between  $E_g$  and geometry did not represent a regular trend. While the orthogonal geometries led to small  $E_g$  values for some molecules, some of them yield large energy differences in favorable geometries. This behavior can be attributed to the large variety of emitters under investigation, where, in some cases, molecules with totally different acceptor moieties may yield same degree of orthogonality, but the difference in acceptor groups may be the reason of different  $E_g$  values

**Table S21** Oscillator strengths for singlet excitations of Group 1 and Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory.

	S0→S1	S0→S2	S0→S3	S0→S4	S0→S5	S0→S6	S0→S7	S0→S8	S0→S9	S0→S10
<i>m</i> -Cz-DPS-Cz	0.0185	0.0587	0.0191	0.1179	0.0371	0.3055	0.0052	0.3728	0.2308	0.0377
<i>p</i> -Cz-DPS-Cz	0.6433	0.2086	0.0743	0.0467	0.0025	0.0113	0.0318	0.0788	0.1359	0.3846
<i>m</i> -PTZ-DPS-PTZ	0.0006	0.0007	0.0002	0.0022	0.0025	0.0066	0.0526	0.0547	0.1105	0.1072
<i>p</i> -PTZ-DPS-PTZ	0.0007	0.0023	0.0002	0.0005	0.0248	0.0380	0.0481	0.0555	0.0856	0.0993
<i>m</i> -DMAC-DPS-DMAC	0.0002	0.0154	0.0005	0.0124	0.0986	0.2999	0.0592	0.1863	0.4185	0.0124
<i>p</i> -DMAC-DPS-DMAC	0.0001	0.0003	0.0011	0.0014	0.1023	0.0484	0.3343	0.4996	0.0016	0.0101
<i>m</i> -PXZ-DPS-PXZ	0.0000	0.0007	0.0061	0.0031	0.0748	0.0965	0.0048	0.0000	0.1892	0.1712
<i>p</i> -PXZ-DPS-PXZ	0.0014	0.0008	0.0000	0.0000	0.1242	0.1707	0.0086	0.0028	0.1300	0.1478
<i>m</i> -DPA-DPS-DPA	0.0052	0.0744	0.1228	0.5341	0.4195	0.2402	0.1032	0.0799	0.0343	0.0378
<i>p</i> -DPA-DPS-DPA	0.9967	0.1901	0.2356	0.0299	0.5097	0.0551	0.0391	0.0832	0.0261	0.0192



**Table S22** Experimental and calculated energy gaps and, and root mean square coupling element ( $|\langle S_1 | H^{SOC} | T_n \rangle|$ ) for  $T_n \rightarrow S_1$  transition.

Compound	$\Delta E_{ST}$ (M/P) <sup>a</sup> (eV)	$\Delta E_{S_1-T_n}$ (M/P) <sup>b</sup> (eV)	$ \langle S_1   H^{SOC}   T_n \rangle $ (cm-1) M/P	$ V_{SOC} ^2$ (cm-2) M/P
<b>Cz-DPS-Cz (m/p)</b>	0.440/0.28±0.03	$S_1-T_1 = \mathbf{0.365}/0.4100$	<b>0.640</b> /0.330	<b>0.123</b> /0.064
		$S_1-T_2 = 0.350/\mathbf{0.2735}$	0.080/ <b>0.330</b>	0.006/ <b>0.109</b>
		$S_1-T_3 = 0.326/\mathbf{0.2365}$	0.040/0.190	0.002/0.036
		$S_1-T_4 = 0.313/\mathbf{0.2335}$	<b>0.490</b> /0.240	0.240/0.058
		$S_1-T_5 = 0.308/0.1985$	<b>0.420</b> /0.140	0.176/0.020
		$S_1-T_6 = 0.245/0.1985$	0.300/0.230	0.090/0.053
		$S_1-T_7 = 0.093$ (M)	0.530	0.281
		$S_1-T_8 = 0.039$ (M)	0.330	0.109
<b>PTZ-DPS-PTZ (m/p)</b>	0.010/0.410	$S_1-T_1 = 0.269/\mathbf{0.205}$	0.410/ <b>1.470</b>	0.079/ <b>0.280</b>
		$S_1-T_2 = 0.219/0.203$	0.260/0.260	0.068/0.068
		$S_1-T_3 = \mathbf{0.040}/0.013$	<b>0.530</b> /0.500	<b>0.281</b> /0.250
		$S_1-T_4 = -/0.0149$	-/0.110	-/0.012
<b>DMAC-DPS-DMAC (m/p)</b>	0.050/0.090	$S_1-T_1 = \mathbf{0.089}/0.006$	<b>0.540</b> /0.720	<b>0.104</b> /0.139
		$S_1-T_2 = \mathbf{0.093}/0.005$	<b>0.420</b> /0.680	<b>0.176</b> /0.462
		$S_1-T_3 = 0.108/0.213$	0.340/0.550	0.116/0.303
<b>PXZ-DPS-PXZ (m/p)</b>	0.060/0.080	$S_1-T_1 = 0.170/0.022$	0.270/0.640	0.052/0.123
		$S_1-T_2 = 0.170/0.019$	<b>0.510</b> / <b>1.610</b>	<b>0.260</b> / <b>2.592</b>
		$S_1-T_3 = 0.030/\mathbf{0.034}$	0.200/0.040	0.040/0.002
		$S_1-T_4 = \mathbf{0.030}/\mathbf{0.035}$	<b>0.260</b> /0.920	<b>0.068</b> /0.846
<b>DPA-DPS-DPA (m/p)</b>	-/0.540	$S_1-T_1 = 0.573/0.587$	0.260/0.150	0.050/0.030
		$S_1-T_2 = 0.396/0.425$	0.580/1.530	0.336/2.341
		$S_1-T_3 = 0.331/0.100$	0.860/1.040	0.740/1.082
		$S_1-T_4 = 0.306/0.079$	0.200/0.190	0.040/0.036
		$S_1-T_5 = 0.186/0.013$	0.350/0.110	0.123/0.012
		$S_1-T_6 = 0.098/0.046$	0.390/0.600	0.152/0.360

**Table S23.** Natures of  $S_1$ ,  $T_1$ - $T_5$  states of the emitters in Group 1 and Group 2 computed at M062X/6-31+G(d,p) level of theory in toluene.

Emitters	$S_1$ ( $\Phi_s$ )	$T_1$ ( $\Phi_s$ )	$T_2$ ( $\Phi_s$ )	$T_3$ ( $\Phi_s$ )	$T_4$ ( $\Phi_s$ )	$T_5$ ( $\Phi_s$ )
<i>m</i> -Cz-DPS-Cz	CT 0.5570	LE 0.7721	LE 0.8095	LE 0.8065	LE 0.9629	LE 0.9618
<i>p</i> -Cz-DPS-Cz	CT-LE 0.7047	CT-LE 0.8405	CT-LE 0.8622	LE 0.7503	LE 0.7622	LE 0.9676
<i>m</i> -PTZ-DPS-PTZ	CT-LE 0.4703	CT-LE 0.7920	LE 0.8164	CT-LE 0.5513	CT 0.5599	LE 0.7030
<i>p</i> -PTZ-DPS-PTZ	CT 0.3310	CT-LE 0.7845	CT-LE 0.7859	CT 0.4534	CT 0.4614	LE 0.6823
<i>m</i> -DMAC-DPS-DMAC	CT 0.3939	CT-LE 0.6062	CT-LE 0.5834	LE 0.8424	LE 0.7313	CT-LE 0.5798
<i>p</i> -DMAC-DPS-DMAC	CT 0.1642	CT 0.1692	CT 0.1677	LE 0.8800	LE 0.8798	LE 0.7097
<i>m</i> -PXZ-DPS-PXZ	CT 0.4383	CT-LE 0.7597	CT-LE 0.7578	CT-LE 0.6758	CT-LE 0.6576	CT-LE 0.5843
<i>p</i> -PXZ-DPS-PXZ	CT 0.2485	CT-LE 0.4301	CT 0.3921	CT-LE 0.7840	CT-LE 0.7951	LE 0.7599
<i>m</i> -DPA-DPS-DPA	CT-LE 0.7416	CT-LE 0.8193	CT-LE 0.7288	CT-LE 0.7987	LE 0.8031	LE 0.8448
<i>p</i> -DPA-DPS-DPA	CT-LE 0.7594	CT-LE 0.8375	CT-LE 0.8465	LE 0.8208	LE 0.8373	LE 0.8241

**Table S24.** Natures of  $S_1$ ,  $T_1$ - $T_5$  states computed at M062X/6-31+G(d,p) level of theory in toluene (TXO2-PXZ, *p*-PXZ-DPS-PXZ, TXO2-DMAC, *p*-DMAC-DPS-DMAC, DBTO-DMAC) and in dichloromethane (DBTO-PXZ).

Emitters	$S_1$ ( $\Phi_s$ )	$T_1$ ( $\Phi_s$ )	$T_2$ ( $\Phi_s$ )	$T_3$ ( $\Phi_s$ )	$T_4$ ( $\Phi_s$ )	$T_5$ ( $\Phi_s$ )
TXO2-PXZ	CT (0.2809)	LE (0.8393)	LE (0.8372)	CT (0.3879)	CT (0.3939)	LE (0.8082)
<i>p</i> -PXZ-DPS-PXZ	CT (0.2485)	CT-LE (0.4301)	CT-LE (0.3921)	CT-LE (0.7840)	CT-LE (0.7951)	CT-LE (0.7599)
DBTO-PXZ	CT (0.1854)	CT (0.3842)	CT (0.4018)	CT-LE (0.6394)	CT-LE (0.6383)	LE (0.9497)
TXO2-DMAC	CT (0.3465)	CT (0.3422)	CT (0.3206)	LE (0.8951)	LE (0.8951)	LE (0.7484)
<i>p</i> -DMAC-DPS-DMAC	CT (0.1642)	CT (0.1692)	CT (0.1677)	LE (0.8800)	LE (0.8798)	LE (0.7097)
DBTO-DMAC	CT (0.1712)	CT (0.2102)	CT (0.2044)	LE (0.9530)	CT-LE (0.4715)	CT-LE (0.4789)

**Table S25.** Natures of  $S_1$ ,  $T_1$ - $T_5$  states computed at M062X/6-31+G(d,p) level of theory in toluene (for Cz-Ph-TTR, DMAC-TTR, DMAC-Ph-TTR, PXZ-TTR, PXZ-Ph-TTR, PTZ-TTR, PTZ-Ph-TTR) and in ethyl ethanoate (Cz-TTR).

Emitters	$S_1$ ( $\Phi_s$ )	$T_1$ ( $\Phi_s$ )	$T_2$ ( $\Phi_s$ )	$T_3$ ( $\Phi_s$ )	$T_4$ ( $\Phi_s$ )	$T_5$ ( $\Phi_s$ )
Cz-TTR	CT-LE (0.5372)	LE (0.6815)	LE (0.9669)	LE (0.7556)	LE (0.6962)	LE (0.9489)
Cz-Ph-TTR	CT-LE (0.7649)	LE (0.9017)	LE (0.7723)	LE (0.9601)	LE (0.9118)	LE (0.9495)
DMAC-TTR (Planar)	CT-LE (0.7150)	LE (0.7941)	LE (0.7471)	LE (0.9543)	LE (0.9551)	LE (0.9622)
DMAC-TTR (Orthogonal)	CT 0.2008	CT 0.2255	CT 0.4256	LE 0.8829	LE 0.9490	LE 0.7289
DMAC-Ph-TTR	CT	CT	LE	LE	LE	LE

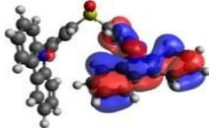
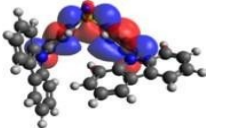
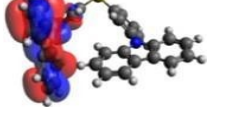
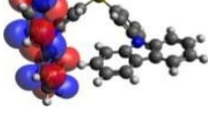
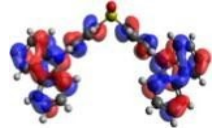
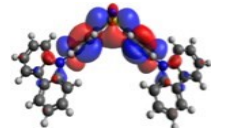
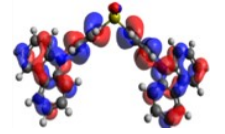
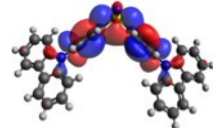
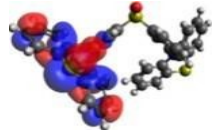
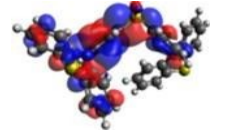
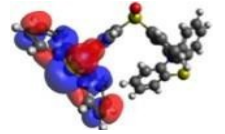
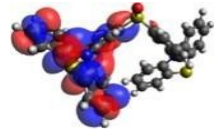



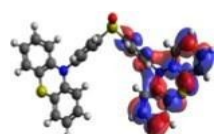
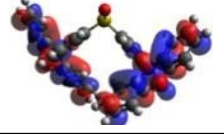
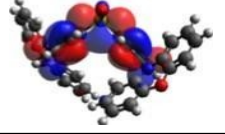


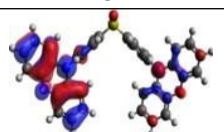
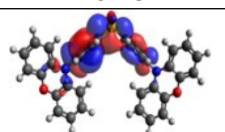
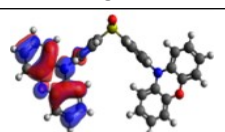
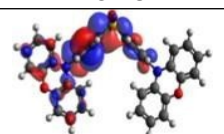
(only orthogonal)	(0.4644)	(0.4545)	(0.9450)	(0.8793)	(0.7088)	(0.7127)
<b>PXZ-TTR</b>	CT-LE (0.5143)	CT-LE (0.5045)	CT (0.4417)	LE (0.7709)	CT-LE (0.5976)	CT-LE (0.5589)
<b>PXZ-Ph-TTR</b>	CT (0.2247)	CT-LE (0.5210)	LE (0.7435)	LE (0.9473)	LE (0.8069)	LE (0.7076)
<b>PTZ-TTR</b> (Planar)	LE (0.6951)	LE (0.8187)	LE (0.7689)	LE (0.9175)	LE (0.8723)	LE (0.9630)
<b>PTZ-TTR</b> (Orthogonal)	CT (0.1588)	CT (0.1974)	LE (0.7363)	CT-LE (0.5658)	LE (0.7236)	LE (0.9450)
<b>PTZ-Ph-TTR</b> (Planar)	CT-LE (0.6631)	LE (0.8496)	LE (0.8313)	LE (0.8525)	LE (0.9040)	LE (0.8741)
<b>PTZ-Ph-TTR</b> (Orthogonal)	CT (0.3481)	LE (0.7746)	CT-LE (0.4652)	LE (0.9449)	LE (0.6797)	LE (0.6983)

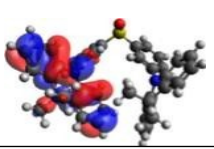
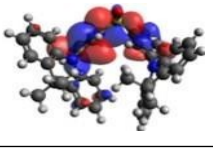
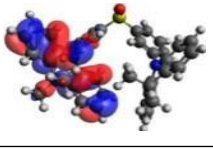
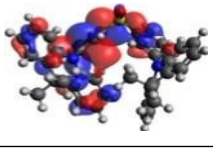
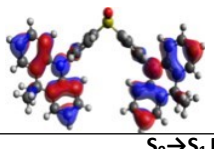
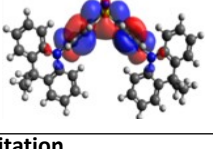
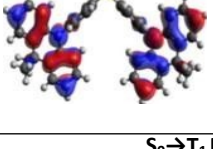
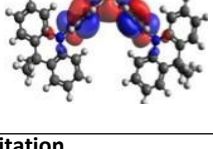
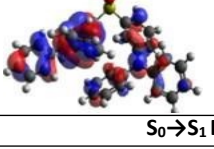
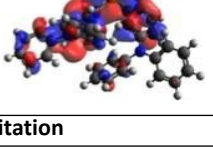
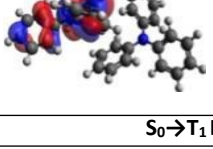
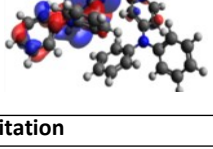
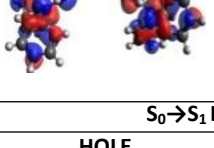
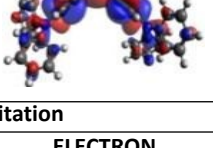
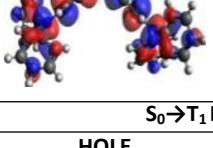
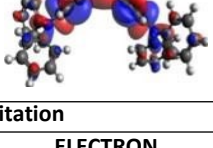
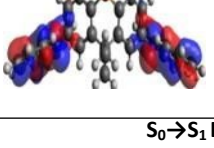
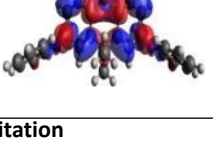
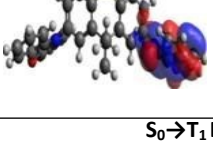
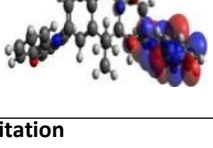
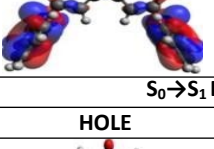
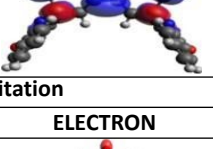
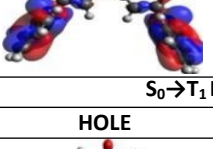
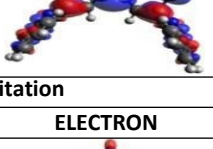
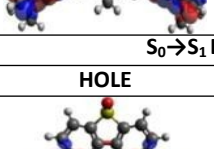
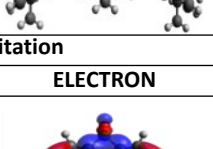
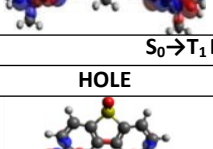
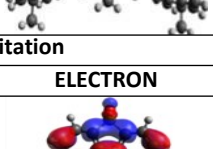

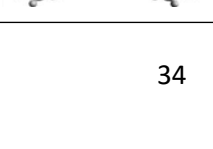


**Table S26** Reorganization energies (kcal/mol) between the  $S_1$  and  $T_1$  geometries of selected compounds.

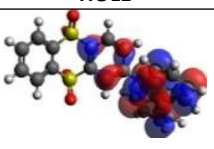
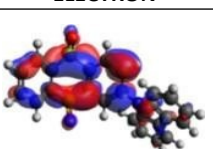
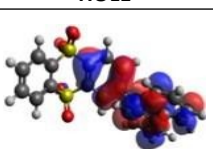
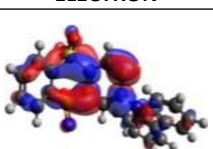
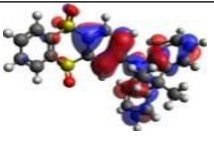
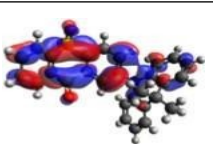
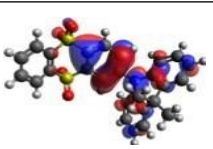
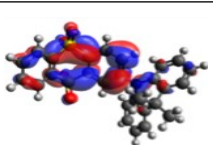
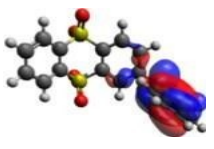

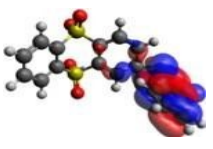

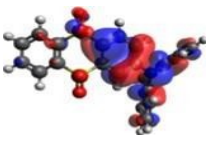
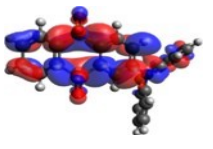
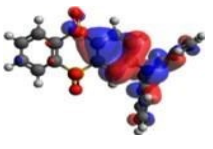

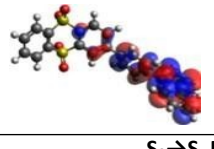
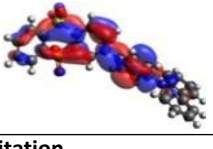
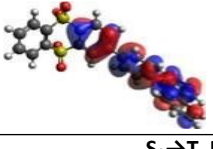
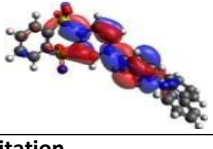
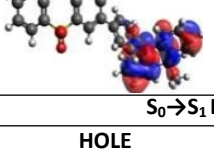
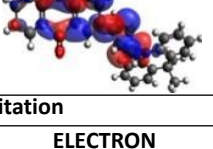
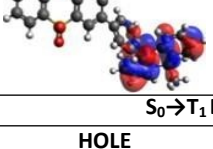
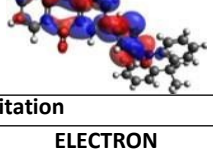
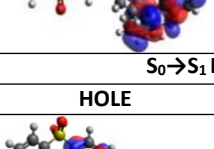
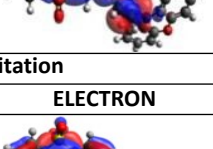
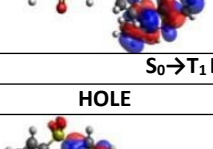
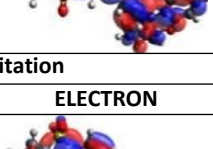
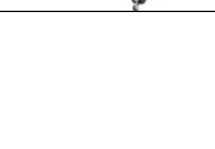
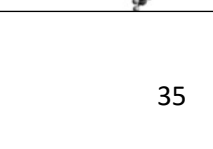

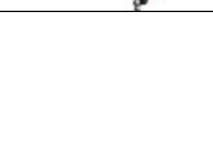
Compound	Reorganization Energy
m-Cz-DPS-Cz	6.51
m-PTZ-DPS-PTZ	6.00
m-PXZ-DPS-PXZ	1.89
m-DMAC-DPS-DMAC	0.32
m-DPA-DPS-DPA	0.08
p-Cz-DPS-Cz	4.36
p-PTZ-DPS-PTZ	1.79
p-PXZ-DPS-PXZ	1.65
p-DMAC-DPS-DMAC	3.54
p-DPA-DPS-DPA	10.24
TXO2-PXZ	0.92
TXO2-DMAC	0.49
DBTO-NO	0.20
DBTO-DMAC	0.37
DMAC-TTR	0.78
PTZ-TTR	5.38
Cz-Ph-TTR	5.43
DMAC-Ph-TTR	2.13
PXZ-Ph-TTR	0.35
PTZ-Ph-TTR	3.60

The reorganization energies of the molecule set under investigation have been calculated at the M062X/6-31+G(d,p) level of theory. As reported in Table S26, reorganization energies lie between 0.08 and 10.24 kcal/mol and it should be noted that the emitters, m-DPA-DPS-DPA, DBTO-NO, m-DMAC-DPS-DMAC, DBTO-DMAC, PXZ-Ph-TTR and TXO2-DMAC represented the smallest reorganization energies which range between 0.08 kcal/mol and 0.49 kcal/mol respectively. On the other hand, some emitters represent values around the 5 - 10 kcal/mol, which are less favorable for RISC. Considering all the data reported in Table S26, no systematic behavior was observed between the group of molecules, thus hampering the use of this parameter in comparisons.

**Table S27** Electron and hole orbitals of sulfone based emitters computed from ground state geometries at M062X/6-31+G(d,p) level of theory.

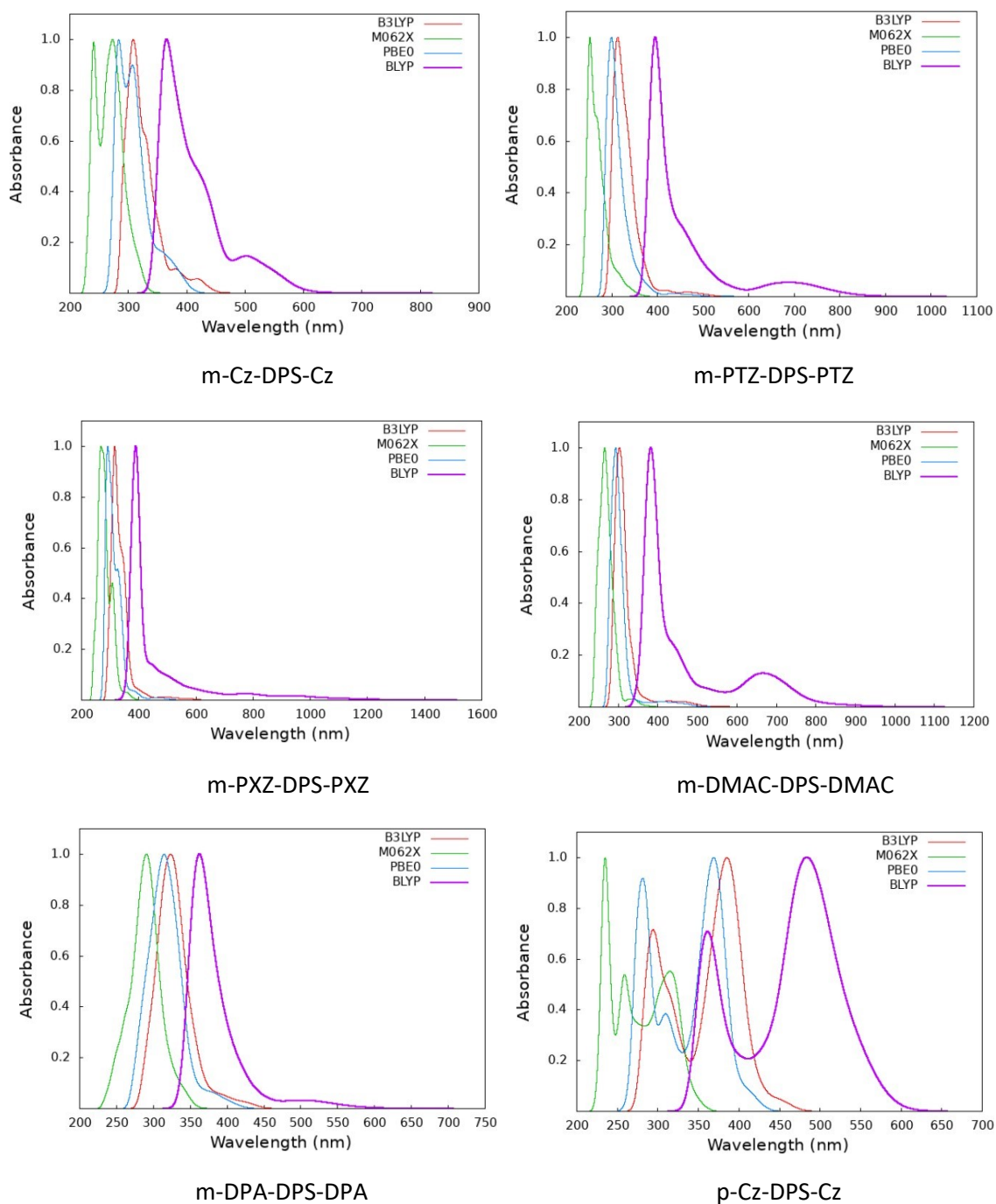
Molecule	M062X/6-31+G(d,p)			
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
m-Cz-DPS-Cz				
p-Cz-DPS-Cz				
m-PTZ-DPS-PTZ				
p-PTZ-DPS-PTZ				
m-PXZ-DPS-PXZ				
p-PXZ-DPS-PXZ				

m-DMAC-DPS-DMAC	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
p-DMAC-DPS-DMAC	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
m-DPA-DPS-DPA	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
p-DPA-DPS-DPA	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
TXO2-NO	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
DBTO-NO	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
TXO2-ACR	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
DBTO-ACR	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				

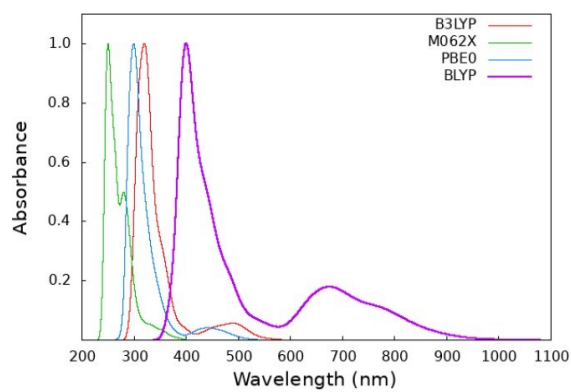
Cz-TTR	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
DMAC-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
PXZ-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
PTZ-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
Cz-Ph-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
DMAC-Ph-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
PXZ-Ph-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON
PTZ-Ph-TTR	HOLE	ELECTRON	HOLE	ELECTRON
				
	$S_0 \rightarrow S_1$ Excitation		$S_0 \rightarrow T_1$ Excitation	
	HOLE	ELECTRON	HOLE	ELECTRON



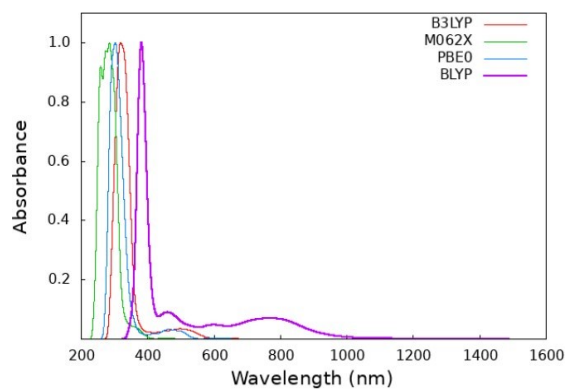
**Figure S7** Absorption Spectra of Sulfone Based TADF Emitters computed at B3LYP/6-31+G(d,p), M06-2X/6-31+G(d,p), PBE0/6-31+G(d,p) and BLYP/6-31+G(d,p) level of theories.



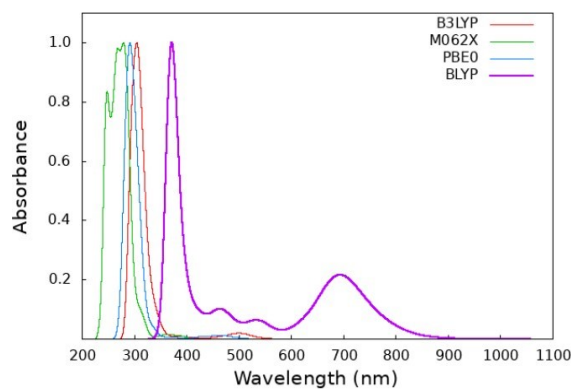




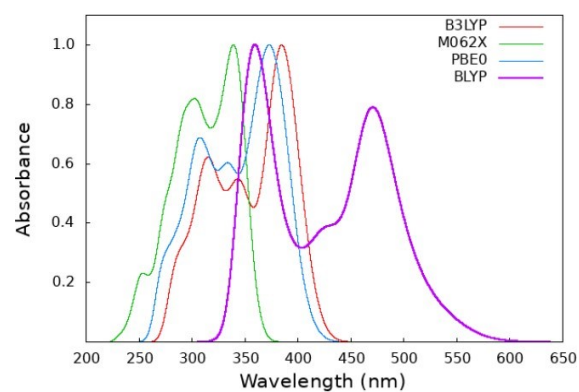
p-PTZ-DPS-PTZ



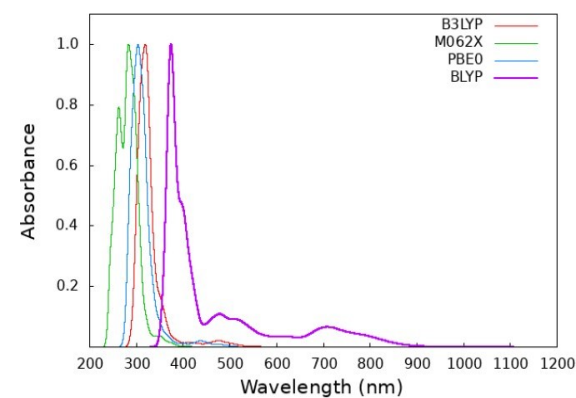
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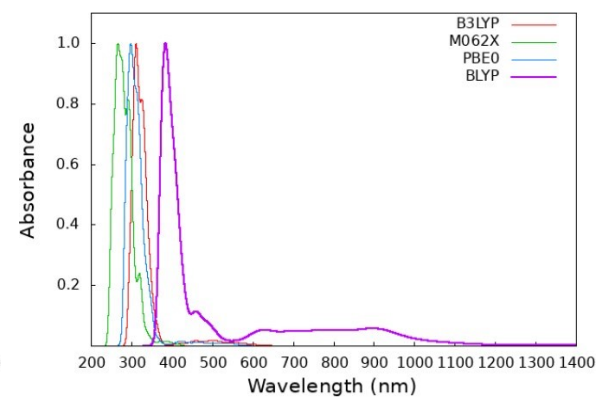
p-DMAD-DPS-DMAC



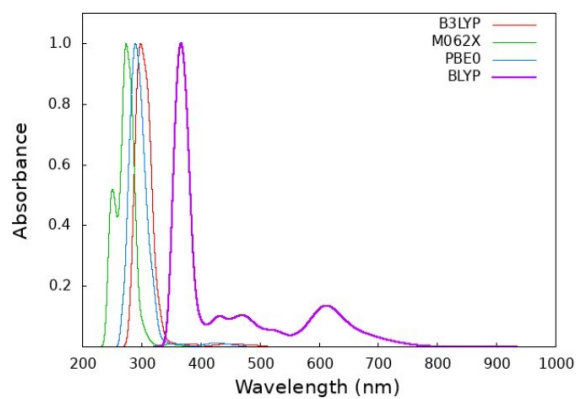
p-DPA-DPS-DPA



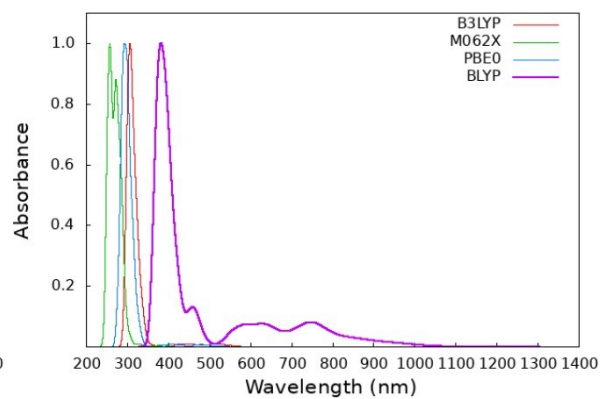
TXO2-NO



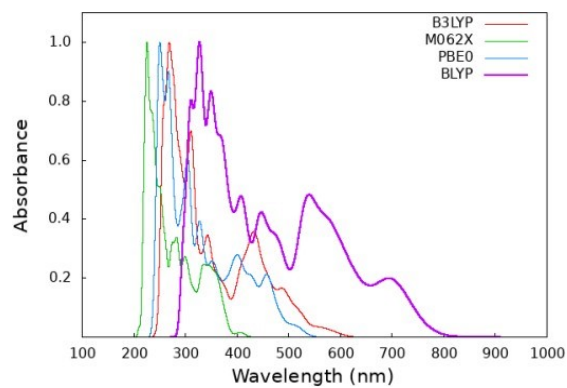
DBTO-NO



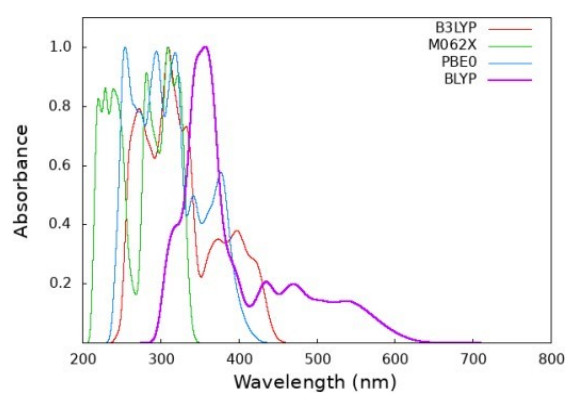
TXO2-ACR



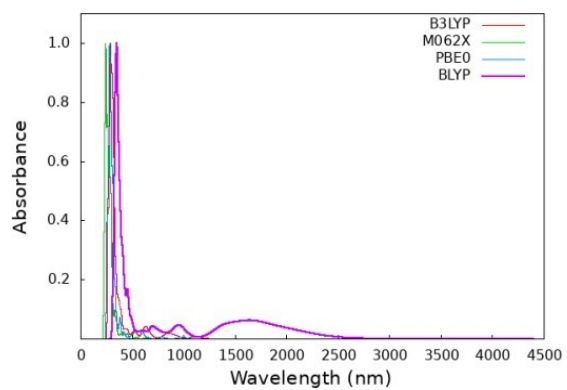
DBTO-ACR



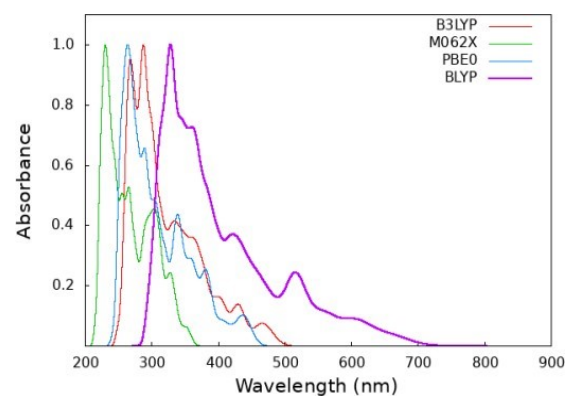
Cz-TTR



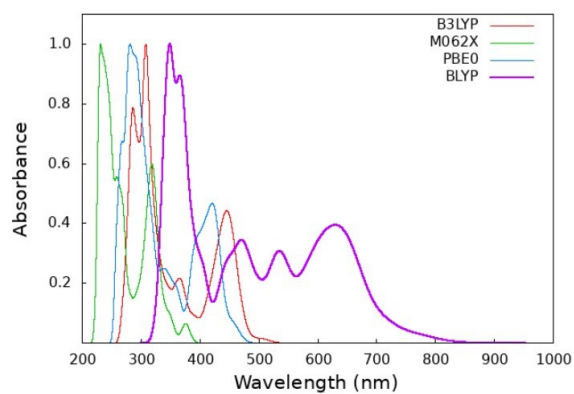
DMAC-TTR



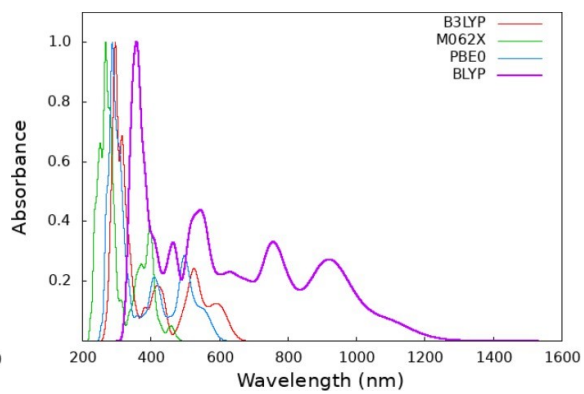
PXZ-TTR



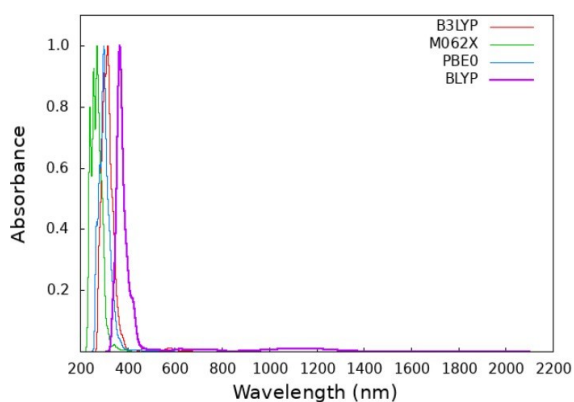
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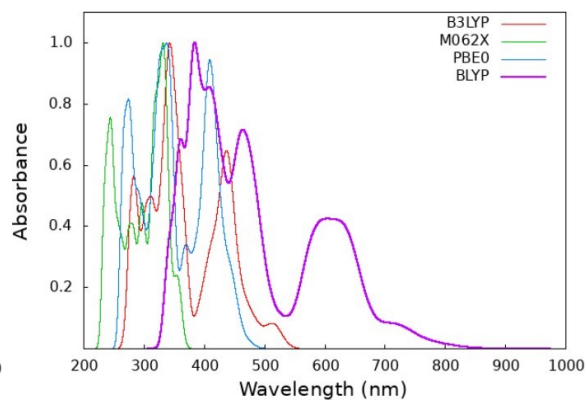
Cz-Ph-TTR



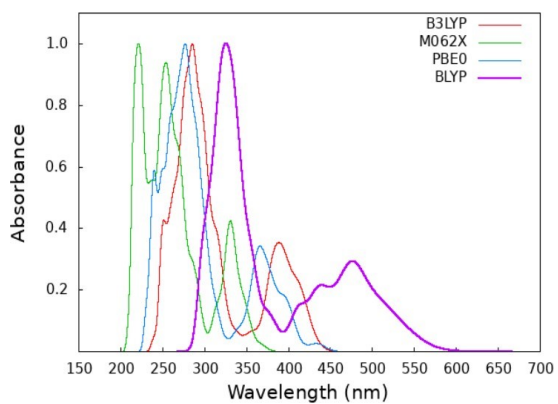
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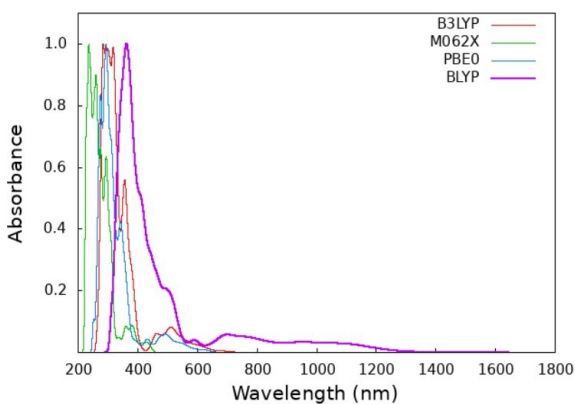
PXZ-Ph-TTR



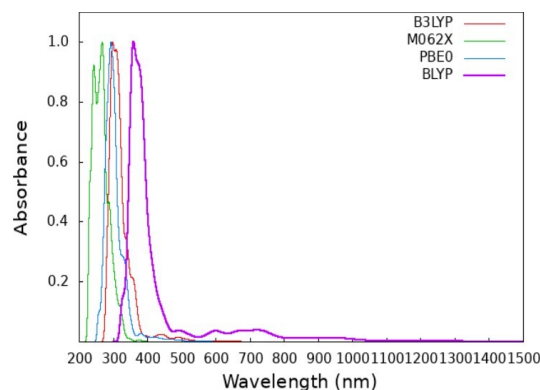
PTZ-Ph-TTR



AC-OSO



CzSOXO



TXO-Ph-Cz

**Table S28** Experimental absorption wavelengths of the modeled sulfone based TADF emitters.

Emitter	Experimental Maximum Absorption Wavelength	Experimental Reference	Theoretical Data*
m-Cz-DPS-Cz	338 nm	1	290 nm
m-PTZ-DPS-PTZ	304 nm	1	315 nm
m-PXZ-DPS-PXZ	308 nm	1	300 nm
m-DMAC-DPS-DMAC	301 nm	1	320 nm
p-Cz-DPS-Cz	350 nm	2	325 nm
p-PTZ-DPS-PTZ	209 nm, 255 nm, 319 nm	3	220 nm, 260 nm, 325 nm
p-PXZ-DPS-PXZ	325 nm	4	300 nm
p-DMAC-DPS-DMAC	286 nm	4	290 nm
p-DPA-DPS-DPA	350 nm	5	345 nm
TXO2-NO	325 nm, 309 nm	6	300 nm
DBTO-NO	240 nm, 320 nm, 400 nm	5	250 nm, 315 nm, 390 nm
TXO2-ACR	290 nm, 365 nm	7	290 nm, 370 nm
DBTO-ACR	284 nm, 376 nm	7	280 nm, 350 nm
Cz-TTR	290 nm, 325 nm, 370 nm	8	290 nm, 330 nm, 360 nm
DMAC-TTR	290 nm, 320 nm, 365 nm	9	280 nm, 305 nm, 310 nm
PXZ-TTR	-	10	-
PTZ-TTR	315 nm, 360 nm	9	302 nm, 350 nm
Cz-Ph-TTR	290 nm, 380 nm	11	305 nm, 380 nm
DMAC-Ph-TTR	290 nm, 390 nm	9	290 nm, 400 nm
PXZ-Ph-TTR	300 nm, 405 nm	12	300 nm, 390 nm
PTZ-Ph-TTR	290 nm, 375 nm	9	300 nm, 325 nm, 370 nm

\*Theoretical data were obtained from calculations at M062X/6-31+G(d,p) level of theory.

### Findings From The Absorption Spectra Analyses

Absorption spectra calculations via Wigner distribution method have been performed with B3LYP,<sup>13</sup> PBE0,<sup>14</sup> M062X and BLYP<sup>13</sup> functionals using the 6-31+G(d,p) basis set. The main purpose of absorption spectra analyses was observing the effect of functional choice in excited state energies and oscillator strengths. Analyses with M062X represented a blue shifted spectra compared to the hybrid B3LYP, PBE0 and BLYP functionals. Additionally, we also observed that while B3LYP and PBE0 behaves highly similar to each other, BLYP represents red shifted absorption spectra for all compounds. The choice of various functionals for spectra analyses gave us the opportunity to observe the effect of different methodologies on absorption spectra.

While comparing experimental and theoretical spectra, we focused on the data obtained from M062X, which is the best performing functional in reproducing TADF descriptors. As reported in Table S28, M062X well reproduced the absorption spectra of emitters with some exceptions such as *m*-Cz-DPS-Cz<sup>1</sup> (~50 nm shift), *p*-Cz-DPS-Cz<sup>1</sup> (~25 nm shift) and *p*-PXZ-DPS-PXZ,<sup>15</sup> (~25 nm shift). For the other emitters, Table S28 represents that the absorption wavelength differences between the calculated and experimental data are in the range of ~ 0 nm -10 nm.

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**Table S29** Relative energies of the different conformers of the emitters *m*-Cz-DPS-Cz and *m*-PTZ-DPS-PTZ computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{\text{rel}}$ (kcal/mol)
<i>m</i> -Cz-DPS-Cz	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.35
	Conf. 4	0.36
	Conf. 5	0.66

	Conf. 6	0.89
	Conf. 7	0.89
	Conf. 8	1.00
	Conf. 9	1.70
<b><i>m</i>-PTZ-DPS-PTZ</b>	Conf. 1	0.00
	Conf. 2	0.04
	Conf. 3	0.05
	Conf. 4	0.17
	Conf. 5	0.17
	Conf. 6	0.67
	Conf. 7	0.83
	Conf. 8	0.91
	Conf. 9	0.93
	Conf. 10	0.98
	Conf. 11	1.04
	Conf. 12	1.25
	Conf. 13	1.25
	Conf. 14	1.32
	Conf. 15	1.33
	Conf. 16	1.51
	Conf. 17	1.63
	Conf. 18	1.88
	Conf. 19	1.95
	Conf. 20	1.95
	Conf. 21	1.98
	Conf. 22	2.05
	Conf. 23	2.29
	Conf. 24	2.29
	Conf. 25	2.42
	Conf. 26	2.42
	Conf. 27	2.58
	Conf. 28	2.90
Conf. 29	2.90	
Conf. 30	3.06	
Conf. 31	3.22	
Conf. 32	3.31	

**Table S30** Relative energies of the different conformers of the emitters *m*-Cz-DPS-Cz and *m*-PTZ-DPS-PTZ computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{\text{rel}}$ (kcal/mol)
<i>m</i> -PXZ-DPS-PXZ	Conf. 1	0.00
	Conf. 2	0.18
	Conf. 3	0.21
	Conf. 4	0.32
	Conf. 5	0.32
	Conf. 6	0.61
	Conf. 7	0.65
	Conf. 8	0.93
	Conf. 9	0.94
	Conf. 10	0.98
	Conf. 11	0.99
	Conf. 12	1.27
	Conf. 13	1.28
	Conf. 14	1.28
	Conf. 15	1.32
	Conf. 16	1.56
	Conf. 17	2.16
<i>m</i> -DMAC-DPS-DMAC	Conf. 1	0.00
	Conf. 2	0.05
	Conf. 3	0.19
	Conf. 4	0.20
	Conf. 5	0.52
	Conf. 6	0.52
	Conf. 7	0.58
	Conf. 8	0.59
	Conf. 9	0.66
	Conf. 10	0.73
	Conf. 11	1.15
	Conf. 12	1.72
	Conf. 13	1.73
	Conf. 14	1.77
	Conf. 15	1.97
	Conf. 16	1.98
	Conf. 17	2.85
	Conf. 18	2.85
	Conf. 19	3.79
	Conf. 20	3.79
	Conf. 21	4.37
	Conf. 22	4.39
	Conf. 23	4.63
	Conf. 24	4.64



**Table S31** Relative energies of the different conformers of the emitter *m*-DPA-DPS-DPA computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{rel}$ (kcal/mol)
<b><i>m</i>-DPA-DPS-DPA</b>	Conf. 1	0.00
	Conf. 2	0.11
	Conf. 3	0.12
	Conf. 4	0.32
	Conf. 5	0.32
	Conf. 6	0.51
	Conf. 7	0.51
	Conf. 8	1.71
	Conf. 9	1.72
	Conf. 10	2.67
	Conf. 11	3.13

**Table S32** Relative energies of the different conformers of Group 2 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{rel}$ (kcal/mol)
<b>p-Cz-DPS-Cz</b>	Conf. 1	0.00
	Conf. 2	0.31
	Conf. 3	1.33
	Conf. 4	1.33
<b>p-PTZ-DPS-PTZ</b>	Conf. 1	0.00
	Conf. 2	0.64
	Conf. 3	0.66
	Conf. 4	0.67
	Conf. 5	0.70
	Conf. 6	0.70
<b>p-PXZ-DPS-PXZ</b>	Conf. 1	0.00
	Conf. 2	0.01
	Conf. 3	0.13
	Conf. 4	0.24
	Conf. 5	1.05
	Conf. 6	1.05
<b>p-DMAC-DPS-DMAC</b>	Conf. 1	0.00
	Conf. 2	1.38
	Conf. 3	1.98
<b>p-DPA-DPS-DPA</b>	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.24
	Conf. 4	0.36
	Conf. 5	1.26

**Table S33** Relative energies of the different conformers of Group 3 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{rel}$ (kcal/mol)
TXO2-NO	Conf. 1	0.00
	Conf. 2	0.11
	Conf. 3	0.15
	Conf. 4	0.16
DBTO-NO	Conf. 1	0.00
	Conf. 2	0.24
	Conf. 3	0.30
	Conf. 4	0.40
TXO2-ACR	Conf. 1	0.00
DBTO-ACR	Conf. 1	0.00

**Table S34** Relative energies of the different conformers of Group 4 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{rel}$ (kcal/mol)
Cz-TTR	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.35
	Conf. 4	0.35
PXZ-TTR	Conf. 1	0.00
	Conf. 2	0.01
	Conf. 3	0.02
	Conf. 4	0.30
	Conf. 5	0.83
	Conf. 6	0.86
	Conf. 7	0.91
	Conf. 8	1.04
PTZ-TTR	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.69
	Conf. 4	0.69
	Conf. 5	3.21
	Conf. 6	3.21
	Conf. 7	3.70
	Conf. 8	3.71
DMAC-TTR	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.15
	Conf. 4	0.15
	Conf. 5	0.25
	Conf. 6	0.26
	Conf. 7	0.29
	Conf. 8	0.29
	Conf. 9	0.35
	Conf. 10	0.36

**Table S35** Relative energies of the different conformers of Group 5 emitters computed at M06-2X/6-31+G(d,p) level of theory.

Compound	Conformer	$\Delta G_{rel}$ (kcal/mol)
<b>Cz-Ph-TTR</b>	Conf. 1	0.00
	Conf. 2	0.01
	Conf. 3	0.01
	Conf. 4	0.05
	Conf. 5	0.05
	Conf. 6	0.08
	Conf. 7	0.22
	Conf. 8	0.23
<b>PXZ-Ph-TTR</b>	Conf. 1	0.00
	Conf. 2	0.00
	Conf. 3	0.03
	Conf. 4	0.04
	Conf. 5	0.05
	Conf. 6	0.40
	Conf. 7	3.45
	Conf. 8	3.46
	Conf. 9	3.47
	Conf. 10	3.56
	Conf. 11	3.56
	Conf. 12	3.80
<b>PTZ-Ph-TTR</b>	Conf. 1	0.00
	Conf. 2	0.04
	Conf. 3	0.04
	Conf. 4	0.05
	Conf. 5	0.06
	Conf. 6	0.08
	Conf. 7	0.16
	Conf. 8	0.19
	Conf. 9	0.20
	Conf. 10	0.29
	Conf. 11	0.33
	Conf. 12	0.33
	Conf. 13	0.43
	Conf. 14	0.43
	Conf. 15	0.48
	Conf. 16	0.48
<b>DMAC-Ph-TTR</b>	Conf. 1	0.00
	Conf. 2	0.02
	Conf. 3	0.24
	Conf. 4	0.24

## Cartesian Coordinates for The Ground State Geometries

***m*-Cz-DPS-Cz**

S	-0.17709	3.66918	-0.84997
O	-0.06718	3.11252	-2.17367
O	-0.27193	5.09173	-0.64594
C	1.18771	3.05995	0.10327
C	3.18614	1.99957	1.68884
C	1.71419	1.81456	-0.22342
C	1.6321	3.7867	1.20437
C	2.64251	3.24483	1.9965
C	2.71918	1.28236	0.58328
H	1.34938	1.26274	-1.08564
H	1.197	4.75655	1.42243
H	3.01447	3.79812	2.85227
H	3.98164	1.57622	2.29471
C	-1.5589	2.90342	-0.04765
C	-3.60797	1.6322	1.29801
C	-2.30205	3.6243	0.8812
C	-1.82811	1.56876	-0.33853
C	-2.85144	0.92594	0.35572
C	-3.34517	2.977	1.54335
H	-2.06766	4.66648	1.07003
H	-1.264	1.03877	-1.10046
H	-3.94208	3.51834	2.26956
H	-4.39441	1.11468	1.83883
N	3.2434	0.00317	0.28845
N	-3.11476	-0.43824	0.1081
C	3.74106	-0.40873	-0.94748
C	4.79632	-1.69192	-3.1596
C	4.01892	-1.79123	-0.89138
C	3.99084	0.34901	-2.09363
C	4.51815	-0.31477	-3.19507
C	4.55301	-2.43483	-2.01148
H	3.78475	1.41394	-2.12692
H	4.7207	0.2463	-4.10175
H	4.77364	-3.49786	-1.98261
H	5.2077	-2.17581	-4.03918
C	3.1724	-1.10426	1.13192
C	3.16324	-3.58174	2.36772
C	2.67837	-1.19207	2.43574
C	3.64927	-2.23835	0.43713
C	3.64549	-3.48574	1.06714
C	2.6829	-2.44494	3.03916
H	2.29004	-0.3222	2.95571
H	4.00261	-4.36722	0.5425
H	2.29619	-2.54598	4.04816
H	3.14811	-4.54382	2.86902
C	-2.17513	-1.47026	0.15969
C	-0.73887	-3.83886	0.16856
C	-2.8203	-2.68724	-0.15096
C	-0.81837	-1.42285	0.49489
C	-0.11465	-2.62258	0.49188
C	-2.0905	-3.87963	-0.14858
H	-0.32523	-0.49108	0.75926
H	0.93911	-2.62007	0.75406
H	-2.57666	-4.82138	-0.38648
H	-0.15475	-4.75337	0.17522
C	-4.35411	-0.97878	-0.23425

C	-6.54506	-2.50815	-0.95934
C	-5.57437	-0.3314	-0.44102
C	-4.21272	-2.37311	-0.40416
C	-5.32283	-3.14095	-0.76736
C	-6.6634	-1.11732	-0.80136
H	-5.67253	0.74416	-0.33589
H	-5.22784	-4.21449	-0.90239
H	-7.62483	-0.64174	-0.96779
H	-7.41647	-3.09001	-1.24068

***m*-DMAC-DPS-DMAC**

S	0.44158	4.08601	0.63037
O	0.58111	5.47677	0.28068
O	0.25568	3.68213	2.00068
C	1.8629	3.22527	0.00414
C	4.07731	1.85316	-0.92792
C	2.84866	3.92388	-0.68435
C	1.95584	1.8531	0.2224
C	3.05872	1.16055	-0.26444
C	3.96805	3.22576	-1.14059
H	2.74022	4.99181	-0.84126
H	1.18971	1.31212	0.76979
H	4.75944	3.75612	-1.65942
H	4.95094	1.30651	-1.27177
C	-0.89434	3.39977	-0.30902
C	-2.86215	2.21605	-1.84559
C	-1.44133	2.18756	0.10809
C	-1.32148	4.03858	-1.46974
C	-2.32731	3.44384	-2.23095
C	-2.41282	1.58531	-0.68363
H	-1.1196	1.71262	1.03065
H	-0.87733	4.98584	-1.75831
H	-2.68449	3.93228	-3.13132
H	-3.62738	1.72797	-2.44225
N	3.11676	-0.24432	-0.03402
N	-2.91774	0.30016	-0.32498
C	2.92147	-1.16323	-1.08354
C	2.70694	-3.08207	-3.10748
C	2.61563	-2.49728	-0.74475
C	3.04162	-0.78913	-2.42802
C	2.93393	-1.74801	-3.43233
C	2.54238	-3.44013	-1.76938
H	3.23547	0.24314	-2.69451
H	3.03888	-1.44441	-4.46941
H	2.32887	-4.47569	-1.52728
H	2.63632	-3.83557	-3.88516
C	3.58544	-0.71584	1.20945
C	4.61361	-1.73397	3.59649
C	4.34906	0.10138	2.051
C	3.28908	-2.04081	1.57847
C	3.83482	-2.53624	2.76239
C	4.8522	-0.40868	3.24434
H	4.5581	1.1282	1.77039
H	3.63461	-3.56104	3.05668
H	5.44405	0.23301	3.88945
H	5.01569	-2.13948	4.519
C	-2.30172	-0.83546	-0.87454

C	-1.06095	-3.07306	-2.03241	H	3.15843	1.10947	2.93602
C	-1.1532	-0.69194	-1.67582	N	-4.18663	0.4851	-0.58958
C	-2.82501	-2.11758	-0.63266	N	4.18659	0.4849	0.58946
C	-2.18636	-3.21119	-1.22793	C	-4.11297	1.43214	0.45439
C	-0.54086	-1.7989	-2.2459	C	-4.10749	3.34851	2.50833
H	-0.73021	0.29114	-1.85109	C	-2.91995	2.02919	0.86495
H	-2.58374	-4.20693	-1.05094	C	-5.30337	1.81514	1.08983
H	0.3542	-1.663	-2.84485	C	-5.30515	2.75176	2.10896
H	-0.58517	-3.94418	-2.47169	C	-2.92066	2.98626	1.88235
C	-4.0613	0.20703	0.48105	H	-1.98859	1.7558	0.38074
C	-6.33835	0.07399	2.11516	H	-6.25325	3.0089	2.56972
C	-4.6215	-1.04641	0.7805	H	-1.98242	3.44375	2.17869
C	-4.64612	1.37644	0.99866	H	-4.11131	4.08902	3.30079
C	-5.77269	1.30846	1.80683	C	-5.3337	-0.33732	-0.63795
C	-5.75501	-1.07788	1.59864	C	-7.69355	-1.85514	-0.71196
H	-4.21333	2.34375	0.77153	C	-5.37786	-1.5433	-1.33762
H	-6.20227	2.22614	2.19618	C	-6.49056	0.09349	0.02636
H	-6.19717	-2.04028	1.84109	C	-7.65517	-0.65421	-0.00036
H	-7.21728	0.00754	2.7474	C	-6.55535	-2.29331	-1.37845
C	-4.04255	-2.35945	0.25669	H	-4.49449	-1.89421	-1.85983
C	2.29327	-2.80435	0.71417	H	-8.52246	-0.27676	0.5313
C	2.29237	-4.30487	1.00597	H	-6.56928	-3.22423	-1.93509
H	2.01921	-4.48888	2.04819	H	-8.60832	-2.43693	-0.73931
H	3.26969	-4.75937	0.81312	C	5.33372	-0.33741	0.63796
H	1.54157	-4.80927	0.39158	C	7.69369	-1.85504	0.71228
C	0.87875	-2.25337	1.03008	C	6.4906	0.09346	-0.02627
H	0.81158	-1.1836	0.80959	C	5.37791	-1.54335	1.33769
H	0.65592	-2.40502	2.09168	C	6.55546	-2.29327	1.37868
H	0.12519	-2.7686	0.42539	C	7.65527	-0.65415	0.00061
C	-5.12713	-3.09916	-0.5558	H	4.49451	-1.89431	1.85982
H	-6.00536	-3.30615	0.06224	H	6.56941	-3.22417	1.93536
H	-4.75074	-4.05553	-0.92938	H	8.52258	-0.27665	-0.53099
H	-5.44223	-2.49488	-1.41147	H	8.6085	-2.43674	0.73975
C	-3.61433	-3.23381	1.45545	C	4.11298	1.43206	-0.45439
H	-4.46584	-3.44209	2.11026	C	4.10755	3.3487	-2.50808
H	-2.84273	-2.72524	2.04136	C	2.91998	2.02918	-0.86489
H	-3.21084	-4.19104	1.11159	C	5.3034	1.81512	-1.08976
<b>m-PXZ-DPS-PXZ</b>				C	5.3052	2.75189	-2.10877
S	-0.00007	-2.49599	-0.00014	C	2.92071	2.98638	-1.88217
O	0.85641	-3.20331	-0.91697	H	1.98861	1.75574	-0.38073
O	-0.85659	-3.20334	0.91663	H	6.25331	3.00907	-2.56947
C	-1.01172	-1.39312	-0.94968	H	1.98248	3.44391	-2.17847
C	-2.54212	0.40321	-2.38894	H	4.11141	4.08931	-3.30044
C	-2.20317	-0.93225	-0.40046	O	-6.51716	1.30469	0.68485
C	-0.57187	-0.98218	-2.20761	O	6.51719	1.30458	-0.68489
C	-1.34954	-0.08086	-2.92905	H	-3.15839	1.10982	-2.93608
C	-2.96574	-0.02147	-1.13092	<b>m-PTZ-DPS-PTZ</b>			
H	-2.53934	-1.27802	0.57357	S	-0.11186	-2.84913	0.14179
H	0.3554	-1.37671	-2.61044	O	0.71035	-3.58068	1.07034
H	-1.02762	0.24514	-3.91215	O	-0.91993	-3.53135	-0.83654
C	1.01161	-1.39322	0.94947	C	-1.17367	-1.78282	1.07624
C	2.54211	0.40293	2.38885	C	-2.75457	0.00847	2.46293
C	0.5718	-0.98235	2.20743	C	-2.2689	-1.21297	0.43569
C	2.20309	-0.93237	0.40027	C	-0.85687	-1.48592	2.40035
C	2.9657	-0.02167	1.13078	C	-1.66499	-0.59028	3.09619
C	1.34952	-0.08112	2.92894	C	-3.05353	-0.29895	1.13625
H	-0.35549	-1.37686	2.61024	H	-2.50792	-1.46991	-0.59332
H	2.53923	-1.27809	-0.57378	H	0.0007	-1.95875	2.86771
H	1.02762	0.24482	3.91206	H	-1.4418	-0.35195	4.13055

H	-3.3847	0.72069	2.98638	C	-0.86261	2.72243	-0.06862
C	0.92266	-1.69912	-0.72606	C	-2.61608	1.29266	-1.63389
C	2.4697	0.17966	-2.03209	C	-1.52763	1.63857	0.49055
C	2.10148	-1.26183	-0.12584	C	-1.05989	3.13355	-1.38368
C	0.50724	-1.22409	-1.9673	C	-1.96108	2.40341	-2.1568
C	1.2927	-0.27592	-2.62126	C	-2.4139	0.89377	-0.30134
C	2.87724	-0.31747	-0.7901	H	-1.34842	1.379	1.5287
H	2.42103	-1.65427	0.83484	H	-0.52561	3.99042	-1.78022
H	-0.40722	-1.60222	-2.41332	H	-2.14443	2.68942	-3.18766
H	0.98693	0.10386	-3.59037	H	-3.29289	0.72178	-2.26158
H	3.08903	0.92015	-2.53161	C	1.86335	2.74643	0.29217
N	-4.16334	0.34714	0.50468	C	4.08799	1.51005	-0.77313
C	-3.87069	1.38437	-0.41882	C	2.91788	3.53707	-0.14825
C	-3.35794	3.47008	-2.24676	C	1.90327	1.3572	0.23627
C	-2.5654	1.66106	-0.84589	C	3.00521	0.72767	-0.34243
C	-4.91297	2.19085	-0.90625	C	4.04873	2.89523	-0.65664
C	-4.66005	3.20147	-1.83048	H	2.84367	4.61769	-0.09898
C	-2.31538	2.70119	-1.74045	H	1.06797	0.76296	0.59694
H	-1.73183	1.07873	-0.47123	H	4.89347	3.48385	-0.99928
H	-5.4928	3.79081	-2.20278	H	4.9526	1.02234	-1.21272
H	-1.29184	2.89864	-2.04373	N	-3.06988	-0.22817	0.22391
H	-3.16601	4.27105	-2.95241	N	3.01078	-0.6748	-0.51131
C	-5.37037	-0.39089	0.38647	C	-2.50759	-0.9537	1.31305
C	-7.79565	-1.80085	0.13497	C	-1.41246	-2.38748	3.45202
C	-6.54297	0.26055	-0.02901	C	-1.1613	-1.33128	1.29065
C	-5.44056	-1.7549	0.69345	C	-3.30574	-1.30308	2.40654
C	-6.64623	-2.4458	0.57983	C	-2.75888	-2.02454	3.46517
C	-7.73411	-0.44464	-0.1785	C	-0.61757	-2.03492	2.36092
H	-4.55854	-2.28439	1.03333	H	-0.5498	-1.08225	0.42782
H	-6.67301	-3.50044	0.8339	H	-4.35153	-1.01034	2.41941
H	-8.61783	0.08483	-0.5222	H	-3.38645	-2.29152	4.3097
H	-8.73109	-2.34048	0.03449	H	0.42982	-2.32139	2.32836
S	-6.53736	2.00852	-0.24885	H	-0.98674	-2.941	4.28267
N	4.08819	0.12963	-0.17186	C	-4.35101	-0.61147	-0.25815
C	4.05358	1.37279	0.50915	C	-6.87605	-1.39075	-1.17975
C	4.03455	3.82746	1.895	C	-5.35184	0.34453	-0.46079
C	5.13534	1.75126	1.32215	C	-4.62133	-1.95998	-0.51221
C	2.95527	2.23755	0.42287	C	-5.88131	-2.34445	-0.96329
C	2.94425	3.44489	1.12041	C	-6.60374	-0.04587	-0.92879
C	5.13471	2.97692	1.98259	H	-5.14404	1.38937	-0.24899
H	2.09483	1.96663	-0.17733	H	-3.84199	-2.69822	-0.34618
H	2.07345	4.08838	1.04553	H	-6.08242	-3.39384	-1.1554
H	5.99613	3.24775	2.58595	H	-7.37315	0.70437	-1.08232
H	4.0319	4.77108	2.42967	H	-7.85501	-1.6935	-1.53655
C	5.31187	-0.38266	-0.6746	C	1.8476	-1.34581	-0.95935
C	7.77138	-1.37835	-1.62528	C	-0.45221	-2.70128	-1.85031
C	5.37283	-1.14092	-1.85013	C	1.59376	-2.66424	-0.55428
C	6.50401	-0.15558	0.03247	C	0.93112	-0.71196	-1.81423
C	7.72152	-0.62457	-0.45456	C	-0.20927	-1.38577	-2.24429
C	6.5899	-1.64194	-2.3102	C	0.45992	-3.33358	-1.00635
H	4.46894	-1.36222	-2.40426	H	2.28918	-3.16182	0.1145
H	8.62697	-0.41189	0.10608	H	1.10682	0.30963	-2.13833
H	6.60361	-2.23803	-3.2168	H	-0.90984	-0.87161	-2.89556
H	8.7201	-1.75798	-1.9887	H	0.28058	-4.3518	-0.67464
S	6.4493	0.61561	1.61575	H	-1.34238	-3.22123	-2.18874
<b>m-DPA-DPS-DPA</b>				C	4.21316	-1.39079	-0.26266
S	0.38519	3.51874	0.90491	C	6.59913	-2.76456	0.24201
O	0.44712	4.91521	0.55274	C	4.66674	-2.36389	-1.15938
O	0.19296	3.128	2.27957	C	4.95909	-1.10869	0.88646
				C	6.15043	-1.78684	1.12929

C 5.84954 -3.05123 -0.8992  
 H 4.08842 -2.57935 -2.05294  
 H 4.60125 -0.35586 1.58278  
 H 6.72171 -1.55723 2.02327  
 H 6.19281 -3.80562 -1.60039  
 H 7.52384 -3.29758 0.4371

**p-Cz-DPS-Cz**

S 0.0001 -3.23095 1.08678  
 O 0.00012 -3.51047 2.50076  
 O 0.00014 -4.29869 0.11821  
 C -1.39539 -2.19968 0.74346  
 C -3.55232 -0.55984 0.19095  
 C -1.92514 -2.1826 -0.54525  
 C -1.93145 -1.41409 1.76204  
 C -3.0213 -0.59758 1.48501  
 C -3.00342 -1.35153 -0.82365  
 H -1.49543 -2.81501 -1.31538  
 H -1.51804 -1.472 2.76381  
 H -3.48094 -0.00461 2.26916  
 H -3.41942 -1.3024 -1.82478  
 C 1.3955 -2.19957 0.74341  
 C 3.55231 -0.5596 0.19083  
 C 1.92588 -2.18325 -0.54503  
 C 1.93086 -1.41312 1.76171  
 C 3.02063 -0.59655 1.48466  
 C 3.00411 -1.35212 -0.82348  
 H 1.49671 -2.81634 -1.31491  
 H 1.51699 -1.47043 2.76333  
 H 3.42059 -1.30361 -1.82444  
 N -4.6516 0.27763 -0.09081  
 C -5.83394 -0.11192 -0.7241  
 C -8.34163 -0.38155 -1.87106  
 C -6.2278 -1.37666 -1.16819  
 C -6.68635 1.00836 -0.82732  
 C -7.94925 0.86862 -1.40959  
 C -7.48845 -1.49 -1.74409  
 H -5.58449 -2.24358 -1.06202  
 H -8.61347 1.72385 -1.49312  
 H -7.81993 -2.46075 -2.09879  
 H -9.31823 -0.50812 -2.3264  
 C -4.73619 1.63818 0.21132  
 C -5.36918 4.31517 0.54195  
 C -5.98395 2.12763 -0.23173  
 C -3.78662 2.47674 0.80019  
 C -4.1247 3.81595 0.96023  
 C -6.30029 3.47787 -0.05979  
 H -2.81745 2.10573 1.11585  
 H -3.40618 4.49023 1.41553  
 H -7.25712 3.86503 -0.39756  
 H -5.59882 5.36586 0.68467  
 H 3.47974 -0.00292 2.26862  
 N 4.65158 0.27791 -0.0909  
 C 5.83429 -0.11181 -0.72341  
 C 8.34257 -0.38165 -1.86904  
 C 6.68652 1.00857 -0.82694  
 C 6.22862 -1.37674 -1.16651  
 C 7.48956 -1.49019 -1.74176  
 C 7.94972 0.86873 -1.40854  
 H 5.58545 -2.24374 -1.06009  
 H 7.8214 -2.46109 -2.09571

H 8.61381 1.72404 -1.4923  
 H 9.3194 -0.50829 -2.32386  
 C 4.73574 1.63867 0.21038  
 C 5.36806 4.316 0.53961  
 C 3.78573 2.47743 0.79825  
 C 5.98361 2.12809 -0.2324  
 C 6.29962 3.47849 -0.06116  
 C 4.12348 3.81681 0.9576  
 H 2.81647 2.10645 1.11367  
 H 7.25653 3.86562 -0.39872  
 H 3.40462 4.49125 1.41213  
 H 5.59744 5.36683 0.68178

**p-DMAC-DPS-DMAC**

S 0. 3.64675 0.00001  
 O 0.00639 4.35575 -1.25415  
 O -0.00639 4.35574 1.25417  
 C 1.39503 2.55405 0.0098  
 C 3.53825 0.81898 0.02474  
 C 1.96328 2.19188 1.22933  
 C 1.88257 2.07029 -1.2034  
 C 2.9632 1.19417 -1.19063  
 C 3.0464 1.3174 1.23139  
 H 1.57118 2.60475 2.15292  
 H 1.43025 2.38996 -2.13662  
 H 3.37421 0.79972 -2.11469  
 H 3.52083 1.01755 2.1606  
 C -1.39503 2.55405 -0.00978  
 C -3.53825 0.81898 -0.02474  
 C -1.88257 2.07028 1.20342  
 C -1.96328 2.19189 -1.22931  
 C -3.0464 1.3174 -1.23138  
 C -2.96321 1.19417 1.19064  
 H -1.43026 2.38995 2.13664  
 H -1.57118 2.60476 -2.1529  
 H -3.37422 0.79972 2.1147  
 N 4.64684 -0.08024 0.03248  
 C 4.40444 -1.45789 0.13072  
 C 5.94631 0.4403 -0.06372  
 C 5.47345 -2.3711 0.13908  
 C 7.0595 -0.4181 -0.06339  
 C 6.93477 -1.93678 0.04245  
 C 7.57013 -2.58282 -1.20781  
 C 7.68629 -2.41621 1.30335  
 C 3.0824 -1.93091 0.22117  
 H 2.25573 -1.23044 0.21378  
 C 2.81929 -3.2904 0.32122  
 H 1.78995 -3.62815 0.3915  
 C 3.86759 -4.20688 0.33237  
 H 3.67601 -5.27157 0.4107  
 C 5.17173 -3.73263 0.24091  
 H 5.98832 -4.44903 0.24927  
 H 7.51497 -3.67374 -1.15287  
 H 8.62439 -2.30544 -1.29595  
 H 7.05069 -2.25617 -2.11327  
 H 8.74284 -2.13754 1.25586  
 H 7.2514 -1.96819 2.20142  
 H 7.63104 -3.50433 1.39904  
 C 6.13677 1.83081 -0.15928  
 H 5.28177 2.49637 -0.15787



C	7.41345	2.36765	-0.25544	H	-3.46427	-0.56376	1.90191
H	7.53204	3.4441	-0.32793	H	-3.3998	-0.7679	-2.3773
C	8.52606	1.53013	-0.25797	N	4.64741	0.29076	-0.36538
H	9.52883	1.93668	-0.3325	C	4.39162	1.67469	-0.26543
C	8.33038	0.15672	-0.16189	C	4.00921	4.45395	-0.1198
H	9.19969	-0.49475	-0.16264	C	5.48333	2.55165	-0.18112
N	-4.64684	-0.08024	-0.03248	C	3.10508	2.21567	-0.27596
H	-3.52083	1.01756	-2.16059	C	2.91774	3.59831	-0.20958
C	-5.94631	0.4403	0.06372	C	5.30014	3.92123	-0.10038
C	-4.40444	-1.45789	-0.13072	H	2.24704	1.55632	-0.34707
C	-7.0595	-0.41811	0.06338	H	1.90874	3.99665	-0.2286
C	-5.47345	-2.3711	-0.13909	H	6.17865	4.55438	-0.03455
C	-6.93477	-1.93678	-0.04246	H	3.86754	5.5277	-0.06636
C	-3.08239	-1.93091	-0.22116	C	5.91991	-0.1682	0.03761
H	-2.25573	-1.23044	-0.21376	C	8.50868	-0.97161	0.77258
C	-5.17172	-3.73263	-0.2409	C	6.19117	-1.50553	0.32981
H	-5.98832	-4.44903	-0.24925	C	6.96982	0.75849	0.11558
C	-2.81928	-3.2904	-0.32119	C	8.24546	0.36965	0.48613
H	-1.78994	-3.62815	-0.39147	C	7.48068	-1.90338	0.69013
C	-3.86758	-4.20689	-0.33235	H	5.39697	-2.24114	0.26578
H	-3.676	-5.27157	-0.41067	H	9.02068	1.12718	0.53342
C	-6.13677	1.8308	0.15927	H	7.66963	-2.94959	0.90554
H	-5.28177	2.49637	0.15787	H	9.51037	-1.27693	1.05414
C	-8.33038	0.15672	0.16185	O	6.77683	2.08004	-0.2246
H	-9.1997	-0.49476	0.16259	N	-4.62277	0.33116	-0.31997
C	-7.41345	2.36764	0.25541	C	-4.3798	1.70106	-0.08608
H	-7.53204	3.44409	0.32789	C	-4.0212	4.45758	0.31984
C	-8.52606	1.53013	0.25793	C	-3.0979	2.24053	0.02952
H	-9.52884	1.93668	0.33244	C	-5.47896	2.56825	0.00282
C	-7.57013	-2.58282	1.20779	C	-5.30808	3.92584	0.21183
C	-7.68629	-2.4162	-1.30337	C	-2.92201	3.61238	0.22547
H	-7.0507	-2.25617	2.11325	H	-2.23371	1.58958	-0.04398
H	-8.62439	-2.30545	1.29593	H	-6.19218	4.55138	0.27555
H	-7.51496	-3.67375	1.15285	H	-1.91584	4.01031	0.30511
H	-8.74284	-2.13751	-1.25588	H	-3.88844	5.52266	0.47435
H	-7.63107	-3.50432	-1.39905	C	-5.91533	-0.15951	-0.03515
H	-7.25139	-1.9682	-2.20144	C	-8.54012	-1.01985	0.47142
<b>p-PXZ-DPS-PXZ</b>				C	-6.97265	0.75778	0.05271
S	-0.00247	-3.41992	-0.05144	C	-6.1967	-1.51591	0.13286
O	-0.00116	-4.03145	1.253	C	-7.50401	-1.94167	0.37925
O	-0.00977	-4.22047	-1.24893	C	-8.26673	0.34025	0.31081
C	1.39632	-2.33514	-0.13944	H	-5.39592	-2.24363	0.0611
C	3.54043	-0.60925	-0.28096	H	-7.70033	-3.00177	0.49873
C	1.8977	-1.78173	1.03913	H	-9.04727	1.09135	0.37112
C	1.95131	-2.04751	-1.38323	H	-9.55572	-1.3472	0.66443
C	3.03649	-1.17558	-1.44959	O	-6.76452	2.10271	-0.16525
C	2.97842	-0.91113	0.96298	<b>p-PTZ-DPS-PTZ</b>			
H	1.45487	-2.0453	1.99414	S	0.00147	-3.41109	0.04852
H	1.54879	-2.5134	-2.27662	O	0.00888	-4.07291	-1.23175
H	3.50174	-0.9302	-2.39858	O	-0.01113	-4.1655	1.27547
H	3.3984	-0.46423	1.8594	C	1.40174	-2.32698	0.10358
C	-1.39197	-2.32222	-0.127	C	3.57489	-0.6286	0.18759
C	-3.52082	-0.57599	-0.24687	C	1.99907	-2.0529	1.32981
C	-1.89711	-1.95667	-1.37201	C	1.87216	-1.76972	-1.08619
C	-1.93606	-1.83723	1.0622	C	2.96602	-0.91433	-1.03908
C	-3.01062	-0.9574	0.99698	C	3.09741	-1.19553	1.36644
C	-2.9734	-1.0738	-1.42766	H	1.61957	-2.51881	2.2333
H	-1.46347	-2.37024	-2.27665	H	1.39755	-2.02221	-2.02918
H	-1.5308	-2.16152	2.01507	H	3.3635	-0.47171	-1.94823

H	3.59744	-0.96542	2.30155	C	-1.39407	-2.21091	-0.07453
C	-1.3909	-2.31589	0.07252	C	-3.56813	-0.46465	-0.18844
C	-3.54832	-0.59694	0.1123	C	-1.86028	-1.76855	-1.3124
C	-1.8537	-1.83823	1.296	C	-2.00445	-1.7901	1.1063
C	-1.99004	-1.95509	-1.13354	C	-3.08257	-0.91908	1.05093
C	-3.08035	-1.09249	-1.10814	C	-2.94368	-0.9046	-1.36972
C	-2.94088	-0.96817	1.31035	H	-1.39239	-2.12665	-2.22413
H	-1.37913	-2.15674	2.21873	H	-1.63419	-2.14941	2.06131
H	-1.61663	-2.36475	-2.06634	H	-3.55759	-0.58702	1.96774
H	-3.58107	-0.80361	-2.02808	H	-3.32273	-0.57419	-2.33076
H	-3.33553	-0.57881	2.24308	C	1.39401	-2.21084	0.07459
N	4.71421	0.23645	0.25722	C	3.56801	-0.46451	0.1884
C	5.96989	-0.31663	-0.10569	C	2.00431	-1.79	-1.10627
C	8.48864	-1.37085	-0.80359	C	1.86024	-1.76846	1.31244
C	7.14748	0.41136	0.13184	C	2.94362	-0.90447	1.36971
C	6.08181	-1.59142	-0.67442	C	3.08239	-0.91894	-1.05095
C	7.33081	-2.11395	-1.00677	H	1.63401	-2.14932	-2.06126
C	8.38789	-0.10055	-0.24014	H	1.39242	-2.12659	2.22419
H	5.19674	-2.191	-0.84938	H	3.3227	-0.57405	2.33073
H	7.38743	-3.10934	-1.43532	H	3.55738	-0.58686	-1.96777
H	9.27669	0.49729	-0.06072	N	-4.66265	0.40824	-0.24705
H	9.45985	-1.77155	-1.07299	N	4.66254	0.40838	0.24695
C	4.48521	1.63201	0.15435	C	-5.6792	0.37064	0.74718
C	4.08406	4.41683	-0.02287	C	-7.70024	0.31327	2.68172
C	3.22804	2.15736	-0.16854	C	-6.20616	-0.85179	1.17721
C	5.53396	2.53041	0.41401	C	-6.17195	1.56376	1.28515
C	5.33945	3.90425	0.2968	C	-7.18319	1.53142	2.24175
C	3.03067	3.53567	-0.24241	C	-7.20426	-0.87612	2.14721
H	2.39093	1.49408	-0.34903	H	-5.82911	-1.77696	0.75125
H	6.17705	4.56979	0.48381	H	-5.76329	2.51036	0.94409
H	2.04177	3.91345	-0.48192	H	-7.56039	2.46347	2.65096
H	3.93473	5.48888	-0.09167	H	-7.60453	-1.82998	2.47641
S	7.07378	1.92939	1.02279	H	-8.48413	0.29003	3.43176
N	-4.68003	0.2793	0.16304	C	-4.7828	1.3486	-1.30758
C	-4.49295	1.62389	-0.24589	C	-5.03406	3.21526	-3.37717
C	-4.17766	4.31252	-1.03462	C	-3.68508	2.12686	-1.6898
C	-3.29933	2.06635	-0.82952	C	-6.00788	1.51244	-1.96125
C	-5.5166	2.56323	-0.03474	C	-6.13079	2.44764	-2.98566
C	-5.36865	3.88315	-0.45298	C	-3.81155	3.04753	-2.72645
C	-3.14293	3.39937	-1.20684	H	-2.73723	2.00386	-1.17393
H	-2.47874	1.3759	-0.98006	H	-6.85849	0.90903	-1.65838
H	-6.18827	4.57785	-0.29525	H	-7.0869	2.56819	-3.48541
H	-2.20253	3.71475	-1.64762	H	-2.95299	3.6453	-3.01628
H	-4.0626	5.34662	-1.34065	H	-5.13192	3.93936	-4.17926
C	-5.96286	-0.32414	0.08735	C	4.78284	1.34865	1.30753
C	-8.53157	-1.47627	-0.03918	C	5.03437	3.21513	3.37725
C	-7.11125	0.44471	0.33737	C	6.00798	1.51235	1.96113
C	-6.12578	-1.68355	-0.2065	C	3.6852	2.12697	1.68988
C	-7.39779	-2.25218	-0.25536	C	3.8118	3.04754	2.7266
C	-8.38045	-0.12122	0.24744	C	6.13102	2.44746	2.98562
H	-5.26143	-2.31137	-0.38658	H	6.85853	0.90891	1.65817
H	-7.49202	-3.31099	-0.47372	H	2.73731	2.00408	1.17407
H	-9.24826	0.50655	0.42751	H	2.95331	3.64535	3.01654
H	-9.52214	-1.91521	-0.08902	H	7.08717	2.56789	3.48532
S	-6.94647	2.10985	0.88879	H	5.13234	3.93915	4.17941
				C	5.67911	0.37064	-0.74727
				C	7.70018	0.31305	-2.68176
				C	6.17201	1.56371	-1.28522
				C	6.20595	-0.85184	-1.17728
				C	7.20407	-0.87628	-2.14726
<b>p-DPA-DPS-DPA</b>							
S	-0.00001	-3.28589	0.00005				
O	-0.06752	-4.00064	1.25259				
O	0.06755	-4.00068	-1.25247				

C	7.18326	1.53126	-2.2418
H	5.76344	2.51036	-0.94415
H	5.82879	-1.77697	-0.75133
H	7.60423	-1.83019	-2.47646
H	7.56058	2.46328	-2.651
H	8.48409	0.28973	-3.43179

**TXO2-PXZ(NO)**

C	-1.264974	-0.999828	-0.009747
C	-3.631053	-0.688572	-1.559449
C	-1.361746	-1.441214	-1.337306
C	-2.408060	-0.384989	0.515257
C	-3.568037	-0.239711	-0.241407
C	-2.508034	-1.285697	-2.114918
H	-2.428044	0.006660	1.524652
H	-2.502865	-1.624437	-3.145862
H	-4.542469	-0.556728	-2.134505
S	-0.000017	-2.252288	-2.108988
O	0.000014	-3.646927	-1.737240
O	-0.000033	-1.929899	-3.513760
C	1.361692	-1.441164	-1.337324
C	3.567973	-0.239627	-0.241441
C	1.264925	-0.999785	-0.009764
C	2.507968	-1.285617	-2.114951
C	3.630981	-0.688477	-1.559487
C	2.408004	-0.384922	0.515231
H	2.502793	-1.624354	-3.145895
H	4.542393	-0.556618	-2.134548
H	2.427994	0.006717	1.524629
C	-0.000015	-1.212719	0.836805
C	-0.000026	-0.289628	2.063132
H	-0.870857	-0.492938	2.688492
H	-0.000021	0.769233	1.787036
H	0.870789	-0.492943	2.688513
C	0.000015	-2.672547	1.366939
H	0.000034	-3.403546	0.558021
H	-0.888665	-2.830341	1.985429
H	0.888697	-2.830303	1.985435
N	-4.700552	0.391664	0.360291
C	-5.008898	1.718193	-0.007205
C	-5.705705	4.368804	-0.622129
C	-6.201486	2.281929	0.470048
C	-4.170151	2.507381	-0.795392
C	-4.516613	3.826927	-1.095499
C	-6.553948	3.584667	0.162954
H	-3.239844	2.093889	-1.168981
H	-3.845976	4.423634	-1.704539
H	-7.488496	3.970942	0.555981
H	-5.978339	5.392177	-0.855061
C	-5.759710	-0.423453	0.812515
C	-7.915573	-1.936151	1.787948
C	-5.686673	-1.816430	0.854907
C	-6.931772	0.198077	1.268032
C	-8.000449	-0.542761	1.741988
C	-6.758210	-2.566108	1.346013
H	-4.788364	-2.317552	0.511368
H	-8.884379	-0.012433	2.080311
H	-6.676272	-3.647353	1.376043
H	-8.749887	-2.515500	2.167645

O	-7.036645	1.571743	1.305064
N	4.700511	0.391699	0.360271
C	5.759554	-0.423517	0.812617
C	7.915179	-1.936370	1.788323
C	5.686377	-1.816483	0.855066
C	6.931639	0.197921	1.268198
C	8.000201	-0.542993	1.742292
C	6.757796	-2.566237	1.346312
H	4.788053	-2.317542	0.511479
H	8.884153	-0.012733	2.080666
H	6.675753	-3.647472	1.376389
H	8.749398	-2.515782	2.168135
C	5.009058	1.718146	-0.007342
C	5.706247	4.368603	-0.622474
C	6.201665	2.281784	0.469970
C	4.170480	2.507354	-0.795692
C	4.517133	3.826823	-1.095904
C	6.554319	3.584447	0.162772
H	3.240154	2.093931	-1.169314
H	3.846630	4.423554	-1.705066
H	7.488873	3.970653	0.555853
H	5.979028	5.391919	-0.855486
O	7.036645	1.571581	1.305152

**DBTO-PXZ(NO)**

C	0.74015	1.78723	0.00067
C	3.50269	2.21995	0.00041
C	1.28487	3.07486	0.00122
C	1.59968	0.69572	-0.00003
C	2.9789	0.92729	-0.00012
C	2.64556	3.32345	0.00109
H	1.22861	-0.32551	-0.00045
H	3.0355	4.33595	0.00155
H	4.57946	2.35059	0.00031
S	0.00004	4.296	0.00238
O	0.00044	5.03817	1.23804
O	-0.00038	5.03983	-1.23229
C	-1.2848	3.07485	0.00198
C	-2.97883	0.92728	0.00125
C	-0.74008	1.78722	0.00106
C	-2.64549	3.32345	0.00251
C	-3.50262	2.21994	0.00217
C	-1.59961	0.69572	0.00065
H	-3.03543	4.33594	0.00321
H	-4.57939	2.35058	0.0026
H	-1.22854	-0.32551	-0.00009
N	-3.87889	-0.18359	0.00084
N	3.87897	-0.18358	-0.00067
C	-4.06116	-0.89468	1.20674
C	-4.53482	-2.37048	3.55006
C	-4.79591	-2.08904	1.17365
C	-3.57102	-0.45067	2.43603
C	-3.81272	-1.18345	3.60064
C	-5.02485	-2.82527	2.3235
H	-3.00809	0.47476	2.48823
H	-3.42835	-0.81473	4.54564
H	-5.59643	-3.74401	2.24281
H	-4.72193	-2.94315	4.45167

C	-4.06344	-0.89184	-1.20639	H	-0.870866	-0.175450	-2.382567
C	-4.54145	-2.36216	-3.55227	C	-0.000004	-2.597705	-1.582078
C	-3.57549	-0.44501	-2.43553	H	0.000007	-3.490435	-0.956123
C	-4.79815	-2.08627	-1.17473	H	0.888944	-2.613937	-2.219952
C	-5.02923	-2.81981	-2.32587	H	-0.888964	-2.613946	-2.219935
C	-3.81937	-1.17507	-3.60141	N	4.709833	0.152476	0.085194
H	-3.01258	0.4805	-2.4866	N	-4.709831	0.152480	0.085197
H	-5.60069	-3.73872	-2.24627	C	-4.853873	1.486481	0.493065
H	-3.4367	-0.80417	-4.54624	C	-5.099701	4.151994	1.340457
H	-4.73024	-2.93272	-4.45486	C	-3.892103	2.066138	1.340679
C	4.06225	-0.89391	1.20554	C	-5.953102	2.249271	0.061220
C	4.53782	-2.36823	3.54941	C	-6.046139	3.573001	0.502030
C	4.79689	-2.08833	1.17259	C	-4.015821	3.384239	1.758750
C	3.57317	-0.44909	2.43496	H	-3.044141	1.481078	1.676501
C	3.81582	-1.18113	3.59984	H	-6.891228	4.173429	0.177322
C	5.02677	-2.82385	2.32272	H	-3.260150	3.806127	2.413843
H	3.01033	0.4764	2.48704	H	-5.208618	5.182621	1.660398
H	3.43227	-0.81178	4.54492	C	-5.635444	-0.467447	-0.767047
H	5.59822	-3.74267	2.24213	C	-7.461679	-1.754045	-2.467760
H	4.72566	-2.94034	4.45122	C	-5.441778	-1.806323	-1.153869
C	4.06238	-0.89267	-1.20759	C	-6.756938	0.238714	-1.235922
C	4.53824	-2.36456	-3.55291	C	-7.647103	-0.431162	-2.081015
C	3.57339	-0.44661	-2.4366	C	-6.346231	-2.440570	-1.994836
C	4.79704	-2.08711	-1.17578	H	-4.580366	-2.355178	-0.792030
C	5.02707	-2.82142	-2.32664	H	-8.518713	0.102150	-2.449791
C	3.81619	-1.17745	-3.6022	H	-6.173493	-3.474554	-2.276206
H	3.01051	0.47891	-2.48778	H	-8.176199	-2.238053	-3.124743
H	5.59855	-3.74031	-2.24694	C	4.853877	1.486474	0.493071
H	3.43272	-0.80715	-4.54694	C	5.099710	4.151980	1.340480
H	4.72621	-2.93572	-4.4553	C	3.892110	2.066127	1.340690
O	-5.35865	-2.54246	-0.00054	C	5.953107	2.249265	0.061230
O	5.35857	-2.54255	-0.0018	C	6.046147	3.572992	0.502048

**TXO2-DMAC**

C	1.265602	-1.274257	0.132421	H	3.044147	1.481065	1.676509
C	3.631647	-1.311548	1.713316	H	6.891236	4.173421	0.177343
C	1.361467	-1.996630	1.332377	H	3.260160	3.806109	2.413866
C	2.409524	-0.564124	-0.244919	H	5.208629	5.182605	1.660427
C	3.571782	-0.588981	0.525628	C	5.635440	-0.467446	-0.767059
C	2.506390	-2.015036	2.124897	C	7.461669	-1.754035	-2.467786
H	2.429345	0.037255	-1.145865	C	6.756936	0.238715	-1.235929
H	2.500146	-2.570226	3.057285	C	5.441768	-1.806317	-1.153894
H	4.542832	-1.306835	2.302593	C	6.346218	-2.440559	-1.994868
S	0.000000	-2.958272	1.904529	C	7.647098	-0.431156	-2.081028
O	-0.000004	-4.235501	1.231583	H	4.580355	-2.355172	-0.792059
O	0.000003	-2.957863	3.346040	H	6.173475	-3.474540	-2.276248
C	-1.361466	-1.996626	1.332383	H	8.518711	0.102156	-2.449800
C	-3.571780	-0.588975	0.525633	H	8.176187	-2.238040	-3.124772
C	-1.265603	-1.274257	0.132425	C	7.038068	1.691890	-0.858335
C	-2.506386	-2.015024	2.124906	C	8.399617	1.768893	-0.134082
C	-3.631643	-1.311535	1.713325	H	8.639475	2.801823	0.133963
C	-2.409524	-0.564125	-0.244917	H	9.202646	1.393910	-0.775062
H	-2.500141	-2.570211	3.057296	H	8.380659	1.170267	0.781120
H	-4.542825	-1.306816	2.302606	C	7.094949	2.544523	-2.144404
H	-2.429346	0.037246	-1.145870	H	7.315123	3.589619	-1.909120
C	-0.000003	-1.293267	-0.739589	H	6.138274	2.504041	-2.673130
C	-0.000013	-0.118391	-1.727596	H	7.876787	2.181829	-2.817658
H	0.870784	-0.175490	-2.382636	C	-7.038064	1.691893	-0.858341
H	0.000029	0.851043	-1.219860	C	-8.399614	1.768906	-0.134089
				H	-8.639469	2.801840	0.133946
				H	-8.380659	1.170288	0.781118

H	-9.202643	1.393920	-0.775067
C	-7.094941	2.544515	-2.144417
H	-7.315112	3.589614	-1.909141
H	-7.876780	2.181819	-2.817669
H	-6.138266	2.504025	-2.673142

**DBTO-DMAC(ACR)**

C	-0.740317	1.906416	0.000027
C	-3.501234	2.338713	0.000058
C	-1.283456	3.193163	0.000053
C	-1.601532	0.813637	0.000011
C	-2.978920	1.042643	0.000031
C	-2.645554	3.440838	0.000068
H	-1.234407	-0.208504	-0.000012
H	-3.032672	4.454627	0.000086
H	-4.578688	2.469356	0.000069
S	-0.000000	4.417530	0.000078
O	-0.000017	5.153707	-1.236865
O	0.000017	5.153607	1.237081
C	1.283455	3.193163	0.000024
C	2.978919	1.042643	-0.000020
C	0.740316	1.906416	0.000014
C	2.645553	3.440837	0.000010
C	3.501234	2.338712	-0.000014
C	1.601531	0.813637	-0.000005
H	3.032672	4.454626	0.000019
H	4.578688	2.469355	-0.000025
H	1.234406	-0.208504	-0.000009
N	3.870157	-0.071526	-0.000038
N	-3.870158	-0.071526	0.000023
C	4.297778	-0.600759	-1.227270
C	5.124124	-1.624605	-3.706961
C	5.177933	-1.696235	-1.262190
C	3.842835	-0.031706	-2.430656
C	4.252730	-0.539666	-3.655996
C	5.569882	-2.181957	-2.513469
H	3.165330	0.813625	-2.408800
H	3.886815	-0.081448	-4.569330
H	6.249626	-3.028276	-2.555422
H	5.452204	-2.031027	-4.657522
C	4.297832	-0.600751	1.227178
C	5.124286	-1.624577	3.706840
C	3.842951	-0.031680	2.430579
C	5.177980	-1.696233	1.262068
C	5.569984	-2.181945	2.513333
C	4.252898	-0.539632	3.655905
H	3.165453	0.813657	2.408746
H	6.249726	-3.028267	2.555265
H	3.887035	-0.081397	4.569252
H	5.452402	-2.030997	4.657390
C	-4.297729	-0.600823	1.227245
C	-5.123998	-1.624778	3.706916
C	-5.177875	-1.696306	1.262144
C	-3.842756	-0.031817	2.430642
C	-4.252610	-0.539834	3.655972
C	-5.569790	-2.182080	2.513413
H	-3.165264	0.813525	2.408803
H	-3.886674	-0.081650	4.569315
H	-5.452050	-2.031241	4.657469
C	-4.297884	-0.600685	-1.227203

C	-5.124416	-1.624401	-3.706884
C	-3.843039	-0.031563	-2.430594
C	-5.178036	-1.696164	-1.262114
C	-5.570075	-2.181824	-2.513389
C	-4.253028	-0.539457	-3.655929
H	-3.165532	0.813767	-2.408744
H	-6.249810	-3.028150	-2.555336
H	-3.887191	-0.081185	-4.569267
H	-5.452561	-2.030780	-4.657442
C	5.715430	-2.368181	-0.000072
C	7.256899	-2.278935	-0.000098
H	7.675041	-2.769218	-0.883790
H	7.675066	-2.769235	0.883574
H	7.579713	-1.233899	-0.000092
C	5.289687	-3.852499	-0.000073
H	5.676224	-4.367924	-0.883895
H	4.199262	-3.938190	-0.000045
H	5.676271	-4.367946	0.883716
H	-6.249537	-3.028398	2.555350
C	-5.715425	-2.368184	0.000012
C	-5.289674	-3.852501	-0.000101
H	-5.676276	-4.367886	-0.883918
H	-5.676187	-4.367992	0.883693
H	-4.199248	-3.938186	-0.000160
C	-7.256894	-2.278948	0.000117
H	-7.675103	-2.769210	-0.883555
H	-7.579715	-1.233913	0.000176
H	-7.674989	-2.769274	0.883809

**Cz-TTR**

H	0.93906	-2.45085	-2.08546
C	0.58437	-1.6094	-1.49997
C	-0.2954	0.5392	0.06969
C	1.49434	-0.68002	-1.01222
C	-0.77413	-1.44248	-1.24392
C	-1.21774	-0.37511	-0.45868
C	1.0476	0.39276	-0.23338
H	-1.49407	-2.14084	-1.65672
H	-0.62075	1.3368	0.73013
S	3.20922	-0.88806	-1.41102
O	3.44181	-2.28467	-1.666
O	3.57608	0.07714	-2.41146
S	2.17731	1.60472	0.41217
O	2.57636	2.47297	-0.66153
O	1.59286	2.17491	1.59606
C	3.56405	0.6108	0.89897
C	5.76897	-0.87769	1.69477
C	4.0087	-0.46044	0.11527
C	4.2082	0.92891	2.08694
C	5.32608	0.18711	2.47405
C	5.10081	-1.21772	0.51651
H	3.8312	1.74057	2.69992
H	5.41403	-2.06499	-0.08408
H	6.62772	-1.46094	2.00813
H	5.83854	0.43644	3.39658
N	-2.58425	-0.22148	-0.17475
C	-3.3127	0.96721	-0.29959
C	-5.18038	3.00896	-0.4198
C	-2.89886	2.21666	-0.76717
C	-4.64839	0.72317	0.08347

C	-5.58747	1.7567	0.02454
C	-3.85089	3.22961	-0.81584
H	-1.88043	2.39998	-1.09216
H	-6.61828	1.58025	0.31677
H	-3.55573	4.21119	-1.17216
H	-5.89524	3.82338	-0.46986
C	-3.44291	-1.22457	0.28894
C	-5.50532	-2.80553	1.25
C	-4.73099	-0.67449	0.46158
C	-3.16277	-2.55343	0.61525
C	-4.21254	-3.33162	1.09248
C	-5.7698	-1.4762	0.94285
H	-2.16674	-2.97049	0.51476
H	-4.02294	-4.36831	1.3514
H	-6.76465	-1.06307	1.07954
H	-6.30021	-3.44257	1.62305

**DMAC-TTR (Planar)**

N	-2.26075	-0.25742	-0.69249
C	-3.29207	-1.1955	-0.37404
C	-5.37573	-2.92322	0.22189
C	-4.16089	-0.86988	0.67701
C	-3.47684	-2.34384	-1.14189
C	-4.5133	-3.21982	-0.83143
C	-5.20717	-1.75083	0.95824
C	-2.7084	1.1016	-0.67591
C	-3.69122	3.69251	-0.64026
C	-2.37796	1.97853	-1.70729
C	-3.56172	1.48695	0.36791
C	-4.05055	2.7946	0.36472
C	-2.85721	3.28534	-1.6789
C	-3.90528	0.43833	1.42762
C	-5.10616	0.85473	2.27865
C	-2.69051	0.25313	2.36938
H	-6.19275	-3.59565	0.46232
H	-2.81599	-2.53706	-1.98169
H	-4.6567	-4.11775	-1.42324
H	-5.906	-1.52601	1.75633
H	-4.07697	4.70648	-0.61756
H	-1.75708	1.63165	-2.5279
H	-4.72152	3.12471	1.15003
H	-2.59311	3.97364	-2.47471
H	-5.31626	0.09479	3.03575
H	-6.00481	1.00345	1.67184
H	-4.88798	1.78215	2.81433
H	-1.79112	-0.04856	1.82696
H	-2.47843	1.19378	2.88701
H	-2.91559	-0.51624	3.11459
C	-0.91556	-0.59175	-0.60714
C	1.82353	-1.2725	-0.43821
C	-0.5003	-1.91664	-0.35622
C	0.08504	0.40319	-0.70163
C	1.41924	0.05008	-0.64234
C	0.84469	-2.24467	-0.26397
H	-1.23352	-2.69626	-0.19906
H	-0.16715	1.45217	-0.79262
H	1.14264	-3.26416	-0.0418
S	3.51957	-1.74342	-0.36697
O	3.61773	-2.94043	0.42713
O	4.0865	-1.73183	-1.68714

S	2.61149	1.35492	-0.83741
O	3.18334	1.262	-2.15149
O	2.00439	2.58978	-0.41753
C	3.8509	0.91913	0.35979
C	5.83344	0.31531	2.20809
C	4.24204	-0.40865	0.56079
C	4.43683	1.94402	1.09133
C	5.44378	1.63673	2.00776
C	5.22191	-0.71716	1.49487
H	4.09696	2.96398	0.94588
H	5.91076	2.43398	2.57573
H	5.48911	-1.75535	1.66191
H	6.60524	0.07972	2.9328

**PXZ-TTR**

H	1.15797	-0.16965	3.30375
C	0.72921	-0.22965	2.30897
C	-0.32747	-0.3026	-0.28896
C	1.56011	-0.43523	1.21664
C	-0.64554	-0.09743	2.10496
C	-1.16894	-0.13235	0.81638
C	1.03178	-0.4747	-0.07898
H	-1.319	0.05396	2.94207
H	-0.73035	-0.29255	-1.29817
S	3.29875	-0.65596	1.51919
O	3.62035	0.01719	2.74824
O	3.61889	-2.04616	1.36618
S	2.06663	-0.75176	-1.5
O	2.43263	-2.13873	-1.53499
O	1.4216	-0.15532	-2.63756
C	3.50381	0.21654	-1.11088
C	5.78051	1.7159	-0.57997
C	4.03227	0.25756	0.1839
C	4.10083	0.9366	-2.13697
C	5.25455	1.67511	-1.86817
C	5.16065	1.01874	0.45857
H	3.6577	0.92112	-3.12712
H	5.53708	1.06644	1.47492
H	6.66751	2.30463	-0.37309
H	5.73053	2.23174	-2.66799
N	-2.56906	0.04936	0.62672
C	-3.33648	-1.03472	0.14228
C	-4.98488	-3.11499	-0.77163
C	-2.83715	-2.33157	0.01797
C	-4.67892	-0.80063	-0.18725
C	-5.49348	-1.82065	-0.64809
C	-3.66007	-3.36538	-0.4341
H	-1.8075	-2.54319	0.2843
H	-6.52384	-1.58524	-0.89276
H	-3.25117	-4.36635	-0.51875
H	-5.6254	-3.91502	-1.12586
C	-3.03612	1.35433	0.34751
C	-4.09771	3.90043	-0.17369
C	-4.38894	1.51895	0.01767
C	-2.22224	2.48624	0.40316
C	-2.75449	3.7528	0.1508
C	-4.916	2.77135	-0.24663
H	-1.17195	2.38423	0.65296
H	-2.10511	4.61971	0.20808
H	-5.96881	2.84342	-0.49824

H -4.51365 4.88202 -0.37197  
O -5.24702 0.44237 -0.01029

**PTZ-TTR (Planar)**

H 5.29108 -1.88227 -1.56922  
C 5.05056 -0.83497 -1.4195  
C 4.33404 1.85217 -1.06298  
C 4.05957 -0.48758 -0.51117  
C 5.7074 0.1712 -2.13004  
C 5.35189 1.50551 -1.95293  
C 3.70265 0.85312 -0.33364  
H 6.48761 -0.09481 -2.83494  
H 5.85425 2.2823 -2.51909  
H 4.02027 2.883 -0.93688  
S 3.27952 -1.79044 0.41479  
O 3.36127 -2.99919 -0.36303  
O 3.81621 -1.77948 1.74752  
S 2.4485 1.33787 0.82864  
O 2.9857 1.24504 2.15738  
O 1.88637 2.58399 0.38051  
C 1.22494 0.0647 0.61959  
C -0.74184 -1.85932 0.33744  
C 1.59508 -1.27207 0.44452  
C -0.10053 0.45405 0.64502  
C -1.11912 -0.5176 0.53903  
C 0.59577 -2.22448 0.27786  
H -0.33222 1.50913 0.72828  
H 0.87221 -3.25666 0.08917  
H -1.4978 -2.62183 0.19947  
N -2.46065 -0.14821 0.61993  
C -3.48319 -1.08065 0.26102  
C -5.44266 -2.89785 -0.5153  
C -3.84071 -2.12118 1.11638  
C -4.14004 -0.91897 -0.96299  
C -5.12608 -1.82895 -1.34944  
C -4.80879 -3.0403 0.7205  
H -3.34008 -2.20883 2.07613  
H -5.64379 -1.69087 -2.29348  
H -5.07486 -3.86007 1.37907  
H -6.20382 -3.60797 -0.82103  
C -2.84119 1.22447 0.48753  
C -3.55127 3.8932 0.14483  
C -2.65942 2.12904 1.53186  
C -3.42536 1.64369 -0.71221  
C -3.78588 2.98156 -0.88118  
C -2.99747 3.46799 1.35336  
H -2.2341 1.77677 2.46697  
H -4.25249 3.29902 -1.80843  
H -2.83523 4.17604 2.15874  
H -3.82239 4.93468 0.00761  
S -3.71618 0.45609 -1.98881

**PTZ-TTR (Orthogonal)**

H -0.1187 0.41835 0.35919  
C -0.0095 0.15159 1.40961  
C 0.27525 -0.50105 4.11343  
C 0.02949 -1.18945 1.80867  
C 0.09748 1.16179 2.36643  
C 0.23956 0.83611 3.71567  
C 0.17108 -1.51405 3.15313

H 0.0722 2.20574 2.0598  
H 0.3248 1.62655 4.45894  
H 0.38783 -0.74279 5.16958  
S -0.13121 -2.44876 0.58468  
O -0.99503 -1.90236 -0.44496  
O 1.20037 -2.92355 0.28359  
S 0.19537 -3.19677 3.68201  
O 1.53606 -3.69116 3.46427  
O -0.41886 -3.21289 4.99592  
C -0.87134 -4.12989 2.63346  
C -2.5864 -5.62112 1.01122  
C -1.01369 -3.80659 1.2881  
C -1.5862 -5.2006 3.18128  
C -2.44599 -5.95419 2.36833  
C -1.87438 -4.54902 0.47102  
H -1.47936 -5.46412 4.23301  
H -1.9921 -4.30595 -0.58425  
H -3.25175 -6.2059 0.37836  
N -3.17504 -7.06339 2.9195  
C -2.54903 -8.37183 2.91144  
C -1.24526 -10.9025 2.85825  
C -1.25028 -8.54586 2.36782  
C -3.1755 -9.51881 3.4282  
C -2.52075 -10.76717 3.39713  
C -0.60808 -9.78775 2.34149  
H -0.69823 -7.7101 1.94636  
H -3.01003 -11.65275 3.7997  
H 0.38901 -9.87466 1.9168  
H -0.75636 -11.87274 2.84428  
C -4.49781 -6.82028 3.4618  
C -7.08531 -6.25368 4.50597  
C -5.05442 -5.51558 3.44549  
C -5.28906 -7.83674 4.02362  
C -6.56915 -7.54523 4.53776  
C -6.32502 -5.23521 3.95781  
H -4.50639 -4.6753 3.02906  
H -7.17801 -8.3365 4.97252  
H -6.71276 -4.22019 3.92562  
H -8.0738 -6.04912 4.90807  
S -4.79351 -9.53199 4.14712

**Cz-Ph-TTR**

H 3.16686 -1.06775 3.09203  
C 2.73295 -0.86667 2.11814  
C 1.64796 -0.27899 -0.39136  
C 3.56588 -0.7142 1.01748  
C 1.35384 -0.76066 1.95336  
C 0.79222 -0.46484 0.70575  
C 3.01747 -0.4228 -0.23522  
H 0.70641 -0.91635 2.81031  
H 1.25597 0.00902 -1.36195  
S 5.31414 -0.90468 1.25444  
O 5.61281 -0.57703 2.62281  
O 5.72213 -2.17588 0.72722  
S 4.04209 -0.22527 -1.67438  
O 4.48512 -1.52118 -2.10437  
O 3.34933 0.63016 -2.5999  
C 5.43161 0.6746 -1.02979  
C 7.63488 2.08964 -0.10499

C	5.97739	0.38312	0.22475	C	2.20835	-0.00412	0.48958
C	5.97389	1.68268	-1.81588	C	1.34947	-0.81619	-0.26711
C	7.09108	2.37996	-1.35319	C	3.28363	-1.99785	-1.1516
C	7.06915	1.09843	0.69881	H	1.81898	0.81373	1.08823
H	5.51615	1.91811	-2.77088	H	3.71412	-2.75011	-1.80415
H	7.45871	0.8826	1.68811	H	1.25354	-2.45036	-1.66653
H	8.49299	2.6453	0.25709	C	-0.11795	-0.6053	-0.21566
H	7.52404	3.16252	-1.96666	C	-2.88638	-0.21085	-0.11736
C	-0.67485	-0.3278	0.54098	C	-0.74683	-0.27702	0.99241
C	-3.44927	-0.06789	0.22644	C	-0.8959	-0.73191	-1.37403
C	-1.30743	-0.78218	-0.62323	C	-2.27212	-0.53504	-1.32601
C	-1.45568	0.25914	1.54482	C	-2.12372	-0.08232	1.04217
C	-2.83209	0.38183	1.39623	H	-0.16147	-0.19848	1.90374
C	-2.68135	-0.64768	-0.78611	H	-0.42051	-0.95982	-2.32336
H	-0.72421	-1.2558	-1.40724	H	-2.8795	-0.62198	-2.22191
H	-0.98413	0.63609	2.44734	H	-2.61823	0.16313	1.97718
H	-3.43496	0.82263	2.18397	N	-4.29969	-0.00924	-0.06893
H	-3.16391	-0.98568	-1.69777	C	-5.13604	-1.10603	0.18213
N	-4.84776	0.06549	0.06819	C	-6.76733	-3.33556	0.69018
C	-5.57334	1.24665	0.21504	C	-4.57458	-2.37766	0.40021
C	-7.43021	3.2985	0.35212	C	-6.53257	-0.94627	0.21952
C	-6.94028	0.97701	-0.01702	C	-7.31603	-2.07603	0.47458
C	-5.11681	2.53704	0.49653	C	-5.38255	-3.47839	0.65102
C	-6.0643	3.55216	0.56387	H	-3.49879	-2.50377	0.37387
C	-7.87331	2.01539	0.05635	H	-8.39634	-1.96589	0.50598
H	-4.06309	2.74486	0.64906	H	-4.92259	-4.44761	0.81643
H	-5.73793	4.56419	0.78154	H	-7.40999	-4.18726	0.88534
H	-8.92708	1.82066	-0.12006	C	-4.81232	1.27632	-0.2927
H	-8.14151	4.11529	0.4141	C	-5.78817	3.8709	-0.74644
C	-5.73228	-0.96214	-0.2562	C	-6.19921	1.50684	-0.26936
C	-7.86591	-2.63246	-0.83385	C	-3.93277	2.34574	-0.54289
C	-5.47493	-2.32017	-0.46145	C	-4.41711	3.62739	-0.7668
C	-7.0421	-0.43697	-0.3179	C	-6.65214	2.8097	-0.49873
C	-8.1147	-1.28367	-0.61255	H	-2.86354	2.17166	-0.56092
C	-6.55839	-3.14116	-0.75289	H	-3.71591	4.43396	-0.95665
H	-4.47064	-2.72409	-0.39043	H	-7.7214	3.0011	-0.48274
H	-9.12629	-0.89177	-0.66323	H	-6.17972	4.86752	-0.91945
H	-6.38756	-4.20012	-0.9187	C	-7.2181	0.40004	-0.00521
H	-8.68686	-3.30281	-1.0654	C	-8.04046	0.7621	1.25056
<b>DMAC-Ph-TTR</b>				H	-7.38737	0.84806	2.12372
H	8.00076	-0.35804	-1.90256	H	-8.79324	-0.00407	1.45701
C	7.61655	0.4175	-1.24843	H	-8.5607	1.71446	1.11382
C	6.53354	2.4164	0.39393	C	-8.16438	0.28645	-1.22017
C	6.53163	0.14094	-0.42718	H	-8.68501	1.23177	-1.39787
C	8.18224	1.6935	-1.2223	H	-8.9206	-0.48599	-1.05367
C	7.64462	2.68567	-0.40722	H	-7.60045	0.0286	-2.12122
C	5.99155	1.13795	0.39206	<b>PXZ-Ph-TTR</b>			
H	9.03536	1.91238	-1.85517	H	7.47497	-0.43839	-2.02779
H	8.07742	3.68009	-0.40302	C	7.12875	0.34493	-1.36182
H	6.08082	3.18641	1.00962	C	6.14259	2.36566	0.31471
S	5.86797	-1.50749	-0.44978	C	6.06882	0.08969	-0.50194
O	6.16192	-2.08695	-1.73304	C	7.71883	1.61012	-1.35794
O	6.2785	-2.18945	0.74465	C	7.22945	2.61305	-0.52579
S	4.61059	0.81596	1.4626	C	5.57686	1.09769	0.33409
O	5.06364	0.04812	2.5875	H	8.55288	1.81228	-2.02108
O	3.9195	2.05772	1.68299	H	7.68097	3.59903	-0.53845
C	3.57747	-0.21551	0.44724	H	5.72675	3.14475	0.94484
C	1.90516	-1.8096	-1.08117	S	5.37502	-1.54633	-0.49629
C	4.12022	-1.20944	-0.37275	O	5.61292	-2.13449	-1.78713



O	5.81419	-2.23212	0.68565	O	4.72581	2.25902	-1.20564
S	4.22865	0.80366	1.45308	O	3.78057	2.4309	1.08281
O	4.70592	0.03037	2.56404	C	5.78853	0.81078	0.70094
O	3.56805	2.05826	1.69319	C	8.05579	-0.39523	1.75792
C	3.14187	-0.21132	0.47794	C	6.25543	-0.3951	0.16799
C	1.3868	-1.7752	-0.98827	C	6.44255	1.40709	1.77104
C	3.63643	-1.21606	-0.35911	C	7.59065	0.80501	2.28826
C	1.77922	0.02447	0.56982	C	7.37936	-1.01056	0.70329
C	0.87956	-0.77238	-0.15456	H	6.04619	2.3245	2.1932
C	2.75838	-1.98901	-1.10724	H	7.70754	-1.96281	0.30011
H	1.42579	0.84913	1.1814	H	8.93903	-0.8678	2.17369
H	3.15157	-2.74949	-1.7737	H	8.11042	1.27054	3.11853
H	0.70259	-2.40373	-1.54942	C	-0.43979	-0.38458	-0.02526
C	-0.58102	-0.53597	-0.04682	C	-3.20029	-0.01644	0.5115
C	-3.33479	-0.09583	0.16038	C	-1.05454	0.86023	-0.2053
C	-1.40273	-0.6302	-1.17916	C	-1.23958	-1.44278	0.42202
C	-1.15834	-0.21655	1.18745	C	-2.59081	-1.2704	0.68855
C	-2.53025	0.00111	1.29188	C	-2.40586	1.04712	0.05013
C	-2.77114	-0.41021	-1.07767	H	-0.47734	1.69854	-0.58537
H	-0.96531	-0.8509	-2.14827	H	-0.79828	-2.42088	0.59171
H	-0.53836	-0.16291	2.07738	H	-3.17133	-2.11627	1.03598
H	-2.9875	0.23925	2.24691	H	-2.84515	2.02121	-0.12714
H	-3.4109	-0.47208	-1.95354	N	-4.56698	0.17439	0.80898
N	-4.74229	0.12921	0.27505	C	-5.41554	-0.97424	0.88887
C	-5.26499	1.36287	-0.16365	C	-7.02202	-3.24965	0.9758
C	-6.41969	3.79493	-0.96828	C	-6.16851	-1.34494	-0.23071
C	-4.4615	2.44183	-0.53559	C	-5.50558	-1.71744	2.06425
C	-6.6581	1.52555	-0.20123	C	-6.29559	-2.86389	2.10373
C	-7.23214	2.71855	-0.60476	C	-6.97637	-2.48272	-0.18561
C	-5.03777	3.65176	-0.92942	H	-4.9347	-1.39536	2.93004
H	-3.38234	2.33943	-0.50665	H	-6.35102	-3.45019	3.01481
H	-8.31467	2.78994	-0.61682	H	-7.56975	-2.75541	-1.05286
H	-4.39261	4.47903	-1.20559	H	-7.64538	-4.13724	1.00695
H	-6.87056	4.73224	-1.27505	C	-5.22127	1.336	0.29111
C	-5.60508	-0.98567	0.265	C	-6.44311	3.59197	-0.79582
C	-7.4221	-3.12896	0.29362	C	-5.14106	2.55804	0.95578
C	-5.14867	-2.30296	0.33269	C	-5.95235	1.23401	-0.8975
C	-6.98934	-0.76207	0.21547	C	-6.56872	2.36347	-1.43937
C	-7.88838	-1.81439	0.22014	C	-5.73793	3.68958	0.40506
C	-6.05399	-3.3665	0.35253	H	-4.58868	2.60887	1.88933
H	-4.08297	-2.49732	0.38112	H	-7.14747	2.27374	-2.35344
H	-8.94803	-1.58535	0.17787	H	-5.65928	4.64375	0.91517
H	-5.67562	-4.38135	0.41399	H	-6.91624	4.47039	-1.22226
H	-8.12777	-3.95225	0.30684	S	-6.09642	-0.34207	-1.68361
O	-7.50193	0.51714	0.2114				

**PTZ-Ph-TTR (Planar)**

H	3.21691	-2.90564	-1.46729
C	2.84332	-1.96315	-1.08083
C	1.91804	0.45247	-0.02234
C	3.73428	-0.9268	-0.83175
C	1.48555	-1.77484	-0.83611
C	0.99942	-0.57302	-0.3046
C	3.26345	0.28001	-0.30412
H	0.79179	-2.57561	-1.07071
H	1.59303	1.37532	0.44789
S	5.44708	-1.18232	-1.20591
O	5.71403	-2.59393	-1.12656
O	5.78	-0.4694	-2.4071
S	4.36189	1.63482	0.0351

**PTZ-Ph-TTR (Orthogonal)**

H	3.47336	-1.20765	-3.11796
C	3.03713	-0.90835	-2.17076
C	1.9391	-0.23633	0.31222
C	3.86781	-0.63774	-1.09123
C	1.65631	-0.81299	-2.01278
C	1.08967	-0.47533	-0.77838
C	3.31362	-0.30473	0.14816
H	1.01039	-1.04173	-2.85444
H	1.53647	0.01701	1.28815
S	5.62301	-0.72102	-1.33953
O	5.87403	-1.63998	-2.41713
O	6.14706	0.61333	-1.4112
S	4.33557	0.06729	1.55477
O	4.89613	1.37758	1.3856

O	3.58112	-0.23391	2.74176	H	1.197	4.75655	1.42243
C	5.6325	-1.13805	1.40851	H	3.01447	3.79812	2.85227
C	7.69238	-2.99493	1.2564	H	3.98164	1.57622	2.29471
C	6.18356	-1.47621	0.1681	C	-1.5589	2.90342	-0.04765
C	6.09782	-1.73778	2.57146	C	-3.60797	1.6322	1.29801
C	7.14425	-2.65811	2.49091	C	-2.30205	3.6243	0.8812
C	7.20235	-2.41602	0.08456	C	-1.82811	1.56876	-0.33853
H	5.63602	-1.48886	3.52107	C	-2.85144	0.92594	0.35572
H	7.59463	-2.69155	-0.88872	C	-3.34517	2.977	1.54335
H	8.49414	-3.72289	1.19766	H	-2.06766	4.66648	1.07003
H	7.51767	-3.12279	3.39689	H	-1.264	1.03877	-1.10046
C	-0.38207	-0.38591	-0.61476	H	-3.94208	3.51834	2.26956
C	-3.16033	-0.2169	-0.31615	H	-4.39441	1.11468	1.83883
C	-0.9515	0.61336	0.18756	N	3.2434	0.00317	0.28845
C	-1.22379	-1.29625	-1.26337	N	-3.11476	-0.43824	0.1081
C	-2.60627	-1.21197	-1.11562	C	3.74106	-0.40873	-0.94748
C	-2.33051	0.69713	0.3373	C	4.79632	-1.69192	-3.1596
H	-0.3124	1.31514	0.71531	C	4.01892	-1.79123	-0.89138
H	-0.80046	-2.05862	-1.91052	C	3.99084	0.34901	-2.09363
H	-3.26643	-1.90704	-1.62444	C	4.51815	-0.31477	-3.19507
H	-2.7734	1.46654	0.96392	C	4.55301	-2.43483	-2.01148
N	-4.58606	-0.14716	-0.1854	H	3.78475	1.41394	-2.12692
C	-5.15699	-0.64233	1.01348	H	4.7207	0.2463	-4.10175
C	-6.34156	-1.62654	3.37657	H	4.77364	-3.49786	-1.98261
C	-6.55199	-0.77597	1.12149	H	5.2077	-2.17581	-4.03918
C	-4.36917	-1.03725	2.10236	C	3.1724	-1.10426	1.13192
C	-4.95815	-1.53483	3.26406	C	3.16324	-3.58174	2.36772
C	-7.1348	-1.23501	2.30008	C	2.67837	-1.19207	2.43574
H	-3.28973	-0.97151	2.04357	C	3.64927	-2.23835	0.43713
H	-4.32037	-1.84281	4.08627	C	3.64549	-3.48574	1.06714
H	-8.21705	-1.30495	2.3564	C	2.6829	-2.44494	3.03916
H	-6.80154	-2.00159	4.28426	H	2.29004	-0.3222	2.95571
C	-5.26103	0.83771	-0.9503	H	4.00261	-4.36722	0.5425
C	-6.64817	2.77167	-2.46322	H	2.29619	-2.54598	4.04816
C	-4.56822	1.81442	-1.6771	H	3.14811	-4.54382	2.86902
C	-6.66471	0.83259	-1.01682	C	-2.17513	-1.47026	0.15969
C	-7.34737	1.80632	-1.7417	C	-0.73887	-3.83886	0.16856
C	-5.25751	2.76107	-2.4338	C	-2.8203	-2.68724	-0.15096
H	-3.48539	1.83238	-1.66806	C	-0.81837	-1.42285	0.49489
H	-8.43304	1.78533	-1.7538	C	-0.11465	-2.62258	0.49188
H	-4.6922	3.49766	-2.99542	C	-2.0905	-3.87963	-0.14858
H	-7.18581	3.51482	-3.04188	H	-0.32523	-0.49108	0.75926
S	-7.57135	-0.48909	-0.28595	H	0.93911	-2.62007	0.75406
				H	-2.57666	-4.82138	-0.38648
				H	-0.15475	-4.75337	0.17522
				C	-4.35411	-0.97878	-0.23425
				C	-6.54506	-2.50815	-0.95934
				C	-5.57437	-0.3314	-0.44102
				C	-4.21272	-2.37311	-0.40416
				C	-5.32283	-3.14095	-0.76736
				C	-6.6634	-1.11732	-0.80136
				H	-5.67253	0.74416	-0.33589
				H	-5.22784	-4.21449	-0.90239
				H	-7.62483	-0.64174	-0.96779
				H	-7.41647	-3.09001	-1.24068

### Cartesian Coordinates for The $S_1$ Geometries

#### m-Cz-DPS-Cz

S	-0.17709	3.66918	-0.84997
O	-0.06718	3.11252	-2.17367
O	-0.27193	5.09173	-0.64594
C	1.18771	3.05995	0.10327
C	3.18614	1.99957	1.68884
C	1.71419	1.81456	-0.22342
C	1.6321	3.7867	1.20437
C	2.64251	3.24483	1.9965
C	2.71918	1.28236	0.58328
H	1.34938	1.26274	-1.08564

#### m-PTZ-DPS-PTZ

S	0.14132	-3.68446	0.13241
O	0.91979	-4.42494	1.10364
O	-0.86161	-4.35468	-0.66534

C	-0.6877	-2.39054	1.01616	H	7.50264	1.78052	0.63781
C	-1.62626	0.00653	2.0632	H	6.95532	-1.83753	-1.61719
C	-1.67372	-1.67323	0.3284	H	8.47199	-0.13577	-0.59247
C	-0.17587	-1.92568	2.23127	S	4.90904	2.60055	1.08193
C	-0.64966	-0.71859	2.74669				
C	-2.15285	-0.48672	0.86117				
H	-2.03834	-2.0247	-0.63519	<b>m-DMAC-DPS-DMAC</b>			
H	0.59546	-2.49673	2.73538	S	0.00582	4.0288	0.7148
H	-0.25561	-0.34243	3.68564	O	0.08223	5.4519	0.45719
H	-2.0151	0.94043	2.45684	O	-0.10207	3.53921	2.07522
C	1.19567	-2.77295	-0.87202	C	1.51185	3.33306	0.07426
C	2.05282	-0.38623	-2.16663	C	3.784	2.15275	-1.02573
C	2.02749	-1.82457	-0.18889	C	2.38601	4.10256	-0.69332
C	0.79551	-2.48086	-2.2096	C	1.74868	1.96839	0.26942
C	1.23017	-1.34036	-2.84463	C	2.87337	1.38123	-0.29475
C	2.42147	-0.69019	-0.85326	C	3.52846	3.50789	-1.23035
H	2.32848	-1.98813	0.84188	H	2.17539	5.15675	-0.83822
H	0.12093	-3.17157	-2.70477	H	1.07305	1.36613	0.87008
H	0.92507	-1.14917	-3.8674	H	4.22933	4.10759	-1.80224
H	2.40589	0.51972	-2.64527	H	4.67847	1.68501	-1.42658
N	-3.15912	0.29176	0.19107	C	-1.25095	3.3385	-0.20826
C	-2.78942	1.07	-0.9306	C	-2.94605	1.88995	-1.97712
C	-2.06041	2.69664	-3.11866	C	-1.71066	2.03681	0.14402
C	-1.64547	0.79197	-1.68696	C	-1.61871	3.88153	-1.48453
C	-3.59841	2.14722	-1.33169	C	-2.44782	3.18388	-2.3249
C	-3.24548	2.93706	-2.42351	C	-2.52948	1.37489	-0.73646
C	-1.26828	1.61524	-2.74766	H	-1.44679	1.59714	1.10067
H	-1.07448	-0.10417	-1.47909	H	-1.2488	4.86447	-1.7583
H	-3.90245	3.7512	-2.71492	H	-2.73969	3.62364	-3.27339
H	-0.3602	1.37472	-3.2942	H	-3.59801	1.32157	-2.62781
H	-1.78299	3.32626	-3.95708	N	3.08928	-0.01553	-0.06633
C	-4.52025	-0.01734	0.41541	N	-3.00419	0.06185	-0.35816
C	-7.24589	-0.57143	0.84675	C	2.96581	-0.94043	-1.11616
C	-5.5064	0.93348	0.10288	C	2.89961	-2.84468	-3.17337
C	-4.91979	-1.23221	0.98295	C	2.92675	-2.31472	-0.79455
C	-6.27033	-1.49818	1.20311	C	2.89651	-0.53606	-2.45787
C	-6.85595	0.6452	0.28981	C	2.86825	-1.4858	-3.47584
H	-4.17782	-1.97183	1.2597	C	2.91867	-3.24278	-1.83593
H	-6.55268	-2.44691	1.64759	H	2.87963	0.51728	-2.70928
H	-7.59562	1.39242	0.01788	H	2.82985	-1.15314	-4.50857
H	-8.29734	-0.78442	1.00603	H	2.91599	-4.30291	-1.6058
S	-5.02559	2.55984	-0.386	H	2.8962	-3.58776	-3.96401
N	3.21789	0.28534	-0.12756	C	3.74369	-0.41445	1.11627
C	2.54798	1.24128	0.6185	C	5.14472	-1.26803	3.37935
C	1.13783	3.15596	2.13865	C	4.42252	0.5132	1.91697
C	3.22017	2.31539	1.24988	C	3.72073	-1.77569	1.47282
C	1.148	1.15204	0.78088	C	4.44717	-2.18314	2.5918
C	0.45749	2.09844	1.50717	C	5.11228	0.08348	3.04628
C	2.50824	3.25568	2.01546	H	4.41786	1.56456	1.65263
H	0.62034	0.32809	0.32976	H	4.45804	-3.23113	2.87133
H	-0.62051	2.00901	1.58537	H	5.63477	0.81241	3.65762
H	3.05409	4.05462	2.50711	H	5.6938	-1.60858	4.25089
H	0.59275	3.88548	2.72664	C	-2.29588	-1.04284	-0.79074
C	4.59607	0.20507	-0.25814	C	-0.85689	-3.23284	-1.72675
C	7.39633	-0.03208	-0.50832	C	-1.13042	-0.84782	-1.57655
C	5.17298	-0.88839	-0.94959	C	-2.73429	-2.34857	-0.45646
C	5.46564	1.17335	0.29735	C	-1.99238	-3.42272	-0.94129
C	6.85953	1.03691	0.17752	C	-0.42426	-1.93963	-2.038
C	6.54123	-0.99427	-1.07662	H	-0.80222	0.15652	-1.81042
H	4.53217	-1.64845	-1.37295	H	-2.29937	-4.43458	-0.69799
				H	0.4694	-1.7906	-2.63302

H	-0.29704	-4.0907	-2.08565	C	-0.81458200	-2.35358600	-1.81543700
C	-4.16431	-0.03735	0.39133	H	-0.68947200	-0.69191800	-0.45863600
C	-6.47817	-0.1726	1.93131	H	-3.71118300	-3.86950800	-2.83104100
C	-4.64966	-1.30519	0.7919	H	0.25947300	-2.40691300	-1.95311600
C	-4.84891	1.14893	0.75389	H	-1.23642700	-3.99721400	-3.15574100
C	-5.9969	1.07339	1.51637	C	-4.67747900	-0.36488000	0.23226500
C	-5.80629	-1.3374	1.56712	C	-7.45820500	-0.37057800	0.48709800
H	-4.46596	2.10714	0.43005	C	-5.30458500	0.56492700	1.08585000
H	-6.51661	1.98341	1.79294	C	-5.47403400	-1.28939200	-0.48046700
H	-6.19772	-2.29304	1.90016	C	-6.85916400	-1.29277100	-0.35616500
H	-7.37595	-0.23732	2.53639	C	-6.67947100	0.55457900	1.20654900
C	-3.94917	-2.59721	0.41683	H	-4.69353900	1.27322300	1.63129100
C	2.80276	-2.69555	0.67703	H	-7.43228200	-2.01685800	-0.92338700
C	3.09986	-4.17471	0.92568	H	-7.16128100	1.27035500	1.86202700
H	2.9641	-4.41704	1.98272	H	-8.53723300	-0.36394400	0.59072300
H	4.12109	-4.43966	0.63355	C	4.72953400	-0.10981000	-0.29459400
H	2.40092	-4.8037	0.36774	C	7.39401100	-0.38374300	-1.15131500
C	1.34719	-2.41386	1.12914	C	5.57399900	-1.07924400	0.26625400
H	1.06389	-1.37527	0.92978	C	5.25000400	0.72494900	-1.28582700
H	1.25114	-2.6014	2.20374	C	6.57255800	0.58893100	-1.71040500
H	0.65448	-3.06733	0.58854	C	6.88560600	-1.22044300	-0.15643800
C	-4.94426	-3.50644	-0.34315	H	4.61539300	1.49077800	-1.71837700
H	-5.81792	-3.71943	0.27679	H	6.95246100	1.25387700	-2.47873100
H	-4.47465	-4.45908	-0.59818	H	7.49432500	-1.98798600	0.31011800
H	-5.27997	-3.02487	-1.26521	H	8.42263600	-0.49424500	-1.47654700
C	-3.48415	-3.30534	1.71341	C	2.92133700	-0.97174200	1.05728000
H	-4.33952	-3.51486	2.36045	C	2.02906300	-2.97332700	2.82646200
H	-2.77588	-2.67923	2.26261	C	1.58207500	-1.03528800	1.45130800
H	-2.99706	-4.25358	1.4727	C	3.80783000	-1.92682700	1.57952000

**m-PXZ-DPS-PXZ**

S	-0.25022500	3.61034900	-0.06261400
O	0.55233300	4.44401700	0.80493000
O	-1.07505000	4.20891400	-1.09130300
C	-1.19246800	2.54167600	0.89472100
C	-2.02722000	0.08708300	2.07614900
C	-2.09247000	1.68268100	0.20352800
C	-0.70699500	2.13501500	2.18207300
C	-1.13221800	0.96141100	2.75549500
C	-2.46237900	0.50506900	0.80448000
H	-2.44544200	1.93565300	-0.79196000
H	-0.00048900	2.77857100	2.69603800
H	-0.76644200	0.68421600	3.73953700
C	0.82325100	2.46476700	-0.88129700
C	2.09042800	0.19082100	-1.87962500
C	0.45449700	1.95437200	-2.13016500
C	1.83967900	1.85376900	-0.13258600
C	2.45081900	0.71245800	-0.62831700
C	1.10633000	0.82782200	-2.63184300
H	-0.33392000	2.44532000	-2.69100500
H	2.11802200	2.23983800	0.84403700
H	0.83109700	0.43499900	-3.60603100
H	2.59197200	-0.70007700	-2.24714300
N	-3.31030700	-0.39685200	0.06306000
N	3.40928200	0.01761200	0.17793800
C	-2.73076400	-1.32429600	-0.77572900
C	-1.66028200	-3.25123400	-2.49307700
C	-1.33504700	-1.39509800	-0.97000400
C	-3.56540600	-2.23476700	-1.46496400
C	-3.03487300	-3.19280800	-2.32195100

**m-DPA-DPS-DPA**

S	0.18645900	3.45934000	0.99708100
O	0.24254500	4.87216600	0.68987700
O	0.01981600	3.02766600	2.36959400
C	-1.02006000	2.68559200	0.04833300
C	-2.57515300	1.02893900	-1.66555900
C	-1.66981900	1.53758100	0.56959000
C	-1.14055400	2.97720000	-1.34425200
C	-1.89421600	2.16721000	-2.16847800
C	-2.41709500	0.74857800	-0.28532800
H	-1.61408100	1.31570100	1.63088900
H	-0.63084200	3.84874600	-1.74532300
H	-1.96517400	2.40471700	-3.22539900
H	-3.10440300	0.33865900	-2.31062300
C	1.71793100	2.77456200	0.39838800
C	3.96169100	1.64043200	-0.77980200
C	2.69415200	3.60519700	-0.14810700
C	1.85211600	1.38642800	0.37083900
C	2.95670800	0.81549900	-0.25547900
C	3.83218800	3.02455900	-0.70966800
H	2.55326300	4.67996300	-0.12653800

H	1.07456600	0.74887400	0.78533900	H	-1.56084500	-2.90282400	-1.54668300
H	4.61045800	3.65670400	-1.12522100	H	-1.54120600	-1.87600700	2.66402600
H	4.82619200	1.18828700	-1.25632200	H	-3.32108200	-0.19352500	2.26950500
N	-3.09365900	-0.38363300	0.24631600	H	-3.32213800	-1.20505900	-1.95973900
N	3.02732200	-0.59612100	-0.40690800	C	1.31996800	-2.46615400	0.58497300
C	-2.44931500	-1.20071900	1.18178000	C	3.38540400	-0.65377700	0.16753600
C	-1.14758600	-2.75095000	3.09007900	C	1.82692300	-2.27790100	-0.70525000
C	-1.07235500	-1.45929800	1.04828800	C	1.84144700	-1.74851000	1.66672800
C	-3.17296800	-1.72128700	2.27208000	C	2.88133300	-0.85161500	1.45839400
C	-2.51553600	-2.49168500	3.21970500	C	2.85419000	-1.36724900	-0.91385700
C	-0.43421800	-2.23851600	2.00345500	H	1.41439500	-2.84924200	-1.53041100
H	-0.53762700	-1.07991600	0.18301600	H	1.45120200	-1.92664400	2.66340100
H	-4.22352900	-1.47573200	2.38479700	H	3.24953500	-1.19867600	-1.91091400
H	-3.06361200	-2.87089900	4.07522600	N	-4.44446400	0.35764700	-0.09778300
H	0.62368700	-2.45040700	1.89193300	C	-5.72473900	0.07565900	-0.54381500
H	-0.63780900	-3.34815200	3.83865900	C	-8.32181500	-0.02360100	-1.41871600
C	-4.41149000	-0.62221500	-0.13629800	C	-6.26353600	-1.17933100	-0.83891700
C	-7.03463200	-1.07609400	-0.95023200	C	-6.46050800	1.28176600	-0.66272900
C	-5.24927000	0.47319700	-0.44088400	C	-7.76797000	1.23278100	-1.10291500
C	-4.89075400	-1.94287600	-0.25069100	C	-7.58521200	-1.20365000	-1.28585200
C	-6.19707500	-2.16156000	-0.65589000	H	-5.67591200	-2.08218100	-0.71517800
C	-6.55921500	0.23061300	-0.83919100	H	-8.36310300	2.13447500	-1.20310700
H	-4.87686500	1.48212600	-0.30907700	H	-8.04799900	-2.15340700	-1.52858800
H	-4.21944700	-2.77302000	-0.05691800	H	-9.34746500	-0.07451800	-1.76778400
H	-6.56366000	-3.17673300	-0.76054700	C	-4.32751500	1.72507700	0.08747900
H	-7.21395500	1.06774600	-1.05509600	C	-4.54230700	4.44846300	0.32959100
H	-8.05689400	-1.25451100	-1.26664700	C	-5.55769900	2.35276100	-0.23344800
C	1.94901200	-1.27802500	-1.01086600	C	-3.19885500	2.43085600	0.51175100
C	-0.21267800	-2.64810400	-2.18835400	C	-3.33407500	3.81460800	0.63142600
C	1.72409000	-2.63532700	-0.73239200	C	-5.66675400	3.72361500	-0.11197700
C	1.07466700	-0.61512900	-1.88933200	H	-2.26835600	1.91748300	0.72703300
C	0.00453400	-1.29738100	-2.46355700	H	-2.48667700	4.40646900	0.95819500
C	0.65861200	-3.30954800	-1.32272600	H	-6.59066900	4.23939200	-0.35261700
H	2.38930600	-3.15796000	-0.05177500	H	-4.61641700	5.52577200	0.43095400
H	1.22622200	0.43476100	-2.11832900	H	3.32459300	-0.31572600	2.29218800
H	-0.65958600	-0.76030500	-3.13330800	N	4.43977500	0.26600000	-0.04491600
H	0.50213500	-4.35815000	-1.08779600	C	5.64436800	-0.01084000	-0.68716000
H	-1.04681300	-3.17494100	-2.64000600	C	8.16498300	-0.06660400	-1.83439200
C	4.26515700	-1.24258400	-0.15896100	C	6.43482400	1.16018900	-0.70925800
C	6.73886200	-2.45716800	0.35305000	C	6.10596600	-1.21989000	-1.21510800
C	4.78810400	-2.18275800	-1.05472300	C	7.37205000	-1.22627200	-1.78873700
C	4.99150400	-0.91065700	0.99092700	C	7.70484800	1.12724800	-1.29193000
C	6.22329700	-1.50999000	1.23780300	H	5.50506200	-2.12196500	-1.17201500
C	6.01318700	-2.79013500	-0.79072500	H	7.75642900	-2.15117000	-2.20693800
H	4.23360400	-2.43274000	-1.95397300	H	8.32290400	2.02002700	-1.31488100
H	4.58525000	-0.17758300	1.68158100	H	9.14805300	-0.10896200	-2.29140800
H	6.77664800	-1.24101600	2.13216000	C	4.44460300	1.60107100	0.34877200
H	6.40799500	-3.51759500	-1.49328400	C	4.91808800	4.27832300	0.88349200
H	7.69617100	-2.92793600	0.55072500	C	3.44495800	2.33637300	0.99214600
<b>p-Cz-DPS-Cz</b>				C	5.66611800	2.19365700	-0.04468200
S	-0.08374400	-3.51729800	0.82675000	C	5.90052200	3.54363500	0.22991100
O	-0.04489300	-3.93174000	2.21380100	C	3.70316700	3.67706400	1.25434600
O	-0.03983400	-4.50356400	-0.23286400	H	2.50149900	1.88045600	1.27299700
C	-1.44245100	-2.50093200	0.58533200	H	6.83503600	4.01088700	-0.06666000
C	-3.42849400	-0.59156800	0.12931900	H	2.94648700	4.27168700	1.75657000
C	-1.94743500	-2.29800600	-0.73298900	H	5.08614600	5.32672600	1.10651000
C	-1.93097700	-1.70786400	1.66526900	<b>p-PTZ-DPS-PTZ</b>			
C	-2.90879700	-0.77095300	1.44725600	S	0.12866300	4.22414300	0.00365500
C	-2.92944400	-1.36839300	-0.96050300	O	0.01019300	4.92349600	1.26629000

O	0.07513200	4.96121900	-1.24167900	H	-5.06836000	2.05745500	0.28450900
C	1.51782600	3.22739400	0.01210600	H	-7.49421400	2.40931600	0.19889600
C	3.19507500	0.98936100	-0.06932300	H	-8.08174400	-1.78550200	-0.53163200
C	2.03564600	2.75885100	-1.23472200	H	-9.03793500	0.48972900	-0.19039000
C	1.85992600	2.53844200	1.21770600	S	-5.40093000	-2.70823800	-0.77986700
C	2.68069600	1.43983600	1.17892000				
C	2.86682900	1.66792200	-1.27529500				
H	1.77148900	3.28626700	-2.14551000	<b>p-DMAC-DPS-DMAC</b>			
H	1.46476600	2.89734100	2.16304600	S	0.04906400	3.79150900	-0.03827600
H	2.94851800	0.91457600	2.09156600	O	-0.00715200	4.50254500	-1.29968100
H	3.27404500	1.31526700	-2.21884700	O	-0.01549400	4.52165700	1.21179200
C	-1.19436200	3.03979000	-0.03407100	C	1.41923100	2.77601800	-0.02309000
C	-2.91960000	0.86320600	-0.03188700	C	3.43776400	0.84020300	0.00846700
C	-1.49342100	2.39285800	-1.23698100	C	1.92758900	2.28756400	1.21992800
C	-1.77111500	2.61598000	1.16731800	C	1.91656000	2.23577000	-1.24924500
C	-2.64464900	1.53377800	1.16254600	C	2.91142900	1.29275200	-1.23831100
C	-2.35696200	1.30176700	-1.23147600	C	2.92435100	1.34663200	1.23970500
H	-1.04507100	2.74404900	-2.16115900	H	1.53422700	2.69140100	2.14725100
H	-1.53191700	3.14072400	2.08630900	H	1.51498200	2.60033300	-2.18932900
H	-3.10928500	1.19333300	2.08439800	H	3.31291400	0.89725300	-2.16675000
H	-2.60341100	0.77815500	-2.15014000	H	3.33591400	0.99226100	2.18029000
N	3.88528900	-0.26196300	-0.13221800	C	-1.35869400	2.70307000	-0.03591700
C	5.26669500	-0.26212400	0.02584500	C	-3.43313000	0.86115000	-0.03312800
C	8.06396000	-0.17377300	0.36152900	C	-1.84004700	2.20814200	1.17904200
C	6.04159000	-1.44833700	0.01474200	C	-1.90673700	2.28036700	-1.24899200
C	5.93719400	0.97013100	0.21156600	C	-2.95039200	1.35928300	-1.24347600
C	7.30569200	1.00892700	0.37359500	C	-2.87991700	1.28413600	1.17671900
C	7.43337200	-1.38938900	0.18369600	H	-1.40871700	2.56293200	2.10956100
H	5.35456300	1.88134700	0.22291200	H	-1.52620200	2.69090600	-2.17849600
H	7.79521200	1.96612200	0.51220400	H	-3.28005400	0.89139400	2.10695100
H	8.00457100	-2.31251000	0.17121200	N	4.50733500	-0.09913200	0.02407600
H	9.13969500	-0.13720900	0.49076200	C	4.21836600	-1.45846200	0.08167500
C	3.12303300	-1.40540900	-0.35071800	C	5.81824400	0.36443700	-0.01630300
C	1.51017300	-3.67507400	-0.80196900	C	5.25451400	-2.42268800	0.10009300
C	1.72396400	-1.27858400	-0.53703600	C	6.90949800	-0.53748900	-0.00491500
C	3.68590900	-2.70621800	-0.39958900	C	6.72180800	-2.04137700	0.05513700
C	2.87056800	-3.82699600	-0.62014800	C	7.36513300	-2.67754900	-1.20073000
C	0.94130600	-2.39056000	-0.76426800	C	7.41860500	-2.58144500	1.32728000
H	1.27339400	-0.29543600	-0.50475700	C	2.86043400	-1.85549400	0.12410500
H	3.32660600	-4.81183000	-0.64798600	H	2.08901800	-1.09713200	0.10895700
H	-0.12676400	-2.26660200	-0.90491700	C	2.53564300	-3.19627400	0.18495000
H	0.88541200	-4.54459700	-0.97331600	H	1.49438500	-3.49533100	0.21996400
S	5.36759300	-3.02084000	-0.19343900	C	3.54994000	-4.15789500	0.20329400
N	-3.77726600	-0.28756300	-0.05409000	H	3.30235500	-5.21283000	0.25105700
C	-3.25996100	-1.50379400	0.44842900	C	4.88581000	-3.76432600	0.16062400
C	-2.27402800	-3.96194700	1.43073500	H	5.65665100	-4.52813000	0.17538100
C	-2.03733200	-1.56947500	1.13162100	H	7.26155100	-3.76487300	-1.17328400
C	-3.96655600	-2.70380300	0.24297100	H	8.43072200	-2.44054400	-1.24566800
C	-3.49111800	-3.90923300	0.75266700	H	6.88671700	-2.30493300	-2.11026800
C	-1.55034500	-2.78715000	1.60683500	H	8.48466100	-2.34305400	1.30905000
H	-1.45129000	-0.67087200	1.28396500	H	6.97822000	-2.14026100	2.22526700
H	-4.07542500	-4.81090400	0.59427700	H	7.31608900	-3.66739800	1.38693200
H	-0.59523300	-2.80329000	2.12315500	C	6.03622200	1.76228800	-0.07060400
H	-1.90332400	-4.90687100	1.81338100	H	5.18510000	2.43006500	-0.07741800
C	-5.17554600	-0.06348200	-0.08765800	C	7.32417900	2.25826500	-0.11354800
C	-7.96426400	0.33906300	-0.16208200	H	7.48526600	3.32933800	-0.15484400
C	-6.05289800	-1.13058800	-0.34244900	C	8.40950300	1.37746600	-0.10376300
C	-5.72149400	1.21163900	0.10670600	H	9.42399000	1.75983100	-0.13753800
C	-7.10061100	1.40815700	0.05639800	C	8.19239700	0.00212600	-0.04974200
C	-7.43157500	-0.93452000	-0.35130000	H	9.05025000	-0.66239000	-0.04208600
				N	-4.50929400	-0.08216800	-0.03045800

H	-3.40422700	1.02443300	-2.17171000	C	-2.43456900	3.44543500	0.27377400
C	-5.82664800	0.38684800	0.06575700	C	-4.79221600	4.01197500	0.22696300
C	-4.21886000	-1.44801300	-0.11953100	H	-1.94716200	1.34762000	0.16574200
C	-6.90842500	-0.51153400	0.08356000	H	-1.40035200	3.76408300	0.33108800
C	-5.25120500	-2.40413800	-0.11125000	H	-5.60667500	4.72696500	0.24228200
C	-6.72717400	-2.02580000	-0.00270200	H	-3.22084000	5.45690400	0.36649500
C	-2.88000400	-1.87250500	-0.21806000	C	-5.74676800	-0.01361000	-0.03291900
H	-2.08349500	-1.13802200	-0.22380200	C	-8.46402700	-0.65347200	-0.14723900
C	-4.89886000	-3.75401600	-0.20416900	C	-6.14879500	-1.36129700	-0.11872500
H	-5.68785100	-4.50097000	-0.19834500	C	-6.73630100	0.99492100	-0.00594900
C	-2.56707000	-3.22161200	-0.31022900	C	-8.08874800	0.67865600	-0.06319700
H	-1.52612000	-3.51995900	-0.38949900	C	-7.49335400	-1.66999300	-0.17465300
C	-3.57843500	-4.17924800	-0.30408400	H	-5.38723700	-2.13086400	-0.13866900
H	-3.34698700	-5.23658800	-0.37606800	H	-8.81435400	1.48347500	-0.04036900
C	-6.06997700	1.77085100	0.14333700	H	-7.79952300	-2.70741100	-0.24035800
H	-5.23871500	2.46538600	0.12646100	H	-9.51660600	-0.90929500	-0.19186700
C	-8.19970200	0.01606100	0.18327300	O	-6.40009900	2.30601100	0.07573700
H	-9.04389000	-0.66774100	0.19884100	N	4.38796000	0.35714200	0.29318400
C	-7.36507300	2.26027300	0.24098800	C	4.08318100	1.69708900	-0.00610200
H	-7.52304100	3.33259700	0.29958900	C	3.59074700	4.41278300	-0.54799500
C	-8.44630700	1.38224800	0.26283300	C	2.78711200	2.14680100	-0.26620200
H	-9.46314700	1.75214400	0.33938900	C	5.12719800	2.63619600	-0.01862800
C	-7.32175100	-2.67816900	1.26429900	C	4.89181000	3.97187800	-0.29374300
C	-7.47516800	-2.55270900	-1.24662100	C	2.54531200	3.49728000	-0.52994900
H	-6.80453000	-2.31785800	2.15820300	H	1.96624600	1.43826200	-0.25572700
H	-8.38495600	-2.44049400	1.36189800	H	5.73619700	4.65321600	-0.29329600
H	-7.22388400	-3.76697200	1.22412100	H	1.52931100	3.82299600	-0.72777500
H	-8.54107400	-2.31413800	-1.18976600	H	3.40659300	5.46100900	-0.75642600
H	-7.37916800	-3.63930000	-1.32771500	C	5.72951600	-0.05208600	0.16363100
H	-7.06893300	-2.10126400	-2.15629900	C	8.44293800	-0.75156300	-0.04420900
<b>p-PXZ-DPS-PXZ</b>				C	6.73172300	0.92956600	0.14784100
S	-0.04181500	-3.63992500	-0.07657900	C	6.11199100	-1.39135600	0.07347100
O	0.06219300	-4.28647500	-1.36879800	C	7.46219100	-1.73623900	-0.02317800
O	-0.01459200	-4.43008800	1.13726200	C	8.06905700	0.59216200	0.03684200
C	-1.41647800	-2.62883200	-0.05931900	H	5.35247400	-2.16517200	0.08822800
C	-3.39601200	-0.65696900	-0.00333600	H	7.73575900	-2.78428100	-0.08382500
C	-1.87302200	-2.03509200	-1.27621000	H	8.80277100	1.39142200	0.02789600
C	-1.94658100	-2.17860800	1.18930900	H	9.49171100	-1.01656200	-0.12115400
C	-2.92335600	-1.21727000	1.22054100	O	6.41663400	2.26487700	0.29396000
C	-2.84944300	-1.07295100	-1.25408200	<b>p-DPA-DPS-DPA</b>			
H	-1.45474500	-2.37361400	-2.21863600	S	-0.00008800	3.64424700	-0.00002000
H	-1.58482300	-2.62584100	2.10951300	O	0.10496500	4.36207100	1.25228600
H	-3.34955900	-0.88819700	2.16376400	O	-0.10518000	4.36211600	-1.25229300
H	-3.21994100	-0.63528200	-2.17640900	C	1.35041700	2.55795600	-0.11396400
C	1.34838100	-2.53561000	0.02889600	C	3.27853900	0.53842900	-0.27798500
C	3.35364300	-0.62769900	0.19610600	C	1.73425800	2.04928800	-1.37624000
C	1.78578700	-2.10335200	1.28253400	C	1.93308400	2.04008400	1.06582400
C	1.91157000	-2.02334500	-1.14388100	C	2.88547800	1.04694700	0.98489400
C	2.92076200	-1.07095700	-1.05660400	C	2.68900300	1.05877400	-1.45705100
C	2.79218700	-1.14428200	1.36286700	H	1.29445500	2.47009900	-2.27453000
H	1.34547100	-2.52869400	2.17854100	H	1.62864700	2.43898500	2.02794600
H	1.56594600	-2.38829700	-2.10561900	H	3.33794700	0.64416100	1.88592400
H	3.38293900	-0.66558400	-1.95266300	H	3.01481000	0.68638800	-2.42347400
H	3.15669600	-0.79358700	2.32348000	C	-1.35053900	2.55788600	0.11391800
N	-4.40882400	0.34093500	0.02505800	C	-3.27860400	0.53830200	0.27793800
C	-4.07072400	1.68134300	0.11355300	C	-1.93356100	2.04035200	-1.06584500
C	-3.46377800	4.40276600	0.29514200	C	-1.73405200	2.04889700	1.37616700
C	-5.09226100	2.65744900	0.13780200	C	-2.68875200	1.05834100	1.45697900
C	-2.72672400	2.09901600	0.18318700	C	-2.88593400	1.04719000	-0.98491300

H	-1.62939100	2.43951900	-2.02794100	H	-4.62421800	2.35797900	0.00631600
H	-1.29402400	2.46948600	2.27445000	S	0.00616400	4.15167000	-0.03556800
H	-3.01427000	0.68567000	2.42338900	O	-0.02221500	4.93942300	-1.26271700
H	-3.33865200	0.64463100	-1.88592100	O	-0.00801700	4.97057700	1.17120400
N	4.24371100	-0.48078900	-0.36197300	C	1.23063200	2.94092800	-0.02777000
N	-4.24369800	-0.48098800	0.36193400	C	2.88882200	0.74090400	-0.01334200
C	5.39981800	-0.41581600	0.44281400	C	0.65938700	1.61560300	-0.00995600
C	7.66335700	-0.26572200	2.08073100	C	2.61590900	3.14531000	-0.03996200
C	5.98441500	0.82980900	0.72642000	C	3.46470400	2.05529700	-0.03306200
C	5.94898100	-1.58477200	0.99698100	C	1.50759200	0.52427000	-0.00196400
C	7.07550400	-1.50307300	1.80483500	H	3.02410300	4.15219500	-0.05465400
C	7.10979400	0.89565000	1.53941200	H	4.54218900	2.17361900	-0.04264200
H	5.55731600	1.72977000	0.29618300	H	1.12215700	-0.49248200	0.01157200
H	5.47917400	-2.54299000	0.80006700	N	3.76837000	-0.38254400	-0.00964500
H	7.48981900	-2.40994000	2.23346100	N	-4.01199100	-0.20740000	0.02305100
H	7.56047200	1.86114000	1.74504500	C	4.18285600	-0.94493700	-1.20443600
H	8.54094700	-0.20800600	2.71581100	C	5.05317000	-2.15753800	-3.56483300
C	4.04126600	-1.55771300	-1.24695500	C	5.04704400	-2.06285200	-1.17490000
C	3.61658100	-3.66423700	-3.04154200	C	3.76318000	-0.43797900	-2.45009100
C	2.74103400	-2.04242400	-1.47370500	C	4.19892800	-1.04156200	-3.61303800
C	5.12552600	-2.12812000	-1.93726600	C	5.47847800	-2.66967800	-2.34877000
C	4.90776900	-3.17573600	-2.82171100	H	3.10485800	0.42150300	-2.47386700
C	2.53942000	-3.08941500	-2.36526500	H	3.87696300	-0.64912000	-4.57033800
H	1.90623900	-1.59963000	-0.94034200	H	6.13736000	-3.52752400	-2.28197900
H	6.12480700	-1.73365300	-1.78423200	H	5.38524700	-2.62374000	-4.48535000
H	5.74981500	-3.60505500	-3.35498600	C	4.23501700	-0.89517900	1.18814300
H	1.53326200	-3.46257900	-2.52728800	C	5.21080100	-2.00733600	3.55657400
H	3.45265700	-4.47999300	-3.73758600	C	3.86839300	-0.33711900	2.42868200
C	-4.04094500	-1.55809200	1.24662300	C	5.09966800	-2.01291200	1.16741300
C	-3.61559900	-3.66495700	3.04065000	C	5.58386100	-2.56964100	2.34550700
C	-5.12497100	-2.12873800	1.93710200	C	4.35599600	-0.89145800	3.59562900
C	-2.74061300	-2.04272900	1.47292400	H	3.20918700	0.52184500	2.44519900
C	-2.53867300	-3.08991000	2.36418900	H	6.24099600	-3.42937200	2.28594200
C	-4.90688400	-3.17651000	2.82128400	H	4.07487700	-0.45988900	4.54893000
H	-6.12432700	-1.73432700	1.78440800	H	5.58434800	-2.43413100	4.48031700
H	-1.90600000	-1.59972700	0.93944600	C	-4.28109100	-0.88590200	-1.17955200
H	-1.53243900	-3.46302300	2.52586300	C	-4.92264700	-2.29308000	-3.52863700
H	-5.74874700	-3.60600100	3.35470800	C	-5.10956400	-2.01864900	-1.14355800
H	-3.45141400	-4.48083900	3.73648400	C	-3.78260700	-0.47057300	-2.41619300
C	-5.40003900	-0.41590100	-0.44250700	C	-4.10814400	-1.16763700	-3.58258400
C	-7.66407800	-0.26560700	-2.07970700	C	-5.42117400	-2.72068400	-2.29507400
C	-5.94926800	-1.58477000	-0.99678700	H	-3.14671600	0.40626800	-2.46692800
C	-5.98482800	0.82974100	-0.72562500	H	-3.71580700	-0.81943500	-4.53225300
C	-7.11044600	0.89568300	-1.53828000	H	-6.06432300	-3.59062500	-2.21084300
C	-7.07604300	-1.50297600	-1.80427900	H	-5.17594300	-2.83772000	-4.43154300
H	-5.47932600	-2.54299600	-0.80022700	C	-4.26139800	-0.88480500	1.23038400
H	-5.55767000	1.72963400	-0.29530500	C	-4.86444300	-2.29051500	3.59054800
H	-7.56126500	1.86118400	-1.74355200	C	-3.74409100	-0.46778000	2.45865400
H	-7.49041600	-2.40977600	-2.23298900	C	-5.08996800	-2.01790100	1.20860600
H	-8.54186500	-0.20781400	-2.71450800	C	-5.38247300	-2.71931000	2.36548600
<b>DBTO-PXZ</b>				C	-4.05032000	-1.16419800	3.63062700
C	-0.78947800	1.64659400	-0.00312500	H	-3.10858100	0.40988000	2.49857300
C	-3.55277400	2.18997700	0.00362700	H	-6.02646600	-3.58962500	2.29224900
C	-1.29440900	2.96455500	-0.01406200	H	-3.64335500	-0.81479900	4.57367200
C	-1.70784000	0.58860700	0.01049700	H	-5.10271200	-2.83477400	4.49775700
C	-3.06779200	0.87018900	0.01343800	O	5.48129700	-2.58136100	-0.00133900
C	-2.65467700	3.25206100	-0.01068300	O	-5.68369400	-2.44113800	0.03751100
H	-1.37770300	-0.44714000	0.01783800	<b>DBTO-DMAC</b>			
H	-3.00600900	4.27953800	-0.01933800	C	0.74290400	1.84024900	-0.00873500



C	3.54377500	2.33256900	-0.02733000	H	5.54596600	-1.90828300	4.64876000
C	1.29326700	3.17511400	-0.02672900	C	-5.77342800	-2.34345000	0.02357600
C	1.61886200	0.76562300	0.00211600	C	-7.31533000	-2.26239900	0.02149600
C	2.98934700	1.01014300	-0.00702600	H	-7.73294900	-2.74848100	0.90773800
C	2.66684300	3.40585400	-0.03680800	H	-7.73120200	-2.76078600	-0.85871000
H	1.25377900	-0.25887800	0.01567900	H	-7.64257700	-1.21884400	0.01389500
H	3.05126900	4.42217900	-0.05215900	C	-5.34182800	-3.82614300	0.03446400
H	4.61822700	2.47315700	-0.03532100	H	-5.72658000	-4.33616400	0.92265800
S	0.04053400	4.37075300	-0.03845400	H	-4.25082400	-3.90643500	0.03593800
O	0.01405400	5.17395300	1.17267800	H	-5.72509800	-4.34876800	-0.84702800
O	0.00819400	5.14271500	-1.26966200	H	6.24062000	-3.07645800	-2.56053100
C	-1.23365500	3.15261300	-0.02058000	C	5.75193100	-2.37787900	0.00927300
C	-2.96539300	1.01995900	0.00188200	C	5.32003700	-3.86413300	0.04316300
C	-0.70197600	1.84461300	-0.00641300	H	5.72413200	-4.35790400	0.92999600
C	-2.59957800	3.41064400	-0.02280000	H	5.69619800	-4.39014900	-0.83741300
C	-3.47683100	2.33240300	-0.01115000	H	4.23055300	-3.95034100	0.06184500
C	-1.60313000	0.76741900	0.00516300	C	7.29739000	-2.28793600	-0.01763200
H	-2.96797800	4.43221000	-0.03403200	H	7.72235300	-2.76515800	0.86841800
H	-4.55174900	2.47972900	-0.01311200	H	7.62357900	-1.24497200	-0.04245300
H	-1.25732600	-0.26267600	0.01508500	H	7.69352400	-2.79819400	-0.89861200
N	-3.87977200	-0.08311200	0.00944100				
N	3.89712100	-0.10099000	-0.00174200				
C	-4.33632400	-0.58174100	1.23527500	<b>TXO2-PXZ</b>			
C	-5.20763200	-1.55237300	3.72463500	C	1.31063100	-1.14649000	0.00655000
C	-5.23873200	-1.66004700	1.28076700	C	3.56871800	-0.87104000	1.76364400
C	-3.88627900	-0.00069000	2.43606800	C	1.34597700	-1.74792200	1.31715000
C	-4.31868400	-0.48131200	3.66422500	C	2.41056100	-0.42164700	-0.38858500
C	-5.65063800	-2.12070700	2.53527400	C	3.55263200	-0.29465500	0.45858800
H	-3.19640100	0.83396900	2.40235800	C	2.47051000	-1.57504000	2.17740400
H	-3.95737900	-0.01173200	4.57386900	H	2.43570300	0.08159100	-1.34828200
H	-6.34418300	-2.95571100	2.58311900	H	2.43366600	-2.00325600	3.17349300
H	-5.55247700	-1.93767800	4.67825800	H	4.42889700	-0.73752500	2.41203100
C	-4.33369800	-0.59928700	-1.21019600	S	0.01700900	-2.63587400	1.91565200
C	-5.19999300	-1.60560800	-3.68723500	O	-0.06512800	-3.99904700	1.41508600
C	-3.88075700	-0.03594300	-2.41837800	O	-0.05062500	-2.51049100	3.36096200
C	-5.23624000	-1.67796200	-1.24213000	C	-1.32561800	-1.72963300	1.20388900
C	-5.64566500	-2.15655900	-2.49071800	C	-3.46834200	-0.31646600	0.21206600
C	-4.31066400	-0.53419900	-3.64035600	C	-1.19728400	-1.15138500	-0.07104600
H	-3.19052700	0.79878500	-2.39554000	C	-2.48089400	-1.60259400	1.97412200
H	-6.33934100	-2.99198700	-2.52797500	C	-3.56871000	-0.89887000	1.47389800
H	-3.94711400	-0.07798400	-4.55589300	C	-2.30279300	-0.43460600	-0.54205300
H	-5.54296300	-2.00450200	-4.63593100	H	-2.50520200	-2.04818800	2.96343000
C	4.31434900	-0.63182400	-1.21334900	H	-4.48248900	-0.78828100	2.05044500
C	5.08972800	-1.66302600	-3.67996200	H	-2.28644000	0.05937000	-1.50637200
C	5.20284600	-1.73456300	-1.24947300	C	0.08407000	-1.31903600	-0.90251800
C	3.83243800	-0.05148300	-2.41281100	C	0.10735500	-0.33169000	-2.07578100
C	4.22199800	-0.56729300	-3.63209000	H	1.00669300	-0.48724100	-2.67569200
C	5.56692800	-2.22818600	-2.49913300	H	0.07979000	0.71070100	-1.74364700
H	3.16354000	0.79702200	-2.36230500	H	-0.74022300	-0.51354300	-2.74056200
H	3.85169100	-0.11889600	-4.54665600	C	0.09666200	-2.74038400	-1.52616000
H	5.39635300	-2.07562900	-4.63493500	H	0.09963700	-3.52428300	-0.76948600
C	4.35227700	-0.58926200	1.21403700	H	0.99277300	-2.84492600	-2.14659700
C	5.20796000	-1.53059200	3.68990400	H	-0.78644000	-2.86742500	-2.16129000
C	3.90646700	0.03243800	2.40671600	N	4.69515400	0.40020400	-0.02184500
C	5.24357800	-1.68925300	1.26114100	C	4.82299900	1.76619200	0.17272500
C	5.64845900	-2.13733400	2.51544400	C	5.14329100	4.51942300	0.52436100
C	4.33585000	-0.43893900	3.63067000	C	5.96461200	2.43719400	-0.32010900
H	3.23353500	0.87712500	2.34694700	C	3.83660100	2.50785100	0.85245300
H	6.32532300	-2.98240700	2.58573800	C	4.00179300	3.86812800	1.02290900
H	3.99336100	0.04106500	4.54002600	C	6.12555300	3.80708700	-0.14674700
				H	2.96500300	1.98741800	1.22955200



C	-7.00335200	1.74041600	-0.81217400	N	-2.13714100	-0.05280900	0.28948800
C	-8.33559300	1.85454600	-0.03244600	C	-2.97091600	-1.12788900	0.01795900
H	-8.54993400	2.89911000	0.20569300	C	-4.58235300	-3.32591800	-0.54556300
H	-8.28682300	1.28717800	0.90063800	C	-4.35260100	-0.92467500	-0.22012800
H	-9.16281400	1.46797300	-0.63254800	C	-2.41354200	-2.42972300	-0.02168700
C	-7.10073700	2.55204200	-2.12621600	C	-3.21880000	-3.51529500	-0.30024700
H	-7.30207400	3.60415400	-1.91120600	C	-5.12895200	-2.04477500	-0.50302400
H	-7.91470200	2.17361600	-2.74907400	C	-2.61230300	1.24817100	0.37806400
H	-6.16814000	2.48410700	-2.69244800	C	-3.49382200	3.88273200	0.55034500

**Cz-TTR**

H	0.94628000	1.37024000	2.88325700
C	0.58507900	0.83181500	2.01255700
C	-0.28006300	-0.51997400	-0.30786700
C	1.50954000	0.11158700	1.24178000
C	-0.75443200	0.86262800	1.68461300
C	-1.17979100	0.16076300	0.50332200
C	1.05652500	-0.58145000	0.05448900
H	-1.47830100	1.38009700	2.30275700
H	-0.61202900	-0.99855800	-1.22499800
S	3.18177300	0.15078800	1.66125500
O	3.43655900	1.29924000	2.50594000
O	3.65131600	-1.12977500	2.13999900
S	2.16508600	-1.41285500	-0.98993600
O	2.66576800	-2.61920000	-0.37422000
O	1.57396100	-1.53899700	-2.30499800
C	3.48753900	-0.23808300	-1.07277100
C	5.53143400	1.64308500	-1.25683900
C	3.92677300	0.44067200	0.07779300
C	4.06023700	0.03913400	-2.31168400
C	5.09473200	0.96751000	-2.39867700
C	4.93732500	1.39462700	-0.02205100
H	3.68581000	-0.47089300	-3.19302000
H	5.24382600	1.93280200	0.86871500
H	6.32899700	2.37464300	-1.32975900
H	5.55114400	1.17295900	-3.36090800
N	-2.55809000	0.15430000	0.18239400
C	-3.38612900	-0.95581600	0.18913000
C	-5.36936600	-2.84416100	0.06555700
C	-3.04207300	-2.27916200	0.47546200
C	-4.70328600	-0.55268700	-0.14724000
C	-5.70229600	-1.50157200	-0.21102000
C	-4.06883200	-3.22231500	0.40458700
H	-2.02774900	-2.55356100	0.74267100
H	-6.72177400	-1.23183800	-0.46529600
H	-3.85084600	-4.26234100	0.61733800
H	-6.14601800	-3.59929500	0.01617000
C	-3.29690500	1.27481400	-0.13794700
C	-5.12855700	3.20359700	-0.78938500
C	-4.64883100	0.89862900	-0.34641000
C	-2.83818400	2.59023300	-0.26172000
C	-3.79187000	3.55508700	-0.58948100
C	-5.57200300	1.86846700	-0.67452500
H	-1.79274100	2.83696200	-0.11438000
H	-3.48852500	4.59010400	-0.69511500
H	-6.61473700	1.62226700	-0.84353000
H	-5.84668400	3.97466800	-1.04555800

**DMAC-TTR**

C	-2.13714100	-0.05280900	0.28948800
C	-2.97091600	-1.12788900	0.01795900
C	-4.58235300	-3.32591800	-0.54556300
C	-4.35260100	-0.92467500	-0.22012800
C	-2.41354200	-2.42972300	-0.02168700
C	-3.21880000	-3.51529500	-0.30024700
C	-5.12895200	-2.04477500	-0.50302400
C	-2.61230300	1.24817100	0.37806400
C	-3.49382200	3.88273200	0.55034500
C	-1.70131000	2.28621400	0.69237100
C	-3.98176000	1.53107400	0.15358200
C	-4.38844300	2.85941200	0.24410000
C	-2.14566500	3.59009400	0.77781400
C	-4.99063900	0.45050800	-0.18433100
C	-5.60160000	0.75453300	-1.57427300
C	-6.10769300	0.45567800	0.88756200
H	-5.21965700	-4.17432800	-0.76987600
H	-1.35734600	-2.56517500	0.16754600
H	-2.78713100	-4.50893000	-0.32960200
H	-6.18914400	-1.92209100	-0.69838100
H	-3.84867900	4.90576700	0.61126100
H	-0.66069000	2.04863700	0.86616900
H	-5.42953600	3.11031700	0.06970400
H	-1.44458700	4.38052100	1.01926100
H	-6.35020700	0.00234400	-1.83383500
H	-4.82672300	0.75563000	-2.34517700
H	-6.09043000	1.73162500	-1.56979400
H	-5.69452500	0.24422700	1.87718500
H	-6.60367900	1.42845300	0.91766000
H	-6.86184800	-0.29997000	0.65642500
C	-0.74484700	-0.29969400	0.51781500
C	1.95559100	-0.80956400	1.00061800
C	-0.30104400	-0.55435700	1.85904200
C	0.13807100	-0.26419700	-0.55125900
C	1.47883600	-0.54140400	-0.34151800
C	1.04596800	-0.77819900	2.06640800
H	-1.00737700	-0.54697700	2.68054700
H	-0.20666000	-0.01912700	-1.55224000
H	1.42605400	-0.93429500	3.07130000
S	3.63452800	-1.04774600	1.31512800
O	3.90484400	-0.74363200	2.70425400
O	4.11004400	-2.31086300	0.80624500
S	2.56539400	-0.45014500	-1.69327800
O	3.07162500	-1.75063000	-2.05195700
O	1.95018600	0.34065300	-2.73780400
C	3.89208800	0.49111400	-0.98661500
C	5.94294400	2.02963600	0.09628600
C	4.35267600	0.23403000	0.31557400
C	4.44649100	1.52643400	-1.73494900
C	5.48527500	2.28291000	-1.19858300
C	5.36611200	1.01868500	0.86080500
H	4.05326900	1.72748900	-2.72603500
H	5.92944100	3.07852700	-1.78727400
H	5.68639700	0.82734000	1.87973300
H	6.74411800	2.62848200	0.51648700

**PXZ-TTR**

H	0.99718300	-0.73707900	3.10744200
C	0.63425100	-0.62534800	2.09042200
C	-0.22417700	-0.23178500	-0.56667900

C	1.55735500	-0.73233300	1.04088000	O	-2.82982800	-1.85512100	-1.98313000
C	-0.70399500	-0.38321300	1.85091100	O	-1.74291500	0.22235100	-2.76057300
C	-1.12284900	-0.19212100	0.49095000	C	-1.24153500	-0.55345300	-0.33597300
C	1.10579100	-0.52620400	-0.32095300	C	0.55268900	-0.45311700	1.85133100
H	-1.42163500	-0.31902400	2.66000100	C	-1.70349300	-0.77708400	1.01946300
H	-0.54929100	-0.03637300	-1.58495900	C	0.09584200	-0.25837400	-0.56233300
S	3.22505200	-0.99691000	1.39237700	C	0.98194300	-0.23742200	0.50084100
O	3.48560500	-0.61908100	2.76506400	C	-0.79018200	-0.69231300	2.07712000
O	3.67015300	-2.30056100	0.96505000	H	0.43174400	-0.04609100	-1.57370800
S	2.21263500	-0.54739700	-1.65946900	H	-1.16240500	-0.81863500	3.08906000
O	2.68562500	-1.88151500	-1.92882700	H	1.26418600	-0.40544400	2.66712600
O	1.63381000	0.19461500	-2.75892600	N	2.37253400	0.02770400	0.25557300
C	3.55666500	0.39709900	-0.99126900	C	3.20177800	-1.06047500	0.01569400
C	5.64208900	1.93204200	0.02741100	C	4.82532200	-3.30766900	-0.49904800
C	3.99303800	0.20309400	0.32996800	C	2.66140800	-2.36833600	0.04654400
C	4.15211400	1.36846600	-1.79163900	C	4.58222700	-0.91618900	-0.27347000
C	5.20762800	2.12313700	-1.28587300	C	5.37798000	-2.04356900	-0.53148000
C	5.02492300	0.98589300	0.84194300	C	3.45974300	-3.46350000	-0.20411800
H	3.77767500	1.52266200	-2.79829300	H	1.61188800	-2.50184200	0.26922200
H	5.32804400	0.84434900	1.87414600	H	6.43092200	-1.90442500	-0.75627700
H	6.45707800	2.52926000	0.42260400	H	3.02076000	-4.45403600	-0.17389600
H	5.68347700	2.86887900	-1.91376700	H	5.44501300	-4.17408400	-0.69980700
N	-2.50634000	0.05727600	0.22960100	C	2.79882900	1.34771600	0.31874300
C	-3.36383200	-0.99778700	-0.02306700	C	3.59525700	4.05055000	0.43561000
C	-5.16652300	-3.06172900	-0.56855100	C	1.86932200	2.36520300	0.64195100
C	-2.91482600	-2.33342100	-0.05164400	C	4.14021000	1.72790300	0.06222800
C	-4.73014100	-0.72998800	-0.26928200	C	4.52190300	3.07767300	0.12073600
C	-5.62805200	-1.75515300	-0.54338400	C	2.26404700	3.68443600	0.69938300
C	-3.81186800	-3.34731500	-0.32042800	H	0.84244300	2.09605200	0.84625800
H	-1.86943300	-2.54226500	0.13718400	H	5.55450500	3.34154500	-0.08551000
H	-6.66560300	-1.50409200	-0.73062700	H	1.53265500	4.44362500	0.95140900
H	-3.46344000	-4.37305100	-0.34239000	H	3.89683000	5.09079400	0.47910500
H	-5.85841000	-3.86840800	-0.78224400	S	5.38077400	0.60703300	-0.34735000
C	-2.99991000	1.34791400	0.27320800				
C	-4.08467800	3.92233100	0.32769300				
C	-4.37411800	1.56794200	0.02488900	<b>Cz-Ph-TTR</b>			
C	-2.17247600	2.45301000	0.55623700	H	3.18533300	1.97689500	2.61146400
C	-2.71615900	3.72150500	0.58220100	C	2.74968400	1.27133800	1.91156100
C	-4.91525100	2.84836900	0.04901500	C	1.67170500	-0.51639100	0.04659000
H	-1.12072000	2.28555900	0.75054900	C	3.60637600	0.41388800	1.19909500
H	-2.07800500	4.56952600	0.80077300	C	1.38576300	1.21289900	1.73358800
H	-5.97326600	2.97137500	-0.15139200	C	0.78368600	0.30490100	0.79749600
H	-4.49690300	4.92470900	0.34922200	C	3.02979300	-0.47964700	0.25723900
O	-5.20961500	0.53723200	-0.24857900	H	0.76711000	1.86261100	2.34000600
				H	1.30783200	-1.16272100	-0.74393600
				S	5.32306900	0.51998900	1.43718400
<b>PTZ-TTR</b>				O	5.63649000	1.82871800	1.96295300
H	-5.45416700	0.83097800	1.86513400	O	5.83428300	-0.62963700	2.13896200
C	-5.14289100	0.98935000	0.83780400	S	4.04124400	-1.53987100	-0.72761800
C	-4.24691600	1.41414400	-1.78127100	O	4.56788400	-2.60340900	0.08522600
C	-4.12204700	0.19894800	0.31450100	O	3.32256400	-1.88487900	-1.93039900
C	-5.73863500	1.96345300	0.04103100	C	5.36791200	-0.44736700	-1.17093800
C	-5.29225500	2.17556500	-1.26553300	C	7.43728000	1.24938600	-1.91840200
C	-3.67334400	0.41381800	-1.00002500	C	5.91799600	0.44178600	-0.23628000
H	-6.54565000	2.56599800	0.44438000	C	5.83936400	-0.47679400	-2.47819800
H	-5.75117700	2.94299400	-1.87978000	C	6.88975300	0.36353700	-2.84590900
H	-3.86334400	1.58397400	-2.78195400	C	6.94274400	1.30300100	-0.61618400
S	-3.37741100	-1.03202400	1.35566600	H	5.37566000	-1.14833600	-3.19317600
O	-3.64347500	-0.68106900	2.73449200	H	7.33558100	2.00738700	0.10951300
O	-3.82915200	-2.32313600	0.89861300	H	8.24429000	1.91256500	-2.21144200
S	-2.33849900	-0.53457600	-1.67977700	H	7.26837900	0.33552800	-3.86197000

C	-0.63747800	0.24426800	0.59449100
C	-3.45020700	0.13507900	0.19762100
C	-1.25402900	-0.81717800	-0.14226400
C	-1.51391000	1.24506000	1.12548100
C	-2.87181000	1.20228300	0.92629800
C	-2.61131300	-0.88083800	-0.32977800
H	-0.64506200	-1.60776400	-0.56420600
H	-1.10894300	2.07135100	1.69649800
H	-3.51414600	1.95740800	1.36869900
H	-3.04536200	-1.67891800	-0.92363500
N	-4.82808600	0.08120800	0.00171600
C	-5.63518200	1.14595400	-0.40458600
C	-7.59824300	2.89744900	-1.22347100
C	-6.97661400	0.70486100	-0.48429700
C	-5.25085100	2.43781700	-0.77361700
C	-6.26167800	3.30998600	-1.17237300
C	-7.96490600	1.58614300	-0.89262700
H	-4.21176100	2.74546300	-0.77013100
H	-6.00310800	4.32294000	-1.46012800
H	-8.99967800	1.26759500	-0.96652000
H	-8.36072500	3.59993700	-1.54190000
C	-5.63346600	-1.04546700	0.18033300
C	-7.60909700	-2.94741900	0.44596200
C	-5.26978300	-2.30876300	0.65451800
C	-6.97420600	-0.70687200	-0.11701700
C	-7.96785500	-1.66374700	0.01334500
C	-6.28308500	-3.25844600	0.76854300
H	-4.25001700	-2.53822900	0.94059500
H	-9.00406100	-1.42443900	-0.20282200
H	-6.03839500	-4.25217400	1.12669400
H	-8.37518600	-3.70803600	0.55006600

**DMAC-Ph-TTR**

H	7.99353300	0.56476100	-1.81033300
C	7.59473700	0.96986300	-0.88618000
C	6.47566000	2.02276200	1.45577900
C	6.51927000	0.33220800	-0.27818500
C	8.13018100	2.11852800	-0.30430900
C	7.57460000	2.64290100	0.86158100
C	5.96190500	0.86056700	0.89277900
H	8.97552700	2.61147800	-0.77275800
H	7.98515400	3.54447300	1.30341000
H	6.00631800	2.43247700	2.34396200
S	5.87902200	-1.15027900	-1.02885200
O	6.21878900	-1.11907800	-2.43333200
O	6.35883400	-2.26300300	-0.24760600
S	4.58133400	0.07527200	1.69097300
O	5.05532700	-1.10194200	2.36994800
O	3.88742800	1.07849200	2.46243300
C	3.58278200	-0.39283600	0.31395300
C	1.95103800	-1.06971500	-1.82157400
C	4.16994000	-0.92602600	-0.86235400
C	2.22744000	-0.19338900	0.41787400
C	1.33678200	-0.55875600	-0.63270900
C	3.31486800	-1.23211500	-1.93412300
H	1.86401500	0.28445000	1.31999000
H	3.74904400	-1.60578900	-2.85580400
H	1.34073000	-1.35276200	-2.67022500
C	-0.08553500	-0.39296600	-0.50118000
C	-2.89574000	-0.09652600	-0.24469900

C	-0.70125100	-0.06543900	0.74634500
C	-0.96990600	-0.56089400	-1.61279600
C	-2.33472100	-0.41751400	-1.49372300
C	-2.06398300	0.07869300	0.87881300
H	-0.09622400	0.05025000	1.63819600
H	-0.57222400	-0.79100800	-2.59414800
H	-2.98030800	-0.54564100	-2.35844400
H	-2.50273200	0.31383300	1.84455500
N	-4.31665700	0.03008800	-0.10806200
C	-5.05629600	-1.08465900	0.25810700
C	-6.47772700	-3.36203400	0.99802800
C	-4.37862600	-2.31010600	0.47711900
C	-6.46275100	-1.00011600	0.40905600
C	-7.14230900	-2.15699900	0.77988200
C	-5.08922500	-3.43432100	0.84389300
H	-3.30485100	-2.35403600	0.35377500
H	-8.21966600	-2.12449500	0.90343300
H	-4.56579700	-4.36856100	1.01060500
H	-7.04166400	-4.24224700	1.28654300
C	-4.90819200	1.26259500	-0.34346600
C	-6.02786100	3.76381200	-0.83705600
C	-6.31019000	1.42607900	-0.21960500
C	-4.08295300	2.35489000	-0.70904600
C	-4.64443500	3.59137700	-0.95268700
C	-6.83708900	2.68935100	-0.47403500
H	-3.01437000	2.20867700	-0.79258000
H	-4.00860700	4.42358200	-1.23153900
H	-7.90703900	2.84713700	-0.38720300
H	-6.47520400	4.73325800	-1.02718900
C	-7.22911200	0.28806400	0.18006600
C	-7.96198000	0.67354500	1.48856900
H	-7.24676500	0.83863400	2.29844600
H	-8.64986300	-0.12070000	1.78763300
H	-8.54292600	1.58743900	1.34476500
C	-8.26620000	0.06006000	-0.94669600
H	-8.84815900	0.96838300	-1.11859400
H	-8.95968100	-0.73753000	-0.67032700
H	-7.76907800	-0.21762000	-1.87975400

**PXZ-Ph-TTR**

H	7.53518800	0.54850500	-1.83519600
C	7.14228300	0.95440900	-0.90888000
C	6.03812100	2.00944200	1.43926100
C	6.07052400	0.31748900	-0.29362200
C	7.68159800	2.10342700	-0.33120700
C	7.13342500	2.62888500	0.83767200
C	5.52068900	0.84691500	0.88041100
H	8.52411100	2.59579400	-0.80532100
H	7.54696100	3.53071600	1.27617000
H	5.57445100	2.41997900	2.33003800
S	5.42498900	-1.16538700	-1.03909400
O	5.75549000	-1.13508000	-2.44571600
O	5.90824200	-2.27807100	-0.26013200
S	4.14512400	0.06256300	1.68796200
O	4.62289500	-1.11480500	2.36383600
O	3.45645400	1.06626400	2.46338300
C	3.13741000	-0.40525400	0.31736200
C	1.49206000	-1.08217300	-1.80775400
C	3.71657000	-0.94023900	-0.86188000
C	1.78305200	-0.20270500	0.42862400

C	0.88612000	-0.56663300	-0.61688500	H	5.65605900	2.71213100	1.91856100
C	2.85504700	-1.24714100	-1.92798800	H	7.56206200	-1.80100800	1.07468400
H	1.42560500	0.27733000	1.33196700	H	8.42179400	-0.42230000	2.96514400
H	3.28326000	-1.62357500	-2.85132100	H	7.47310700	1.83591800	3.38640800
H	0.87606700	-1.36669700	-2.65180600	C	-0.30910000	-0.54830800	-0.33353400
C	-0.53488500	-0.39316400	-0.47916200	C	-3.11660200	-0.17748800	0.08629800
C	-3.33979100	-0.07157200	-0.21283400	C	-0.93312800	0.72638000	-0.49403500
C	-1.42364600	-0.54979200	-1.58913300	C	-1.17990600	-1.64425800	-0.05290900
C	-1.14299200	-0.06680900	0.77261200	C	-2.52696400	-1.47297400	0.14743500
C	-2.50360300	0.09071300	0.91003600	C	-2.27587900	0.91222600	-0.30066500
C	-2.78653400	-0.39402900	-1.46565800	H	-0.34329800	1.57327800	-0.82528500
H	-1.03019400	-0.77876800	-2.57240800	H	-0.77742100	-2.64677300	0.02477500
H	-0.53348500	0.03748600	1.66276500	H	-3.14176400	-2.34363800	0.33100400
H	-2.93687600	0.32592800	1.87818700	H	-2.70169700	1.88812700	-0.49053900
H	-3.43555900	-0.51170100	-2.32924800	N	-4.46455200	0.00803100	0.30314300
N	-4.75622100	0.07741200	-0.07389300	C	-5.34728200	-1.06116300	0.62534400
C	-5.35120900	1.30514800	-0.29511300	C	-7.10658600	-3.14925400	1.17477900
C	-6.63991500	3.74820400	-0.72506500	C	-6.52187400	-1.20435400	-0.12908700
C	-4.60070400	2.44154100	-0.65756200	C	-5.09351700	-1.92167200	1.69990600
C	-6.75310000	1.42873500	-0.15458700	C	-5.96750300	-2.96789200	1.96400700
C	-7.39578100	2.64265400	-0.36836400	C	-7.39414400	-2.25853400	0.14503700
C	-5.24433800	3.64425800	-0.86798300	H	-4.21756500	-1.75771500	2.31923500
H	-3.52714100	2.34813100	-0.76303600	H	-5.76659200	-3.63576100	2.79445200
H	-8.47186700	2.69123000	-0.24884300	H	-8.30103900	-2.36418400	-0.44158200
H	-4.66463700	4.51655700	-1.14574000	H	-7.78851900	-3.96661700	1.38251300
H	-7.13117100	4.69963700	-0.89348700	C	-5.09536400	1.27883800	0.19139300
C	-5.53569800	-1.00563800	0.28628500	C	-6.36874600	3.73865800	-0.10073300
C	-7.19024200	-3.13911900	1.01132300	C	-4.62791500	2.39389500	0.89743500
C	-4.97812500	-2.27765400	0.52642900	C	-6.24587500	1.38204900	-0.60593000
C	-6.93387000	-0.83681600	0.41819700	C	-6.87355200	2.61909800	-0.75529000
C	-7.75817500	-1.89653200	0.77840400	C	-5.25851100	3.62082900	0.73997800
C	-5.80168300	-3.32578300	0.88439600	H	-3.77813500	2.28583700	1.56370600
H	-3.90809500	-2.40885900	0.42542300	H	-7.76260900	2.69329600	-1.37317900
H	-8.82404300	-1.72152300	0.86688000	H	-4.89086300	4.48424300	1.28341800
H	-5.37000000	-4.30232300	1.06918200	H	-6.86069500	4.69759600	-0.22160800
H	-7.82408400	-3.97202000	1.29315100	S	-6.87913400	-0.05030700	-1.40852800
O	-7.51713200	0.36580200	0.19537900				

**PTZ-Ph-TTR**

H	3.49167200	-3.15898300	-1.00014500
C	3.05702700	-2.17655900	-0.84643900
C	1.99361600	0.37662800	-0.38736400
C	3.91520900	-1.06356400	-0.80071300
C	1.69592600	-2.02323500	-0.70814200
C	1.11492500	-0.72540000	-0.48878200
C	3.35467700	0.22541600	-0.55631800
H	1.06494800	-2.89897700	-0.79875100
H	1.62557200	1.36451100	-0.13039100
S	5.63206200	-1.29095600	-0.93723600
O	5.94325400	-2.67043300	-0.63744900
O	6.13977600	-0.73524800	-2.16570400
S	4.37645700	1.64447500	-0.37193800
O	4.92456100	2.02872000	-1.64547700
O	3.65556000	2.63935000	0.38837800
C	5.66766500	0.99054500	0.64678000
C	7.64863800	-0.02751200	2.31450000
C	6.20500000	-0.28666000	0.40438300
C	6.10985900	1.74484400	1.72955800
C	7.11597600	1.24249300	2.55162900
C	7.18250900	-0.80068900	1.25494900

**Cartesian Coordinates for The T<sub>1</sub> Geometries****m-Cz-DPS-Cz**

S	0.14931300	3.79213100	1.01002300
O	-0.03486400	3.26764900	2.34212400
O	0.27531300	5.21500500	0.80794600
C	-1.09622200	3.14110500	-0.05621100
C	-2.51412000	1.81410900	-2.02642500
C	-1.61812300	1.89576100	0.26443800
C	-1.25511800	3.75695200	-1.29393000
C	-2.00656000	3.07091900	-2.29636300
C	-2.34829900	1.21574000	-0.76239000
H	-1.45619000	1.45449200	1.24232800
H	-0.81457500	4.73034000	-1.47456300
H	-2.16897600	3.52816000	-3.26533800
H	-3.08152100	1.27879600	-2.78387000
C	1.52915200	2.97787500	0.25564600
C	3.31586100	1.52477100	-1.27915200
C	2.16760700	3.60513500	-0.80478200
C	1.74562500	1.64930700	0.60041100
C	2.65501000	0.90937900	-0.20426800

C	3.10052300	2.86314000	-1.57055200	H	-0.55109600	-0.42402200	3.83651700
H	1.94328900	4.64248800	-1.02722200	H	-2.32784300	0.85629300	2.62572400
H	1.27563100	1.21767400	1.47665900	C	1.04168900	-2.58315100	-0.86663000
H	3.60681300	3.32446200	-2.41020100	C	1.96441900	-0.21670800	-2.15052900
H	3.97389500	0.92845200	-1.90449900	C	2.03122100	-1.76196100	-0.24255500
N	-2.86589600	-0.07195300	-0.51715600	C	0.52106500	-2.17989600	-2.13823200
N	2.87854400	-0.44950800	0.08037000	C	0.99309100	-1.04844800	-2.76507400
C	-3.72001400	-0.42063100	0.52952600	C	2.43720900	-0.62171000	-0.89016000
C	-5.41829600	-1.56489300	2.37981000	H	2.42355200	-2.01316800	0.73882600
C	-4.05955700	-1.78784000	0.41634000	H	-0.24697700	-2.79047500	-2.60201100
C	-4.23824100	0.39534100	1.53759100	H	0.60138500	-0.77738800	-3.74131800
C	-5.08574200	-0.20397400	2.46444300	H	2.33613500	0.68890900	-2.61613600
C	-4.91508000	-2.36372100	1.35311300	N	-3.33209800	0.31270100	0.27530300
H	-3.99287300	1.45054900	1.59079400	C	-2.88811300	1.18076500	-0.74973400
H	-5.50153100	0.39738000	3.26607100	C	-2.04290400	2.97069600	-2.75824000
H	-5.19191900	-3.41124200	1.28177700	C	-1.63224200	1.04049700	-1.35515200
H	-6.08410400	-1.99773300	3.11886700	C	-3.71599400	2.23481100	-1.17364900
C	-2.64113700	-1.19609600	-1.29541300	C	-3.30636600	3.10152700	-2.18416300
C	-2.36662200	-3.70404100	-2.42155200	C	-1.21073900	1.93870400	-2.33439700
C	-1.76256900	-1.34423700	-2.37561200	H	-0.98009100	0.21919900	-1.07902500
C	-3.36701400	-2.28969300	-0.76059500	H	-3.97903300	3.89299900	-2.50130300
C	-3.22824700	-3.54965000	-1.33102500	H	-0.22564100	1.80546400	-2.77197000
C	-1.64356900	-2.61518000	-2.92981200	H	-1.72153500	3.66254900	-3.52937300
H	-1.18685600	-0.50465100	-2.75063500	C	-4.69174100	-0.06652900	0.35267400
H	-3.76349300	-4.40362200	-0.92678600	C	-7.41525300	-0.76765200	0.47781900
H	-0.96861600	-2.76693500	-3.76559200	C	-5.69080100	0.86053700	0.01185500
H	-2.24762900	-4.68196200	-2.87586900	C	-5.08179400	-1.34205700	0.77738500
C	1.89468700	-1.38404500	0.36735900	C	-6.43219700	-1.68013000	0.85019500
C	0.32946200	-3.56534600	1.01672300	C	-7.03607500	0.50264600	0.04766700
C	2.50724400	-2.62911600	0.65590200	H	-4.33080100	-2.07064200	1.05930600
C	0.50039900	-1.22886500	0.34309900	H	-6.70827100	-2.67274900	1.19085100
C	-0.26288500	-2.33819600	0.70830700	H	-7.78348000	1.23566100	-0.24132900
C	1.72306600	-3.72622500	0.97231400	H	-8.46527300	-1.03574500	0.52217600
H	0.03401800	-0.28828200	0.06386800	S	-5.24064600	2.52948600	-0.33881300
H	-1.34226400	-2.24719400	0.74860900	N	3.36623000	0.25957200	-0.20332200
H	2.17406000	-4.68990800	1.18751000	C	2.80945200	1.25465900	0.58597500
H	-0.29925300	-4.40657300	1.28859200	C	1.62977300	3.27805000	2.15890700
C	4.12932700	-1.06962500	0.17722200	C	3.60436600	2.18920300	1.29255000
C	6.32297800	-2.70611000	0.53889700	C	1.40027800	1.35555500	0.70136500
C	5.40009600	-0.50598900	0.04659900	C	0.82882300	2.35178300	1.46192200
C	3.94297200	-2.42636100	0.52246600	C	3.00216200	3.19215800	2.07790600
C	5.04797900	-3.25105800	0.70135300	H	0.77124000	0.64037300	0.18809700
C	6.49234300	-1.35057400	0.22475600	H	-0.25330200	2.41122400	1.51612600
H	5.53561900	0.54812200	-0.16602300	H	3.63666500	3.89408300	2.61026600
H	4.92369000	-4.29470400	0.97255200	H	1.17087300	4.05639500	2.75821100
H	7.49404500	-0.94593300	0.12731400	C	4.72058200	0.06905400	-0.41380200
H	7.19611600	-3.33570800	0.67283600	C	7.46853600	-0.37999600	-0.85656000
<b>m-PTZ-DPS-PTZ</b>				C	5.15486700	-0.97044600	-1.27257200
S	0.08500000	-3.57285200	0.15880800	C	5.70293000	0.87704800	0.20807500
O	0.92665400	-4.24006900	1.13039300	C	7.07170600	0.63952200	-0.01978600
O	-0.83981000	-4.33811800	-0.64908400	C	6.49827400	-1.18430100	-1.48590000
C	-0.83897800	-2.35602800	1.05568900	H	4.41616800	-1.59550000	-1.75756200
C	-1.89698300	-0.04492400	2.20045300	H	7.80352400	1.27241600	0.47275200
C	-1.84125900	-1.64657500	0.38243100	H	6.80660000	-1.98641600	-2.14700000
C	-0.36192500	-1.91017400	2.29436600	H	8.52363600	-0.55980900	-1.02893600
C	-0.90597400	-0.76379900	2.86829100	S	5.32400900	2.18126600	1.26316300
C	-2.35275500	-0.48596700	0.95324900	<b>m-DMAC-DPS-DMAC</b>			
H	-2.19405000	-1.98333300	-0.58985400	S	0.28419800	4.10783700	0.67355300
H	0.42002300	-2.47371400	2.79227300	O	0.46026900	5.51429200	0.37589200

O	0.10203100	3.67110700	2.04395100	H	-6.02348500	2.29342400	2.05626000
C	1.74279100	3.28571200	0.08748700	H	-5.92273500	-1.99476700	2.08437600
C	3.90222800	1.88319600	-0.98446000	H	-6.90946100	0.10781000	2.87349100
C	2.68727000	3.95971200	-0.69008400	C	-3.87440800	-2.38975500	0.35600600
C	1.85203600	1.90699300	0.29897600	C	2.24347500	-2.78442100	0.73882500
C	2.91660900	1.20779600	-0.25697800	C	2.28250900	-4.28211100	1.04296500
C	3.77352200	3.25509600	-1.20671500	H	2.00821700	-4.46567100	2.08502000
H	2.57450800	5.02598900	-0.85477900	H	3.27405300	-4.70929200	0.86163100
H	1.12373100	1.37815500	0.90644400	H	1.55279800	-4.81443800	0.42614400
H	4.53263100	3.78008300	-1.77800400	C	0.80987600	-2.27188100	1.03463800
H	4.75580100	1.33314200	-1.36907600	H	0.71046700	-1.20753900	0.79646900
C	-0.98932100	3.46820300	-0.26730600	H	0.57972700	-2.41425000	2.09597200
C	-2.60862500	2.00737500	-2.09822900	H	0.08231500	-2.82766700	0.43304800
C	-1.51460900	2.19007600	0.09584500	C	-5.00936700	-3.21050300	-0.30029100
C	-1.26348400	3.97693500	-1.57988900	H	-5.81173300	-3.39757100	0.41670400
C	-2.06260000	3.27353900	-2.44902600	H	-4.63646900	-4.17866500	-0.64147200
C	-2.29075400	1.51707300	-0.81791800	H	-5.42578100	-2.67544100	-1.15769900
H	-1.33155200	1.77803100	1.08366300	C	-3.30634100	-3.16427800	1.57266000
H	-0.84767800	4.93893800	-1.86285200	H	-4.09139000	-3.33893500	2.31287900
H	-2.28595700	3.69176500	-3.42583200	H	-2.49876500	-2.59885500	2.04595500
H	-3.23445000	1.43560600	-2.77281000	H	-2.91252400	-4.13300800	1.25414200
N	2.98481100	-0.20118200	-0.01763800				
N	-2.82504700	0.22681300	-0.43219400				
C	2.82002400	-1.12807100	-1.05962400	<b>m-PXZ-DPS-PXZ</b>			
C	2.71811600	-3.07596600	-3.07485600	S	0.00000200	-3.55943800	-0.00001100
C	2.56992800	-2.47547900	-0.71829500	O	0.84597500	-4.27903100	-0.92806600
C	2.91782800	-0.76006100	-2.40997700	O	-0.84598800	-4.27903300	0.92802800
C	2.87281500	-1.73221300	-3.40608700	C	-0.96877900	-2.44066300	-0.91214600
C	2.55373700	-3.43000200	-1.73505100	C	-1.94178000	-0.02791400	-2.00341400
H	3.05166400	0.27918800	-2.68348600	C	-1.95914800	-1.70049700	-0.22186200
H	2.97154800	-1.42989700	-4.44426600	C	-0.47956700	-1.95899900	-2.15207300
H	2.39616300	-4.47370000	-1.48412900	C	-0.97881800	-0.78322700	-2.68982700
H	2.70659000	-3.83854500	-3.84677100	C	-2.40500200	-0.51438500	-0.76984200
C	3.46570700	-0.65560700	1.22624500	H	-2.33589200	-2.04054000	0.73861800
C	4.52669200	-1.63344800	3.61893000	H	0.28225800	-2.52998100	-2.67236100
C	4.20815600	0.18663700	2.06379400	H	-0.60743100	-0.43394600	-3.64909200
C	3.21018600	-1.98641000	1.60431700	C	0.96879800	-2.44067900	0.91213000
C	3.76978700	-2.46128200	2.79070900	C	1.94182000	-0.02795000	2.00342900
C	4.72736000	-0.30336800	3.25770400	C	0.47960300	-1.95903400	2.15207200
H	4.38486500	1.21708800	1.77574300	C	1.95915600	-1.70049900	0.22184400
H	3.59987700	-3.49012500	3.08967700	C	2.40501800	-0.51439700	0.76984000
H	5.30149900	0.35859700	3.89819600	C	0.97886000	-0.78327000	2.68983800
H	4.94224200	-2.02232400	4.54260800	H	-0.28221000	-2.53002800	2.67236400
C	-2.23441200	-0.91131200	-0.95535300	H	2.33588500	-2.04052700	-0.73864700
C	-1.06026900	-3.15840900	-2.09961800	H	0.60748900	-0.43400600	3.64911600
C	-1.10129600	-0.77176900	-1.79802300	H	2.33545900	0.90161000	2.40142300
C	-2.74941200	-2.19158400	-0.64049800	N	-3.34978700	0.28369200	-0.03518400
C	-2.14505000	-3.29763000	-1.23984600	N	3.34978900	0.28369900	0.03518100
C	-0.52943600	-1.88985000	-2.36577200	C	-2.89129900	1.17506300	0.92630600
H	-0.68584400	0.21168700	-1.98192500	C	-2.06403400	3.02535300	2.86666600
H	-2.51640100	-4.29272500	-1.01816800	C	-1.53749900	1.26436900	1.28971100
H	0.34472500	-1.78457200	-2.99772000	C	-3.81646100	2.03052400	1.56043200
H	-0.60470100	-4.03810600	-2.54361200	C	-3.40975000	2.94521400	2.52105500
C	-3.91868100	0.17776900	0.42264800	C	-1.13410900	2.18399000	2.24807700
C	-6.07566900	0.13501200	2.18007200	H	-0.81609900	0.59478300	0.83434500
C	-4.43801500	-1.06847100	0.84137700	H	-4.15973900	3.58054500	2.97908500
C	-4.50974500	1.39048200	0.85317200	H	-0.08345100	2.23694900	2.51348000
C	-5.57680700	1.36246000	1.72629100	H	-1.74349200	3.74024400	3.61627200
C	-5.51220700	-1.05434700	1.73200000	C	-4.70242100	0.23976100	-0.35334500
H	-4.11926500	2.33356200	0.49282700	C	-7.44634900	0.21723700	-0.92159000
				C	-5.21902300	-0.64919800	-1.30732600



C	-5.58878900	1.11040600	0.30913900	C	-3.66098900	-1.18057000	2.18013900
C	-6.94791700	1.10148000	0.02963300	C	-3.35984300	-1.85352700	3.35717800
C	-6.57899900	-0.65559100	-1.58591800	C	-1.00813200	-1.73464800	2.83497800
H	-4.54396800	-1.32801700	-1.81581500	H	-0.50279300	-0.77689900	0.97176200
H	-7.59061600	1.79072900	0.56620600	H	4.69034900	-0.94688400	1.92760900
H	-6.96528800	-1.34943300	-2.32420700	H	-4.16408400	-2.14889300	4.02301900
H	-8.50791800	0.20707300	-1.14186100	H	0.02692600	-1.95284400	3.07851100
C	4.70242700	0.23976100	0.35332000	H	-1.80123700	-2.65303000	4.61567200
C	7.44636300	0.21723000	0.92152200	C	-4.10828800	-0.51959400	-0.59064400
C	5.58878300	1.11042200	-0.30915800	C	-6.37511900	-1.37684900	-1.97264700
C	5.21904500	-0.64921900	1.30727200	C	-5.05900500	0.41436200	-1.01899800
C	6.57902400	-0.65561600	1.58584300	C	-4.30064300	-1.88286600	-0.84146000
C	6.94791500	1.10149300	-0.02967300	C	-5.43177400	-2.30620500	-1.53189900
H	4.54399900	-1.32805100	1.81575600	C	-6.18534300	-0.01903900	-1.71132500
H	6.96532600	-1.34947400	2.32411100	H	-4.91102100	1.46683300	-0.79897800
H	7.59060400	1.79075500	-0.56624000	H	-3.56374800	-2.59648600	-0.48610300
H	8.50793500	0.20706400	1.14177700	H	-5.57468500	-3.36369800	-1.72887800
C	2.89128400	1.17508900	-0.92628200	H	-6.92318700	0.70682500	-2.03712400
C	2.06398800	3.02543300	-2.86657800	H	-7.25685500	-1.70935700	-2.51028700
C	1.53747500	1.26441400	-1.28965500	C	1.71318000	-1.53790600	-0.48427500
C	3.81643500	2.03056400	-1.56040400	C	-0.58887500	-3.07236200	-0.88152700
C	3.40971000	2.94528100	-2.52099600	C	1.55735600	-2.76202900	0.18625100
C	1.13407100	2.18406100	-2.24798900	C	0.69386500	-1.07097300	-1.33447500
H	0.81607900	0.59482600	-0.83428700	C	-0.44506100	-1.84263200	-1.53142800
H	4.15969200	3.58062200	-2.97902200	C	0.41162200	-3.52154200	-0.01797200
H	0.08340800	2.23703300	-2.51336700	H	2.33569900	-3.10352500	0.86135400
H	1.74343300	3.74034500	-3.61615800	H	0.81100800	-0.11652700	-1.84008000
O	-5.14659000	1.99670200	1.25120300	H	-1.22154900	-1.48326000	-2.20108300
O	5.14656800	1.99673800	-1.25119400	H	0.29313600	-4.46197800	0.51034600
H	-2.33541200	0.90165500	-2.40139500	H	-1.47311900	-3.67870000	-1.04832900
<b>m-DPA-DPS-DPA</b>				C	4.15666200	-1.43154100	-0.29928900
S	0.53428400	3.50951000	1.10355600	C	6.67671300	-2.63613500	-0.22976800
O	0.68592900	4.93122800	0.87781300	C	4.39301400	-2.60814500	-1.02725400
O	0.32960500	3.00346100	2.44470000	C	5.19024000	-0.85726600	0.45663900
C	-0.76618900	2.89925900	0.11538800	C	6.44222000	-1.46101700	0.48511400
C	-2.25164200	1.36450200	-1.70399400	C	5.64761900	-3.20380500	-0.98454600
C	-1.46256500	1.77088200	0.56904600	H	3.60077900	-3.03512500	-1.63339300
C	-0.83154800	3.28235700	-1.24730900	H	4.99530300	0.04832700	1.02220900
C	-1.56860700	2.50576900	-2.13186700	H	7.23503400	-1.01506200	1.07656300
C	-2.21728500	1.00746000	-0.33057300	H	5.82693000	-4.10874600	-1.55588500
H	-1.43489900	1.52619800	1.62442200	H	7.65459800	-3.10507200	-0.20254500
H	-0.30155400	4.16764700	-1.58367600	<b>p-Cz-DPA-Cz</b>			
H	-1.61225600	2.78404500	-3.18031200	S	-0.01776500	-4.24383800	0.74874500
H	-2.80315000	0.75756800	-2.41181400	O	-0.01335000	-4.72881500	2.10851600
C	1.87570300	2.70480900	0.37055400	O	-0.03055700	-5.16111700	-0.36634700
C	3.67021300	1.29974600	-1.30273500	C	-1.29084500	-3.09748600	0.55501000
C	2.61801400	3.38284200	-0.64197100	C	-2.83405900	-0.79559400	0.14567100
C	1.97774100	1.29854800	0.47509600	C	-1.71354600	-2.74167700	-0.76318400
C	2.84788200	0.61782200	-0.36454300	C	-1.66797000	-2.27911700	1.66545500
C	3.51277800	2.68263200	-1.43664300	C	-2.41952000	-1.15056700	1.45667800
H	2.50039700	4.45610100	-0.74295900	C	-2.47465200	-1.61747700	-0.95638600
H	1.38747900	0.75530700	1.20850700	H	-1.42284400	-3.37003800	-1.59798000
H	4.09650800	3.21702600	-2.17989000	H	-1.38455400	-2.58431700	2.66697500
H	4.34134400	0.73596100	-1.94027400	H	-2.75307500	-0.54984400	2.29730000
N	-2.95169200	-0.09665100	0.11878500	H	-2.77837000	-1.32599900	-1.95692400
N	2.89904400	-0.79492300	-0.33493700	C	1.26989100	-3.11545300	0.54430800
C	-2.62892100	-0.77831900	1.31779800	C	2.83563700	-0.82701900	0.14293200
C	-2.03259900	-2.13185100	3.69269200	C	1.66704800	-2.74011900	-0.77645500
C	-1.29821300	-1.06790300	1.64921900	C	1.68721900	-2.32614000	1.66088000

C	2.45213300	-1.20584700	1.45641100	H	2.35030200	-0.95028700	-1.93423500
C	2.43655700	-1.62107700	-0.96628700	H	2.87782500	-1.46853200	2.32742300
H	1.34691500	-3.34673600	-1.61661400	C	-1.20314700	-3.49320600	0.08780000
H	1.42501800	-2.64869800	2.66265900	C	-2.50431100	-1.03636800	-0.07549200
H	2.71610800	-1.31204600	-1.96850300	C	-1.40363200	-2.73155900	1.24965800
N	-3.59728500	0.35616300	-0.05970400	C	-1.72005400	-3.05602900	-1.14088200
C	-4.74811200	0.44848000	-0.85106400	C	-2.38761500	-1.83919100	-1.21337500
C	-7.05407000	1.12064000	-2.22203500	C	-2.04906900	-1.50396400	1.16121700
C	-5.42929900	-0.56162300	-1.53401100	H	-1.01494700	-3.08690300	2.19897800
C	-5.22778600	1.77557700	-0.81293000	H	-1.56895200	-3.66399700	-2.02682500
C	-6.38729000	2.11354800	-1.50757500	H	-2.78059500	-1.48043700	-2.16158700
C	-6.58206000	-0.20038600	-2.22496700	H	-2.19119400	-0.88573300	2.04375200
H	-5.08932500	-1.59083500	-1.51589500	N	3.09646700	0.29895400	0.31411600
H	-6.76880700	3.12973200	-1.48442900	C	4.40579500	0.59290200	-0.04332700
H	-7.13084300	-0.96219200	-2.76874900	C	7.07589200	1.11358400	-0.79480000
H	-7.95721700	1.36647500	-2.77035000	C	4.91917900	1.91253600	-0.05576300
C	-3.33725000	1.61624000	0.48763500	C	5.27650800	-0.46152800	-0.41162900
C	-3.21722300	4.26916500	1.26163600	C	6.57946500	-0.20230200	-0.77675800
C	-4.32592400	2.52340000	0.04734500	C	6.25072400	2.15787200	-0.43445900
C	-2.26204300	2.02623500	1.27957900	H	4.90043600	-1.47635700	-0.39590100
C	-2.22615900	3.36297400	1.66577800	H	7.22572700	-1.02886500	-1.05050200
C	-4.26614100	3.85793000	0.44127700	H	6.61684400	3.18008700	-0.43359500
H	-1.47696800	1.33772700	1.57117900	H	8.10216600	1.30902400	-1.08457600
H	-1.40743400	3.71156600	2.28645000	C	2.17206900	1.24000000	0.75403600
H	-5.01798600	4.56670200	0.10789700	C	0.24651600	3.10571000	1.64028700
H	-3.15710000	5.30433600	1.58020700	C	0.87118400	0.82173900	1.12682500
H	2.81885300	-0.63076800	2.30102400	C	2.47124100	2.62483100	0.83502400
N	3.60381200	0.32209600	-0.05725200	C	1.50395000	3.54218300	1.27743400
C	4.72452000	0.42755500	-0.88947000	C	-0.06207200	1.73703900	1.56339300
C	6.98324800	1.12020300	-2.32787000	H	0.60226900	-0.22533700	1.04683400
C	5.21640000	1.74952300	-0.83397800	H	1.75979500	4.59655200	1.32089500
C	5.37195700	-0.56848100	-1.62404800	H	-1.05935400	1.39413800	1.82421900
C	6.50096100	-0.19694200	-2.34789500	H	-0.50340900	3.81675800	1.97023800
C	6.35177600	2.09796600	-1.56247600	S	3.99022600	3.29451800	0.37940900
H	5.02578200	-1.59571400	-1.61998900	N	-3.03352800	0.29494200	-0.15407200
H	7.02317400	-0.94787800	-2.93147200	C	-2.23166600	1.28622800	-0.77051800
H	6.74227700	3.11032900	-1.52615400	C	-0.61686700	3.32104900	-1.87847100
H	7.86725300	1.37427200	-2.90296400	C	-1.07171200	0.97247300	-1.49203000
C	3.37730900	1.56835800	0.53575300	C	-2.55882600	2.64417900	-0.60496900
C	3.31619700	4.19856600	1.39201900	C	-1.77682800	3.64519400	-1.17715700
C	2.34144400	1.96395000	1.38555500	C	-0.26883000	1.98125800	-2.02262600
C	4.35548400	2.47991000	0.08137800	H	-0.76087600	-0.05983400	-1.60514300
C	4.32489600	3.80290800	0.51558600	H	-2.07088900	4.68220000	-1.04207800
C	2.33555200	3.28864500	1.81267600	H	0.63438000	1.70364500	-2.55850700
H	1.56447300	1.27359300	1.69383000	H	0.00145300	4.10552500	-2.30208100
H	5.06888500	4.51474000	0.17122900	C	-4.43465900	0.46736300	-0.06773800
H	1.54982000	3.62388500	2.48157200	C	-7.21616200	0.85867000	0.11390700
H	3.28009600	5.22414200	1.74352200	C	-4.96943800	1.74664200	0.15429000
<b>p-PTZ-DPS-PTZ</b>				C	-5.31615300	-0.61435700	-0.17737500
S	0.10910700	-4.67735100	0.07591700	C	-6.69207800	-0.41746500	-0.07400100
O	0.01805700	-5.40286100	-1.17350100	C	-6.34656600	1.94288400	0.21709600
O	0.09912600	-5.39691100	1.33193300	H	-4.92378700	-1.61297700	-0.33117700
C	1.45394600	-3.59963300	0.04987500	H	-7.35394200	-1.27395600	-0.15100300
C	2.65241100	-1.07113400	0.20996000	H	-6.72952700	2.94748300	0.37026900
C	1.92109800	-3.09218300	1.30286800	H	-8.28749100	1.01260100	0.18338700
C	1.64430100	-2.80858800	-1.12877400	S	-3.87652000	3.09346500	0.47470200
C	2.22133200	-1.56202800	-1.04387700	<b>p-DMAC-DPS-DMAC</b>			
C	2.52027000	-1.85481500	1.37582900	S	0.00006400	4.98132400	0.00021000
H	1.79072200	-3.69382700	2.19634600	O	-0.07661500	5.70354700	1.25210400
H	1.30281200	-3.19010000	-2.08621200				

O	0.07671700	5.70366100	-1.25162000	H	1.87483000	-4.41055200	1.20112300
C	-1.30540100	3.83513900	-0.09949600	C	-0.07832600	-1.70438500	1.74089800
C	-2.46125800	1.30295100	-0.33183700	H	-1.07404300	-1.42513200	2.07358200
C	-1.63377200	3.31305300	-1.37578300	C	0.30716000	-3.03967300	1.69265600
C	-1.62996900	3.09049000	1.06451800	H	-0.37800400	-3.82612100	1.99244300
C	-2.19291800	1.83486700	0.94328500	C	5.13077400	0.75966100	-0.26415100
C	-2.21836500	2.06431200	-1.48412000	H	4.77017700	1.77635900	-0.16967300
H	-1.40920400	3.89845700	-2.26112100	C	6.05545800	-1.84296000	-0.45773000
H	-1.39892700	3.50008100	2.04269900	H	6.43214300	-2.85800400	-0.53849500
H	-2.42941800	1.24683400	1.82706000	C	6.43234400	0.52180800	-0.67224800
H	-2.47483000	1.65526900	-2.45803100	H	7.08046500	1.36084300	-0.90201600
C	1.30557500	3.83518500	0.09980700	C	6.90179400	-0.78783900	-0.78071800
C	2.46147000	1.30300200	0.33193100	H	7.91763500	-0.98558500	-1.10561700
C	1.63013900	3.09063700	-1.06427100	C	3.64383300	-3.67100000	-0.97932300
C	1.63398200	3.31300900	1.37604900	C	4.57799400	-3.70624500	1.36378000
C	2.21859100	2.06426800	1.48428000	H	3.13801800	-3.07275300	-1.74354800
C	2.19309700	1.83500900	-0.94314500	H	4.60036600	-4.01096200	-1.38664900
H	1.39906400	3.50029600	-2.04241600	H	3.03032800	-4.55158000	-0.76633900
H	1.40940600	3.89833600	2.26143700	H	5.53912800	-4.06771600	0.99019800
H	2.42957100	1.24704000	-1.82696900	H	3.97392900	-4.58066700	1.61857500
N	-2.95330900	-0.03967300	-0.43956900	H	4.75470500	-3.12980100	2.27584100
C	-2.10112200	-1.04401300	-0.87630500				
C	-4.27007200	-0.31430000	-0.04157500				
C	-2.50800600	-2.39955100	-0.84200000	<b>p-PXZ-DPS-PXZ</b>			
C	-4.73924100	-1.63941300	0.03566300	S	-0.05275000	-4.18096000	0.05096100
C	-3.86494800	-2.83803300	-0.30471000	O	0.04964500	-4.87303500	-1.21673500
C	-3.64442700	-3.67104500	0.97901900	O	0.02709300	-4.92076600	1.29306900
C	-4.57820800	-3.70597200	-1.36423700	C	-1.45920500	-3.20161100	0.06383500
C	-0.79596000	-0.71282400	-1.32364400	C	-3.11173100	-0.94629400	0.13532900
H	-0.47071000	0.32126100	-1.32710100	C	-1.85912500	-2.56009900	-1.15211500
C	0.07847900	-1.70482100	-1.74040400	C	-1.91195500	-2.67459100	1.31687400
H	1.07430500	-1.42571300	-2.07288300	C	-2.72256000	-1.56682700	1.34858200
C	-0.30722200	-3.04004900	-1.69229800	C	-2.67155000	-1.45377900	-1.11578400
H	0.37787900	-3.82659200	-1.99198200	H	-1.51482700	-2.96102300	-2.10018900
C	-1.59227900	-3.36321700	-1.24620300	H	-1.61759800	-3.17016600	2.23615900
H	-1.87519100	-4.41070100	-1.20110200	H	-3.07836800	-1.16823300	2.29557000
H	-3.03100100	-4.55168700	0.76606500	H	-2.97723600	-0.96047100	-2.03531300
H	-4.60107400	-4.01091700	1.38615400	C	1.24177100	-2.97252800	0.08034000
H	-3.13866500	-3.07292800	1.74338100	C	2.88772400	-0.73654600	0.09686700
H	-5.53945200	-4.06734200	-0.99083900	C	1.58454400	-2.37383500	1.29819600
H	-4.75469400	-3.12942900	-2.27627900	C	1.73194100	-2.46446200	-1.12924500
H	-3.97421900	-4.58045400	-1.61900500	C	2.56448600	-1.35160800	-1.11601700
C	-5.13063900	0.75988900	0.26386100	C	2.40894100	-1.25245400	1.30161100
H	-4.76989300	1.77654200	0.16946900	H	1.20426600	-2.79037000	2.22549300
C	-6.43230000	0.52219300	0.67176300	H	1.46028900	-2.95116400	-2.06029000
H	-7.08034300	1.36130500	0.90146800	H	2.96204500	-0.94342200	-2.04151900
C	-6.90193800	-0.78739500	0.78011800	H	2.68969500	-0.76714200	2.23164100
H	-7.91785100	-0.98502000	1.10486300	N	-3.80218300	0.31128900	0.17814400
C	-6.05569500	-1.84261400	0.45720700	C	-3.13238100	1.45186500	0.58757900
H	-6.43252700	-2.85761200	0.53787400	C	-1.86322300	3.80329800	1.42221400
N	2.95343600	-0.03965700	0.43955900	C	-3.82786800	2.67996600	0.64560100
H	2.47505200	1.65514000	2.45815600	C	-1.76547000	1.42942800	0.94091700
C	4.27011200	-0.31442800	0.04137300	C	-1.14874300	2.59223000	1.35524500
C	2.10120000	-1.04389500	0.87640200	C	-3.19965700	3.85055800	1.06377900
C	4.73909300	-1.63960100	-0.03598800	H	-1.21985000	0.49455600	0.87870600
C	2.50788700	-2.39948500	0.84197900	H	-0.09649300	2.57139700	1.61683400
C	3.86468100	-2.83812400	0.30443800	H	-3.77514300	4.76889200	1.09009300
C	0.79618500	-0.71251100	1.32400800	H	-1.36190400	4.70852500	1.74644800
H	0.47111500	0.32163400	1.32757800	C	-5.12676500	0.40558300	-0.20936200
C	1.59208600	-3.36302600	1.24631000	C	-7.80279700	0.68416900	-0.97505900
				C	-5.85621100	-0.72046800	-0.64288700

C	-5.77539400	1.65890700	-0.16061400	C	-3.19074500	-2.45006800	-0.31448600
C	-7.10747100	1.80016200	-0.54158600	C	-4.24219300	-3.04054000	-1.00813400
C	-7.17530500	-0.57452900	-1.02108900	C	-5.61010500	-1.09299000	-0.61508600
H	-5.36182100	-1.68430400	-0.66406400	H	-4.69090700	0.48720100	0.53147500
H	-7.56452000	2.78140600	-0.48358500	H	-2.24155400	-2.96586800	-0.20435000
H	-7.73265100	-1.44288700	-1.35337100	H	-4.10865400	-4.02900000	-1.43627500
H	-8.84028400	0.78275600	-1.27424600	H	-6.55162600	-0.56424600	-0.72277200
O	-5.13012200	2.76707600	0.27849500	H	-6.26994200	-2.82912300	-1.70975700
N	3.70484200	0.43829500	0.11384800	C	-1.46388400	-1.35438400	1.78705600
C	3.15172000	1.65702600	-0.31609700	C	0.14902500	-2.88665500	3.48238200
C	2.15531700	4.16287800	-1.12021600	C	-0.07786300	-1.14647900	1.81744500
C	1.80773200	1.81051600	-0.66430600	C	-2.03792600	-2.33805000	2.60360200
C	3.98580400	2.78639100	-0.37558200	C	-1.23035100	-3.10119000	3.43929700
C	3.50310100	4.01877000	-0.77871800	C	0.71782700	-1.90548200	2.67050700
C	1.31532900	3.05753400	-1.05965200	H	0.36565200	-0.38452100	1.18162700
H	1.14537800	0.95183700	-0.62600200	H	-3.11239400	-2.49100000	2.58311800
H	4.19275600	4.85583800	-0.80935900	H	-1.68382200	-3.85656100	4.07299600
H	0.26588400	3.15003000	-1.32197700	H	1.79008300	-1.73317300	2.68907700
H	1.77730200	5.13043100	-1.43207700	H	0.77275000	-3.47604000	4.14622800
C	5.10524700	0.30029800	0.05245900	C	1.46324100	-1.35496800	-1.78708000
C	7.90904500	0.15377500	-0.03176800	C	-0.15041000	-2.88644900	-3.48239200
C	5.88962100	1.46122000	-0.01604000	C	2.03680100	-2.33896100	-2.60357400
C	5.75100900	-0.93648600	0.07805400	C	0.07733300	-1.14632900	-1.81751700
C	7.14577000	-1.00558900	0.04279200	C	-0.71872600	-1.90495600	-2.67056200
C	7.27068400	1.39610200	-0.06696500	C	1.22885500	-3.10170100	-3.43927200
H	5.16094600	-1.84458200	0.13425800	H	3.11118700	-2.49247100	-2.58305500
H	7.62672400	-1.97755900	0.07182400	H	-0.36580100	-0.38412800	-1.18172600
H	7.82919000	2.32474000	-0.12121900	H	-1.79089400	-1.73210200	-2.68915700
H	8.99185800	0.10220400	-0.06153600	H	1.68195200	-3.85733000	-4.07293000
O	5.30407000	2.71086800	0.01709200	H	-0.77442900	-3.47553500	-4.14622500
<b>p-DPA-DPS-DPA</b>				C	3.35037000	-1.17393000	-0.23727100
S	0.00109000	4.65312500	0.00004100	C	5.45266100	-2.36843500	1.16542600
O	-0.40314800	5.36874500	-1.18677100	C	3.18960700	-2.45155100	0.31433700
O	0.40568000	5.36849600	1.18687800	C	4.56861200	-0.49840100	-0.08829000
C	-1.18273200	3.46040800	0.41333700	C	5.60952700	-1.09551900	0.61517800
C	-2.00118500	0.79506300	0.77960500	C	4.24076700	-3.04252600	1.00798600
C	-1.08753900	2.84763400	1.70209100	H	2.24020300	-2.96693900	0.20411000
C	-1.83368000	2.75253200	-0.64803500	H	4.69105500	0.48516400	-0.53128600
C	-2.22209500	1.45028400	-0.46706800	H	6.55126400	-0.56718000	0.72296100
C	-1.48434200	1.54867600	1.87314500	H	4.10678500	-4.03096700	1.43603200
H	-0.68192600	3.41963200	2.52988300	H	6.26856900	-2.83203400	1.70972700
H	-1.96524000	3.24180000	-1.60735300	<b>DBTO-PXZ</b>			
H	-2.67346600	0.90052200	-1.28810800	C	-0.71386800	1.54453500	-0.03305900
H	-1.41235800	1.07896400	2.84922800	C	-3.50799200	2.03825500	-0.04971100
C	1.18440200	3.45991800	-0.41330600	C	-1.25996100	2.86754600	-0.06951200
C	2.00155800	0.79418900	-0.77960000	C	-1.61859100	0.46491800	-0.00454100
C	1.83504500	2.75172200	0.64807400	C	-2.97299200	0.72329100	-0.01362700
C	1.08895200	2.84721200	-1.70210700	C	-2.63295500	3.11320600	-0.07772900
C	1.48508000	1.54806700	-1.87316100	H	-1.26946000	-0.56420000	0.02300500
C	2.22280400	1.44929400	0.46709600	H	-3.01172000	4.13118200	-0.10621500
H	1.96687600	3.24092300	1.60738900	H	-4.58319600	2.18035800	-0.05521400
H	0.68367700	3.41944000	-2.52990600	S	0.00001100	4.06872900	-0.10678800
H	1.41292300	1.07841300	-2.84925800	O	-0.00012000	4.83577600	-1.34866400
H	2.67389800	0.89930300	1.28813500	O	0.00014000	4.91500500	1.08232900
N	-2.28304100	-0.56202600	0.94191000	C	1.25998600	2.86754300	-0.06978300
N	2.28277500	-0.56301900	-0.94192900	C	2.97302100	0.72328400	-0.01415500
C	-3.35093600	-1.17242900	0.23724500	C	0.71389600	1.54453300	-0.03320400
C	-5.45380900	-2.36592200	-1.16545500	C	2.63297900	3.11319600	-0.07832100
C	-4.56890000	-0.49637600	0.08838500	C	3.50801800	2.03824400	-0.05044700

C	1.61862100	0.46491700	-0.00476300	O	-0.00000500	5.16175500	-1.22204700
H	3.01174000	4.13117000	-0.10694500	C	-1.26320600	3.16517800	-0.00004500
H	4.58322000	2.18034200	-0.05623000	C	-2.97419800	1.02274700	-0.00001500
H	1.26949000	-0.56419700	0.02297000	C	-0.71229000	1.84271200	-0.00002500
N	3.88708900	-0.38581400	0.01182400	C	-2.62965300	3.41113600	-0.00004900
N	-3.88706100	-0.38580600	0.01240800	C	-3.51091900	2.33527600	-0.00003400
C	4.32811500	-0.95234200	-1.17830300	C	-1.62141700	0.76214400	-0.00001100
C	5.26528300	-2.16918900	-3.52540700	H	-3.00367500	4.43131300	-0.00006300
C	5.22167300	-2.04134200	-1.12802000	H	-4.58585400	2.47777000	-0.00003500
C	3.91429400	-0.48177000	-2.43386900	H	-1.27500700	-0.26836600	0.00000600
C	4.38133000	-1.08711200	-3.59272200	N	-3.89248700	-0.08914300	0.00000900
C	5.68571300	-2.64576700	-2.28773600	N	3.89248700	-0.08914000	-0.00000800
H	3.22950700	0.35674300	-2.48477200	C	-4.33108500	-0.59916700	1.21813600
H	4.05349500	-0.71157600	-4.55566900	C	-5.16693600	-1.59229300	3.69583000
H	6.37091700	-3.48150900	-2.19738600	C	-5.22361000	-1.69237000	1.25846300
H	5.62643400	-2.63888500	-4.43333700	C	-3.87263000	-0.01217100	2.41909400
C	4.35863900	-0.87124700	1.22581000	C	-4.28969500	-0.50621900	3.64156700
C	5.35584500	-1.92799400	3.62497600	C	-5.61848500	-2.16506100	2.51109200
C	3.97503200	-0.31773400	2.45684500	H	-3.19375900	0.83038300	2.37719900
C	5.25198200	-1.96151800	1.22631900	H	-3.93028600	-0.04287500	4.55413900
C	5.74581200	-2.48680100	2.41202000	H	-6.30101500	-3.00769600	2.56515900
C	4.47187200	-0.84394400	3.64171200	H	-5.49738800	-1.98725500	4.65048300
H	3.29005500	0.52210800	2.46836300	C	-4.33121300	-0.59911600	-1.21809400
H	6.42951400	-3.32709100	2.36092000	C	-5.16731100	-1.59215400	-3.69574100
H	4.16742200	-0.40478700	4.58520600	C	-3.87286500	-0.01208700	-2.41907800
H	5.74046300	-2.33557100	4.55307400	C	-5.22374800	-1.69231200	-1.25837200
C	-4.32879500	-0.95178200	-1.17772300	C	-5.61874600	-2.16496100	-2.51097700
C	-5.26735700	-2.16753200	-3.52484100	C	-4.29005600	-0.50608900	-3.64152700
C	-5.22237100	-2.04076500	-1.12742000	H	-3.19397400	0.83045300	-2.37722100
C	-3.91565000	-0.48068100	-2.43331400	H	-6.30128100	-3.00759500	-2.56500500
C	-4.38337900	-1.08547800	-3.59217400	H	-3.93072900	-0.04272100	-4.55411800
C	-5.68710300	-2.64464700	-2.28714400	H	-5.49785800	-1.98708200	-4.65037500
H	-3.23083600	0.35781100	-2.48423200	C	4.33107200	-0.59921500	-1.21811900
H	-4.05606300	-0.70953300	-4.55513800	C	5.16687900	-1.59246500	-3.69578200
H	-6.37229500	-3.48039900	-2.19677800	C	5.22359800	-1.69241900	-1.25841100
H	-5.62905100	-2.63680100	-4.43277700	C	3.87260000	-0.01227600	-2.41909900
C	-4.35794800	-0.87175900	1.22644200	C	4.28964500	-0.50638400	-3.64155600
C	-5.35384900	-1.92951700	3.62570800	C	5.61844700	-2.16517600	-2.51102400
C	-3.97366600	-0.31877100	2.45750200	H	3.19373000	0.83028100	-2.37723400
C	-5.25131900	-1.96201000	1.22697500	H	3.93022100	-0.04308300	-4.55414400
C	-5.74449900	-2.48779400	2.41272500	H	5.49731100	-1.98747500	-4.65042200
C	-4.46985700	-0.84548300	3.64241900	C	4.33122700	-0.59906300	1.21811000
H	-3.28868200	0.52106600	2.46899700	C	5.16737100	-1.59198200	3.69579100
H	-6.42824900	-3.32804600	2.36164300	C	3.87289600	-0.01198100	2.41907400
H	-4.16488800	-0.40672900	4.58593400	C	5.22376300	-1.69225800	1.25842500
H	-5.73796000	-2.33748700	4.55384300	C	5.61878800	-2.16484300	2.51104700
O	5.66330000	-2.54636000	0.06211300	C	4.29010800	-0.50592500	3.64154000
O	-5.66331500	-2.54632200	0.06274200	H	3.19400300	0.83055700	2.37718900
<b>DBTO-DMAC</b>				H	6.30133100	-3.00746900	2.56510400
C	0.71228800	1.84271300	-0.00002800	H	3.93079500	-0.04251500	4.55411600
C	3.51091700	2.33527900	-0.00003900	H	5.49793700	-1.98686200	4.65043900
C	1.26320300	3.16517900	-0.00004900	C	-5.75655900	-2.36177100	0.00005800
C	1.62141600	0.76214600	-0.00000900	C	-7.30055000	-2.27506500	0.00014200
C	2.97419800	1.02275000	-0.00001600	H	-7.71419700	-2.76783900	0.88382200
C	2.62965000	3.41113900	-0.00005500	H	-7.71429000	-2.76777900	-0.88352700
H	1.27500800	-0.26836500	0.00000600	H	-7.62664900	-1.23146300	0.00019500
H	3.00367100	4.43131600	-0.00007400	C	-5.32680600	-3.84742600	-0.00000900
H	4.58585300	2.47777400	-0.00004500	H	-5.71482800	-4.35997000	0.88428500
S	-0.00000200	4.37465600	-0.00006400	H	-4.23665600	-3.93250300	-0.00005000
O	-0.00000100	5.16179200	1.22189500	H	-5.71489000	-4.35990600	-0.88431300

H	6.30096900	-3.00782000	-2.56506000
C	5.75656100	-2.36177000	0.00001500
C	5.32680800	-3.84742500	0.00013500
H	5.71492800	-4.35988600	0.88443400
H	5.71479400	-4.35998800	-0.88416400
H	4.23665700	-3.93250000	0.00022300
C	7.30055200	-2.27506300	-0.00008800
H	7.71430000	-2.76773900	0.88360100
H	7.62665100	-1.23146100	-0.00018900
H	7.71419100	-2.76787600	-0.88374900

**TXO2-PXZ**

C	1.22790000	-1.43534800	-0.34404700
C	3.44955200	-1.33830000	1.44527500
C	1.31077600	-2.28168500	0.80782500
C	2.28080500	-0.55367900	-0.55154200
C	3.38225000	-0.50868800	0.31236400
C	2.41053000	-2.21117100	1.69197200
H	2.27151800	0.13308100	-1.39166900
H	2.41298700	-2.84406000	2.57297300
H	4.30242200	-1.27720200	2.11491100
S	-0.00000400	-3.32674400	1.23912500
O	-0.00000600	-4.55525400	0.46016300
O	-0.00000100	-3.53022900	2.67935800
C	-1.31078100	-2.28168100	0.80783000
C	-3.38225100	-0.50867700	0.31236200
C	-1.22790700	-1.43534900	-0.34404600
C	-2.41053200	-2.21115600	1.69197900
C	-3.44955100	-1.33828100	1.44527900
C	-2.28080800	-0.55367900	-0.55154700
H	-2.41299000	-2.84403900	2.57298500
H	-4.30241800	-1.27717400	2.11491800
H	-2.27151600	0.13307300	-1.39168200
C	-0.00000700	-1.47493000	-1.26020400
C	-0.00002900	-0.30251200	-2.24877400
H	0.87652800	-0.36229700	-2.89889300
H	-0.00001000	0.67077200	-1.74713900
H	-0.87662600	-0.36228600	-2.89884100
C	-0.00001100	-2.76179500	-2.12615800
H	-0.00000900	-3.67142700	-1.52865200
H	0.88954500	-2.76108600	-2.76522800
H	-0.88957100	-2.76108500	-2.76522100
N	4.43600700	0.42474100	0.04818300
C	4.24976300	1.78037700	0.29936400
C	3.96043600	4.53340700	0.77091100
C	5.29286100	2.68456500	0.01186100
C	3.05972300	2.28693500	0.84585100
C	2.92120300	3.64908400	1.07541300
C	5.15072300	4.04561000	0.24088800
H	2.25793200	1.59933500	1.08854500
H	1.99609100	4.02268200	1.50054700
H	5.98332300	4.69826800	0.00219500
H	3.84766800	5.59648300	0.95182300
C	5.65251500	-0.01473500	-0.46819700
C	8.13502500	-0.81261700	-1.50521200
C	5.89836800	-1.36483400	-0.76119200
C	6.67267500	0.92339200	-0.72182100
C	7.90171200	0.53155900	-1.23243700
C	7.12931600	-1.75497400	-1.27142200
H	5.11512800	-2.09280900	-0.58555800

H	8.65324900	1.29297600	-1.41018700
H	7.30306400	-2.80258800	-1.49086800
H	9.09467200	-1.12209900	-1.90383200
O	6.48916000	2.25821600	-0.49052900
N	-4.43600400	0.42475400	0.04817500
C	-5.65252600	-0.01472500	-0.46816900
C	-8.13506600	-0.81261300	-1.50510900
C	-5.89839800	-1.36483000	-0.76112300
C	-6.67268400	0.92340400	-0.72179600
C	-7.90173500	0.53156900	-1.23237500
C	-7.12936000	-1.75497200	-1.27131600
H	-5.11516000	-2.09280700	-0.58548800
H	-8.65326800	1.29298800	-1.41013000
H	-7.30312100	-2.80259000	-1.49073100
H	-9.09472400	-1.12209600	-1.90370000
C	-4.24974100	1.78039600	0.29931100
C	-3.96037800	4.53343900	0.77076500
C	-5.29283700	2.68458500	0.01180300
C	-3.05968600	2.28696100	0.84575800
C	-2.92114700	3.64911500	1.07527300
C	-5.15068100	4.04563600	0.24078400
H	-2.25789500	1.59936100	1.08845700
H	-1.99602200	4.02271800	1.50037500
H	-5.98328000	4.69829400	0.00208900
H	-3.84759600	5.59651900	0.95164100
O	-6.48915200	2.25823200	-0.49054400

**TXO2-DMAC**

C	1.22692000	-1.69337800	-0.30070400
C	3.44562600	-1.59323900	1.49059800
C	1.31049700	-2.54300900	0.84909600
C	2.27602900	-0.80502400	-0.50207500
C	3.37558100	-0.75865800	0.36215500
C	2.40916200	-2.47020900	1.73457200
H	2.26411600	-0.11287500	-1.33770500
H	2.41350200	-3.10568300	2.61374900
H	4.29892500	-1.53207000	2.15968800
S	0.00000000	-3.58867600	1.27866700
O	-0.00000300	-4.81697300	0.49867500
O	0.00000100	-3.79496500	2.17886400
C	-1.31049600	-2.54300500	0.84910000
C	-3.37558000	-0.75865400	0.36215800
C	-1.22691900	-1.69337500	-0.30070000
C	-2.40915900	-2.47020200	1.73457800
C	-3.44562200	-1.59323100	1.49060400
C	-2.27603000	-0.80502300	-0.50207500
H	-2.41349900	-3.10567500	2.61375600
H	-4.29892000	-1.53206100	2.15969500
H	-2.26411800	-0.11288000	-1.33771000
C	-0.00000200	-1.73317300	-1.21792200
C	-0.00000400	-0.56019300	-2.20570500
H	0.87691500	-0.61979200	-2.85544300
H	0.00004900	0.41258200	-1.70331400
H	-0.87698000	-0.61973600	-2.85537100
C	-0.00000600	-3.01941400	-2.08464100
H	0.00000600	-3.92946800	-1.48777000
H	0.88962000	-3.01821700	-2.72372700
H	-0.88964900	-3.01822600	-2.72370400
N	4.42629700	0.18504000	0.10361800

N	-4.42629600	0.18504200	0.10361900	<b>Cz-TTR</b>			
C	-4.23408200	1.52149000	0.44564700	H	0.96178000	-2.57448100	-1.93650700
C	-3.77921100	4.19646400	1.13777500	C	0.60625900	-1.69899800	-1.40372900
C	-3.02941000	1.90789600	1.07657100	C	-0.27742900	0.54489000	0.02240900
C	-5.23245000	2.48479400	0.18058900	C	1.51696900	-0.74083100	-0.97440700
C	-4.97175800	3.80958900	0.53417800	C	-0.75153700	-1.52058700	-1.15873000
C	-2.80849800	3.23089800	1.41395200	C	-1.20139400	-0.40261900	-0.44682500
H	-2.28060300	1.15857900	1.30107800	C	1.06572900	0.37815700	-0.26388900
H	-5.72574400	4.56550300	0.33674800	H	-1.46750900	-2.24623800	-1.52791300
H	-1.87862500	3.50873100	1.89901800	H	-0.60266600	1.38222200	0.63132600
H	-3.61418700	5.23649500	1.39785500	S	3.22910000	-0.97304300	-1.35398800
C	-5.60802100	-0.25941500	-0.48878700	O	3.46269500	-2.38273400	-1.52497800
C	-7.95889000	-1.21788500	-1.66603900	O	3.60551800	-0.07111000	-2.40883700
C	-5.73513100	-1.62307200	-0.83438700	S	2.19357800	1.62318900	0.31811800
C	-6.66310100	0.63907900	-0.75584700	O	2.60263500	2.42955500	-0.79962400
C	-7.82310300	0.12796300	-1.34076300	O	1.60365000	2.26238500	1.46388900
C	-6.90071700	-2.09332100	-1.41246600	C	3.57612500	0.65685600	0.86869000
H	-4.91131800	-2.30003500	-0.64641400	C	5.77547400	-0.78768100	1.75692700
H	-8.64723100	0.80227100	-1.55304400	C	4.02298300	-0.45700700	0.14818700
H	-6.98178600	-3.14423300	-1.66891900	C	4.21573500	1.04010300	2.04006700
H	-8.87667000	-1.57753100	-2.11868800	C	5.33064200	0.31968200	2.47337800
C	4.23408300	1.52148700	0.44564900	C	5.11220400	-1.19182100	0.59655000
C	3.77921100	4.19646000	1.13778500	H	3.83738600	1.88558400	2.60462700
C	3.02941100	1.90789100	1.07657600	H	5.42655300	-2.07187400	0.04572000
C	5.23245000	2.48479200	0.18059300	H	6.63185100	-1.35364200	2.10640300
C	4.97175700	3.80958700	0.53418500	H	5.83929000	0.61971600	3.38281800
C	2.80849900	3.23089300	1.41396100	N	-2.56364700	-0.23273400	-0.17620000
H	2.28060500	1.15857300	1.30108400	C	-3.27518200	0.97248900	-0.31268600
H	5.72574300	4.56550200	0.33675700	C	-5.19748700	3.01727200	-0.41888200
H	1.87862700	3.50872400	1.89902900	C	-2.87961100	2.18400800	-0.78880100
H	3.61418600	5.23649100	1.39786700	C	-4.65470900	0.70699000	0.09909300
C	5.60802100	-0.25941500	-0.48879000	C	-5.61721500	1.79650600	0.04967300
C	7.95889000	-1.21788100	-1.66604900	C	-3.86440500	3.23068100	-0.84412000
C	6.66310200	0.63908000	-0.75584800	H	-1.86949700	2.37592500	-1.13149000
C	5.73513100	-1.62307000	-0.83439600	H	-6.63813500	1.63089500	0.37446700
C	6.90071600	-2.09331800	-1.41248000	H	-3.57046700	4.20358700	-1.21927400
C	7.82310400	0.12796600	-1.34076700	H	-5.89906900	3.84380000	-0.46923300
H	4.91131800	-2.30003400	-0.64642600	C	-3.43853600	-1.23065600	0.28632400
H	6.98178500	-3.14422800	-1.66893800	C	-5.60570100	-2.73701700	1.24913600
H	8.64723100	0.80227500	-1.55304600	C	-4.75561200	-0.60977000	0.44187500
H	8.87667000	-1.57752500	-2.11870000	C	-3.20482200	-2.52869900	0.62396800
C	6.57079300	2.12661400	-0.44905900	C	-4.31257200	-3.29776800	1.12009200
C	7.70353500	2.51076200	0.53109000	C	-5.85777600	-1.42700900	0.92309600
H	7.67710300	3.58130400	0.75082300	H	-2.22511600	-2.98448500	0.54409100
H	8.68087700	2.28006500	0.09909700	H	-4.14732700	-4.33226800	1.39651100
H	7.60108800	1.96112500	1.47076500	H	-6.84729500	-0.99539500	1.02184600
C	6.73949100	2.92099800	-1.76500600	H	-6.41187400	-3.36432100	1.61594900
H	6.69319100	3.99658700	-1.57487000				
H	5.95018700	2.65996300	-2.47530500	<b>DMAC-TTR</b>			
H	7.70643300	2.70237100	-2.22574800	N	-2.17147600	-0.21875800	-0.50744500
C	-6.57079300	2.12661400	-0.44906300	C	-3.18256300	-1.20910000	-0.33501900
C	-7.70353400	2.51076500	0.53108400	C	-5.22071700	-3.03975200	-0.00006300
H	-7.67710100	3.58130800	0.75081500	C	-4.18871000	-0.92688500	0.60272700
H	-7.60108900	1.96113100	1.47076100	C	-3.20656400	-2.35626700	-1.12952100
H	-8.68087700	2.28007000	0.09909100	C	-4.23009200	-3.28136300	-0.94882000
C	-6.73948900	2.92099400	-1.76501200	C	-5.20362200	-1.86799800	0.76023400
H	-6.69319100	3.99658300	-1.57488100	C	-2.69222100	1.11185000	-0.57961400
H	-7.70643100	2.70236400	-2.22575600	C	-3.81588300	3.63253100	-0.68348600
H	-5.95018400	2.65995700	-2.47531000	C	-2.31344200	1.98682400	-1.59729800
				C	-3.67574000	1.44763100	0.36435200

C	-4.22052800	2.72887100	0.30000800	O	1.61992400	-0.44252900	-2.73744000
C	-2.87493700	3.25902400	-1.63961600	C	3.54393800	0.18448900	-1.07317600
C	-4.08513000	0.38340000	1.38156700	C	5.58682500	1.96736500	-0.43433900
C	-5.39696200	0.73523000	2.08448700	C	3.98915300	0.30149900	0.25568000
C	-2.97813000	0.25209400	2.45728200	C	4.11106400	0.97352500	-2.07243100
H	-6.02427400	-3.75529200	0.13921800	C	5.14432700	1.84998400	-1.75476800
H	-2.44457600	-2.50264500	-1.88838900	C	4.99837400	1.20904900	0.57335800
H	-4.25972100	-4.17675600	-1.55995700	H	3.73069200	0.89149200	-3.08535700
H	-5.99854000	-1.69236300	1.47609000	H	5.30623800	1.30876600	1.60910500
H	-4.25538400	4.62397100	-0.71300600	H	6.38482600	2.65990900	-0.18779600
H	-1.61095300	1.66605600	-2.35876000	H	5.59761700	2.45089000	-2.53615300
H	-4.97798900	3.03085300	1.01420900	N	-2.50444400	0.09025700	0.22413900
H	-2.58386000	3.94737800	-2.42527300	C	-3.32133100	-1.00999100	0.04213300
H	-5.65454200	-0.03861400	2.81195100	C	-5.05379000	-3.16765400	-0.36557900
H	-6.22428000	0.84185000	1.37629000	C	-2.83460600	-2.33049800	0.13652500
H	-5.28900800	1.66866600	2.64220600	C	-4.68962900	-0.80758300	-0.24572700
H	-2.00541600	0.00726900	2.02241100	C	-5.55343400	-1.88070200	-0.45291100
H	-2.88062800	1.19709300	2.99958700	C	-3.69533500	-3.38845500	-0.06605600
H	-3.24622500	-0.53581200	3.16734200	H	-1.78859600	-2.49239900	0.36763900
C	-0.82333700	-0.51178600	-0.50188200	H	-6.59453700	-1.67626400	-0.67510700
C	1.90363200	-1.26137200	-0.49763500	H	-3.31693900	-4.40155000	0.00661000
C	-0.40637000	-1.89004500	-0.17713700	H	-5.71558500	-4.01137000	-0.52580800
C	0.15773300	0.47191500	-0.67885200	C	-3.03914500	1.36258500	0.15456600
C	1.50488200	0.13466300	-0.73244800	C	-4.21011600	3.89541500	-0.01878800
C	0.92798000	-2.21214300	-0.17263300	C	-4.41540900	1.51545000	-0.12202100
H	-1.13643900	-2.61793300	0.14500500	C	-2.24851600	2.51609500	0.33756500
H	-0.09884500	1.51983300	-0.76740800	C	-2.83485600	3.76167300	0.25296200
H	1.25128200	-3.20815500	0.11162000	C	-5.00126000	2.77651000	-0.20902200
S	3.58988700	-1.70236900	-0.40612900	H	-1.19023800	2.40192100	0.53989600
O	3.70697200	-2.93261500	0.34024200	H	-2.22511900	4.64665300	0.39402700
O	4.18807300	-1.63345800	-1.71203200	H	-6.06097000	2.84486600	-0.42658100
S	2.68777200	1.37372100	-0.92688700	H	-4.65407800	4.88237900	-0.08442300
O	3.38796900	1.24812700	-2.17939300	O	-5.21278300	0.43962400	-0.32386600
O	2.08023800	2.64912600	-0.61574600	<b>PTZ-TTR</b>			
C	3.81848900	0.95266700	0.37108700	H	-5.21254200	-1.81825800	1.71065000
C	5.54517800	0.32396200	2.46875200	C	-4.96793400	-0.77320800	1.55230300
C	4.20827800	-0.38012400	0.59535100	C	-4.23409700	1.90277300	1.16009800
C	4.28192100	1.96215800	1.21264500	C	-4.07893700	-0.43342100	0.53434000
C	5.15936600	1.64811500	2.24638900	C	-5.52009900	0.22922900	2.34428400
C	5.05385400	-0.69458900	1.65765300	C	-5.15343700	1.56276400	2.14840000
H	3.94593400	2.98013200	1.04530800	C	-3.70840500	0.90900500	0.33701500
H	5.53462300	2.43802300	2.88848200	H	-6.22741700	-0.03203400	0.312403800
H	5.31283400	-1.73320100	1.83443800	H	-5.57628400	2.33995000	2.77623800
H	6.21959100	0.08280300	3.28338100	H	-3.91288500	2.92889800	1.01499200
<b>PXZ-TTR</b>				S	-3.38415600	-1.73544400	-0.44356000
H	1.02482600	-0.00412600	3.18661200	O	-3.51059100	-2.97293100	0.28869600
C	0.65644500	-0.13114400	2.17337600	O	-3.91841400	-1.66932100	-1.77695800
C	-0.22682500	-0.37325500	-0.49478900	S	-2.52698000	1.36354600	-0.90321000
C	1.57565400	-0.47913100	1.16938100	O	-3.16301100	1.22900300	-2.18837700
C	-0.68089300	0.04772000	1.88838600	O	-1.96291600	2.64980800	-0.55805200
C	-1.10645700	-0.08591400	0.52728100	C	-1.32667600	0.14939000	-0.65776200
C	1.11841400	-0.60130300	-0.20077300	C	0.60062100	-1.84069200	-0.03529900
H	-1.39732200	0.29352100	2.66454300	C	-1.70544000	-1.25843700	-0.45100700
H	-0.56343100	-0.42605800	-1.52701700	C	0.00827200	0.51486700	-0.54710700
S	3.24933900	-0.64114500	1.56299900	C	1.00018300	-0.44950800	-0.33197900
O	3.50755200	0.03604000	2.81622000	C	-0.72499500	-2.19123800	-0.09023100
O	3.70370500	-2.00423900	1.43693400	H	0.24631800	1.56814600	-0.62427000
S	2.21696200	-0.90762200	-1.50239800	H	-1.03906200	-3.19595000	0.17292500
O	2.71377100	-2.26071300	-1.47482100	H	1.33366000	-2.55320900	0.31409400
				N	2.34367600	-0.13465600	-0.28340100



C	3.35187700	-1.13166200	-0.16233600
C	5.31407600	-3.06923600	0.16809400
C	3.39596100	-2.22604000	-1.03114900
C	4.32563300	-0.97123800	0.83338100
C	5.30316400	-1.95248500	0.99971200
C	4.37242400	-3.19914900	-0.85502900
H	2.66440400	-2.30090600	-1.82960600
H	6.05639700	-1.82935000	1.77111000
H	4.40402500	-4.05325500	-1.52228900
H	6.07827400	-3.82719300	0.30237700
C	2.83415400	1.20616800	-0.33234100
C	3.80051500	3.81190200	-0.31224500
C	2.48577900	2.08106700	-1.36403900
C	3.73385400	1.60708400	0.66391800
C	4.20448300	2.92113400	0.67652300
C	2.96120500	3.38657100	-1.34393700
H	1.85200000	1.73396600	-2.17310500
H	4.90038500	3.22983300	1.44983000
H	2.68081400	4.06890600	-2.13845500
H	4.16877000	4.83196200	-0.29664500
S	4.28512200	0.44969700	1.87100800

**Cz-Ph-TTR**

H	3.16680800	2.85595300	1.63227900
C	2.73400700	1.93426000	1.25786900
C	1.67972900	-0.43982400	0.17543200
C	3.59435000	0.87093700	0.92121900
C	1.37602400	1.80908700	1.10863200
C	0.76971500	0.60496400	0.56902500
C	3.02439600	-0.31979600	0.37224100
H	0.75801300	2.65269400	1.38576700
H	1.32544900	-1.35115700	-0.29063200
S	5.31667700	1.06313200	1.12176800
O	5.62259100	2.47221500	1.08749200
O	5.79458500	0.28428700	2.23287200
S	4.05094200	-1.68064200	-0.09374100
O	4.55179500	-2.32745700	1.08771400
O	3.35487900	-2.46937600	-1.07892300
C	5.39759200	-0.84993700	-0.90002000
C	7.51962700	0.39740100	-2.18682500
C	5.94075500	0.32948100	-0.37489000
C	5.90195300	-1.39633900	-2.07369200
C	6.97856100	-0.77594400	-2.70783100
C	6.99181700	0.96389300	-1.02640700
H	5.44490200	-2.29201800	-2.48092500
H	7.37933800	1.89403700	-0.62430400
H	8.34712100	0.88494100	-2.69101600
H	7.38283100	-1.20469100	-3.61840300
C	-0.61930100	0.46328500	0.42272000
C	-3.45882100	0.19197500	0.12699600
C	-1.22888700	-0.72008300	-0.16898100
C	-1.54945900	1.49672500	0.85908500
C	-2.89660800	1.36691400	0.70649300
C	-2.57661900	-0.84872100	-0.29956200
H	-0.60343200	-1.51630300	-0.55036100
H	-1.17623300	2.38191600	1.35589200
H	-3.56115200	2.13469400	1.08931100
H	-2.99192300	-1.72186000	-0.79211300
N	-4.82742800	0.06090800	-0.02116500
C	-5.71007200	1.06467700	-0.45962600

C	-7.80588800	2.64208700	-1.33355400
C	-7.01960300	0.54374400	-0.48210200
C	-5.42244100	2.35164100	-0.91540800
C	-6.49337700	3.13387700	-1.34003500
C	-8.07601900	1.34054700	-0.91715600
H	-4.40811700	2.73051400	-0.96131300
H	-6.30169100	4.14127900	-1.69407900
H	-9.08856100	0.95006300	-0.94188900
H	-8.61641000	3.27754400	-1.67392400
C	-5.57752200	-1.10078700	0.23692500
C	-7.47406600	-3.06594000	0.66591600
C	-5.15692100	-2.31814500	0.77356100
C	-6.93486400	-0.83900000	-0.03803200
C	-7.88953000	-1.83113500	0.17277200
C	-6.12581200	-3.29872900	0.97029700
H	-4.12441100	-2.49728900	1.04990000
H	-8.93847100	-1.64121400	-0.03243700
H	-5.82796200	-4.25807400	1.37996100
H	-8.20309300	-3.85126400	0.83440400

**DMAC-Ph-TTR**

H	7.92974800	-0.24310200	-1.96350300
C	7.53526100	0.51216800	-1.29178900
C	6.42795100	2.44865400	0.40319100
C	6.49531400	0.17542500	-0.43251300
C	8.04201800	1.81142400	-1.28012300
C	7.49234900	2.77543700	-0.43668100
C	5.94343900	1.14591900	0.41396500
H	8.86030800	2.07234800	-1.94299400
H	7.88076700	3.78827800	-0.44090000
H	5.96347900	3.19132900	1.04343900
S	5.88489200	-1.49766100	-0.45252700
O	6.20556200	-2.07316500	-1.73884900
O	6.39525200	-2.15446600	0.72442100
S	4.60400000	0.75036800	1.51290600
O	5.12639200	-0.02573600	2.60642700
O	3.89789700	1.97267000	1.81428600
C	3.59208800	-0.26267300	0.48560500
C	1.95097900	-1.79366900	-1.15530500
C	4.17334800	-1.24842400	-0.36496800
C	2.23855300	-0.04301400	0.50708200
C	1.34341300	-0.82115700	-0.28519900
C	3.31183000	-1.98590200	-1.19913400
H	1.87906300	0.76830500	1.12945200
H	3.74436100	-2.71142700	-1.88044600
H	1.33634100	-2.40601200	-1.80324000
C	-0.07108900	-0.61422000	-0.23186700
C	-2.88998800	-0.20854500	-0.13697100
C	-0.68385500	0.25706200	0.73174600
C	-0.96799100	-1.27548800	-1.13881100
C	-2.32811100	-1.08884100	-1.08438200
C	-2.03995300	0.46552700	0.76876500
H	-0.07705000	0.75311200	1.47901600
H	-0.57776500	-1.92603400	-1.91091100
H	-2.97805700	-1.59185800	-1.79547900
H	-2.47240200	1.11808700	1.52240700
N	-4.29544900	-0.01032600	-0.08629400
C	-5.12992700	-1.09600800	0.20586500
C	-6.74080100	-3.31541800	0.72779400
C	-4.54972200	-2.33864600	0.55120600

C	-6.53354000	-0.94421900	0.20289300	H	-0.52899600	0.53528700	1.61570800
C	-7.30993100	-2.07677400	0.45269700	H	-2.93107600	0.91751600	1.69215400
C	-5.35072500	-3.43766400	0.79571900	H	-3.42084800	-1.25898000	-1.99511800
H	-3.47530600	-2.42521100	0.64287000	N	-4.74582500	0.06520600	-0.08476300
H	-8.39142600	-1.98821400	0.44627500	C	-5.27714700	1.32070800	-0.32734200
H	-4.89255800	-4.38537300	1.05568200	C	-6.44689200	3.81987100	-0.79728500
H	-7.37744200	-4.17304800	0.91679000	C	-4.46875400	2.42506000	-0.66812800
C	-4.81623900	1.26615500	-0.33083000	C	-6.67575300	1.50163200	-0.25369300
C	-5.78594800	3.84768200	-0.76525000	C	-7.25985100	2.74505100	-0.48312300
C	-6.20504500	1.50411800	-0.24274300	C	-5.05273400	3.65441500	-0.89459000
C	-3.93916400	2.30712500	-0.71407600	H	-3.39741900	2.28926800	-0.75158900
C	-4.42171300	3.58636500	-0.91437700	H	-8.33796200	2.83400000	-0.41365200
C	-6.65529800	2.80847200	-0.45202200	H	-4.42626100	4.49952800	-1.15584700
H	-2.88899400	2.09857200	-0.86849300	H	-6.89026800	4.79253200	-0.97841300
H	-3.73712600	4.37625500	-1.20255200	C	-5.59131700	-0.98809000	0.22055700
H	-7.71766100	3.01856000	-0.38191600	C	-7.38322100	-3.05389900	0.81801100
H	-6.17358600	4.84881900	-0.92014900	C	-5.10622700	-2.27844700	0.51900300
C	-7.21388000	0.39737600	0.00284800	C	-6.98512700	-0.76330800	0.25511600
C	-8.03477700	0.72762900	1.27218400	C	-7.87890800	-1.79062700	0.54733300
H	-7.38429200	0.78174600	2.14918300	C	-5.99614200	-3.29192200	0.80957100
H	-8.79316900	-0.03865200	1.44899500	H	-4.03721500	-2.45287300	0.52235900
H	-8.54614000	1.68655300	1.15904600	H	-8.93984800	-1.56871000	0.56048800
C	-8.15870200	0.31208600	-1.21965700	H	-5.61716100	-4.28099000	1.03993500
H	-8.68350000	1.25908600	-1.36647400	H	-8.06944300	-3.86104700	1.04824600
H	-8.90880600	-0.46831800	-1.06982500	O	-7.50446900	0.46645800	0.02398300
H	-7.59459100	0.08297800	-2.12773600				

**PXZ-Ph-TTR**

H	7.48170700	-0.15388700	-1.97033000
C	7.08992900	0.56181600	-1.25505000
C	5.99042100	2.39823100	0.55114700
C	6.04795500	0.17723400	-0.41738700
C	7.60210300	1.85539300	-1.16656800
C	7.05585500	2.77054100	-0.26732700
C	5.50016500	1.09870000	0.48547300
H	8.42201900	2.15163800	-1.81249600
H	7.44845400	3.78027000	-0.21122700
H	5.52881800	3.10334600	1.23455300
S	5.42699400	-1.48726700	-0.54348600
O	5.74318300	-1.98018900	-1.86623000
O	5.94795900	-2.22252700	0.58286600
S	4.15883000	0.64629500	1.55919000
O	4.68137500	-0.18605500	2.61180200
O	3.45806500	1.85339700	1.93152200
C	3.14574000	-0.30245500	0.47854600
C	1.49340800	-1.71021600	-1.25839400
C	3.72236100	-1.23596300	-0.43366700
C	1.79107100	-0.07548700	0.51004400
C	0.89488900	-0.79146000	-0.32935200
C	2.85273500	-1.90979800	-1.31418000
H	1.43452200	0.70284200	1.17556400
H	3.27929700	-2.59677000	-2.03807800
H	0.87117500	-2.28210800	-1.93643000
C	-0.52583200	-0.57036000	-0.26648800
C	-3.32544000	-0.14372100	-0.14932800
C	-1.41036500	-1.07779200	-1.26726300
C	-1.13508300	0.15813900	0.80049700
C	-2.49611500	0.37212400	0.85872600
C	-2.77449700	-0.87238700	-1.21105500
H	-1.01416500	-1.61832400	-2.11813000

**PTZ-Ph-TTR**

H	3.44635000	-3.31622600	-0.23115200
C	3.02011500	-2.32069700	-0.29708800
C	1.98508200	0.29630200	-0.36666000
C	3.88712700	-1.22809500	-0.50761600
C	1.66815900	-2.12880300	-0.17439500
C	1.07558300	-0.80162000	-0.22027800
C	3.32566500	0.09550700	-0.53191600
H	1.04450000	-3.00036500	-0.02494200
H	1.63826400	1.32270300	-0.33682100
S	5.60000700	-1.49633600	-0.63047500
O	5.91340500	-2.75643100	0.00033000
C	6.06851600	-1.27160500	-1.97261200
S	4.35785700	1.50737700	-0.72833300
O	4.85716500	1.56631000	-2.07542700
O	3.67701400	2.66106200	-0.19264800
C	5.70457400	1.10401600	0.35676200
C	7.80966600	0.52017100	2.07398700
C	6.23790300	-0.19187300	0.39807600
C	6.21145900	2.10060100	1.18276400
C	7.27931600	1.80853700	2.03068400
C	7.27981700	-0.48853800	1.27007400
H	5.76212400	3.08783600	1.15823700
H	7.65900200	-1.50414200	1.31352600
H	8.63081600	0.29284900	2.74548300
H	7.68579900	2.58650700	2.66797700
C	-0.31521600	-0.59591100	-0.10301100
C	-3.14802200	-0.18201100	0.24706800
C	-0.92299900	0.71622600	-0.17708900
C	-1.24590000	-1.69159400	0.06774800
C	-2.58662900	-1.49437200	0.23278300
C	-2.26058200	0.91254400	-0.01022200
H	-0.31157400	1.58330600	-0.39065700
H	-0.88628000	-2.71161600	0.05380200

H	-3.23131100	-2.35855800	0.33206500	C	-5.09871700	1.31538100	0.34631500
H	-2.65529900	1.91640800	-0.10358400	C	-6.30181100	3.80665500	0.07637100
N	-4.49712600	0.02279500	0.43874100	C	-4.72864200	2.35704900	1.19730600
C	-5.42812200	-1.05391900	0.56375600	C	-6.11380500	1.49902000	-0.59894400
C	-7.26631200	-3.13439000	0.70980800	C	-6.71352200	2.75213900	-0.73354900
C	-6.47654000	-1.12243100	-0.36038100	C	-5.32139700	3.60690000	1.05025400
C	-5.33564600	-1.98639800	1.59742100	H	-3.97459000	2.18060100	1.95818700
C	-6.24775100	-3.03496800	1.65967900	H	-7.50546700	2.89027000	-1.46264300
C	-7.39522300	-2.17060600	-0.28610300	H	-5.02488700	4.42133500	1.70204200
H	-4.54644300	-1.88593300	2.33615600	H	-6.76729600	4.78007700	-0.03491700
H	-6.16938100	-3.76781600	2.45524900	S	-6.62770700	0.13312400	-1.59177100
H	-8.21131400	-2.21759500	-0.99997700				
H	-7.98024100	-3.94945900	0.76126600				