

Electronic Supplementary Information

Theoretical Design and Validation of [1,2,4]Triazolo[1,5-a]Pyridine-Based TADF Emitters Through Donor and Linkage Variations

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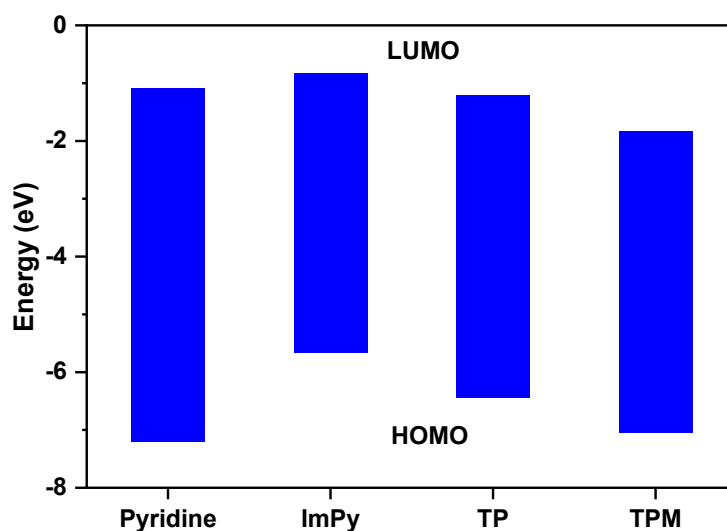


Figure S1. HOMO and LUMO energies (eV) of the acceptor molecules collected from literature. (Manuscript references =10-12)

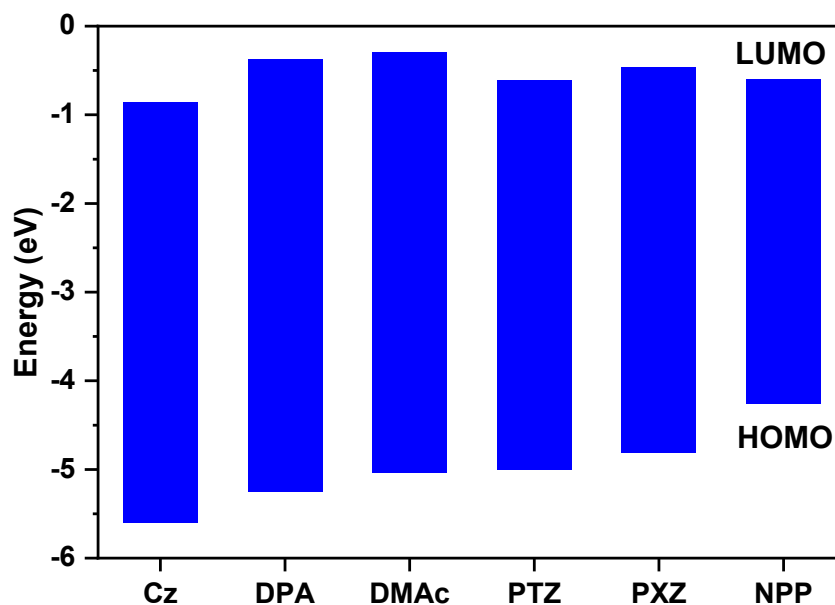


Figure S2. HOMO and LUMO energies (eV) of the donor molecules calculated using B3LYP/def2-SVP level of theory.

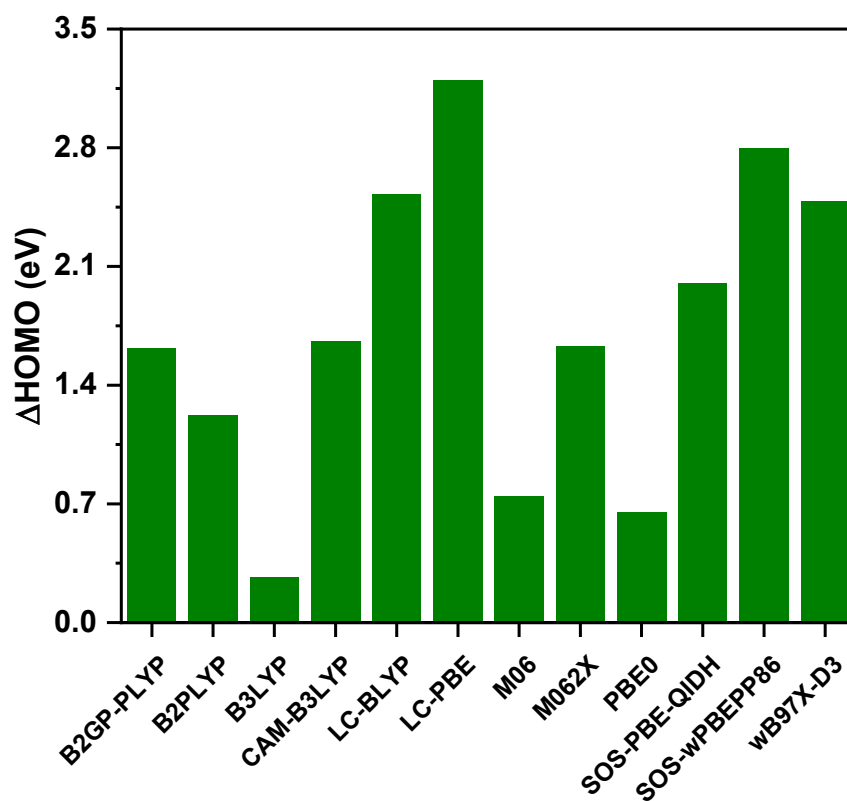


Figure S3. Change in the HOMO values of the *o*-2CZ-TP molecules respective to the various functional and def2-SVP basis sets.

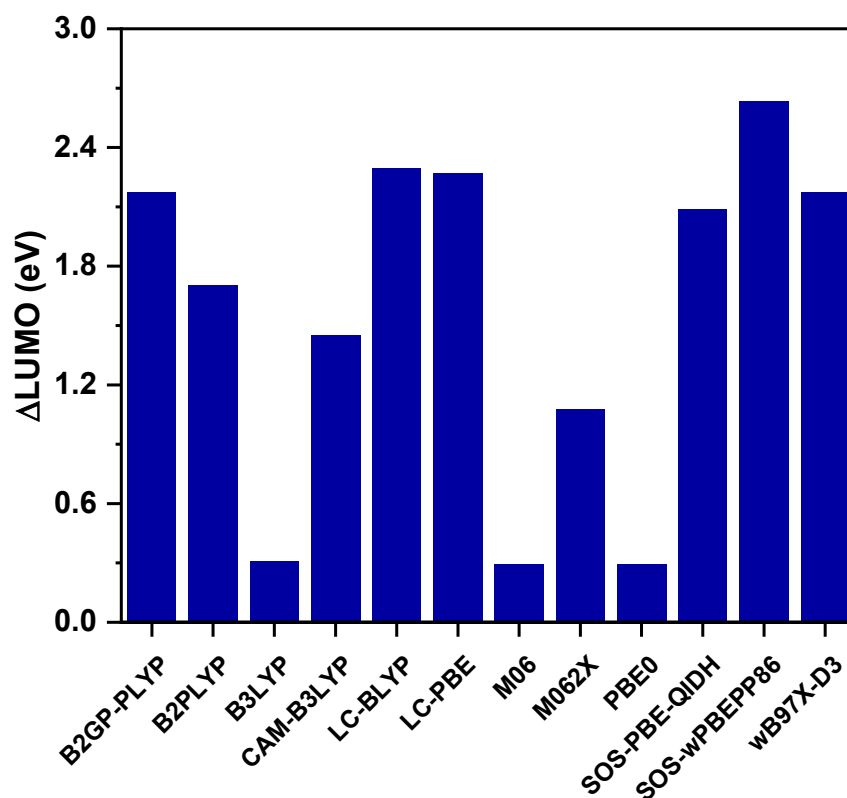


Figure S4. Change in the LUMO values of the *o*-2CZ-TP molecules respective to the various functional and def2-SVP basis sets.

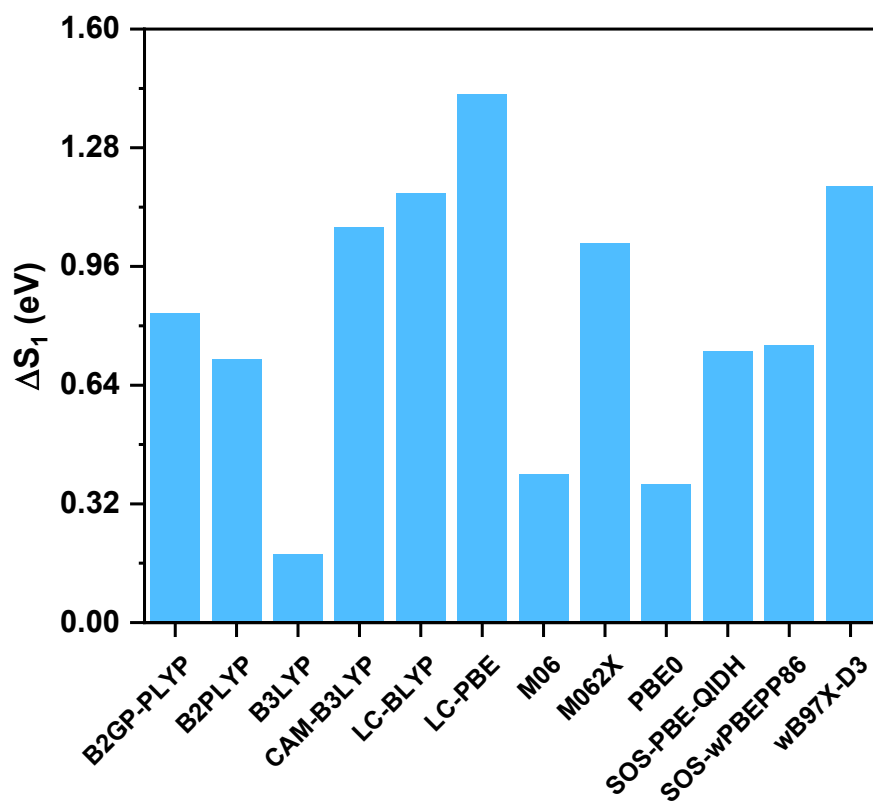


Figure S5. Change in the S_1 (eV) values of the *o*-2CZ-TP molecules respective to the various functional and def2-SVP basis sets.

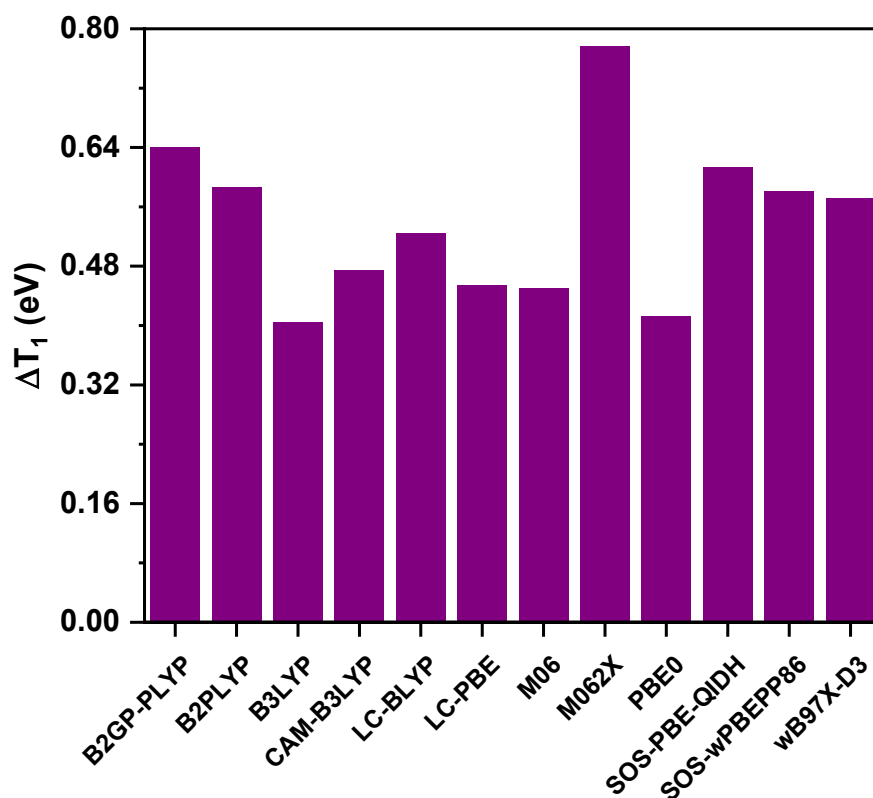


Figure S6. Change in the T_1 (eV) values of the *o*-2CZ-TP molecules respective to the various functional and def2-SVP basis sets.

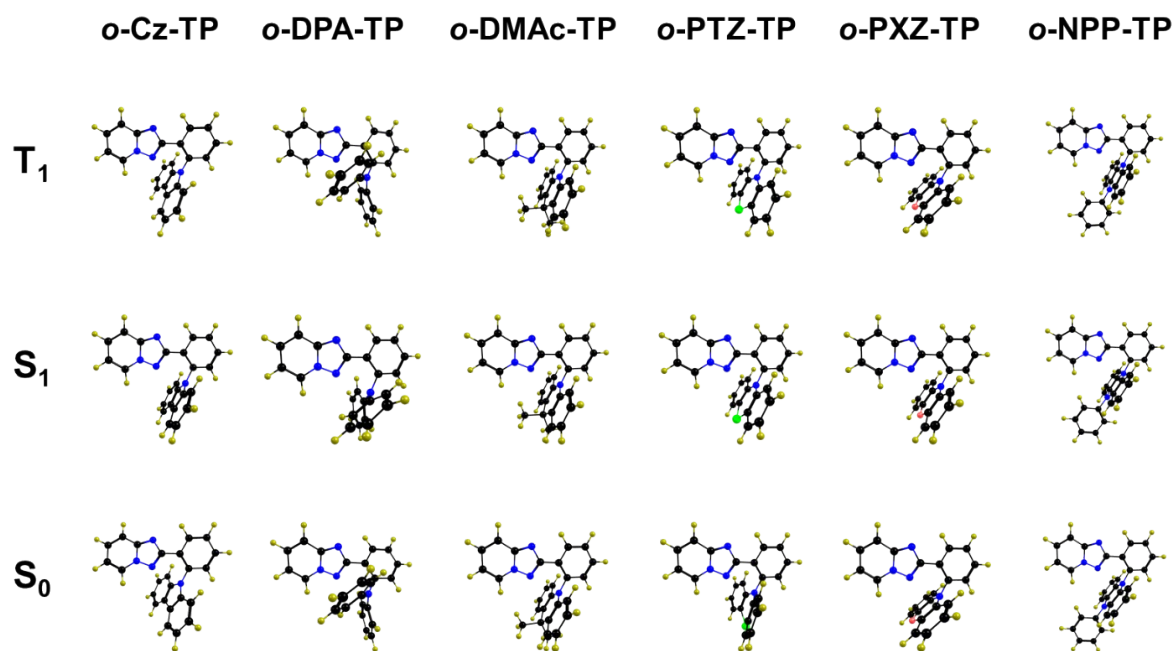


Figure S7. S₀, S₁ and T₁ optimized geometries in the gaseous state of the *ortho*-molecules.

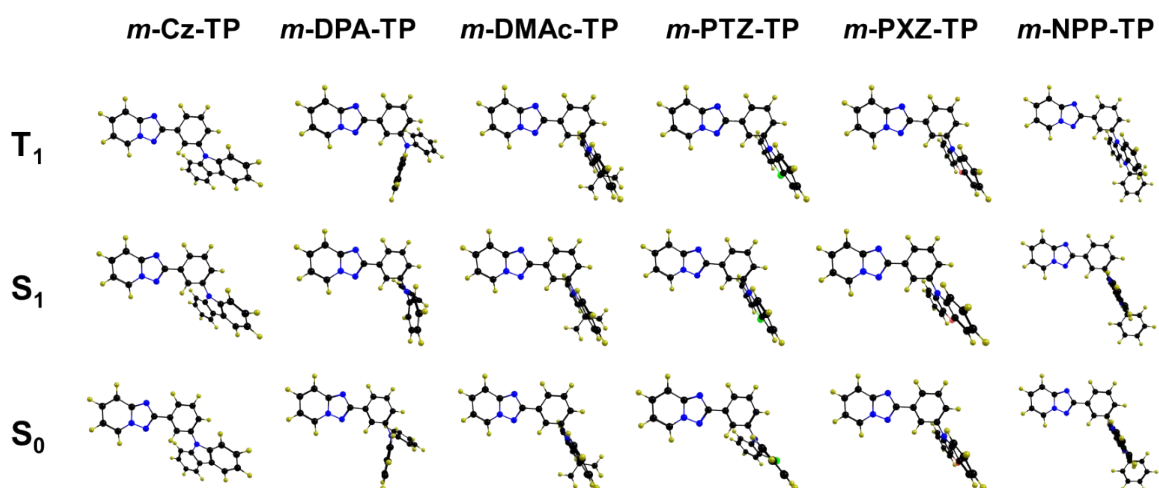


Figure S8. S₀, S₁ and T₁ optimized geometries in the gaseous state of the *meta*-molecules.

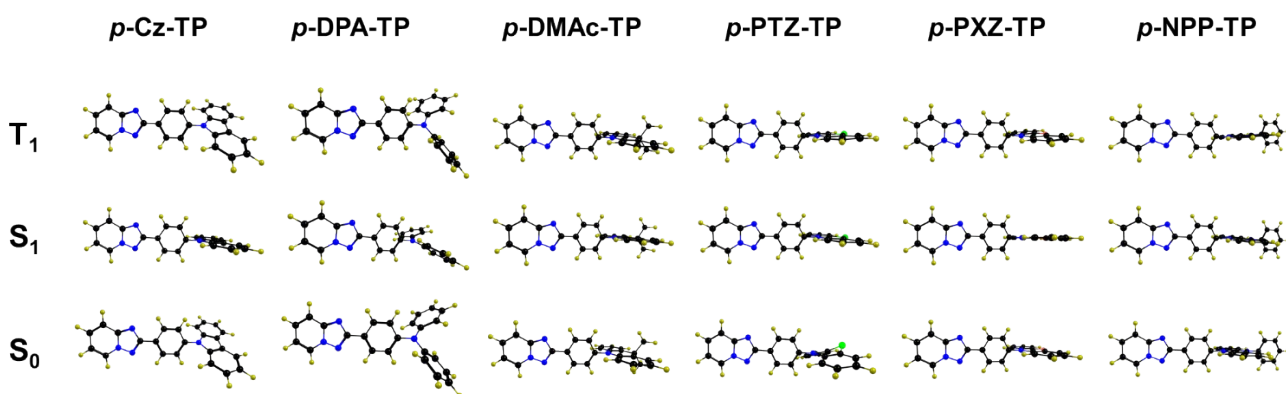


Figure S9. S₀, S₁ and T₁ optimized geometries in the gaseous state of the *para*-molecules.

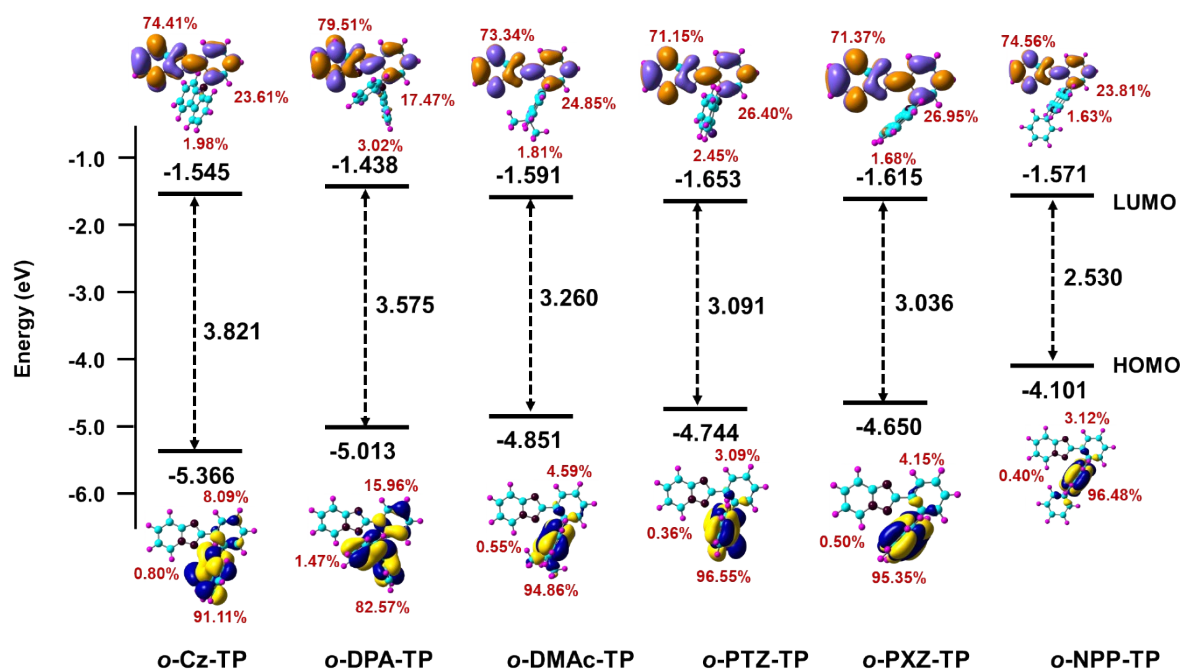


Figure S10. Frontier orbital distribution at the optimized S_0 geometries for the *ortho*-molecules

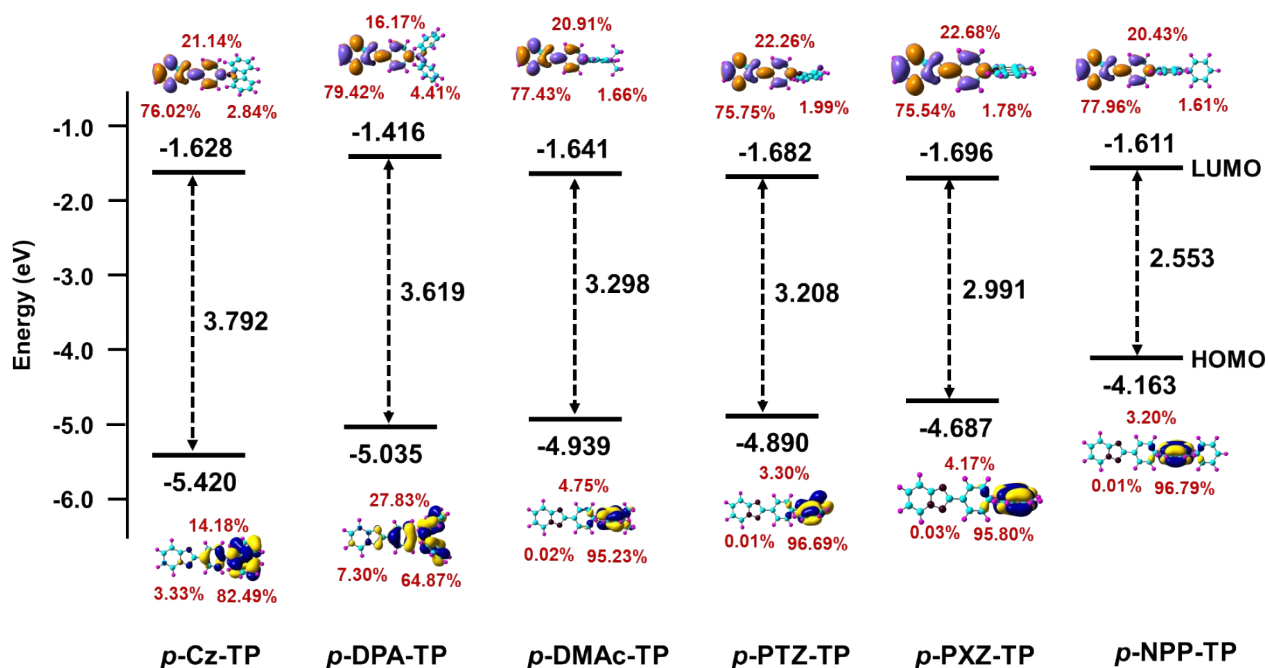


Figure S11. Frontier orbital distribution at the optimized S_0 geometries for the *para*-molecules.

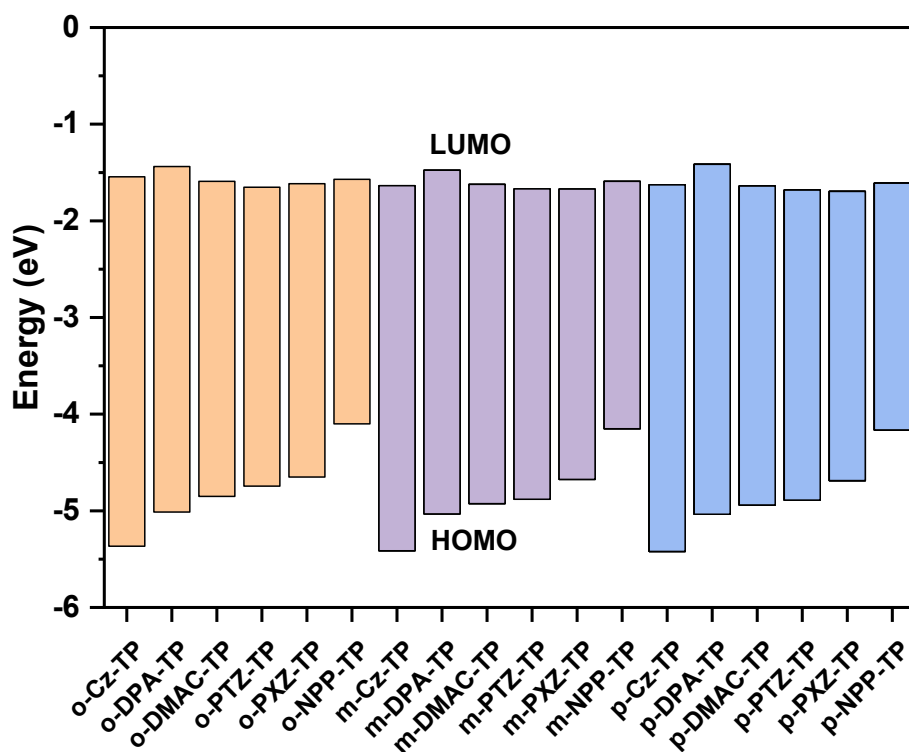


Figure S12. Energy level diagram of the studied molecules.

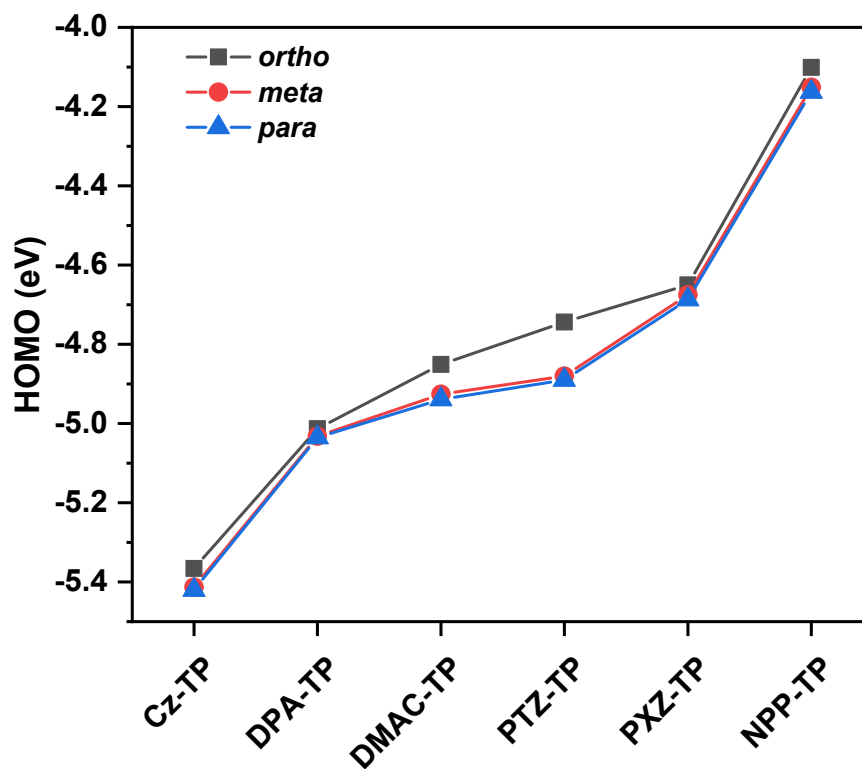


Figure S13. Change in the HOMO (eV) values respective to the molecule's donor strength and linkage variation of the studied molecules.

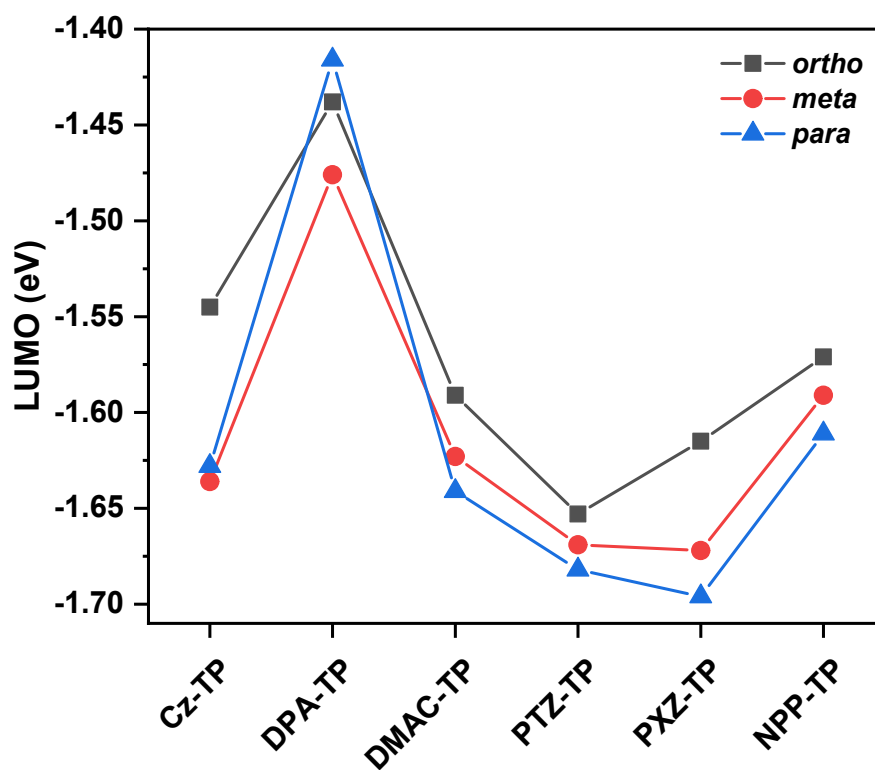


Figure S14. Change in the LUMO (eV) values respective to the molecule's donor strength and linkage variation of the studied molecules.

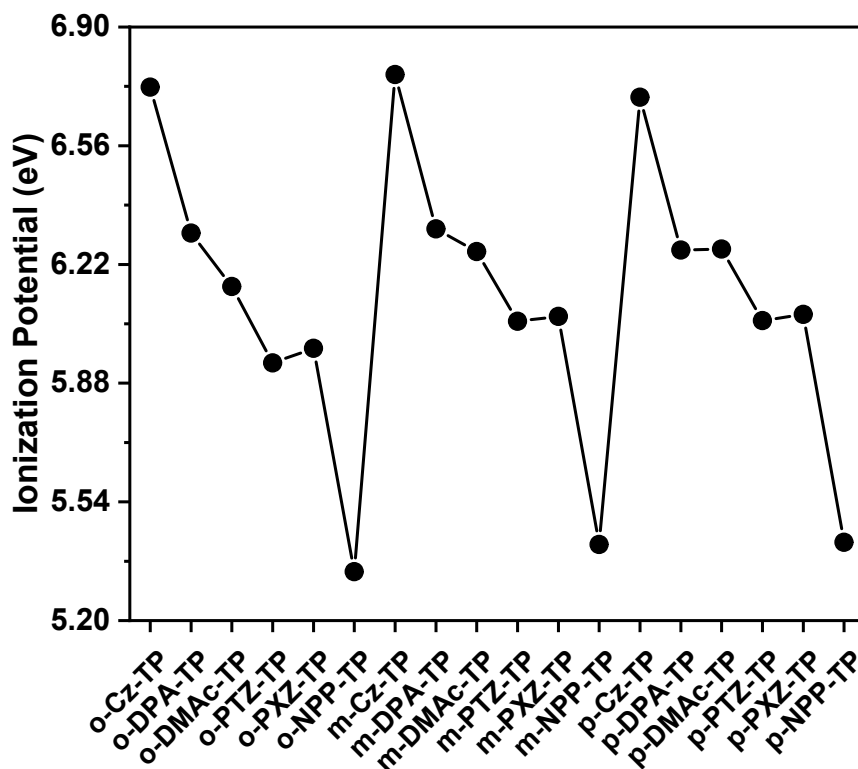


Figure S15. Plotted graph of Ionization potential (IP) for studied molecules

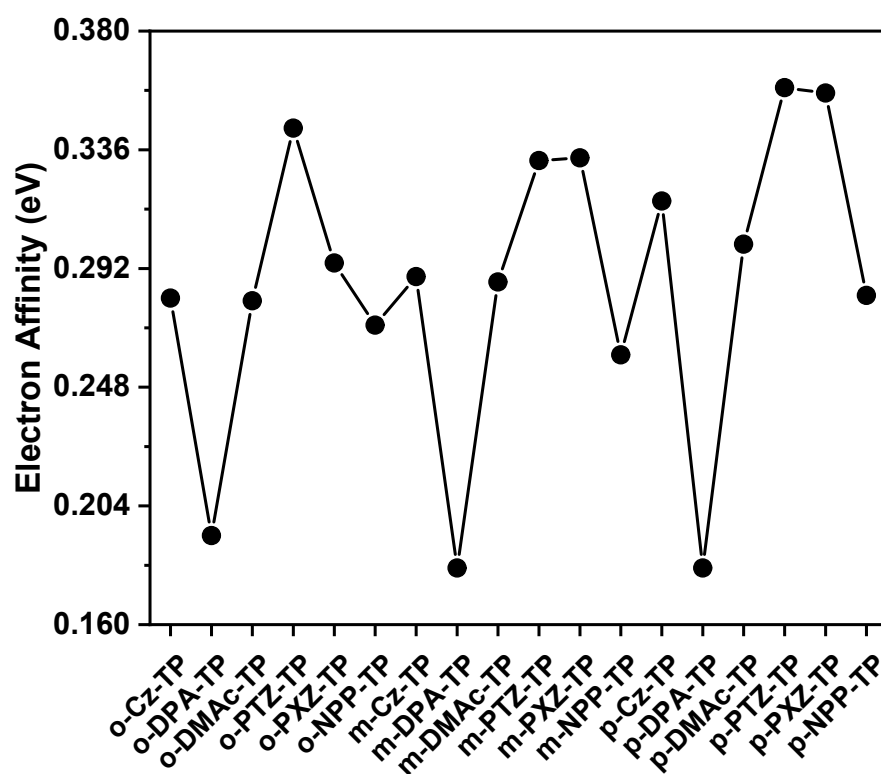


Figure S16. Plotted graph of electron affinity (EA) for studied molecules.

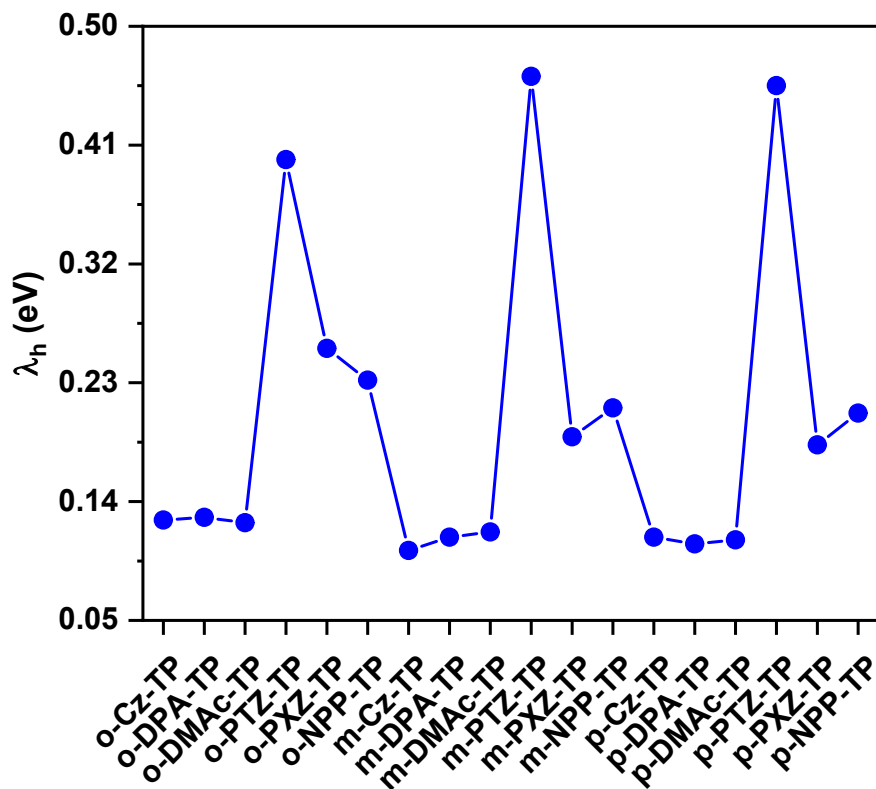


Figure S17. Plotted graph of hole reorganization energies (λ_h) for studied molecules.

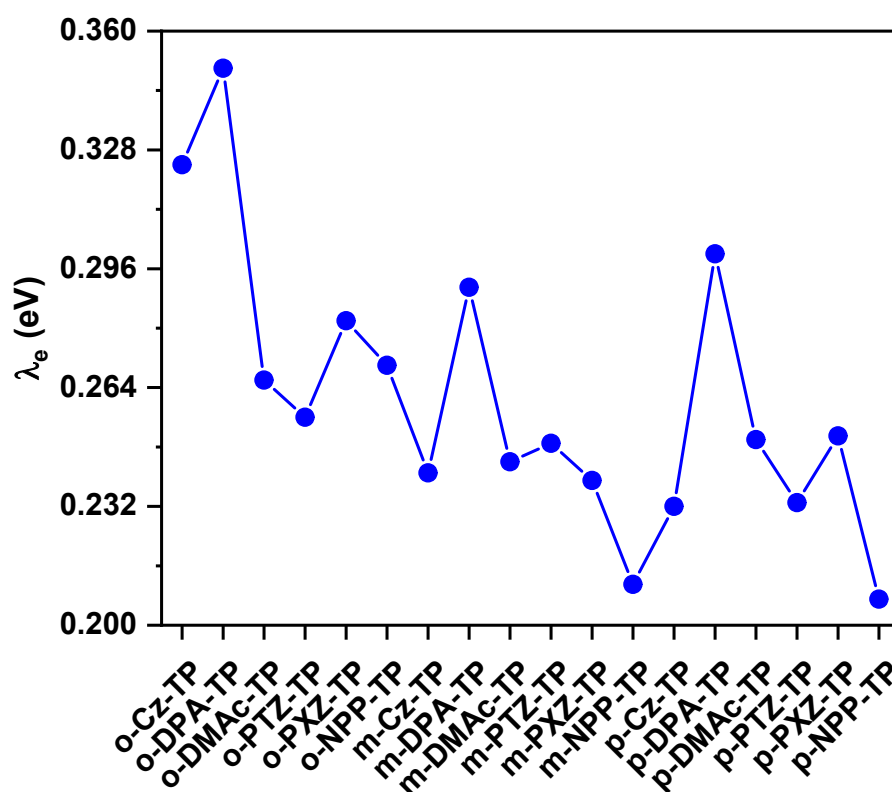


Figure S18. Plotted graph of electron reorganization energies (λ_e) for studied molecules.

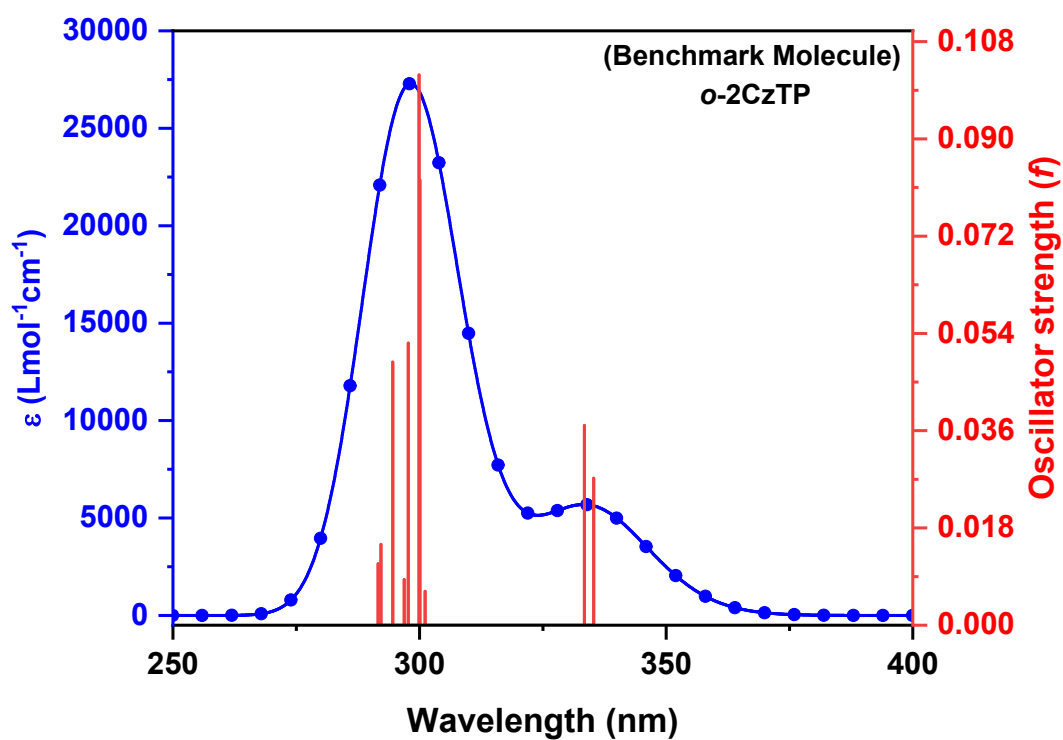


Figure S19. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for benchmarked molecule (*o*-2Cz-TP).

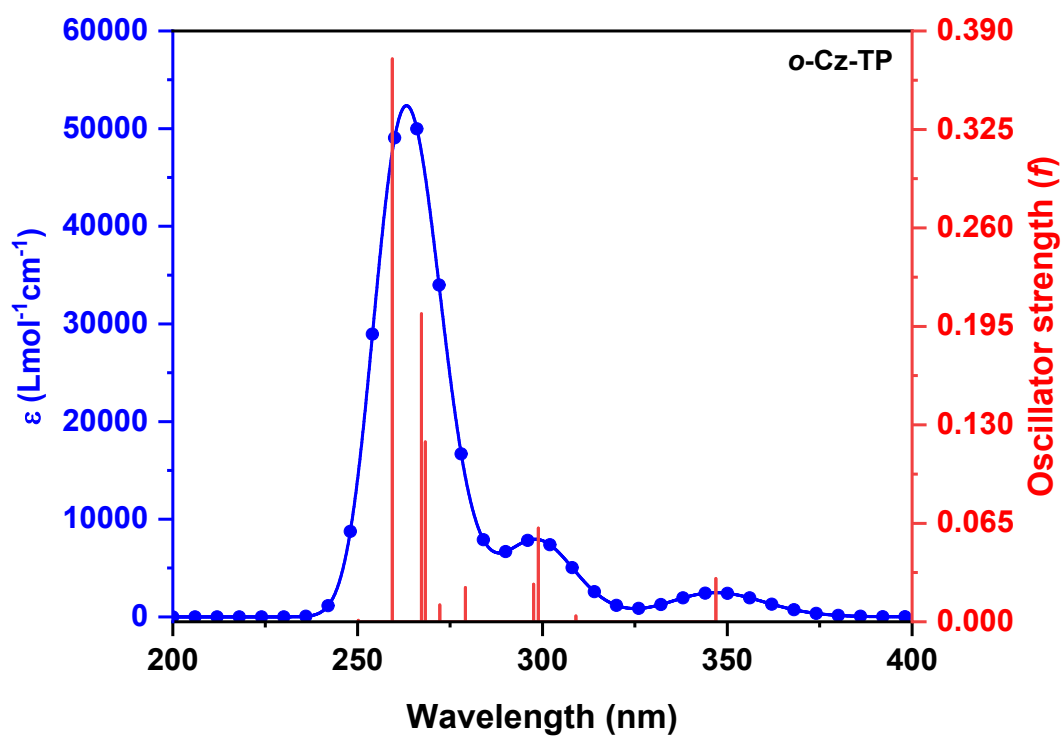


Figure S20. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-Cz-TP molecule.

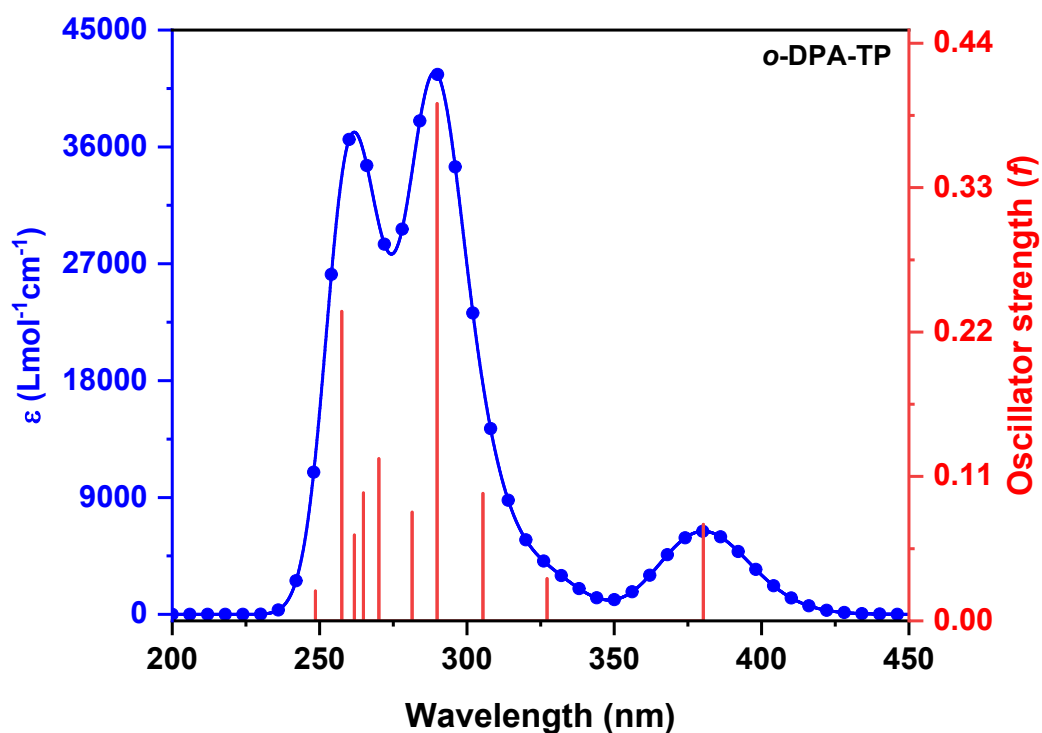


Figure S21. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-DPA-TP molecule.

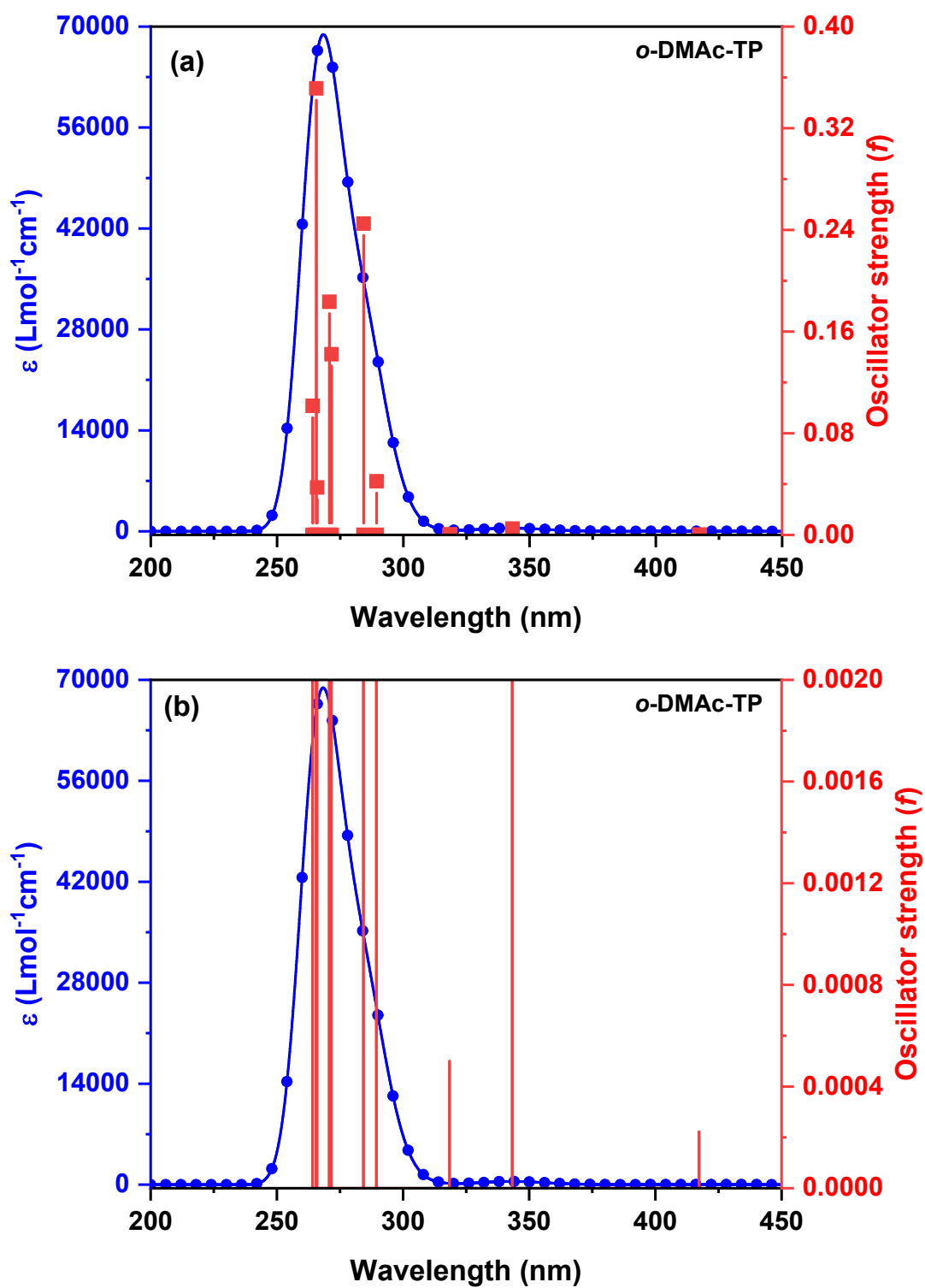


Figure S22(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-DMAc-TP molecule.

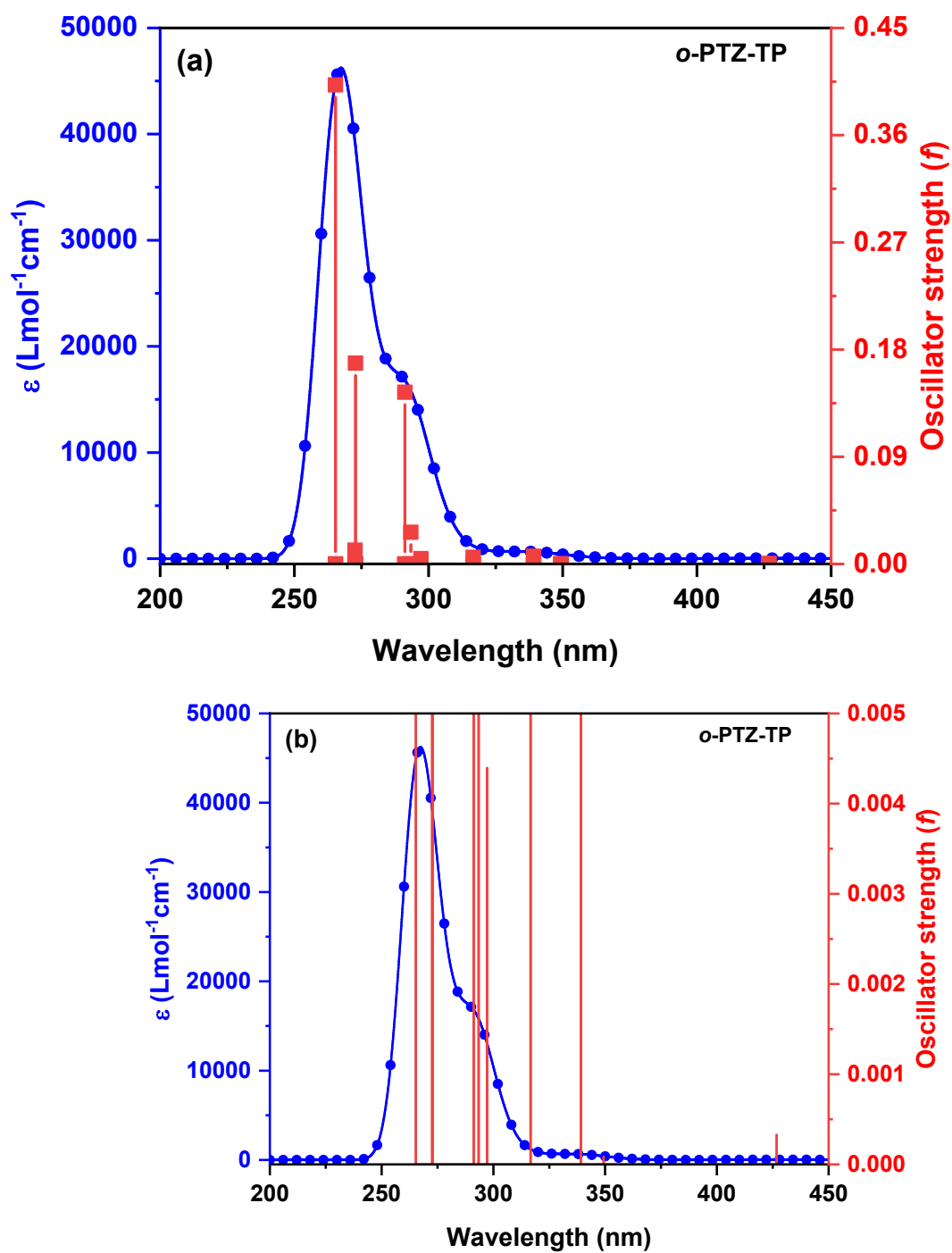


Figure S23(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-PTZ-TP molecule.

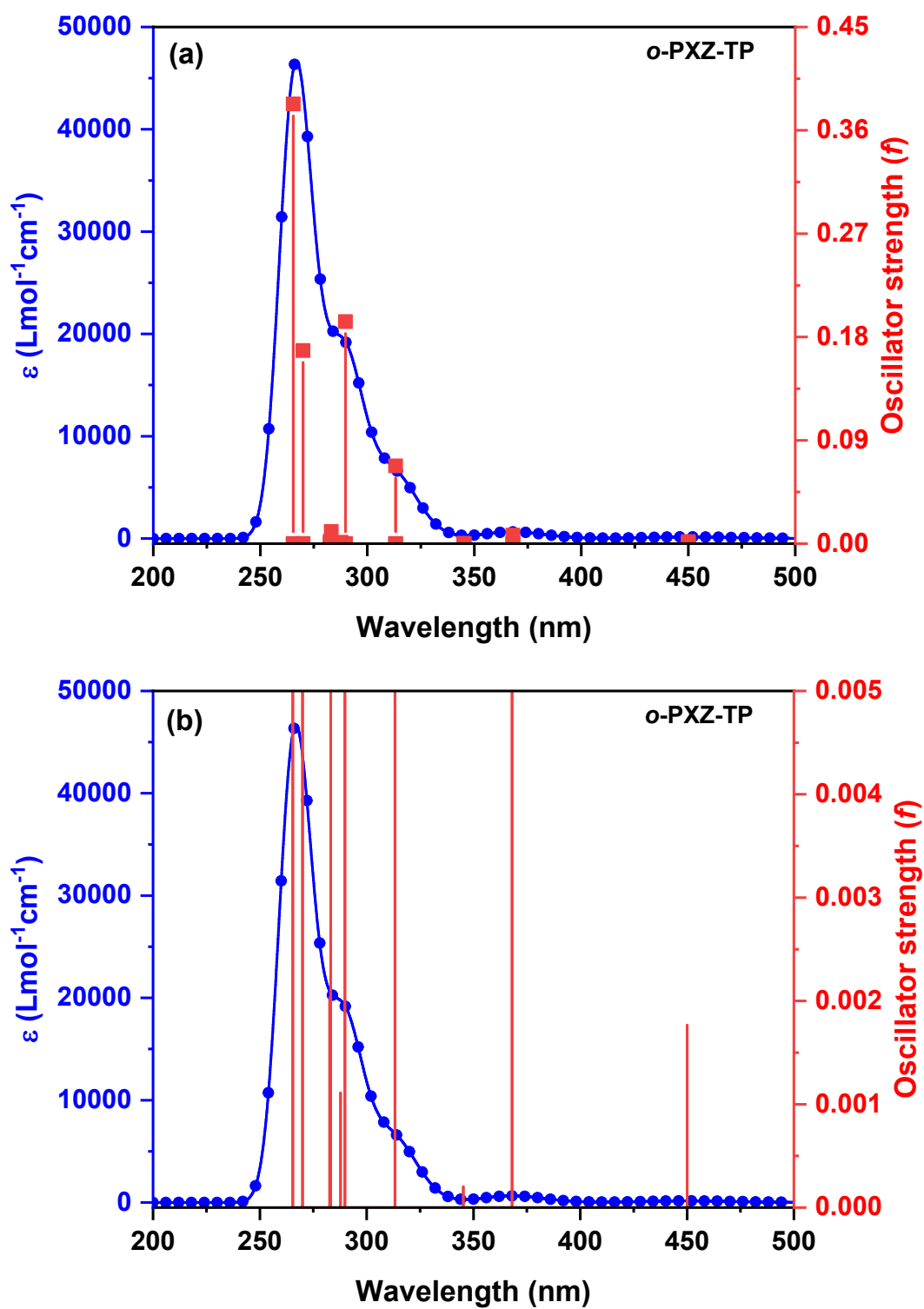


Figure S24(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-PXZ-TP molecule.

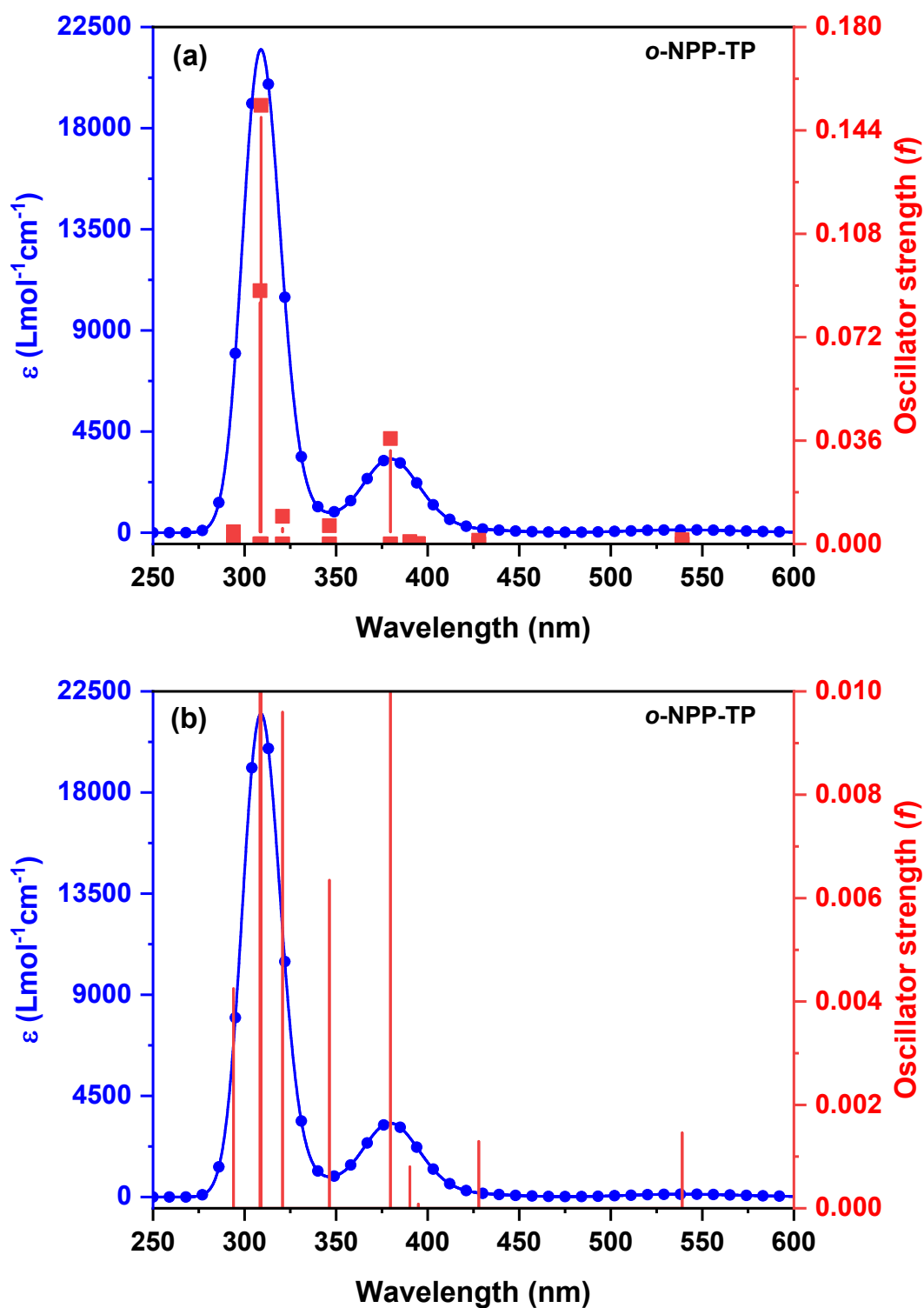


Figure S25(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *o*-NPP-TP molecule.

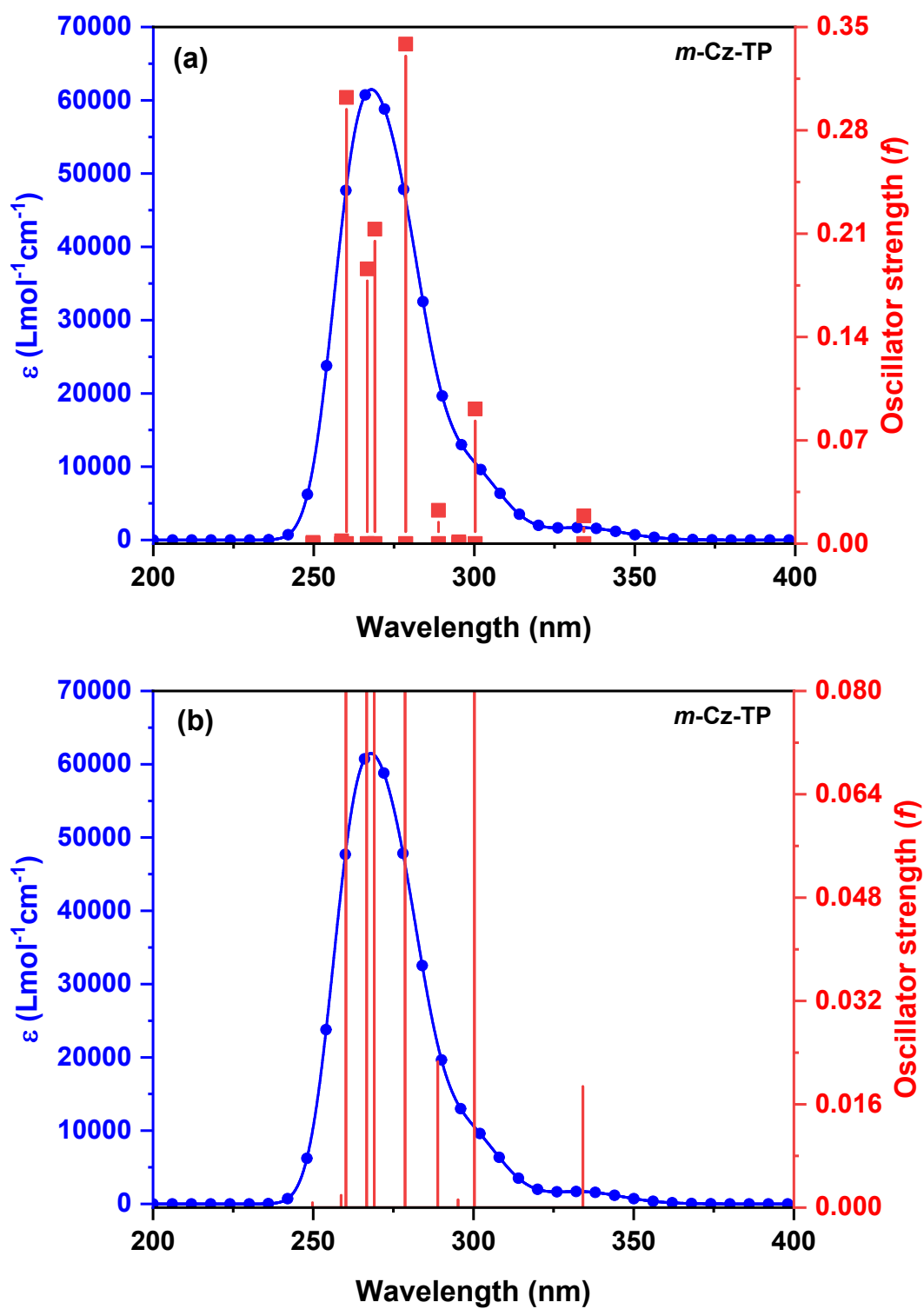


Figure S26(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-Cz-TP molecule.

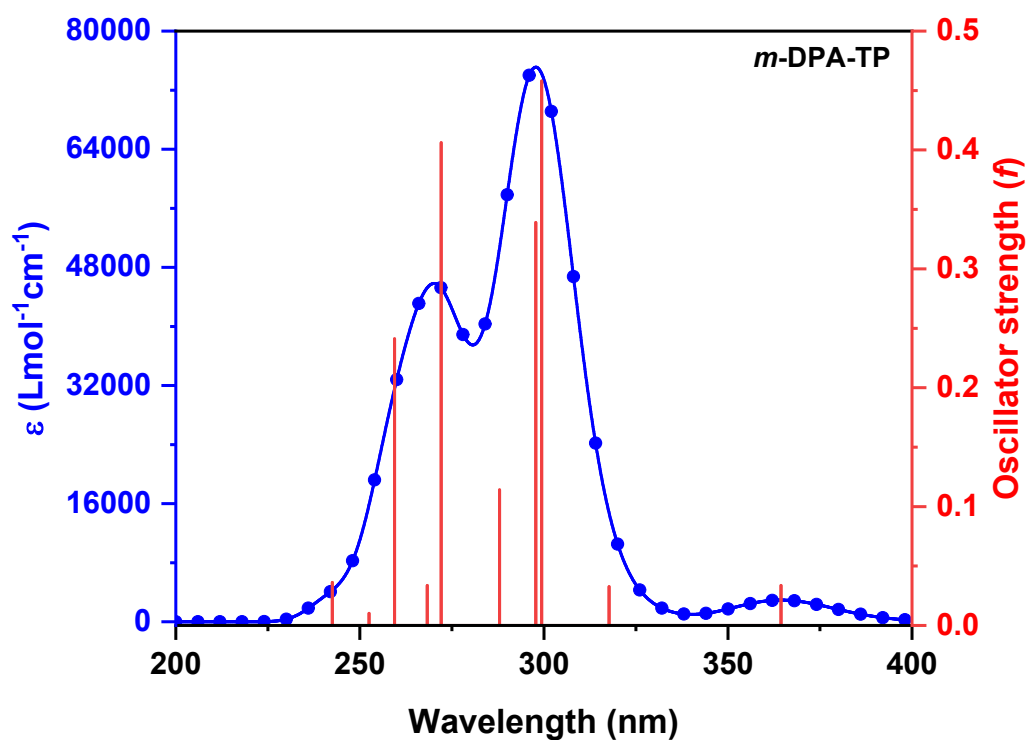
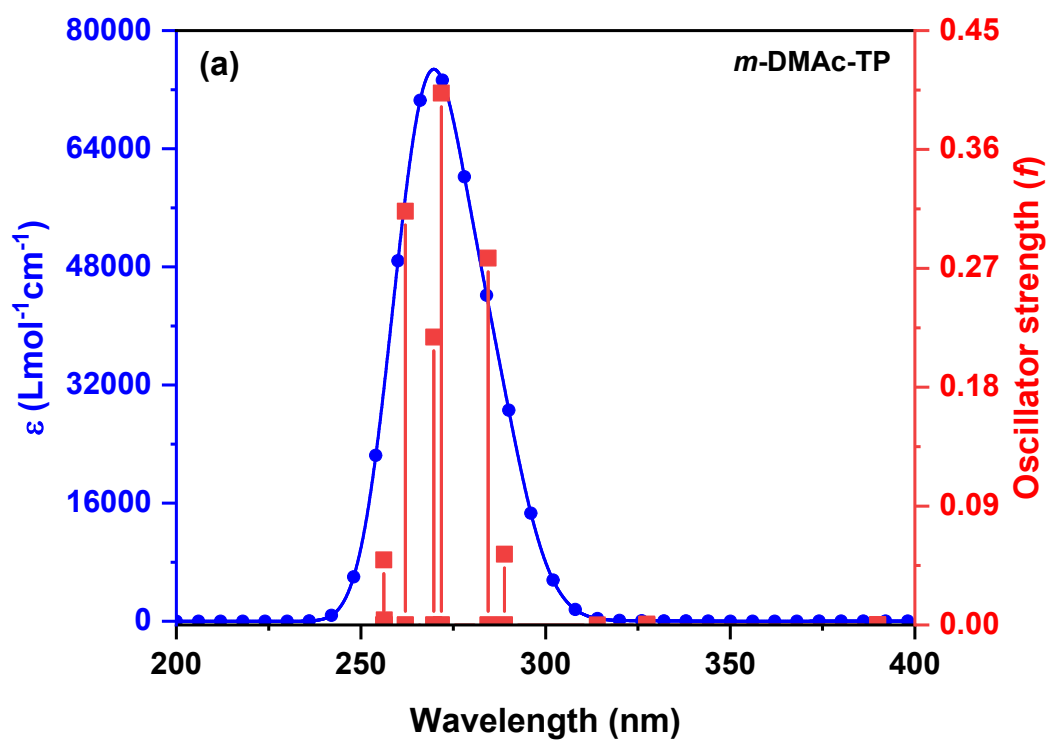


Figure S27. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-DPA-TP molecule.



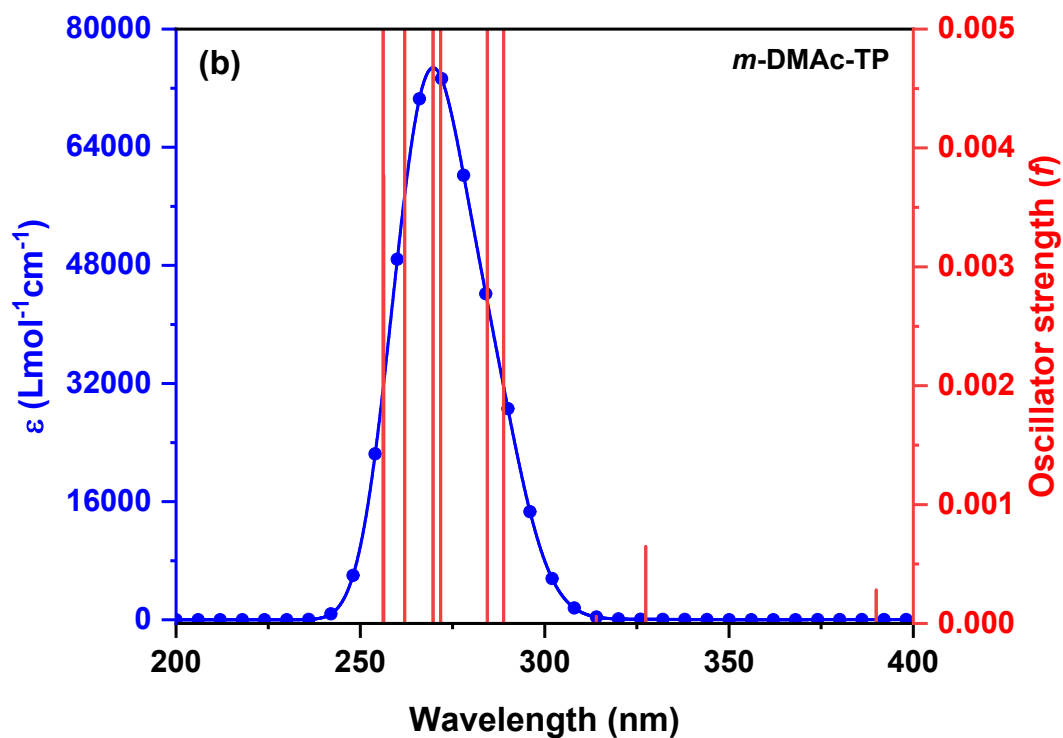
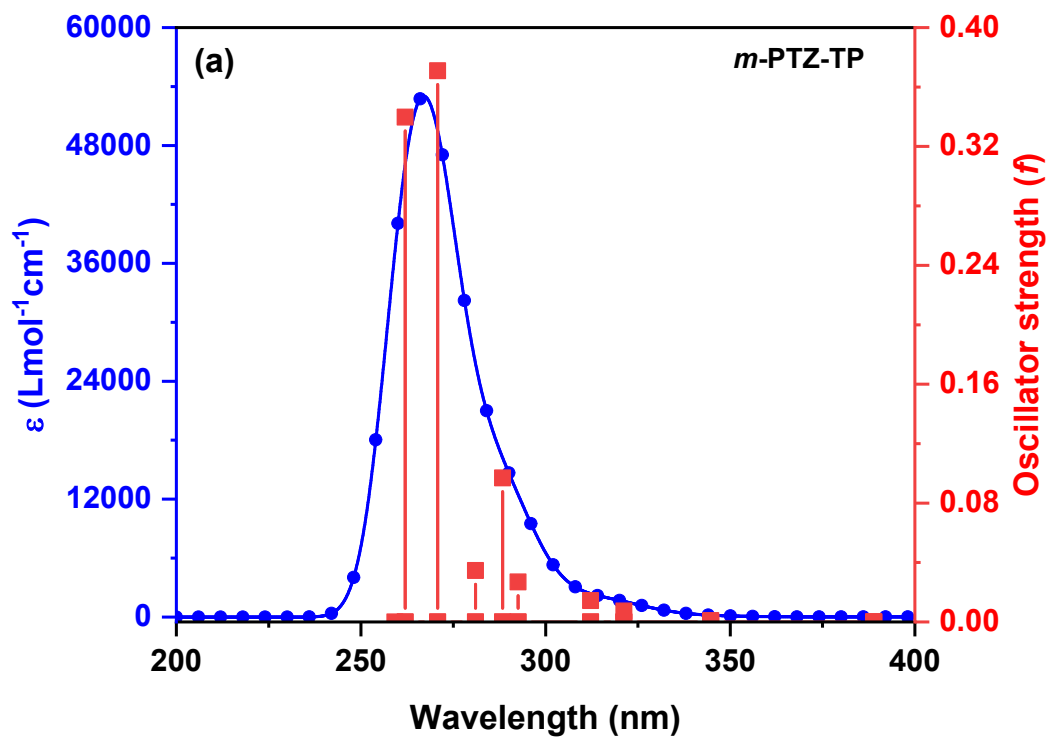


Figure S28(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-DMAc-TP molecule.



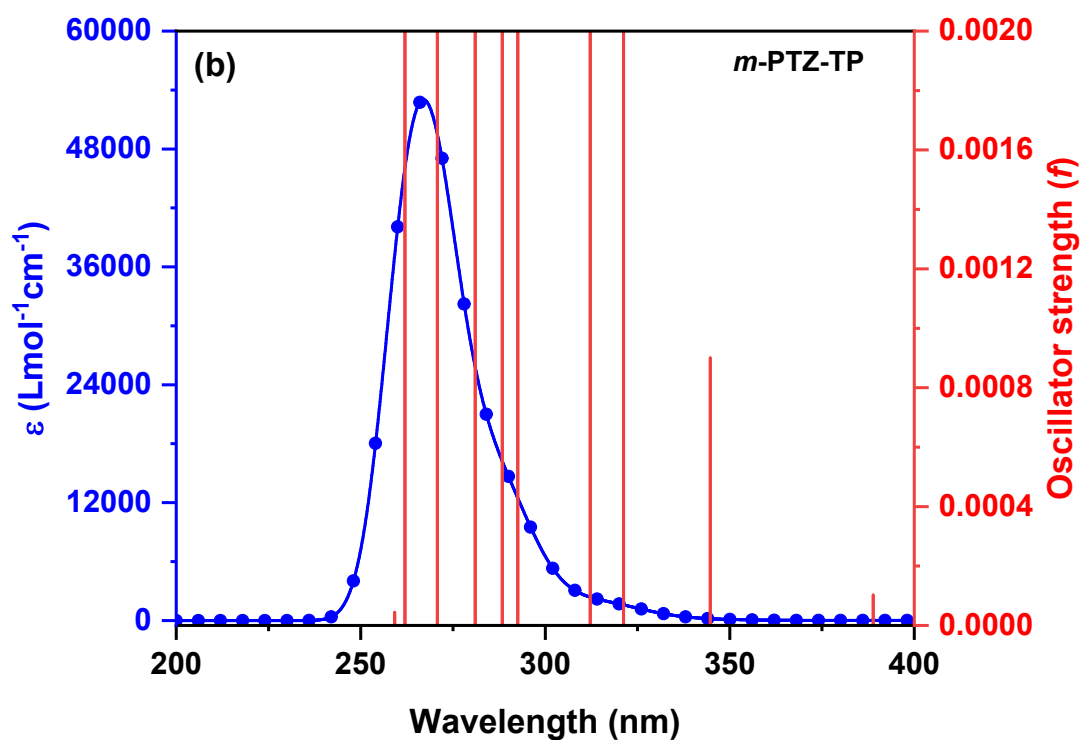
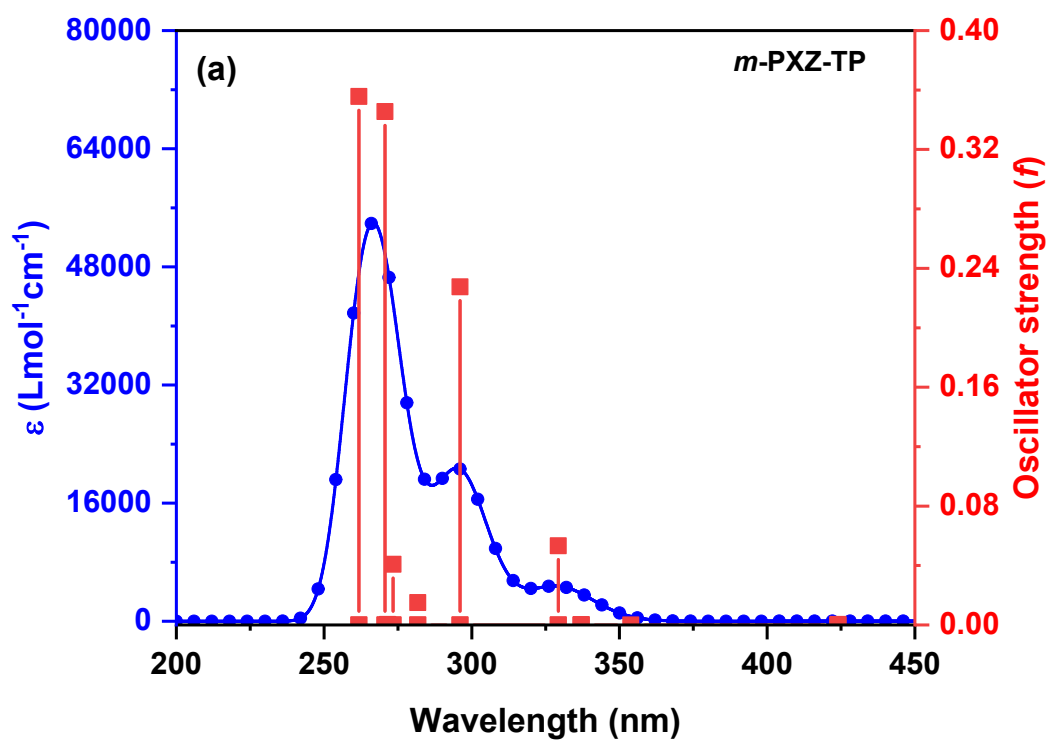


Figure S29(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-PTZ-TP molecule.



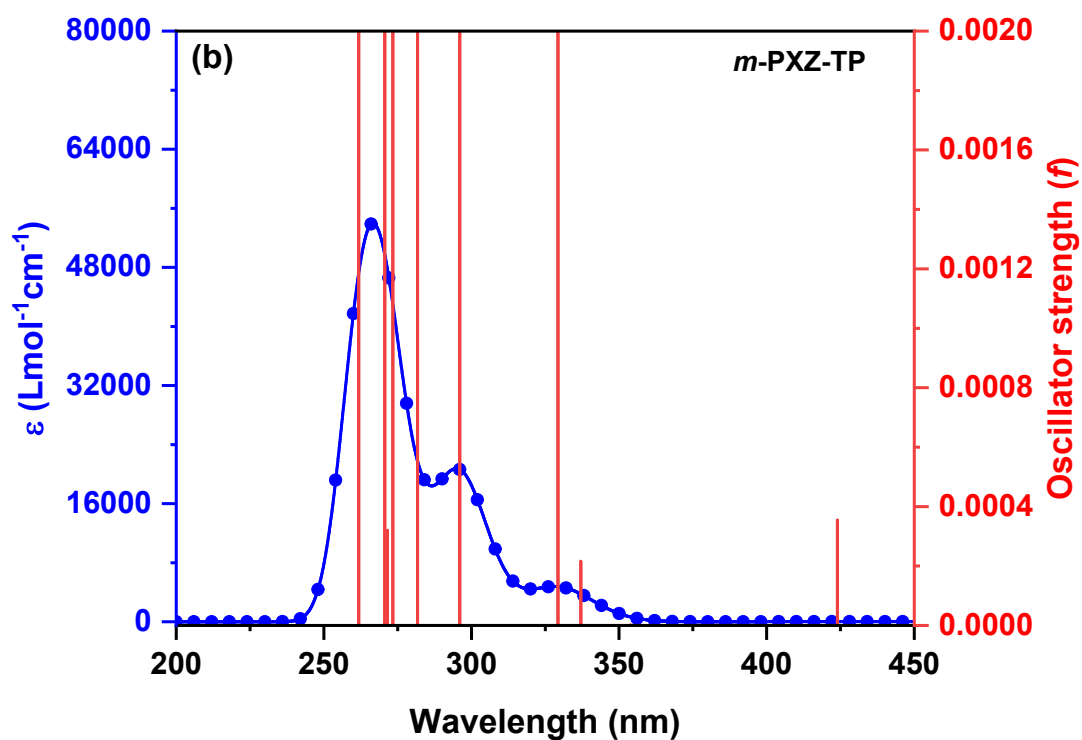
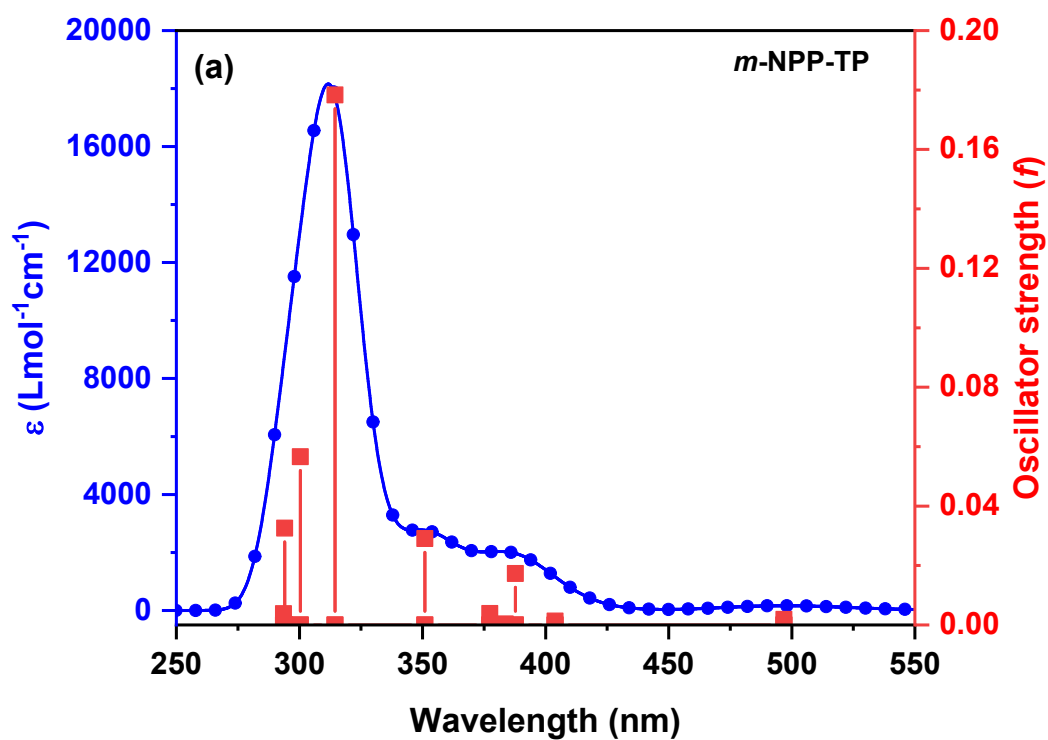


Figure S30(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-PXZ-TP molecule.



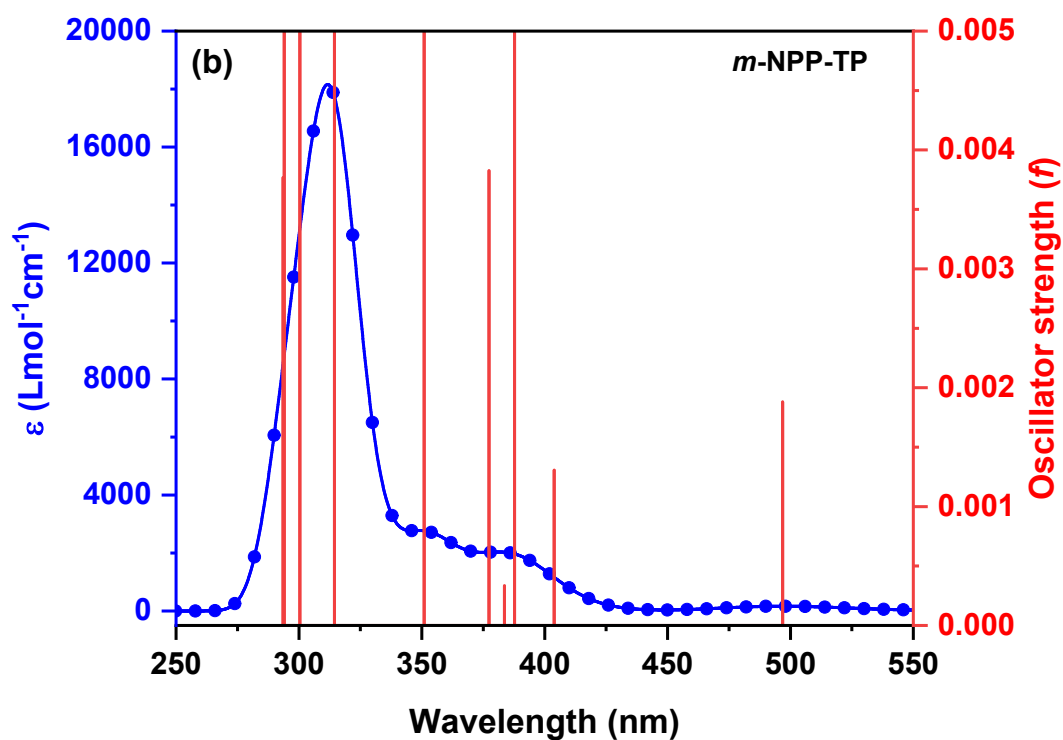


Figure S31(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *m*-NPP-TP molecule.

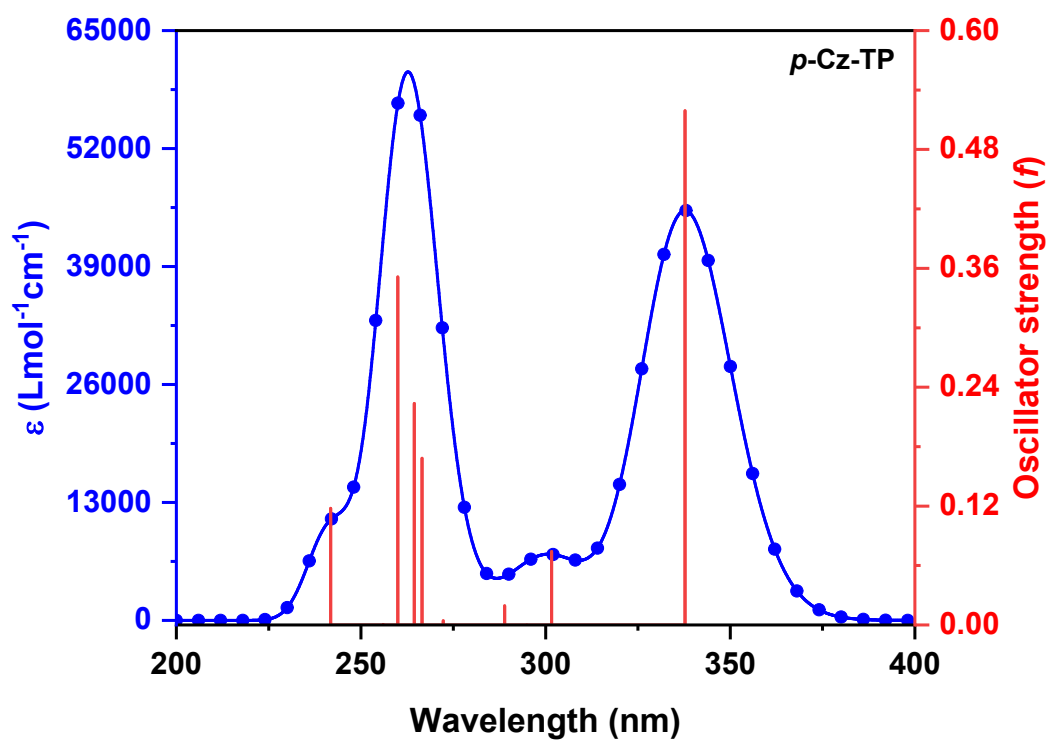


Figure S32. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-Cz-TP molecule.

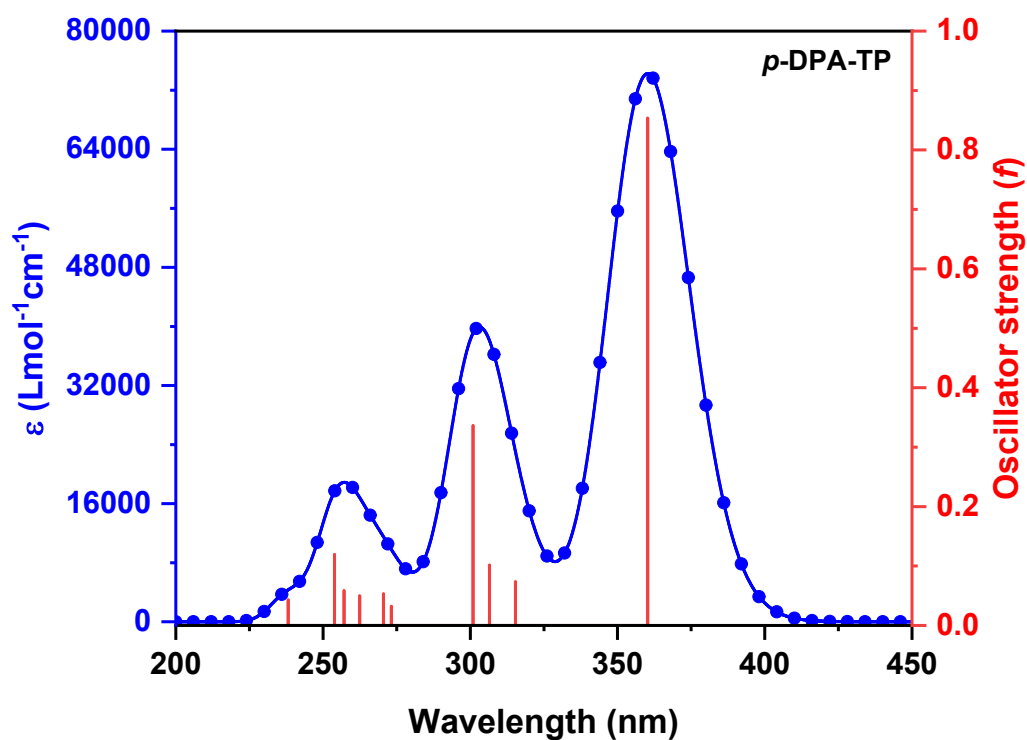
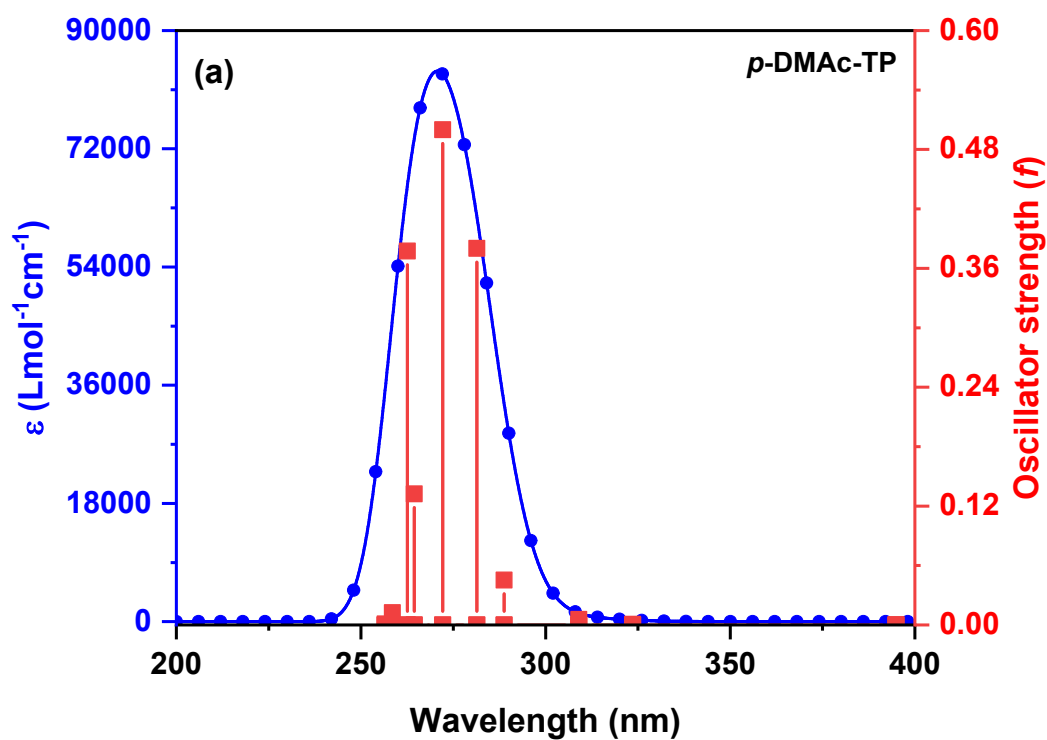


Figure S33. Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-DPA-TP molecule.



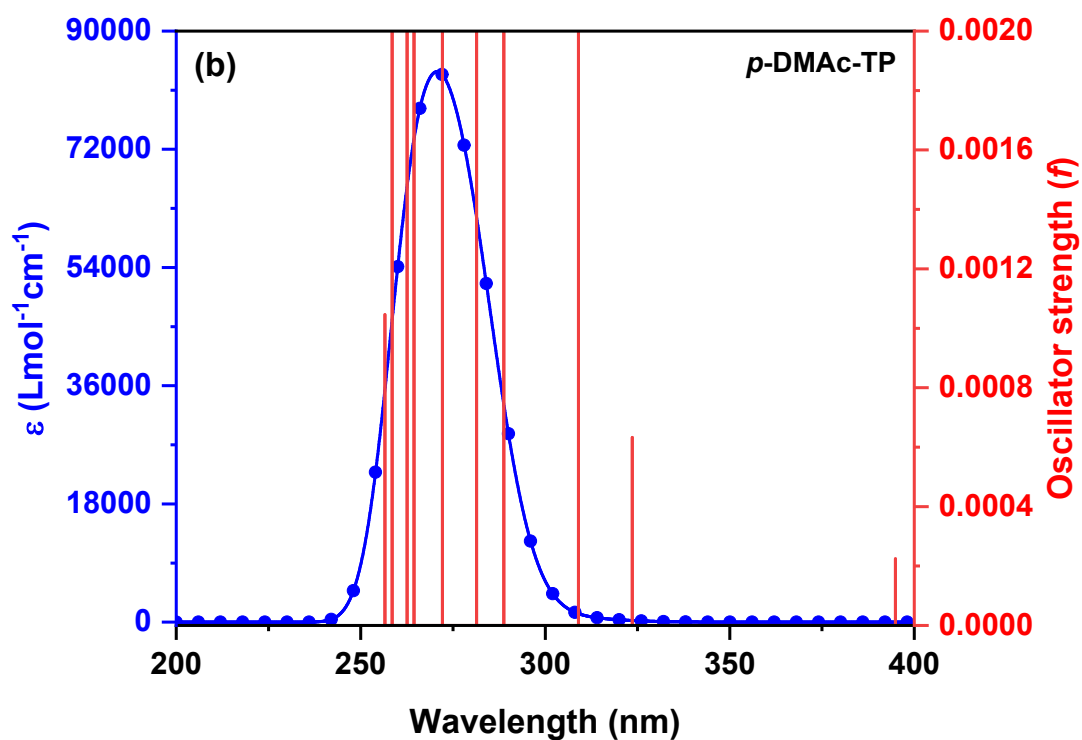
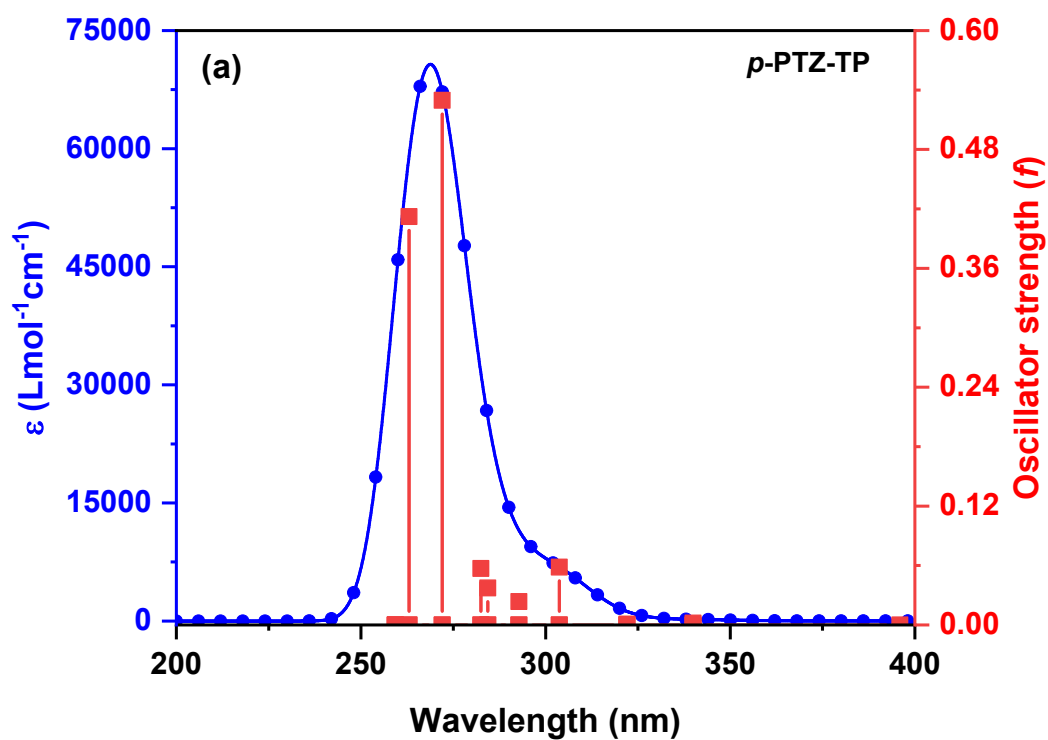


Figure S34(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-DMAc-TP molecule.



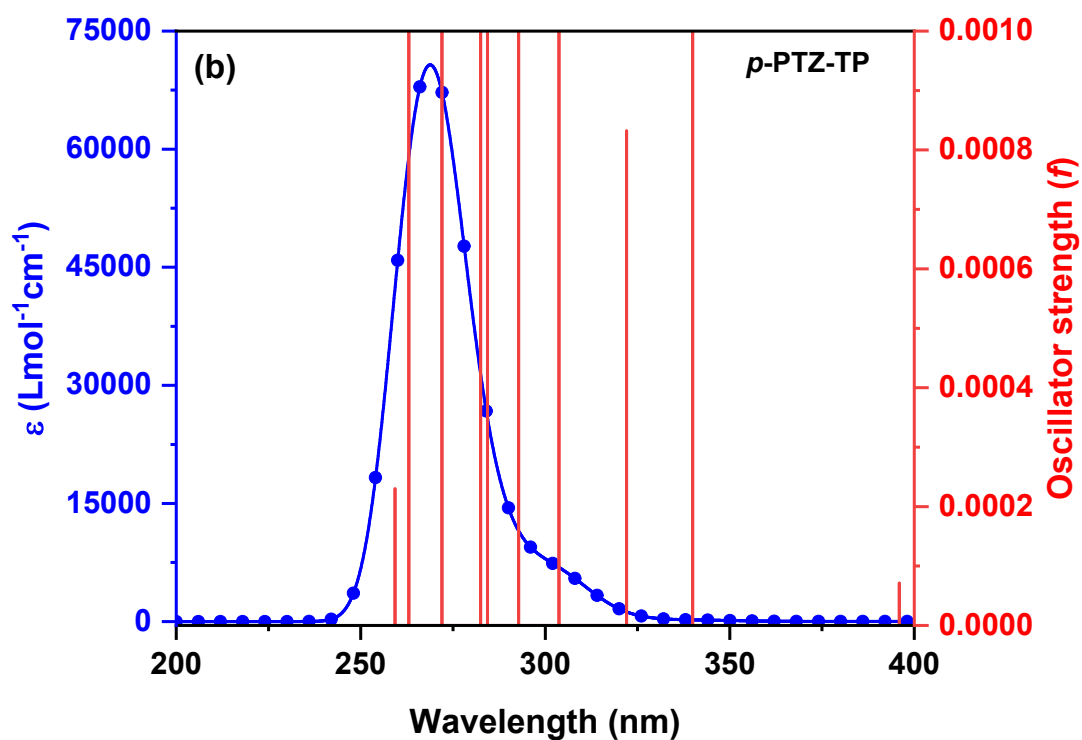
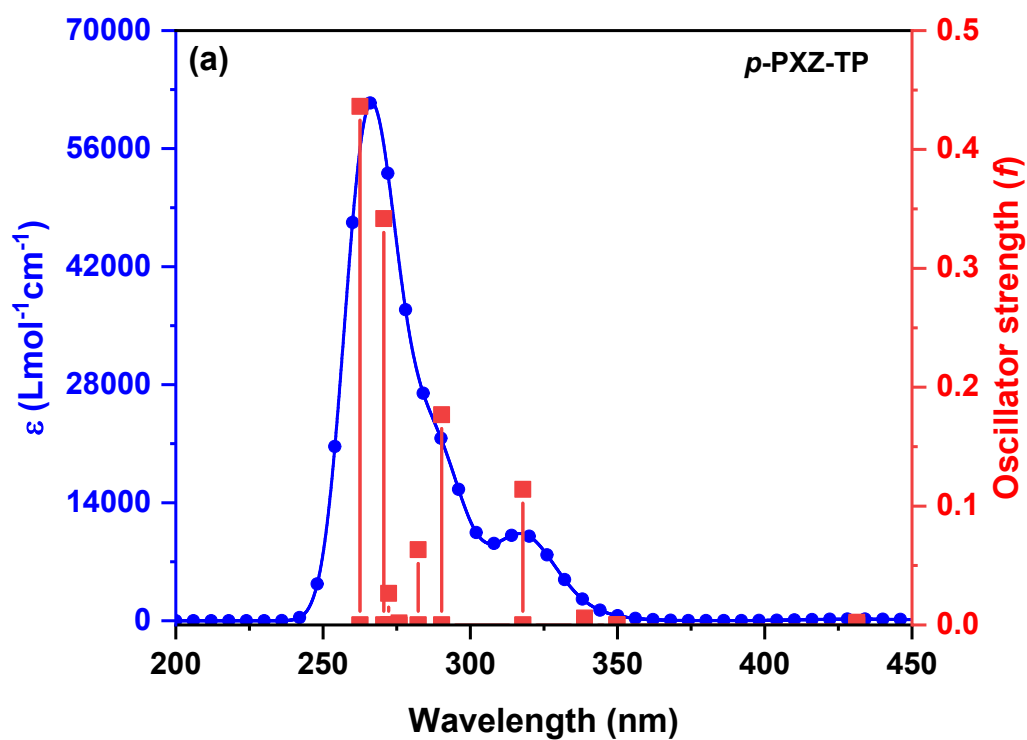


Figure S35(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-PTZ-TP molecule.



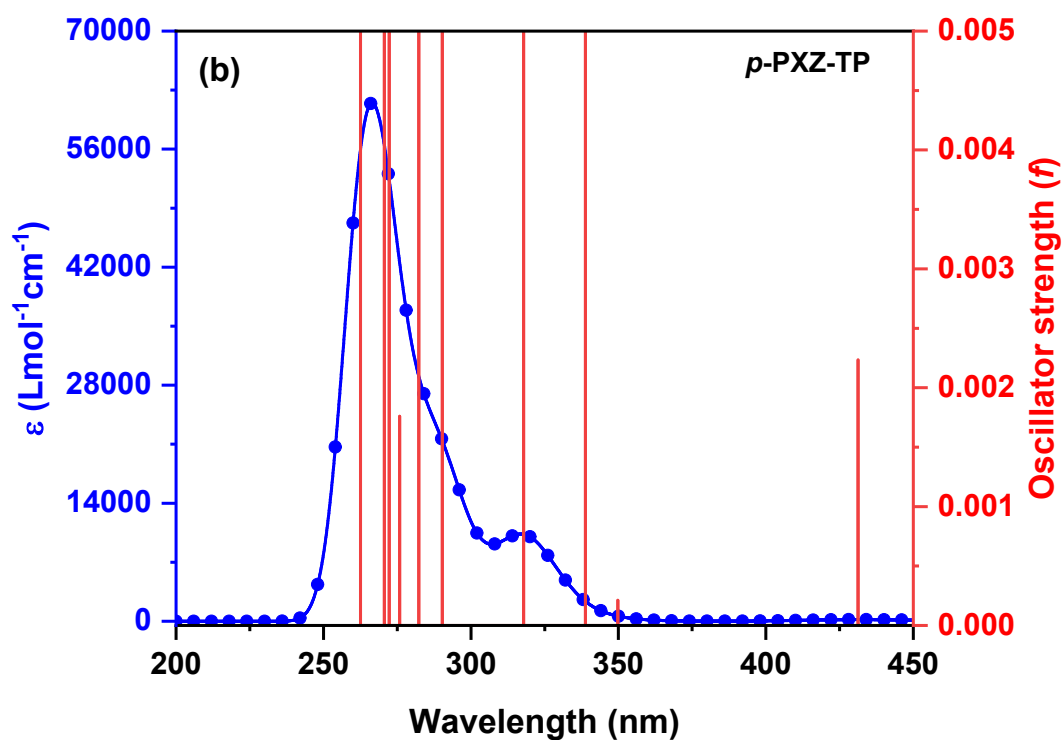
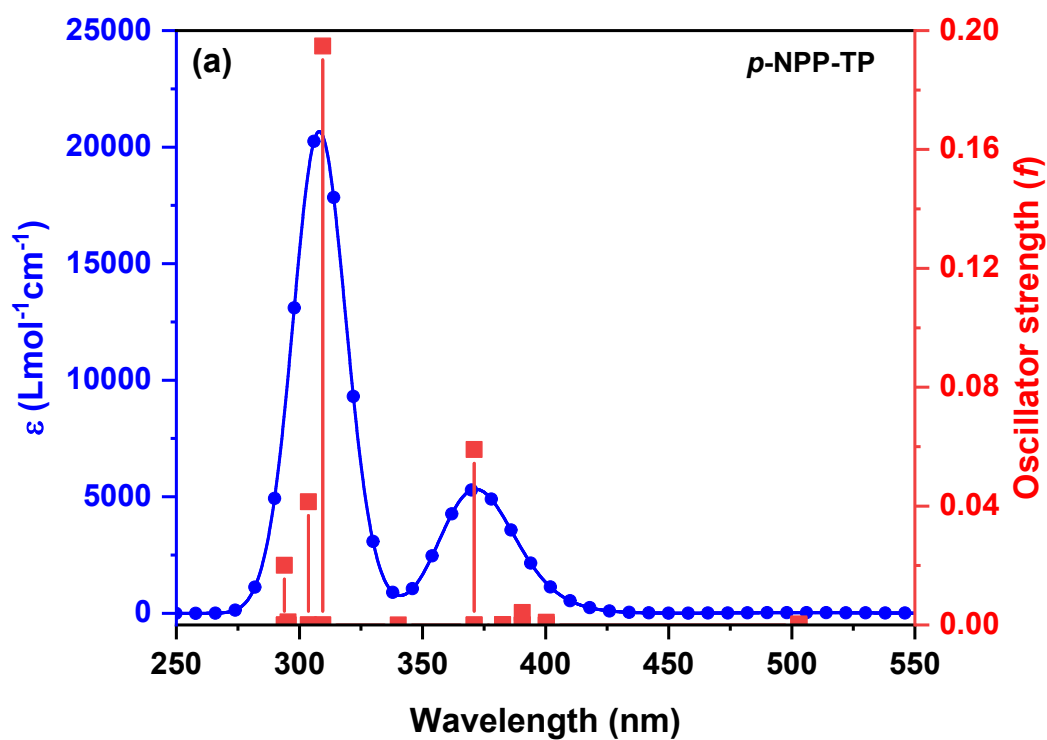


Figure S36(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-PXZ-TP molecule.



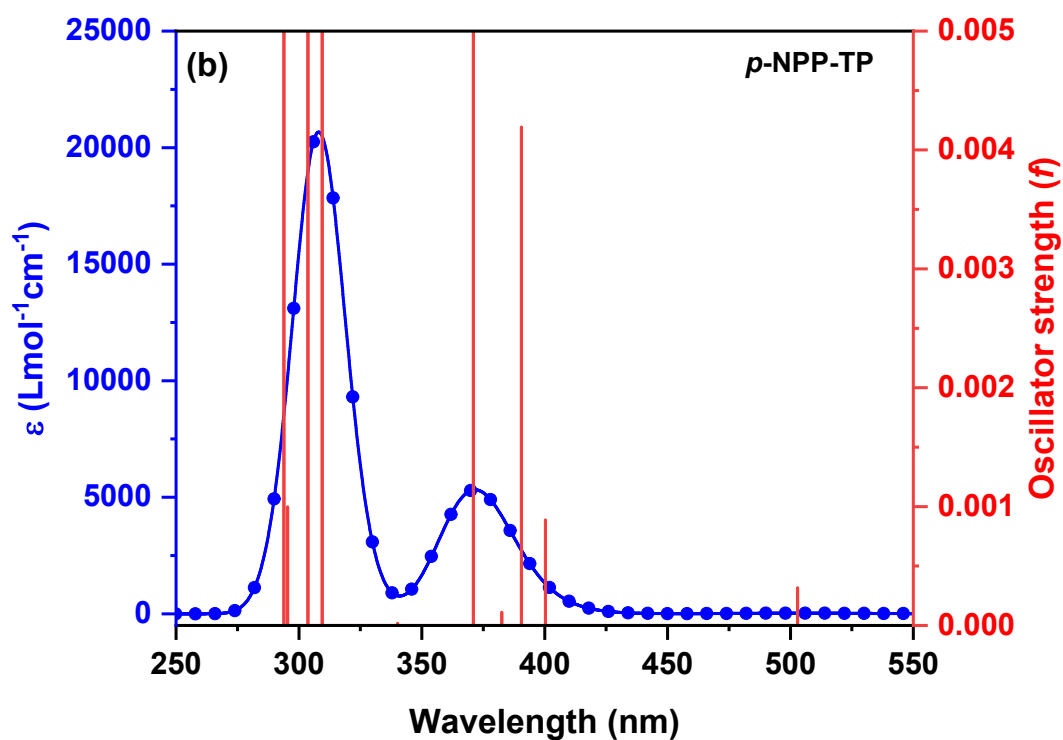


Figure S37(a,b). Theoretical absorption spectra are generated using the Molden program with FWHM of 0.31 eV for *p*-NPP-TP molecule.

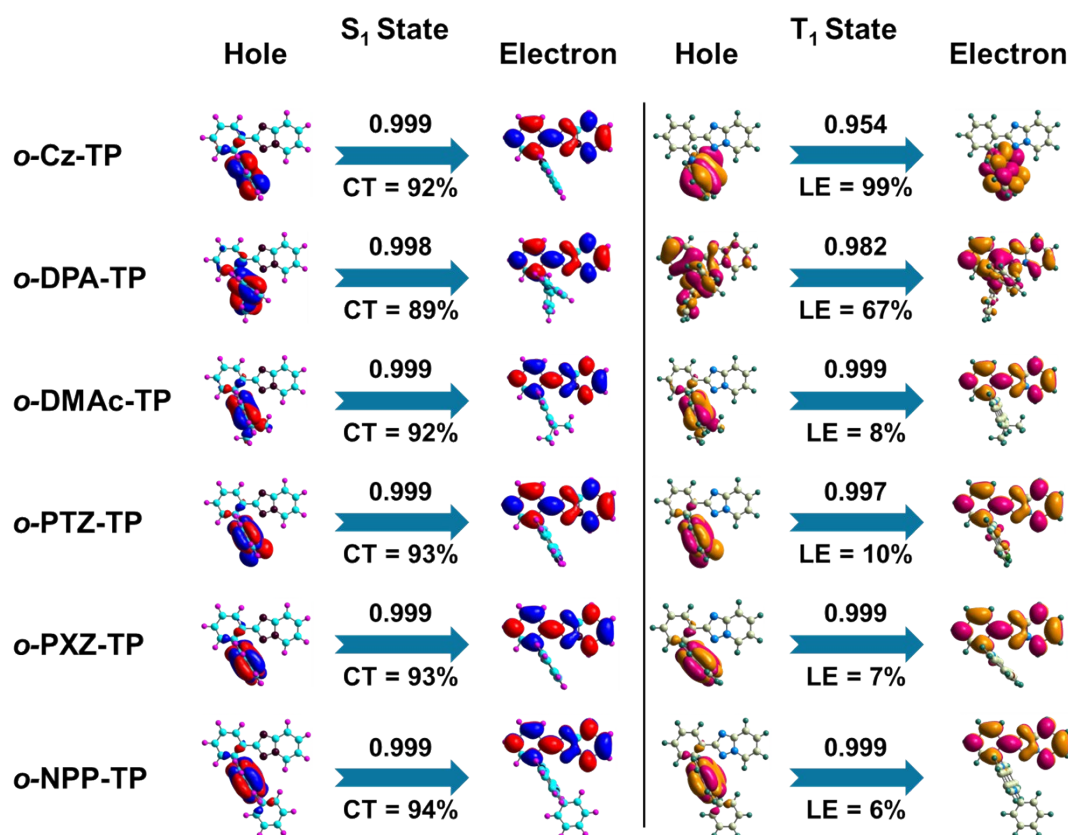


Figure S38. Natural transition orbitals (NTOs) of the S_1 and T_1 states for the *ortho*-molecules at S_1 and T_1 geometry, respectively.

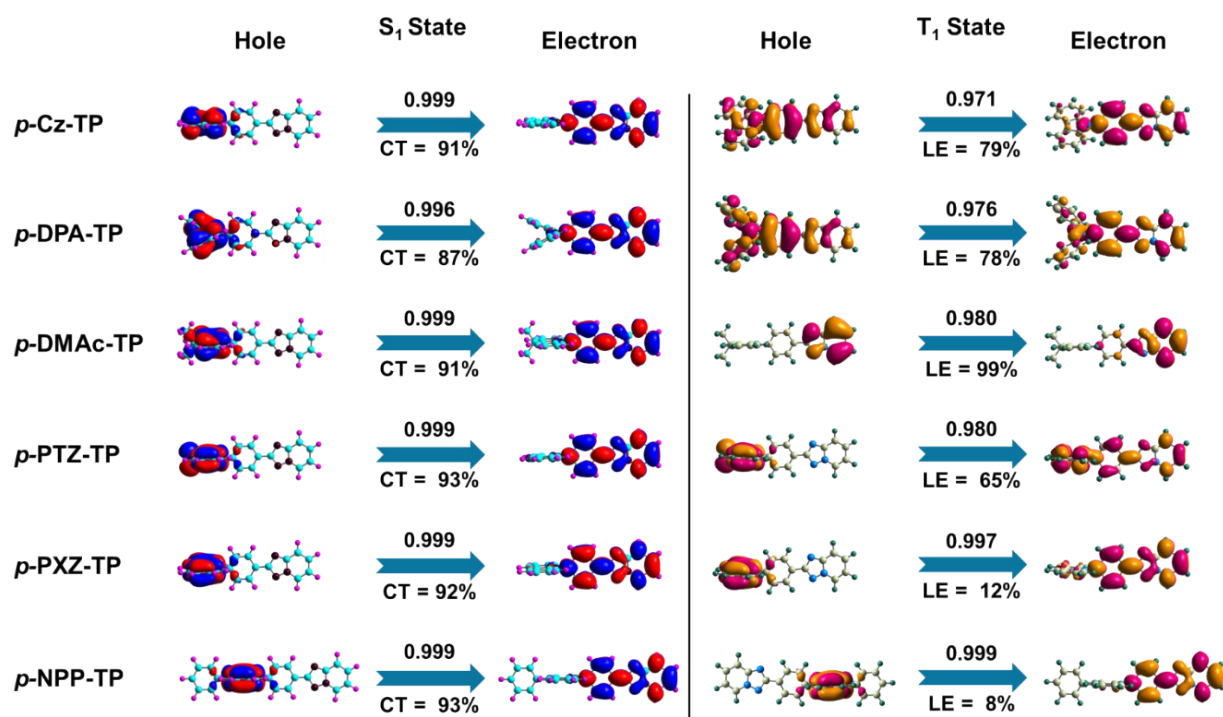


Figure S39. Natural transition orbitals (NTOs) of the S_1 and T_1 states for the *para*- molecules at S_1 and T_1 geometry, respectively.

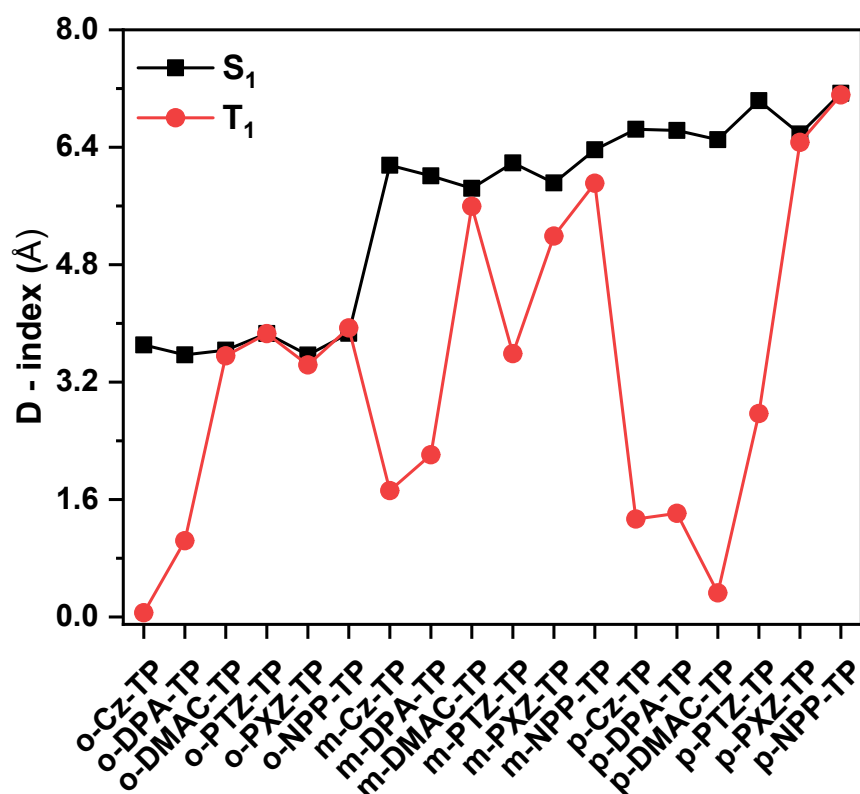


Figure S40. D index at S_1 and T_1 geometry of the proposed molecules.

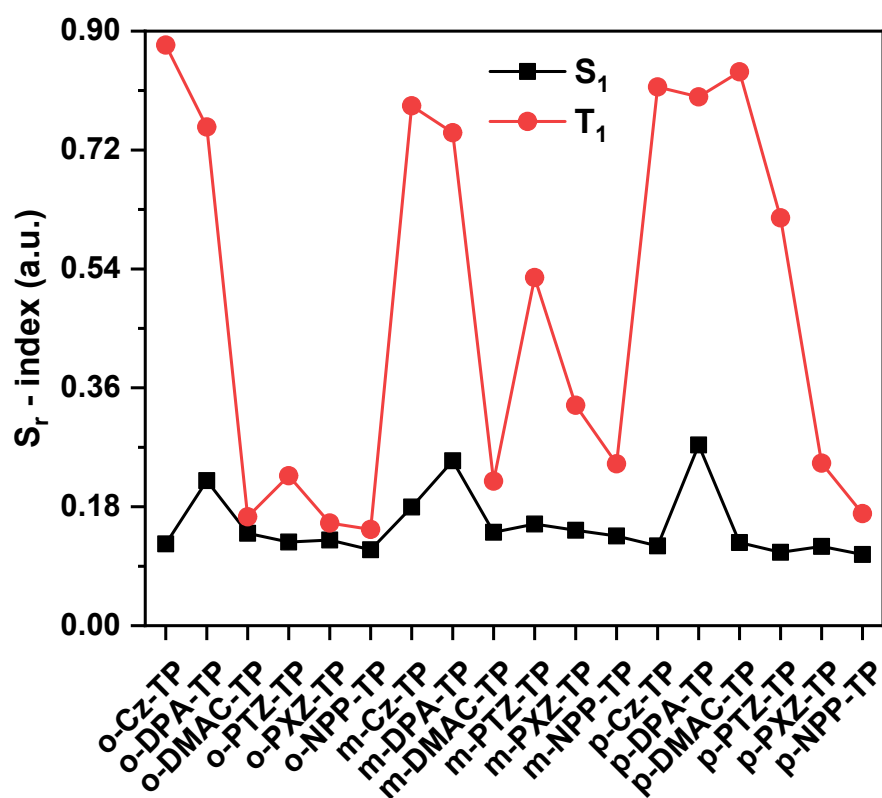


Figure S41. S_r index at S_1 and T_1 geometry of the proposed molecules.

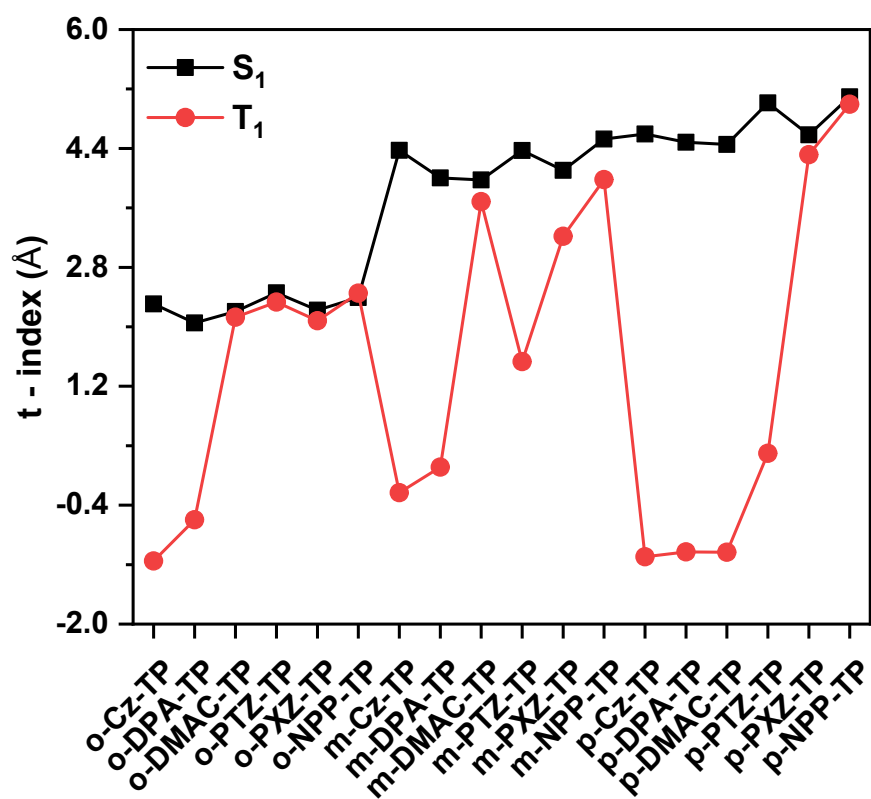


Figure S42. t index at S_1 and T_1 geometry of the proposed molecules.

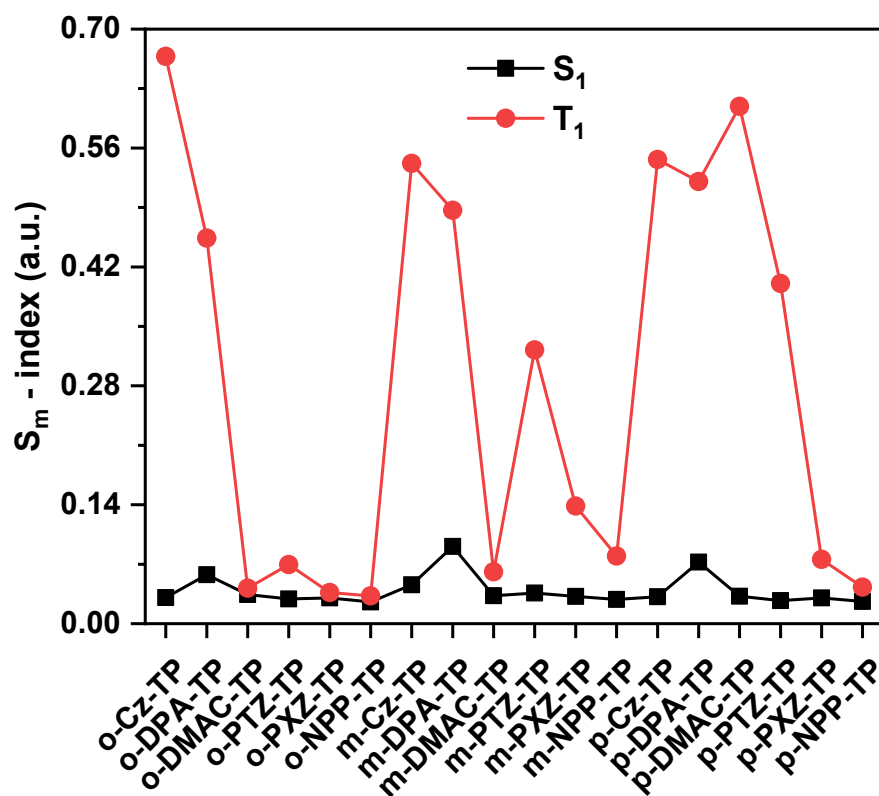


Figure S43. S_m index at S_1 and T_1 geometry of the proposed molecules.

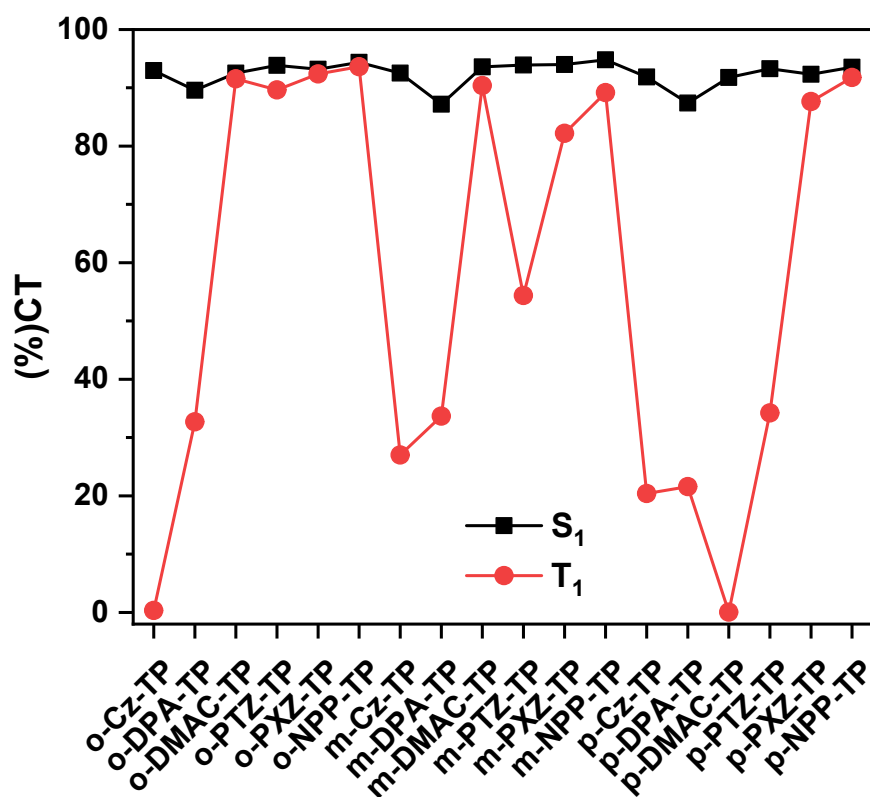


Figure S44. %CT at S_1 and T_1 geometry of the proposed molecules.

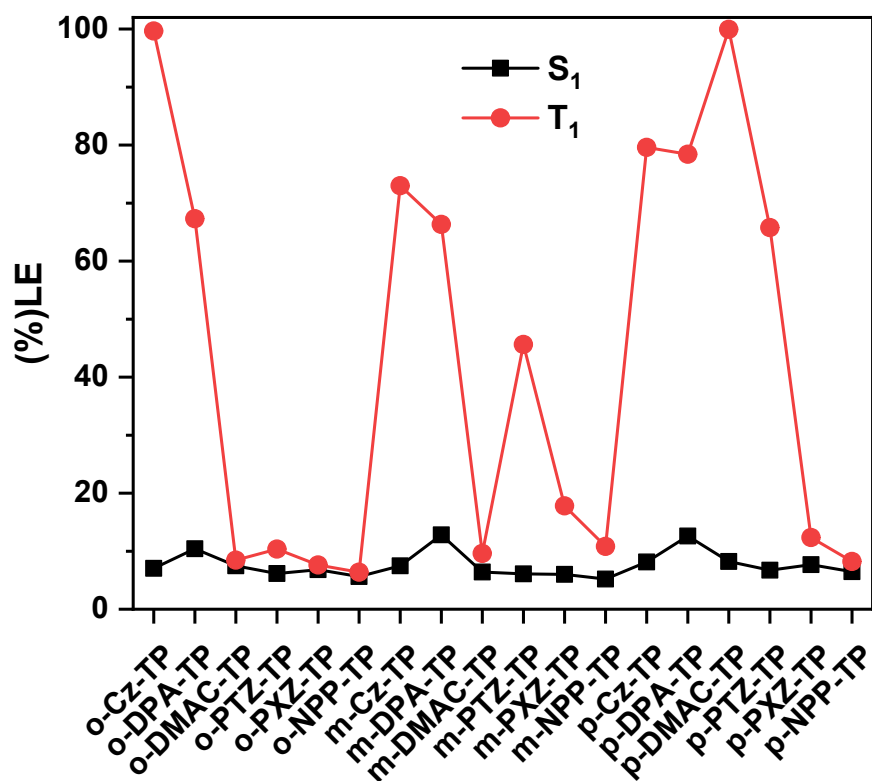


Figure S45. %LE at S_1 and T_1 geometry of the proposed molecules.

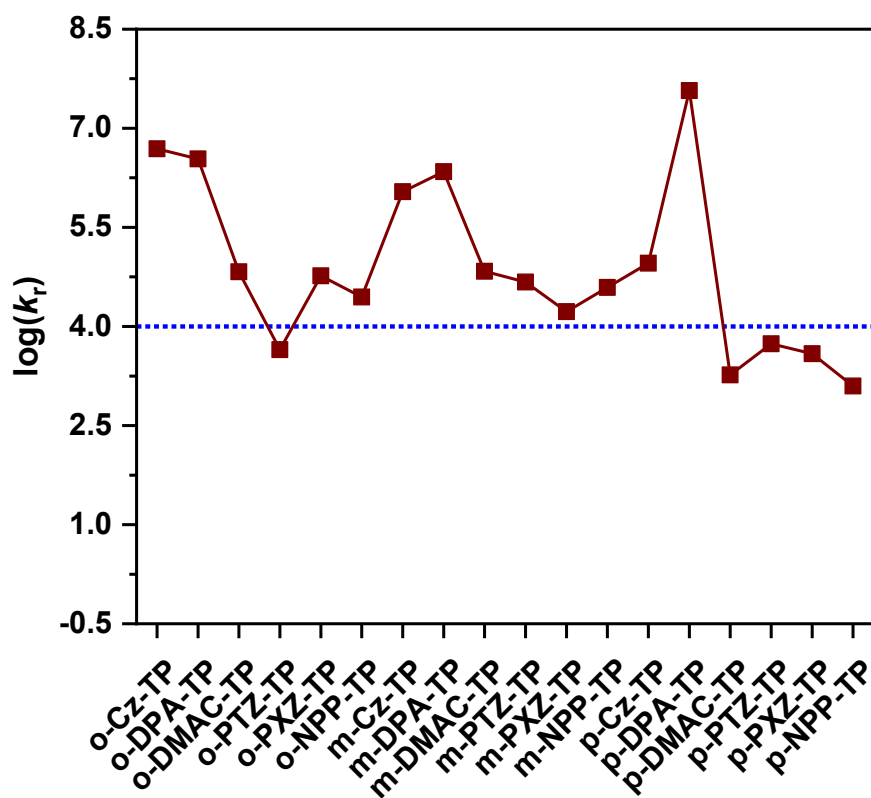


Figure S46. Radiative rates (k_r) of the proposed molecules.

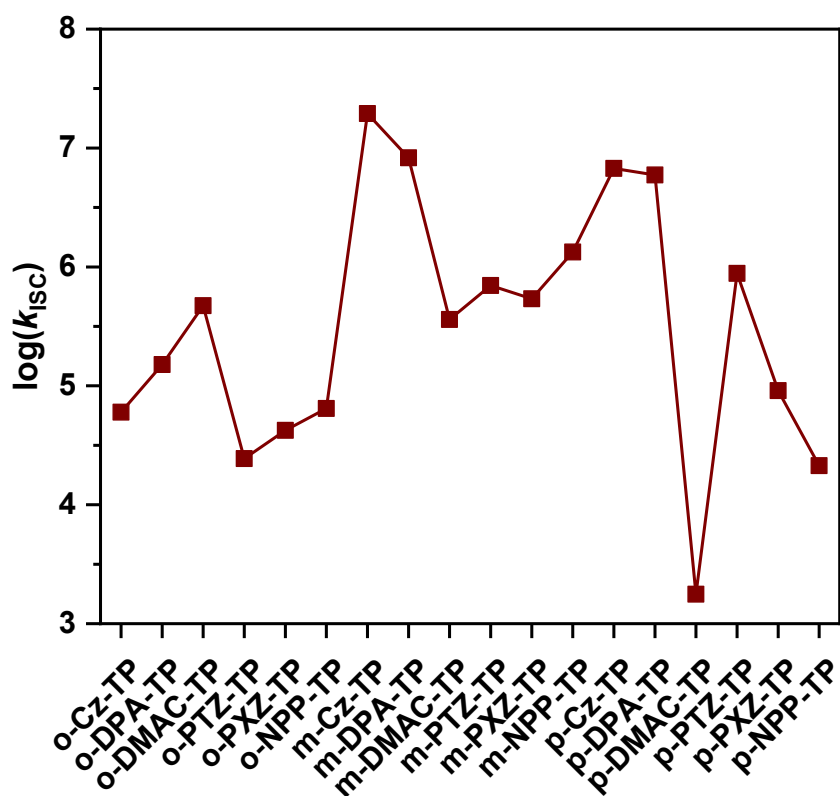


Figure S47. Inter system crossing rates (k_{isc}) of the proposed molecules

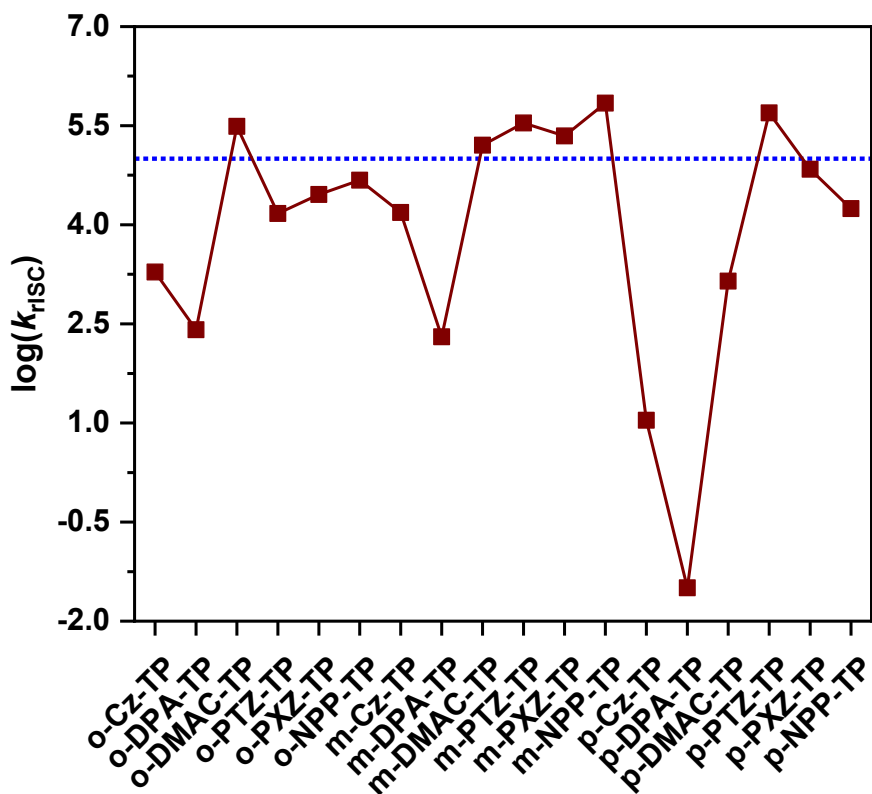


Figure S48. Reverse inter system crossing rates (k_{isc}) of the proposed molecules.

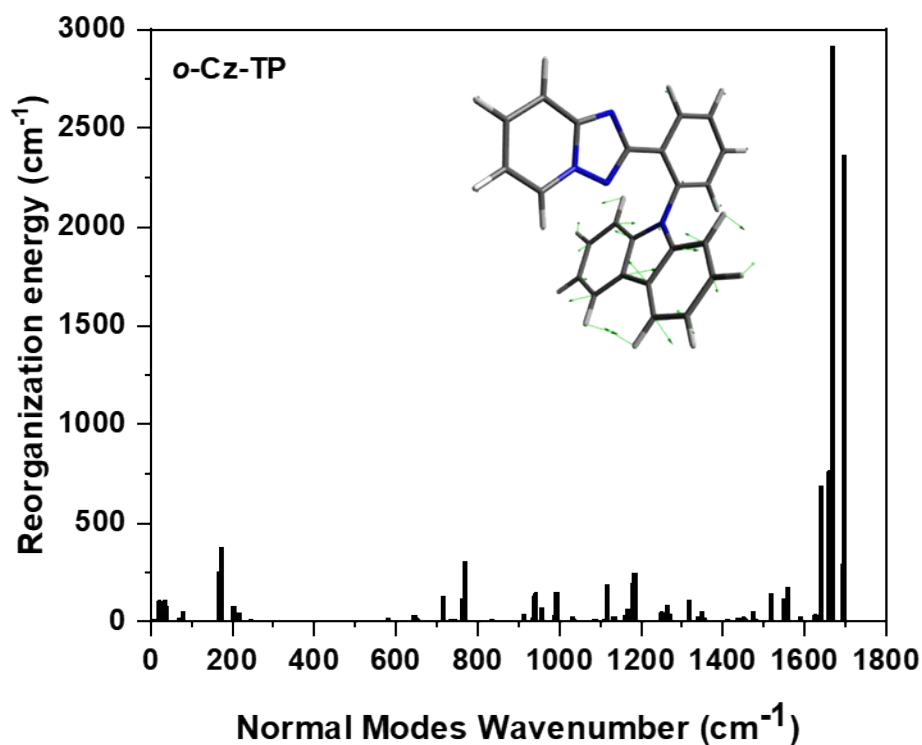


Figure S49. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies for *o*-Cz-TP molecule. Representative vibrational modes are shown in the insets.

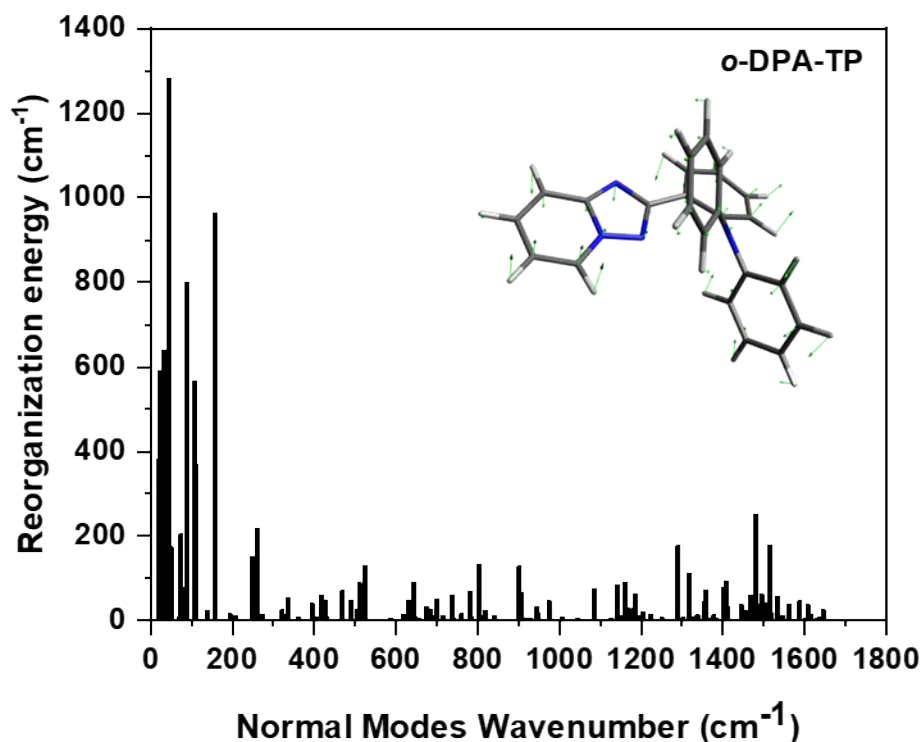


Figure S50. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies for *o*-DPA-TP molecule. Representative vibrational modes are shown in the insets.

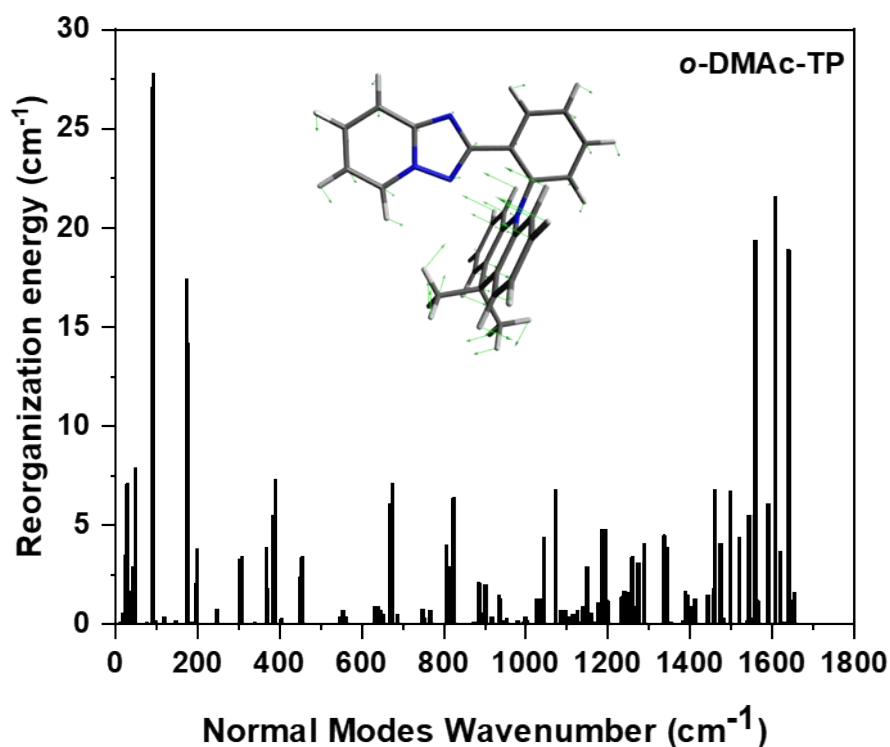


Figure S51. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies for *o*-DMAc-TP molecule. Representative rotational modes are shown in the insets.

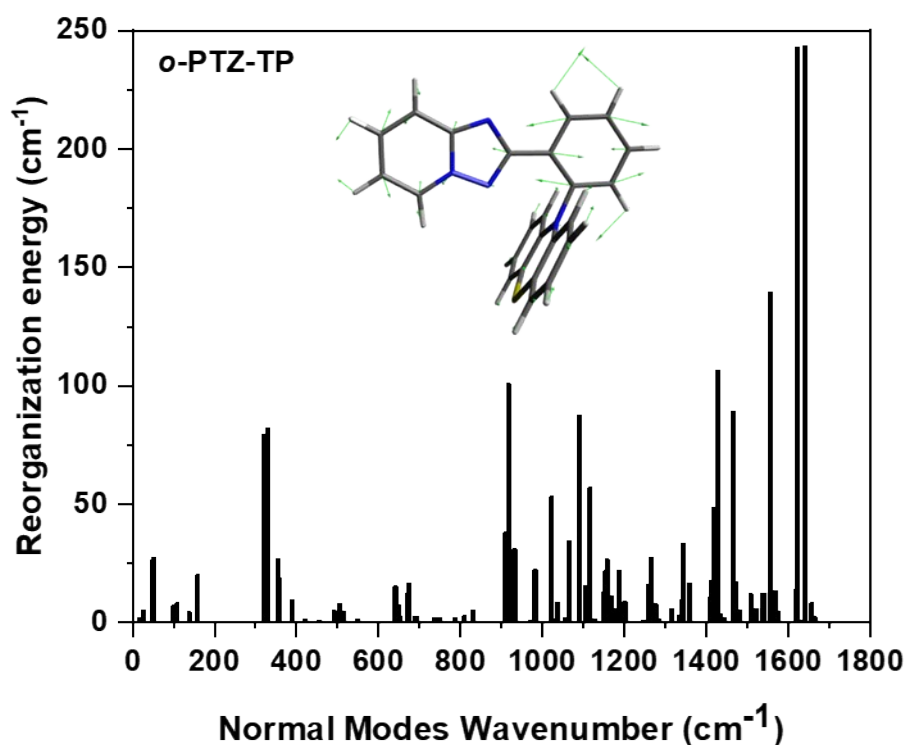


Figure S52. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies for *o*-PTZ-TP molecule. Representative vibrational modes are shown in the insets.

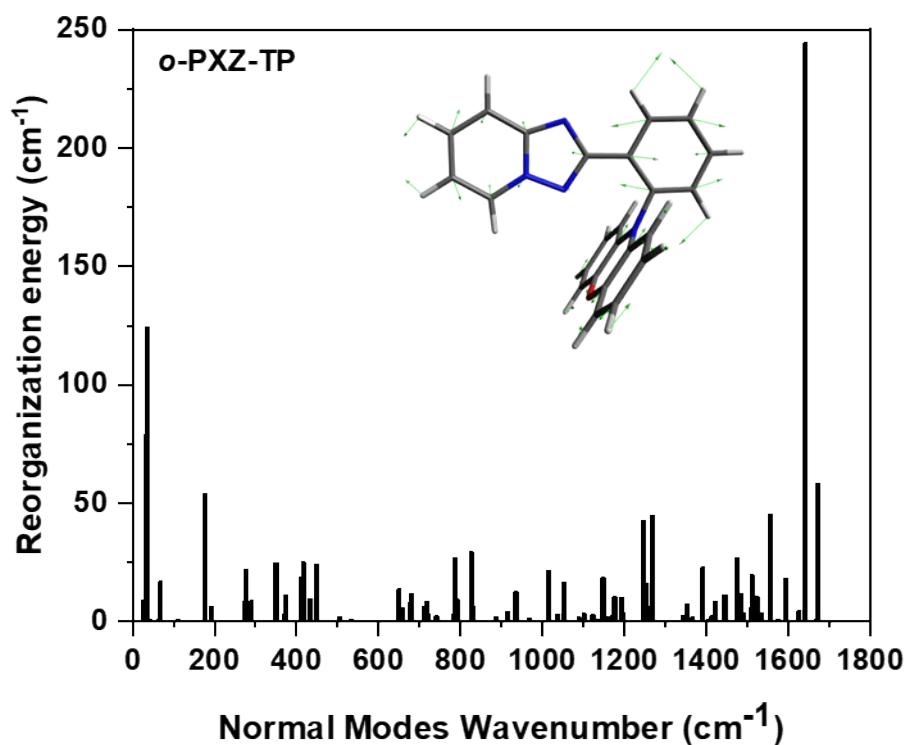


Figure S53. Reorganization energies for the S_1 state in the S_1-T_1 transition versus the normal mode frequencies for *o*-PXZ-TP molecule. Representative vibrational modes are shown in the insets.

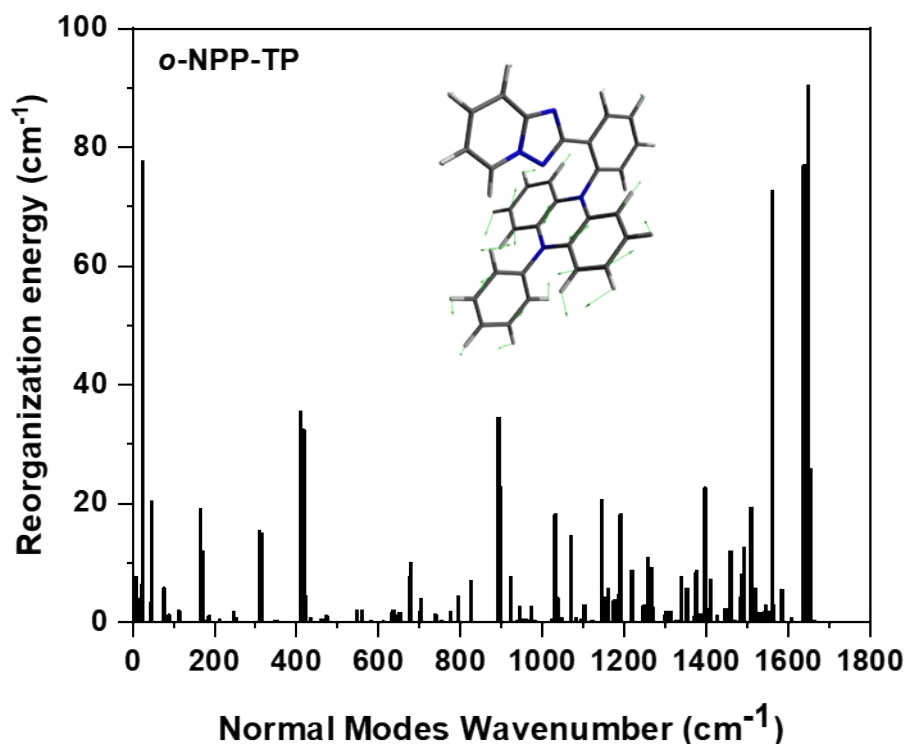


Figure S54. Reorganization energies for the S_1 state in the S_1-T_1 transition versus the normal mode frequencies for *o*-NPP-TP molecule. Representative vibrational modes are shown in the insets.

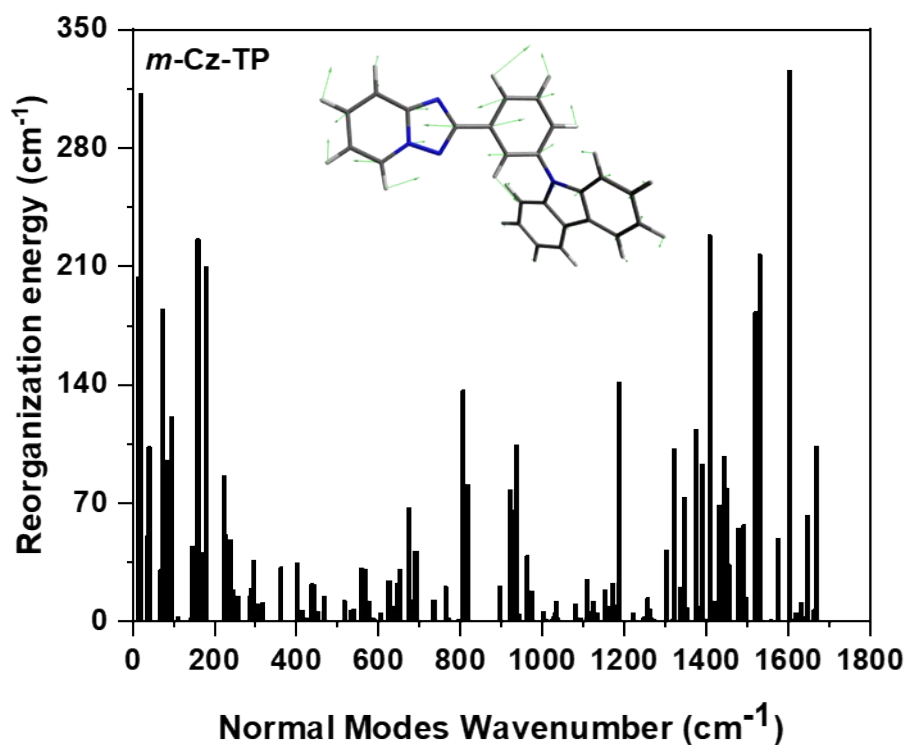


Figure S55. Reorganization energies for the S_1 state in the S_1-T_1 transition versus the normal mode frequencies for *m*-Cz-TP molecule. Representative vibrational modes are shown in the insets.

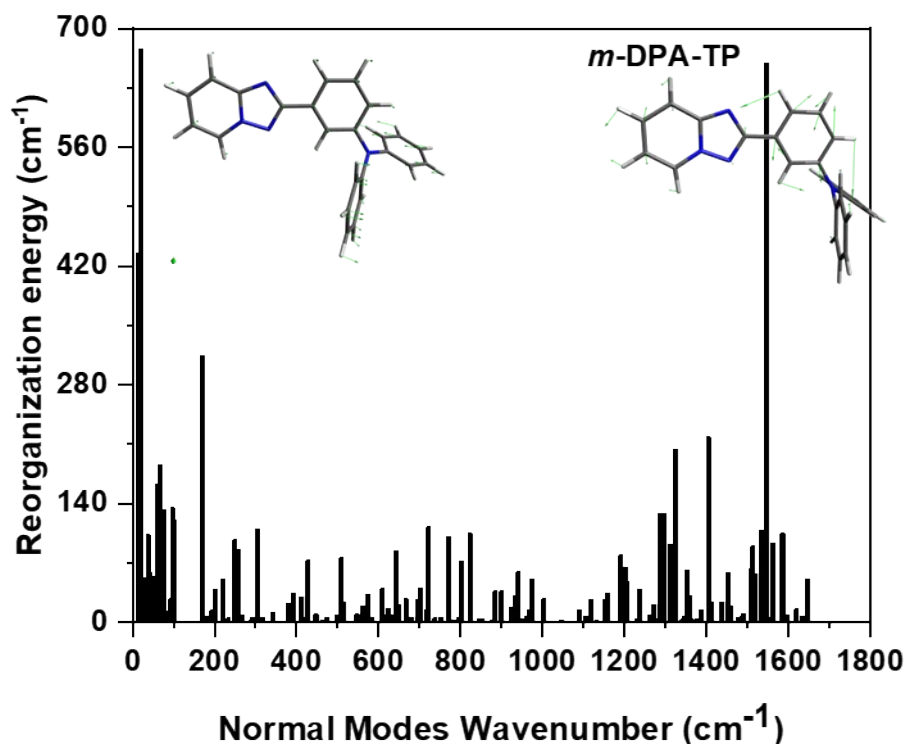


Figure S56. Reorganization energies for the S_1 state in the S_1-T_1 transition versus the normal mode frequencies *m*-DPA-TP molecule. Representative vibrational and rotational modes are shown in the insets.

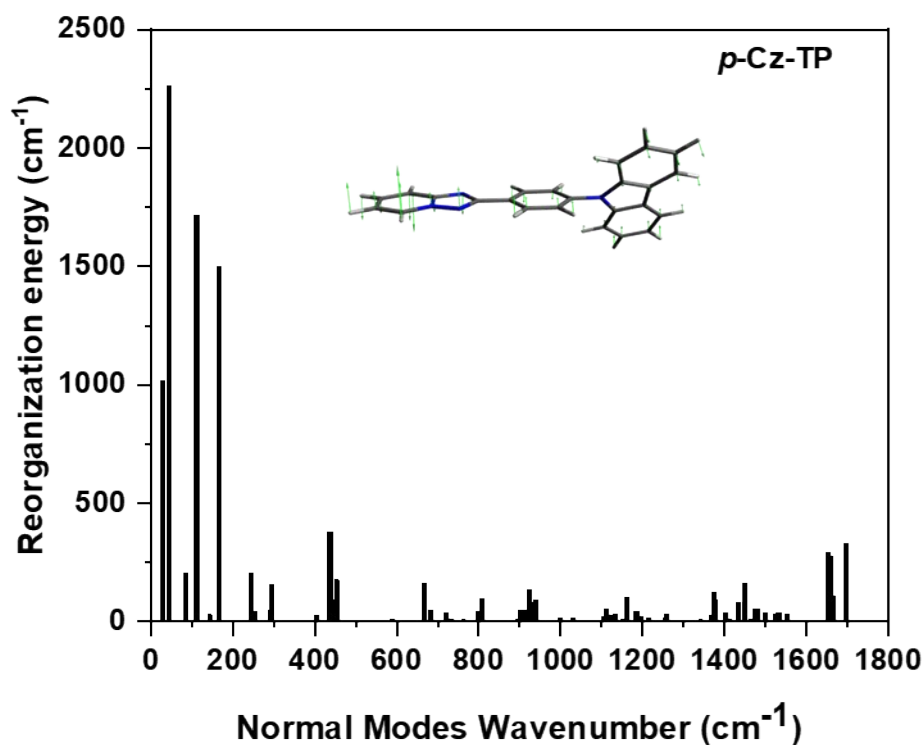


Figure S57. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies *p*-Cz-TP molecule. Representative rotational modes are shown in the insets.

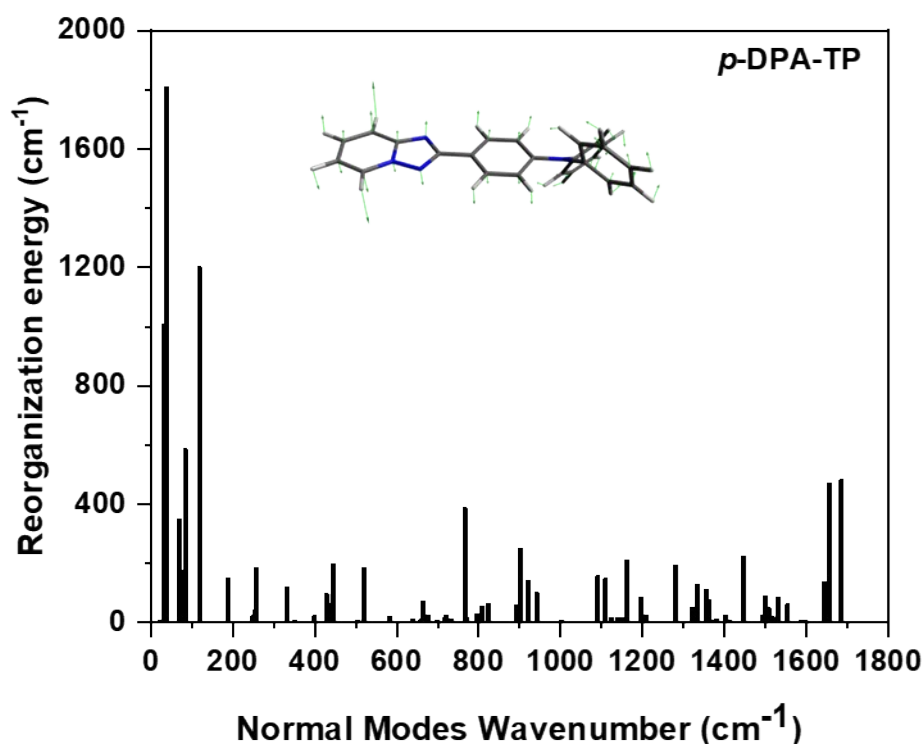


Figure S58. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies *p*-DPA-TP molecule. Representative rotational modes are shown in the insets.

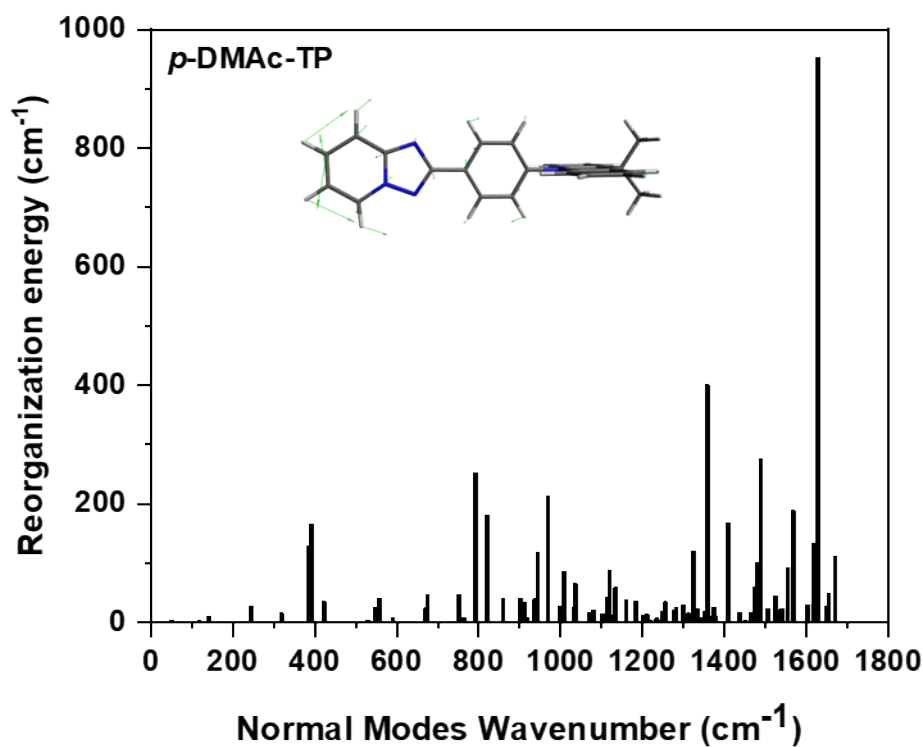


Figure S59. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies p -DMAc-TP molecule. Representative vibrational modes are shown in the insets.

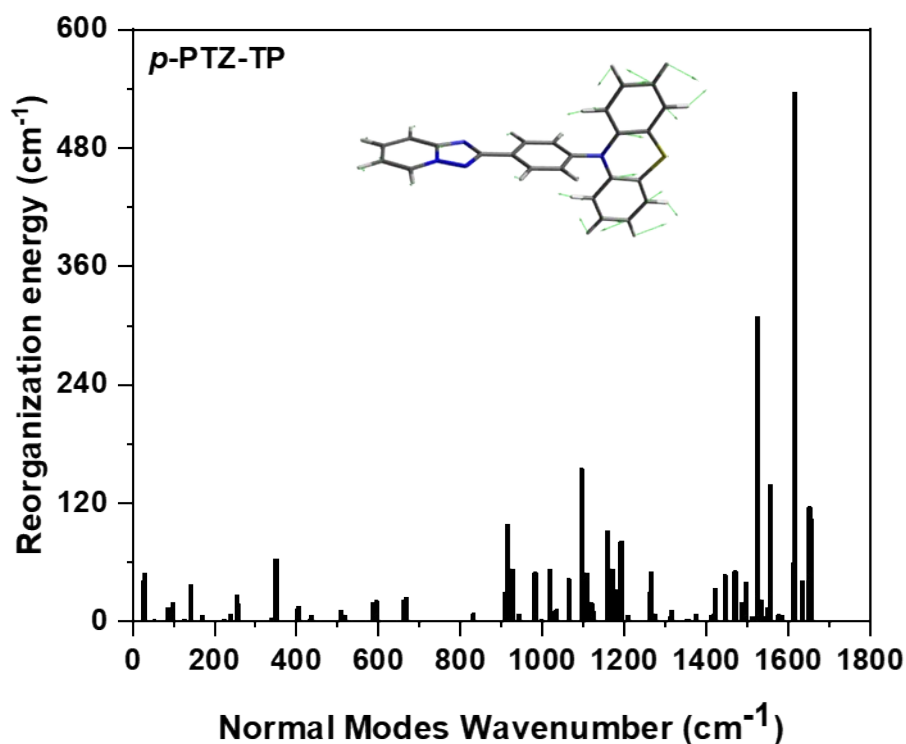


Figure S60. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies p -PTZ-TP molecule. Representative vibrational modes are shown in the insets.

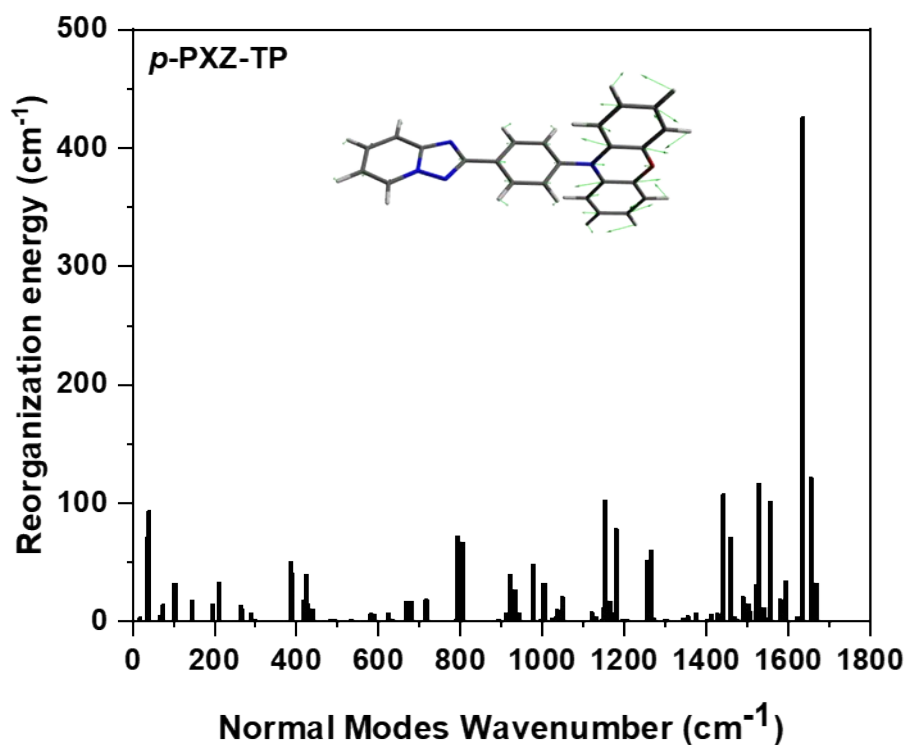


Figure S61. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies p -PXZ-TP molecule. Representative vibrational modes are shown in the insets.

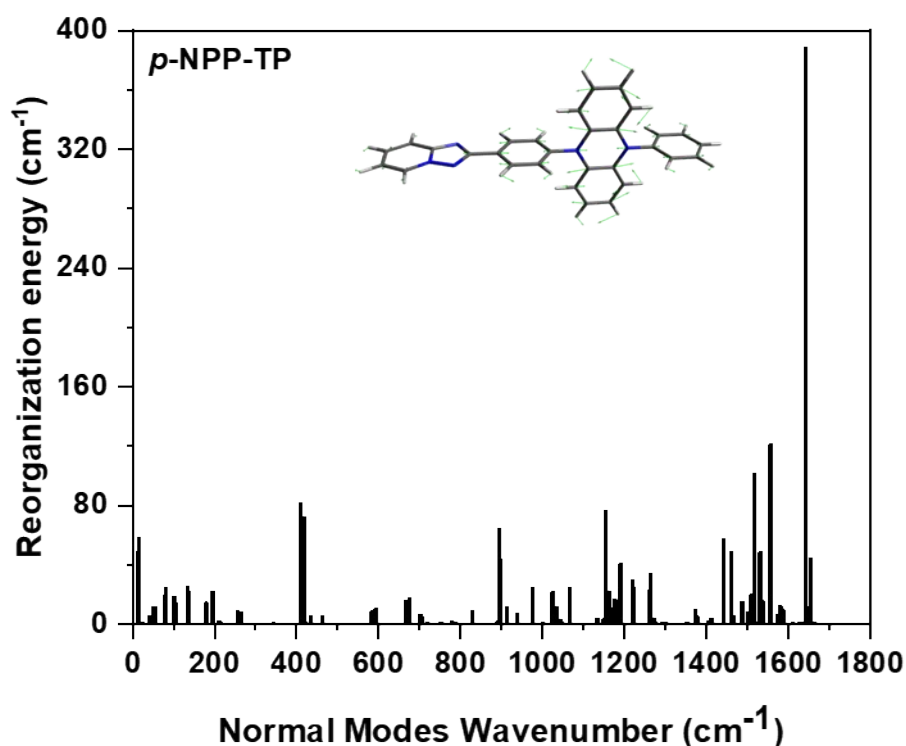


Figure S62. Reorganization energies for the S_1 state in the S_1 - T_1 transition versus the normal mode frequencies p -NPP-TP molecule. Representative vibrational modes are shown in the insets.

Table S1. HOMO and LUMO values of the different donors (def2-svp)

Molecule	HOMO (eV)	LUMO (eV)	Gap (eV)
Cz	-5.603	-0.864	4.739
DPA	-5.247	-0.373	4.874
DMAc	-5.032	-0.291	4.741
PTZ	-4.997	-0.608	4.389
PXZ	-4.816	-0.466	4.35
NPP	-4.253	-0.599	3.654

Table S2. Comparison of calculated HOMO, LUMO, lowest singlet (S_1) and lowest triplet (T_1) state energies at different basis sets at benchmark B3LYP functional in the DCM solvent. (All values are in eV.)

Functional	Basis sets	HOMO	LUMO	S_1	T_1	ΔE_{ST}
Exp.	Exp.	-5.38	-1.78	3.39	2.93	0.460
B3LYP	def2-TZVP	-5.701	-1.558	3.539	3.308	0.231
B3LYP	def2-QZVP	-5.718	-1.582	3.533	3.299	0.234
B3LYP	TZVP	-5.716	-1.565	3.549	3.320	0.229
B3LYP	def2-SVP	-5.648	-1.469	3.575	3.335	0.240

Table S3. Calculated λ_{abs} of the functionals used for benchmarking study at def2-SVP basis sets.

Functionals	λ_{abs} (nm)	$\Delta\lambda$
Experimental	338	0
B2GP-PLYP	293.7	44.3
B2PLYP	311.7	26.3
B3LYP	353.9	15.9
CAM-B3LYP	280.1	57.9
LC-BLYP	272.8	65.2
LC-PBE	257.6	80.4
M06	332.6	5.4
M062X	284	54
PBE0	335.3	2.7

SOS-PBE-QIDH	301	37
SOS-ωPBEPP86	300	38
ωB97X-D3	271.7	66.3

Table S4. Calculated λ_{abs} of the studied molecules using PBE0/def2-SVP functional.

Compound	λ_{abs} (nm)
<i>o</i> -Cz-TP	346.9
<i>o</i> -DPA-TP	380.2
<i>o</i> -DMAC-TP	417.3
<i>o</i> -PTZ-TP	426.8
<i>o</i> -PXZ-TP	450.0
<i>o</i> -NPP-TP	539.0
<i>m</i> -Cz-TP	334.2
<i>m</i> -DPA-TP	364.4
<i>m</i> -DMAC-TP	389.9
<i>m</i> -PTZ-TP	388.9
<i>m</i> -PXZ-TP	424.0
<i>m</i> -NPP-TP	496.8
<i>p</i> -Cz-TP	337.8
<i>p</i> -DPA-TP	360.3
<i>p</i> -DMAC-TP	394.9
<i>p</i> -PTZ-TP	395.9
<i>p</i> -PXZ-TP	431.3
<i>p</i> -NPP-TP	502.9

Table S5. Calculated λ_{em} of the functionals used for benchmarking study at def2-SVP basis sets.

Functional	λ_{abs}	$\Delta\lambda$
Experimental	397	0
B3LYP	460	63
PBE0	427	30
ωB97X	278.8	118.2
CAM-B3LYP	340	57
M06-2X	346.2	50.8
PBE	617	220
LC-PBE	257.6	139.4

Table S6. Calculated λ_{em} of the studied molecules using PBE0/def2-SVP functional.

Compound	λ_{em} (nm)	f
<i>o</i>-Cz-TP	400.4	0.00002
<i>o</i>-DPA-TP	450.6	0.02081
<i>o</i>-DMAC-TP	481.3	0.00007
<i>o</i>-PTZ-TP	560.5	0.00115
<i>o</i>-PXZ-TP	557.2	0.00100
<i>o</i>-NPP-TP	686.8	0.00093
<i>m</i>-Cz-TP	372.6	0.00597
<i>m</i>-DPA-TP	415.9	0.01558
<i>m</i>-DMAC-TP	445.3	0.00026
<i>m</i>-PTZ-TP	517.9	0.00100
<i>m</i>-PXZ-TP	508.9	0.00025
<i>m</i>-NPP-TP	617.4	0.00115
<i>p</i>-Cz-TP	375.6	0.00041
<i>p</i>-DPA-TP	409.8	0.17297
<i>p</i>-DMAC-TP	441.3	0.00002
<i>p</i>-PTZ-TP	510.6	0.00001
<i>p</i>-PXZ-TP	505.6	0.00003
<i>p</i>-NPP-TP	610.7	0.00001

Table S7. Charge transfer indices of TADF emitters at Singlet (S₁) and Triplet (T₁) optimized geometries.

Mol.	States	$\Delta r(\text{\AA})$	S_m(a.u.)	S_r(a.u.)	D (Å)	t (Å)	HDI	EDI	Λ	%CT	%LE
<i>o</i>-Cz-TP	S₁	3.996419	0.03065	0.12381	3.708	2.308	9.00	6.81	0.105656	92.952	7.048
	T₁	0.180811	0.66789	0.87880	0.059	-1.151	6.91	7.03	0.812383	0.334	99.666
<i>o</i>-DPA-TP	S₁	3.96618	0.05758	0.21962	3.572	2.052	9.80	6.74	0.18685	89.58	10.42
	T₁	2.28855	0.45397	0.75482	1.039	-0.596	7.89	6.92	0.57771	32.702	67.298
<i>o</i>-DMAC-TP	S₁	3.98993	0.03426	0.13984	3.637	2.205	9.34	6.77	0.12208	92.513	7.487
	T₁	3.96943	0.04173	0.16469	3.557	2.130	9.37	6.71	0.13117	91.535	8.465
<i>o</i>-PTZ-TP	S₁	4.08551	0.02906	0.12656	3.863	2.458	8.12	6.75	0.114	93.845	6.155
	T₁	4.28335	0.06961	0.22701	3.861	2.332	7.90	6.40	0.13375	89.635	10.365
<i>o</i>-PXZ-TP	S₁	3.82092	0.03040	0.12973	3.569	2.223	9.52	6.78	0.11511	93.195	6.805
	T₁	3.75016	0.03668	0.15540	3.434	2.082	9.41	6.73	0.11582	92.38	7.62
<i>o</i>-NPP-TP	S₁	4.12755	0.02548	0.11492	3.866	2.393	8.70	6.81	0.10293	94.372	5.628

	T₁	4.28506	0.03275	0.14564	3.938	2.453	8.72	6.73	0.11209	93.611	6.389
<i>m</i>-Cz-TP	S₁	6.90632	0.04573	0.17950	6.154	4.374	8.82	6.74	0.14799	92.528	7.472
	T₁	4.16105	0.54193	0.78684	1.723	-0.233	6.99	7.42	0.51028	27.014	72.986
<i>m</i>-DPA-TP	S₁	6.69234	0.09095	0.24959	6.010	4.004	9.53	6.80	0.20551	87.192	12.808
	T₁	4.68894	0.48671	0.74621	2.211	0.113	8.12	6.96	0.48747	33.686	66.314
<i>m</i>-DMAC-TP	S₁	6.66874	0.03297	0.14128	5.841	3.976	9.37	6.66	0.11547	93.584	6.416
	T₁	6.7455	0.06094	0.21868	5.595	3.685	9.09	6.42	0.12762	90.383	9.617
<i>m</i>-PTZ-TP	S₁	6.9778	0.03600	0.15378	6.188	4.373	7.98	6.59	0.11688	93.911	6.089
	T₁	5.64972	0.32228	0.52682	3.587	1.532	7.92	4.86	0.27181	54.373	45.627
<i>m</i>-PXZ-TP	S₁	6.72028	0.03206	0.14451	5.914	4.106	9.61	6.67	0.1147	94.003	5.997
	T₁	6.68479	0.13836	0.33355	5.190	3.217	9.38	5.86	0.15037	82.188	17.812
<i>m</i>-NPP-TP	S₁	7.13589	0.02854	0.13571	6.366	4.526	8.84	6.69	0.10233	94.814	5.186

	T₁	7.11246	0.07967	0.24500	5.909	3.981	8.67	6.25	0.12085	89.163	10.837
<i>p</i>-Cz-TP	S₁	7.88653	0.03178	0.12077	6.645	4.594	8.98	6.86	0.09225	91.858	8.142
	T₁	4.27194	0.54641	0.81554	1.334	-1.094	6.67	7.28	0.61528	20.395	79.605
<i>p</i>-DPA-TP	S₁	7.66497	0.07247	0.27354	6.630	4.483	9.76	6.74	0.23334	87.383	12.617
	T₁	3.94106	0.52047	0.80050	1.413	-1.028	7.32	6.93	0.64521	21.591	78.409
<i>p</i>-DMAC-TP	S₁	7.76279	0.03236	0.12578	6.504	4.454	9.28	6.86	0.09441	91.779	8.221
	T₁	0.93209	0.60907	0.83839	0.329	-1.034	9.36	9.73	0.78681	0.059	99.941
<i>p</i>-PTZ-TP	S₁	8.17346	0.02715	0.11098	7.035	5.013	8.00	6.87	0.08485	93.264	6.736
	T₁	4.2759	0.40056	0.61739	2.771	0.298	7.56	5.25	0.42075	34.232	65.768
<i>p</i>-PXZ-TP	S₁	7.77461	0.03039	0.11985	6.582	4.583	9.64	6.89	0.09416	92.334	7.666
	T₁	7.99085	0.07567	0.24590	6.467	4.315	9.48	6.44	0.12172	87.658	12.342
<i>p</i>-NPP-TP	S₁	8.26628	0.02619	0.10779	7.136	5.094	8.85	6.82	0.08118	93.547	6.453

	T₁	8.3962	0.04297	0.16950	7.112	4.995	8.67	6.65	0.09437	91.773	8.227
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XYZ Coordinates of *o*-Cz-TP in S₀ optimized geometry

C	-1.205347	5.872238	4.770857
C	-1.853152	4.638752	4.852977
C	-3.028005	4.397174	4.127992
C	-3.574804	5.415177	3.311637
C	-2.885316	6.636697	3.208816
C	-1.717617	6.869508	3.934162
H	-1.450011	3.833225	5.470458
H	-0.291008	6.046084	5.343929
H	-3.300289	7.405677	2.55465
H	-1.207163	7.832168	3.849101
N	-5.792721	4.393888	2.930566
N	-5.112998	5.985014	1.451064
N	-6.729071	4.569311	1.987106
C	-4.835468	5.255829	2.562448
C	-6.313422	5.547754	1.079636
C	-7.17406	5.869321	0.002075
C	-8.375878	5.201304	-0.106297
C	-8.749333	4.207155	0.844287
C	-7.913452	3.89877	1.889072
H	-6.857698	6.632229	-0.710012
H	-9.053639	5.431378	-0.931718
H	-9.698746	3.67801	0.750511
H	-8.102722	3.150863	2.659741
N	-3.627342	3.113038	4.21672
C	-3.801061	2.223081	3.158641
C	-4.277217	2.602431	5.339449
C	-4.559128	1.108949	3.608902
C	-3.350072	2.321035	1.837868

C	-4.862162	1.350013	5.006324
C	-4.403074	3.156017	6.618303
C	-4.862679	0.07395	2.712798
C	-3.669334	1.280156	0.964264
H	-2.777705	3.188468	1.503298
C	-5.570351	0.637965	5.984521
C	-5.115399	2.427946	7.573327
H	-3.961311	4.125687	6.855965
H	-5.443008	-0.790664	3.046245
C	-4.417496	0.16568	1.39335
H	-3.331246	1.332946	-0.07422
C	-5.69173	1.179963	7.264946
H	-6.022662	-0.327872	5.743281
H	-5.228003	2.837409	8.580912
H	-4.649382	-0.632934	0.684025
H	-6.240815	0.634853	8.036932

XYZ Coordinates of *o*-Cz-TP in S₁ optimized geometry

C	-0.976014914	5.674529823	4.42366266
C	-1.661142525	4.458324721	4.51463664
C	-2.92438356	4.312809543	3.947420251
C	-3.597424783	5.372082422	3.247662822
C	-2.862401953	6.599968258	3.178374569
C	-1.608505647	6.743855342	3.741226467
H	-1.21442288	3.605036585	5.033104614
H	0.01403179	5.789605281	4.867308338
H	-3.341325203	7.428948299	2.654608219
H	-1.095420141	7.706364077	3.656092865
N	-5.658590537	4.142760962	2.658784041

N	-5.493604957	6.326833441	1.992807901
N	-6.759471237	4.499983996	1.996293006
C	-4.894153657	5.276125343	2.645914312
C	-6.658563608	5.843753272	1.586548477
C	-7.742730198	6.404927466	0.863424566
C	-8.856677843	5.605533648	0.589984178
C	-8.911633917	4.268434513	1.019376456
C	-7.846249523	3.713948096	1.73115362
H	-7.671077899	7.44394496	0.543577464
H	-9.698112749	6.026388425	0.033418326
H	-9.781516282	3.645450549	0.804823517
H	-7.799295085	2.692112618	2.103216132
N	-3.57546561	3.028008435	4.084710957
C	-3.503404607	2.001048698	3.176336587
C	-4.441868163	2.684467312	5.093127968
C	-4.335014708	0.924919516	3.60790191
C	-2.761483533	1.953925921	1.986388537
C	-4.94776201	1.37127469	4.859258857
C	-4.824076141	3.456865073	6.20023928
C	-4.414492503	-0.220719547	2.834906739
C	-2.855952904	0.789391618	1.221327412
H	-2.153360338	2.806957449	1.685665888
C	-5.846297864	0.822593241	5.758229214
C	-5.731420813	2.884893104	7.094727286
H	-4.426066503	4.463217268	6.32998217
H	-5.044223337	-1.062064285	3.132345404
C	-3.66500276	-0.280232492	1.635900141
H	-2.29917443	0.712287676	0.285502489
C	-6.23355913	1.591565001	6.88144818

H	-6.257755758	-0.178030918	5.608641562
H	-6.059644043	3.453213447	7.967063324
H	-3.723686462	-1.17845229	1.017241518
H	-6.944698072	1.168792443	7.594544135

XYZ Coordinates of *o*-Cz-TP in T₁ optimized geometry

C	-1.04042613	5.844397663	4.570673502
C	-1.67082787	4.602931947	4.676149895
C	-2.900581862	4.369705153	4.049932513
C	-3.523998386	5.398173714	3.303578037
C	-2.863535302	6.635216579	3.190129459
C	-1.639194901	6.859899539	3.81849509
H	-1.21712936	3.786567602	5.241990752
H	-0.08149086	6.013845748	5.066960532
H	-3.342841976	7.419171144	2.601354737
H	-1.150836231	7.833019717	3.722041417
N	-5.663776761	4.220726056	2.892483203
N	-5.290515828	6.140377024	1.73026608
N	-6.706990297	4.478516633	2.092220903
C	-4.831808802	5.240526312	2.639567603
C	-6.478761076	5.658563216	1.378620303
C	-7.476673372	6.095194335	0.47329247
C	-8.621541912	5.338327189	0.336650862
C	-8.802765614	4.140444022	1.08781201
C	-7.833918873	3.719452553	1.964975968
H	-7.307555176	7.014536198	-0.088282532
H	-9.403302046	5.655887291	-0.357394763
H	-9.709483913	3.544788499	0.972872568
H	-7.873597867	2.819117779	2.579198894

N	-3.48982225	3.080957016	4.174497588
C	-3.559543127	2.136075834	3.145306813
C	-4.330343498	2.69048278	5.213408703
C	-4.454818688	1.070140994	3.586887748
C	-2.955635126	2.128269499	1.919916322
C	-4.923891617	1.403003791	4.839215632
C	-4.628809062	3.32278938	6.391421751
C	-4.696165365	-0.053906282	2.691570812
C	-3.222850402	0.998899318	1.051456561
H	-2.302460386	2.941275715	1.599419294
C	-5.849644817	0.770626749	5.76597844
C	-5.552108273	2.670743723	7.27925002
H	-4.189321834	4.288952542	6.644234703
H	-5.352631564	-0.868342521	3.003669769
C	-4.075266327	-0.053375159	1.451593137
H	-2.748765731	0.965381469	0.067822217
C	-6.137064177	1.419387725	6.951621359
H	-6.299828552	-0.191860963	5.515177263
H	-5.806812808	3.150430904	8.227096076
H	-4.243765007	-0.88664011	0.763534044
H	-6.831993977	0.962964685	7.662241241

XYZ Coordinates of *o*-DPA-TP in S_0 optimized geometry

C	-0.868948	5.43091	3.92193
C	-1.57378	4.232606	4.029061
C	-2.937106	4.164214	3.699833
C	-3.593624	5.32512	3.22444
C	-2.880453	6.53575	3.168915
C	-1.529482	6.593782	3.507808

H	-1.082028	3.32599	4.388321
H	0.191575	5.46262	4.185647
H	-3.410596	7.4281	2.830328
H	-0.9902	7.54211	3.442876
N	-5.565035	4.243552	2.204866
N	-5.792451	6.414677	2.852168
N	-6.807602	4.672297	1.93569
C	-4.995034	5.319409	2.76792
C	-6.946234	6.00629	2.331151
C	-8.197407	6.637201	2.129028
C	-9.221603	5.910544	1.558178
C	-9.029513	4.550617	1.17884
C	-7.813998	3.942061	1.374804
H	-8.312462	7.677753	2.434464
H	-10.195758	6.377614	1.395373
H	-9.84395	3.978167	0.732481
H	-7.572412	2.908921	1.12385
N	-3.624869	2.932503	3.889192
C	-4.757058	2.885501	4.730857
C	-3.176104	1.793348	3.179026
C	-5.832654	2.018981	4.452862
C	-4.849814	3.740012	5.845043
C	-3.094787	0.536205	3.806168
C	-2.784238	1.911398	1.833785
C	-6.957914	2.003392	5.276139
H	-5.783477	1.371338	3.576765
C	-5.989468	3.729456	6.652366
H	-4.026625	4.420198	6.07126
C	-2.638327	-0.575907	3.097009

H	-3.393828	0.440714	4.852089
C	-2.310849	0.797543	1.138009
H	-2.868258	2.881026	1.340234
C	-7.050067	2.860358	6.379711
H	-7.782236	1.323955	5.040633
H	-6.041112	4.404788	7.510953
C	-2.238094	-0.453082	1.761209
H	-2.58048	-1.545693	3.599239
H	-2.009554	0.906759	0.092382
H	-7.938000	2.8511480	7.016641
H	-1.872879	-1.324435	1.211798

XYZ Coordinates of *o*-DPA-TP in S₁ optimized geometry

C	-1.011776303	5.555990823	4.357397203
C	-1.711668923	4.344047098	4.420731586
C	-2.997351327	4.241032088	3.899652049
C	-3.667789632	5.332999226	3.263309207
C	-2.927769541	6.554802038	3.226238126
C	-1.652060299	6.660870036	3.755293842
H	-1.260471538	3.463669186	4.887080675
H	0.00028871	5.634463876	4.757834641
H	-3.410877288	7.407701633	2.746812557
H	-1.129369874	7.619974967	3.694098344
N	-5.676202615	4.113905709	2.490062278
N	-5.606844569	6.372429708	2.145892887
N	-6.791361867	4.512951916	1.877814729
C	-4.970028063	5.268416365	2.652779534
C	-6.75120211	5.901693896	1.66292699
C	-7.855009092	6.515663948	1.017439689
C	-8.932823214	5.711147464	0.619050327

C	-8.927102423	4.327591604	0.850035705
C	-7.842110104	3.719338194	1.489145258
H	-7.829124712	7.591853519	0.852051277
H	-9.790320164	6.168956973	0.119168083
H	-9.76569217	3.704088395	0.534914238
H	-7.749366343	2.657086639	1.705382513
N	-3.68066652	2.963324944	4.053358669
C	-4.607866456	2.827063649	5.075958604
C	-3.419094173	1.949356916	3.13792359
C	-5.728529278	1.964861266	4.931668729
C	-4.480466552	3.606166844	6.254793079
C	-3.450880285	0.587919361	3.5344969
C	-3.058147909	2.278849393	1.808094976
C	-6.648565675	1.843773415	5.96183704
H	-5.894543962	1.469365953	3.97671025
C	-5.407370074	3.465930903	7.27810069
H	-3.643427943	4.295907147	6.350078478
C	-3.158532256	-0.4126793	2.613966923
H	-3.655937212	0.334707383	4.575395849
C	-2.780653528	1.267444228	0.901164694
H	-3.045332866	3.324149857	1.506382564
C	-6.48943367	2.581595085	7.145145869
H	-7.520691241	1.19931026	5.832062798
H	-5.29211842	4.054281544	8.190955751
C	-2.830453314	-0.081188855	1.293251208
H	-3.164995386	-1.457465914	2.932880059
H	-2.530959647	1.526588129	-0.129944113
H	-7.222130795	2.488994456	7.949972536
H	-2.601962379	-0.869120969	0.571975118

XYZ Coordinates of *o*-DPA-TP in T₁ optimized geometry

C	-0.897493437	5.387474256	3.75030438
C	-1.553703568	4.177662001	3.662641977
C	-2.967653838	4.122053176	3.607409326
C	-3.742533468	5.384966699	3.440818362
C	-3.038189377	6.606577826	3.691671453
C	-1.673723122	6.615561322	3.82653462
H	-0.99657997	3.238540524	3.721255391
H	0.190287269	5.424293547	3.833601042
H	-3.613483649	7.534878876	3.682358944
H	-1.150365926	7.564492113	3.973410325
N	-5.5929659	4.289154412	2.277118434
N	-5.858309498	6.500790135	2.837126009
N	-6.808530927	4.714142994	1.915843528
C	-5.041438973	5.395071082	2.85817273
C	-6.965082236	6.073075578	2.2580016
C	-8.200367335	6.697442309	1.940991863
C	-9.185265773	5.954535851	1.318223522
C	-8.976500417	4.586336928	0.996083502
C	-7.776578594	3.977984217	1.304234584
H	-8.332100465	7.747988217	2.201505282
H	-10.14072439	6.42239205	1.068190378
H	-9.756686249	4.00300337	0.505062621
H	-7.525375686	2.937138843	1.098759627
N	-3.63571633	2.914859357	3.829759794
C	-4.718201087	2.860868587	4.727968766
C	-3.18916665	1.748971119	3.160414983
C	-5.78219603	1.955574465	4.529014811

C	-4.772545172	3.77215292	5.802774916
C	-2.982660872	0.548650819	3.863369296
C	-2.938535489	1.807276932	1.777864933
C	-6.872140448	1.965665035	5.390726987
H	-5.755595629	1.277070289	3.67550078
C	-5.882891474	3.78141506	6.651176761
H	-3.932847011	4.446008866	5.977163269
C	-2.527313032	-0.581764212	3.183066379
H	-3.172397611	0.51750583	4.938092674
C	-2.481482651	0.672554076	1.109678375
H	-3.136062876	2.741306535	1.249557482
C	-6.93365209	2.883450876	6.454373421
H	-7.695840646	1.266340223	5.224622061
H	-5.916783355	4.492867375	7.480294458
C	-2.272067908	-0.524763165	1.807796902
H	-2.358209234	-1.510875857	3.733689204
H	-2.298777237	0.7181721	0.032907352
H	-7.798832496	2.892416496	7.121906542
H	-1.911512138	-1.411469053	1.280302356

XYZ Coordinates of *o*-DMac-TP in S₀ optimized geometry

C	-1.069241	5.710437	4.442569
C	-1.735745	4.488772	4.54688
C	-2.993964	4.302675	3.962742
C	-3.607583	5.360312	3.253127
C	-2.921094	6.586311	3.156624
C	-1.669224	6.762847	3.743383
H	-1.291606	3.64932	5.086061
H	-0.087294	5.839412	4.904984

H	-3.399813	7.398079	2.606894
H	-1.15942	7.725582	3.654173
N	-5.694341	4.154549	2.635145
N	-5.461363	6.299797	1.913401
N	-6.774283	4.519829	1.927853
C	-4.928025	5.255436	2.602367
C	-6.630234	5.837683	1.484653
C	-7.676372	6.405212	0.716256
C	-8.787158	5.635915	0.441555
C	-8.88541	4.296484	0.918851
C	-7.869183	3.749355	1.662464
H	-7.569604	7.432669	0.366768
H	-9.605955	6.053347	-0.149127
H	-9.766281	3.691515	0.699568
H	-7.854339	2.738497	2.069578
N	-3.621308	3.025105	4.105156
C	-4.500016	2.816786	5.176701
C	-3.440008	2.066827	3.098981
C	-5.201722	1.598452	5.30996
C	-4.687453	3.83339	6.138784
C	-4.103398	0.821599	3.159017
C	-2.583036	2.344174	2.011273
C	-6.055187	1.44655	6.413445
C	-5.065729	0.454501	4.296372
C	-5.545314	3.65112	7.219297
H	-4.153354	4.777231	6.034782
C	-3.869365	-0.100174	2.127173
C	-2.377599	1.408872	1.001459
H	-2.075342	3.306609	1.958162

C	-6.23843	2.447749	7.367657
H	-6.601123	0.507498	6.531415
C	-4.533675	-0.80734	5.024271
C	-6.462244	0.156995	3.690523
H	-5.669377	4.457579	7.947182
C	-3.021084	0.170371	1.053144
H	-4.373483	-1.068942	2.161833
H	-1.708933	1.65435	0.171857
H	-6.913304	2.288722	8.212159
H	-3.54335	-0.609136	5.462076
H	-4.436674	-1.657335	4.331293
H	-5.210443	-1.115412	5.836332
H	-7.186564	-0.123565	4.470281
H	-6.416945	-0.667139	2.96236
H	-6.840913	1.051898	3.174737
H	-2.867424	-0.57539	0.269519

XYZ Coordinates of *o*-DMAc-TP in S₁ optimized geometry

C	-1.06993219	5.700619278	4.434386374
C	-1.748370516	4.480167223	4.528696549
C	-3.000115031	4.316490338	3.945040237
C	-3.669035867	5.35742853	3.223375693
C	-2.94382265	6.591930094	3.150089347
C	-1.699580306	6.755292354	3.730189879
H	-1.303566336	3.636451463	5.06413479
H	-0.087851857	5.828238589	4.892216885
H	-3.422062154	7.40936492	2.608446198
H	-1.194134461	7.721386446	3.640519427
N	-5.734400689	4.128779215	2.591434232

N	-5.526796976	6.309552013	1.926347939
N	-6.81428007	4.500170915	1.898500189
C	-4.955924839	5.254045244	2.596225837
C	-6.686260596	5.841371774	1.490263127
C	-7.740799371	6.420818823	0.738142992
C	-8.859830616	5.639308228	0.433285784
C	-8.945101731	4.304134474	0.860320145
C	-7.907802939	3.732576765	1.600815361
H	-7.64240965	7.458693816	0.422057022
H	-9.679422985	6.072807854	-0.14561284
H	-9.81721698	3.692940514	0.622363898
H	-7.896721986	2.709001134	1.967235511
N	-3.642563537	3.015155045	4.091233494
C	-4.474821778	2.802582647	5.172733616
C	-3.424250924	2.053374003	3.124698357
C	-5.139950488	1.556753825	5.346716516
C	-4.653871259	3.846064767	6.121733723
C	-4.045642663	0.776381135	3.21385716
C	-2.559252713	2.352217909	2.036609348
C	-5.944470841	1.400199613	6.478980949
C	-5.054186692	0.448583434	4.306323663
C	-5.460639979	3.654129799	7.227130589
H	-4.153169772	4.796902345	5.957841249
C	-3.757485398	-0.159332298	2.216274954
C	-2.302232192	1.401640612	1.067154627
H	-2.112745293	3.341534885	1.977074461
C	-6.108012686	2.42250977	7.4157594
H	-6.472261053	0.458130086	6.634136478
C	-4.681123011	-0.892816417	4.988126745

C	-6.452827529	0.340423257	3.62884915
H	-5.594638321	4.464623347	7.946315776
C	-2.897503773	0.132955448	1.155835823
H	-4.225132417	-1.144178327	2.255192594
H	-1.640462101	1.644450123	0.233418371
H	-6.746959605	2.263081455	8.287196064
H	-3.693824292	-0.826073535	5.46978924
H	-4.654395297	-1.71333199	4.257419654
H	-5.420872982	-1.16683445	5.753372978
H	-7.226446796	0.101592448	4.373877329
H	-6.45199509	-0.449131236	2.862502674
H	-6.704511115	1.296843523	3.151421509
H	-2.698638601	-0.624021227	0.393918934

XYZ Coordinates of *o*-DMAc-TP in T₁ optimized geometry

C	-1.07196024	5.652523821	4.453737715
C	-1.766760255	4.441985347	4.54458574
C	-3.016836755	4.30135112	3.946455926
C	-3.652657545	5.355754067	3.221466307
C	-2.912199419	6.579251764	3.147701293
C	-1.672029395	6.720915718	3.741397235
H	-1.343742194	3.588813805	5.082057094
H	-0.09228316	5.764720989	4.921802248
H	-3.369827256	7.404707767	2.600235977
H	-1.146106126	7.676384931	3.658563348
N	-5.741682136	4.157192266	2.6082077
N	-5.492545663	6.315214593	1.899525264
N	-6.817851999	4.534731506	1.910296553
C	-4.947141027	5.26341812	2.587022023

C	-6.663766716	5.86217822	1.47436609
C	-7.708724654	6.442728544	0.714596346
C	-8.838526106	5.681850198	0.433903396
C	-8.948639098	4.351827549	0.895686044
C	-7.924362682	3.783208698	1.638789925
H	-7.592542897	7.471679411	0.373829635
H	-9.6529576	6.116781591	-0.150896587
H	-9.834959303	3.754124559	0.676808947
H	-7.92734568	2.768439703	2.034438316
N	-3.684546718	3.023970375	4.068282171
C	-4.519588993	2.815250495	5.151781801
C	-3.456838559	2.066576041	3.095594822
C	-5.142808666	1.545765723	5.347909867
C	-4.738733036	3.873177131	6.073719384
C	-4.03751226	0.767081827	3.214604229
C	-2.62629058	2.384238254	1.988380376
C	-5.934743538	1.384654237	6.493512996
C	-5.026041448	0.42944683	4.3206362
C	-5.539613016	3.68014687	7.183730123
H	-4.269196763	4.837769614	5.889159932
C	-3.722633943	-0.174526824	2.22359429
C	-2.352963254	1.433431243	1.02242885
H	-2.212793129	3.388172958	1.910950898
C	-6.135868256	2.419184638	7.405192676
H	-6.421149742	0.42440603	6.674656643
C	-4.612766409	-0.891872169	5.017793174
C	-6.426003083	0.269305836	3.653160992
H	-5.708379632	4.502712013	7.881680646
C	-2.896397608	0.135158296	1.145855346

H	-4.146606412	-1.178346388	2.287690238
H	-1.720348715	1.690601016	0.170498112
H	-6.760676885	2.253014164	8.286152429
H	-3.626663482	-0.78785185	5.495243632
H	-4.56212209	-1.721804687	4.298411902
H	-5.341808029	-1.177694947	5.789516743
H	-7.189637252	0.019814096	4.405719159
H	-6.405883901	-0.529910997	2.89647098
H	-6.710585489	1.2111953	3.162690084
H	-2.675680206	-0.626869412	0.394374769

XYZ Coordinates of *o*-PTZ-TP in S₀ optimized geometry

C	-1.0707	5.753562	4.431432
C	-1.71108	4.518515	4.548304
C	-2.969442	4.301071	3.977476
C	-3.611596	5.345844	3.268272
C	-2.951102	6.58421	3.158847
C	-1.697381	6.789647	3.732736
H	-1.245585	3.691252	5.088033
H	-0.087596	5.904362	4.884561
H	-3.452128	7.38273	2.609384
H	-1.208332	7.762102	3.633593
N	-5.673317	4.095048	2.690794
N	-5.500306	6.23161	1.930497
N	-6.767992	4.419153	1.989344
C	-4.935426	5.212223	2.631114
C	-6.662246	5.732267	1.521755
C	-7.731	6.256435	0.753975
C	-8.822449	5.451067	0.504641

C	-8.87996	4.118068	1.006531
C	-7.842298	3.612266	1.749946
H	-7.656917	7.279674	0.384269
H	-9.657781	5.834987	-0.085675
H	-9.746272	3.486112	0.805863
H	-7.790263	2.610186	2.177027
N	-3.5487	2.998996	4.15
C	-4.470154	2.823781	5.208268
C	-3.414361	2.069812	3.092573
C	-4.91464	1.53678	5.585186
C	-4.973435	3.925109	5.924892
C	-3.757352	0.710323	3.267056
C	-2.931558	2.46512	1.831494
S	-4.18521	0.078917	4.87391
C	-5.860405	1.378509	6.604034
C	-5.887929	3.755938	6.967223
H	-4.642701	4.930779	5.668672
C	-3.662616	-0.19207	2.202108
C	-2.803732	1.550046	0.783777
H	-2.646523	3.503002	1.665039
C	-6.347146	2.48330	7.308168
H	-6.197845	0.369728	6.857298
H	-6.247804	4.636239	7.506185
C	-3.177887	0.217038	0.956765
H	-3.954518	-1.232978	2.366241
H	-2.41566	1.895286	-0.178101
H	-7.071162	2.345315	8.114705
H	-3.090445	-0.501318	0.138175

XYZ Coordinates of *o*-PTZ-TP in S₁ optimized geometry

C	-1.102517186	5.760564701	4.388122699
C	-1.752296152	4.525184664	4.505619915
C	-3.005927323	4.32752704	3.939692668
C	-3.705841553	5.347315978	3.214243842
C	-3.011267641	6.596950989	3.115371456
C	-1.763570855	6.792905083	3.678789173
H	-1.282115177	3.69777129	5.044822952
H	-0.118114901	5.916300459	4.832021288
H	-3.513415428	7.397606323	2.570000178
H	-1.279638851	7.768274044	3.571859924
N	-5.733490027	4.042390488	2.647504306
N	-5.622217904	6.212423828	1.927838912
N	-6.838879007	4.353904338	1.970161213
C	-4.998404116	5.19549863	2.610291351
C	-6.771989963	5.688505218	1.527094556
C	-7.865659722	6.202181401	0.783673479
C	-8.956525376	5.365593726	0.523860883
C	-8.978136612	4.03928818	0.986584408
C	-7.902891566	3.531333165	1.718853411
H	-7.819670727	7.234274366	0.437941104
H	-9.805258811	5.749224908	-0.048262921
H	-9.8294889	3.387708358	0.782746239
H	-7.831139144	2.520776981	2.116332079
N	-3.629799935	3.01658262	4.098159864
C	-4.492437215	2.845036174	5.166452446
C	-3.433584544	2.089951405	3.089419179
C	-5.225000538	1.644212886	5.390591084
C	-4.675039888	3.899223006	6.099614417

C	-4.04740065	0.804616715	3.082677415
C	-2.584708394	2.408366983	1.996929129
S	-5.138636234	0.270012938	4.327369608
C	-6.079227613	1.511144123	6.502765804
C	-5.520397389	3.754955148	7.182969701
H	-4.143147058	4.833052639	5.937747954
C	-3.802939038	-0.111870578	2.041151355
C	-2.359161634	1.500490556	0.980102193
H	-2.122198982	3.391441215	1.969009863
C	-6.228989649	2.555877433	7.398269544
H	-6.626622589	0.575960964	6.645690484
H	-5.641636579	4.589944889	7.876255271
C	-2.963473316	0.227255533	0.994212336
H	-4.289467596	-1.090280003	2.066852787
H	-1.705732851	1.782932693	0.15199856
H	-6.895264535	2.45117605	8.256701381
H	-2.779628827	-0.483544551	0.186283513

XYZ Coordinates of *o*-PTZ-TP in T₁ optimized geometry

C	-1.153396953	5.738348465	4.376282142
C	-1.802280896	4.504406221	4.494501047
C	-3.058654815	4.315475041	3.92143199
C	-3.714554715	5.34517584	3.209586471
C	-3.03898678	6.585148251	3.103226484
C	-1.785422179	6.776563861	3.675799312
H	-1.343261261	3.671963949	5.032209355
H	-0.168919219	5.885811979	4.825856859
H	-3.535585434	7.387761061	2.556247566
H	-1.291138244	7.746657044	3.576373998

N	-5.768459215	4.077503647	2.621345564
N	-5.614290727	6.232404293	1.904477487
N	-6.866965751	4.40635343	1.934864341
C	-5.034232489	5.205091323	2.58248531
C	-6.776095618	5.731452122	1.491939703
C	-7.85171408	6.262946271	0.743065185
C	-8.945071065	5.452043407	0.482124263
C	-8.988812181	4.114384328	0.955041888
C	-7.940007635	3.596534447	1.68408838
H	-7.786573718	7.294041072	0.394844323
H	-9.786281219	5.843519006	-0.094676021
H	-9.851672504	3.479499022	0.747482803
H	-7.880116438	2.586353229	2.089235716
N	-3.683660545	3.022790692	4.072415652
C	-4.512505283	2.852635305	5.171776962
C	-3.445979064	2.092863921	3.070915358
C	-5.201755073	1.603096298	5.421568542
C	-4.713755998	3.904947131	6.102152303
C	-4.028117682	0.766815918	3.107931492
C	-2.614090952	2.408746541	1.965673638
S	-5.141253699	0.269091148	4.328734136
C	-6.0067256	1.458447351	6.581818627
C	-5.514046881	3.746528857	7.216785397
H	-4.221098392	4.860745468	5.93097764
C	-3.72764093	-0.166990643	2.081621168
C	-2.346966644	1.488662443	0.970607822
H	-2.175796898	3.403544299	1.903447494
C	-6.165369301	2.497853568	7.470252547
H	-6.504933979	0.500585487	6.758346309

H	-5.647445213	4.582795556	7.906000432
C	-2.903812604	0.171852518	1.032255297
H	-4.167296206	-1.167251222	2.137430922
H	-1.705616981	1.773036562	0.133962603
H	-6.784418901	2.369244431	8.36082954
H	-2.678172038	-0.559435934	0.253048952

XYZ Coordinates of *o*-PXZ-TP in S₀ optimized geometry

C	-0.999741	5.785424	4.408333
C	-1.627485	4.544483	4.539188
C	-2.892193	4.317516	3.985486
C	-3.553291	5.35398	3.281652
C	-2.907659	6.598446	3.161846
C	-1.6468	6.814345	3.717118
H	-1.147382	3.723519	5.075999
H	-0.011451	5.947248	4.846237
H	-3.424032	7.392708	2.620168
H	-1.167326	7.790721	3.609784
N	-5.581508	4.053288	2.697529
N	-5.507923	6.223266	2.025108
N	-6.706129	4.362742	2.040521
C	-4.886451	5.199172	2.668375
C	-6.661799	5.696815	1.626438
C	-7.772746	6.208933	0.912052
C	-8.839853	5.371612	0.661757
C	-8.832767	4.0179	1.109212
C	-7.754758	3.522924	1.800671
H	-7.749989	7.24848	0.583429
H	-9.706954	5.746512	0.112868

H	-9.68115	3.362323	0.907833
H	-7.648296	2.508206	2.18699
N	-3.491251	3.02983	4.150257
C	-4.469537	2.849238	5.145851
C	-3.396738	2.087516	3.109027
C	-5.401643	1.799304	5.013168
C	-4.569256	3.685518	6.264801
C	-4.353741	1.054956	3.026647
C	-2.393328	2.139105	2.133169
O	-5.389743	0.96028	3.924903
C	-6.38423	1.58837	5.974014
C	-5.566582	3.481318	7.227913
H	-3.863878	4.510348	6.376109
C	-4.29388	0.102108	2.015922
C	-2.33896	1.186275	1.10706
H	-1.653452	2.939718	2.174333
C	-6.474834	2.432893	7.088961
H	-7.079712	0.760083	5.821483
H	-5.623439	4.151455	8.089263
C	-3.28478	0.164108	1.045202
H	-5.060039	-0.676206	2.000727
H	-1.547148	1.253016	0.356818
H	-7.253459	2.265433	7.836817
H	-3.247629	-0.583816	0.249708

XYZ Coordinates of *o*-PXZ-TP in S₁ optimized geometry

C	-0.995927368	5.709821951	4.461864573
C	-1.667023365	4.484918336	4.562223343
C	-2.92022655	4.318159685	3.984848129

C	-3.600289265	5.35673437	3.26501613
C	-2.882072284	6.594282781	3.185118893
C	-1.635273059	6.761041889	3.759010434
H	-1.215608822	3.643416644	5.095637221
H	-0.011967498	5.844316248	4.913481266
H	-3.365569377	7.410233592	2.64557067
H	-1.133495667	7.728782922	3.666011637
N	-5.649094858	4.092494194	2.670341976
N	-5.493775462	6.26869858	1.978271848
N	-6.744953881	4.432427121	1.990455216
C	-4.891459858	5.233367879	2.652035428
C	-6.650090727	5.770902228	1.564734221
C	-7.73007794	6.313837643	0.821670606
C	-8.834224547	5.501604429	0.54575747
C	-8.883630257	4.169938095	0.991781973
C	-7.822079698	3.633621798	1.723315701
H	-7.662953018	7.349111681	0.48911097
H	-9.672406956	5.908166071	-0.026087451
H	-9.745768142	3.536987928	0.775339477
H	-7.772211095	2.616804311	2.108632835
N	-3.576301879	3.026945065	4.118546792
C	-4.480350092	2.823541203	5.137197521
C	-3.450508642	2.090306688	3.117107461
C	-5.263377035	1.638195428	5.147133717
C	-4.673260385	3.761788849	6.175297179
C	-4.2488702	0.915868127	3.157760965
C	-2.561443551	2.258091876	2.032427776
O	-5.135955411	0.716392437	4.162389749
C	-6.192157886	1.383985304	6.157987495

C	-5.59663856	3.505376615	7.174877406
H	-4.093027698	4.682373562	6.159200774
C	-4.157560312	-0.064582223	2.168194632
C	-2.475689491	1.283143501	1.052887257
H	-1.965152325	3.167229636	1.984159445
C	-6.357908727	2.317193548	7.174020172
H	-6.768339459	0.458602857	6.11478966
H	-5.740569616	4.238980657	7.970545122
C	-3.26885807	0.117746301	1.115738233
H	-4.796134054	-0.945536319	2.247691945
H	-1.787967161	1.424500473	0.216801603
H	-7.083737531	2.131666014	7.968164962
H	-3.190954219	-0.640066976	0.333684568

XYZ Coordinates of *o*-PXZ-TP in T₁ optimized geometry

C	-0.982142423	5.73874569	4.436358911
C	-1.622483723	4.507723088	4.550026394
C	-2.889608904	4.30969829	3.987741242
C	-3.563105189	5.357410132	3.283968639
C	-2.884380807	6.595929777	3.190223212
C	-1.628423026	6.789360081	3.748748254
H	-1.14977283	3.676355338	5.07923691
H	0.00650541	5.885487757	4.877213588
H	-3.38945146	7.403406939	2.656636978
H	-1.138788236	7.7619736	3.65435724
N	-5.578035448	4.05543332	2.711388841
N	-5.506489356	6.229538119	2.019334986
N	-6.701623353	4.361055876	2.04886969
C	-4.873266877	5.212172512	2.676805507

C	-6.654075349	5.697590888	1.625010416
C	-7.766569455	6.203797951	0.902168253
C	-8.83626819	5.363000576	0.652469499
C	-8.833709674	4.017207922	1.10501372
C	-7.750679536	3.525721821	1.807456513
H	-7.742265601	7.240927331	0.566972486
H	-9.700165384	5.737489402	0.097553866
H	-9.680209568	3.358879583	0.904932082
H	-7.652734123	2.511763762	2.196272838
N	-3.513946664	3.01823966	4.140729415
C	-4.441123768	2.836238812	5.146657857
C	-3.386567846	2.08584479	3.130829157
C	-5.356051949	1.728736937	5.054610111
C	-4.594321259	3.741541095	6.22899725
C	-4.317131124	0.990080398	3.080836311
C	-2.428063578	2.196543958	2.091784676
O	-5.275562478	0.853070257	4.026462655
C	-6.36512919	1.548546792	6.00159152
C	-5.584629535	3.542703712	7.168987992
H	-3.922174087	4.59724893	6.296824657
C	-4.278235576	0.060680487	2.039156572
C	-2.386749336	1.260705507	1.077569001
H	-1.73289226	3.036221923	2.106499459
C	-6.487037363	2.441861016	7.060363224
H	-7.040452346	0.698908006	5.88048414
H	-5.682641162	4.241029906	8.003056259
C	-3.320307546	0.182329215	1.039855742
H	-5.015079357	-0.745349213	2.040115654
H	-1.634759446	1.352874145	0.290888005

H	-7.276214505	2.304637463	7.802211641
H	-3.288128527	-0.541950552	0.223475635

XYZ Coordinates of *o*-NPP-TP in S₀ optimized geometry

C	-1.05845	5.881661	4.410833
C	-1.646616	4.623751	4.556557
C	-2.903117	4.34913	4.005214
C	-3.594404	5.352933	3.286278
C	-2.986815	6.615135	3.147455
C	-1.735561	6.879612	3.702663
H	-1.141547	3.824908	5.103657
H	-0.076659	6.080681	4.848178
H	-3.525281	7.383651	2.590638
H	-1.286898	7.868916	3.581337
N	-5.605053	3.998746	2.741457
N	-5.534353	6.13405	1.960789
N	-6.717537	4.267117	2.044451
C	-4.917606	5.148146	2.66631
C	-6.67446	5.579488	1.564842
C	-7.770577	6.047214	0.79884
C	-8.825067	5.190812	0.561359
C	-8.818333	3.860517	1.073826
C	-7.754545	3.4106	1.816056
H	-7.745265	7.069636	0.42043
H	-9.679836	5.531024	-0.027904
H	-9.654865	3.187116	0.881933
H	-7.653717	2.415438	2.249142
N	-3.455292	3.044649	4.187442
C	-4.356359	2.833888	5.249224

C	-3.311947	2.099514	3.153445
C	-5.110439	1.632768	5.296181
C	-4.532012	3.785115	6.259466
C	-4.068251	0.899709	3.195276
C	-2.445779	2.318941	2.077535
C	-5.99953	1.427172	6.357477
N	-4.94455	0.675556	4.275547
C	-5.429553	3.568644	7.315803
H	-3.959725	4.712199	6.221331
C	-3.922964	-0.033609	2.162644
C	-2.311261	1.376505	1.047001
H	-1.867682	3.242524	2.041183
C	-6.16195	2.389039	7.366093
H	-6.578007	0.504032	6.39603
C	-5.659254	-0.558246	4.35358
H	-5.543207	4.331628	8.089751
C	-3.049232	0.200019	1.089736
H	-4.503457	-0.955886	2.193691
H	-1.625805	1.578161	0.220198
H	-6.864728	2.199837	8.181303
C	-5.092196	-1.656746	5.012311
C	-6.930398	-0.674225	3.776717
H	-2.957922	-0.54748	0.297853
C	-5.793291	-2.863133	5.093211
H	-4.100753	-1.550017	5.457922
C	-7.631289	-1.880699	3.857969
H	-7.358222	0.192151	3.268063
C	-7.063026	-2.976767	4.516346
H	-5.347159	-3.71761	5.608978

H	-8.623229	-1.96587	3.406449
H	-7.610751	-3.920717	4.579917

XYZ Coordinates of *o*-NPP-TP in S₁ optimized geometry

C	-1.035777154	5.874492337	4.395313612
C	-1.640045049	4.61952431	4.537602394
C	-2.892414238	4.370655581	3.986478419
C	-3.630414241	5.354408018	3.255539423
C	-2.983422994	6.623528461	3.130842604
C	-1.736429056	6.871466916	3.679296221
H	-1.137121088	3.816487351	5.083765501
H	-0.053005178	6.070826393	4.827226019
H	-3.519007928	7.397541961	2.579027827
H	-1.287587723	7.861258538	3.553493665
N	-5.629619222	3.985208541	2.719018791
N	-5.581678127	6.146200145	1.975544541
N	-6.747358235	4.258822394	2.047807451
C	-4.927231691	5.154558395	2.663345945
C	-6.721951819	5.587584061	1.588903307
C	-7.833420484	6.066070663	0.848249549
C	-8.90673337	5.194617522	0.605695157
C	-8.888934699	3.876338449	1.082335325
C	-7.794060282	3.401938775	1.813469761
H	-7.816863299	7.094873417	0.491275891
H	-9.769740965	5.548917311	0.036099434
H	-9.724565001	3.200496074	0.89176305
H	-7.691986679	2.399178203	2.220556986
N	-3.472026411	3.049489728	4.165491101
C	-4.339454055	2.834032186	5.215495568

C	-3.295372119	2.099926158	3.181461671
C	-5.057836262	1.603863956	5.303261763
C	-4.544298465	3.816250669	6.207834699
C	-4.004123164	0.86304126	3.251778121
C	-2.430985329	2.330163499	2.089984119
C	-5.938876556	1.385566527	6.381011541
N	-4.875108614	0.64788626	4.312214422
C	-5.417237026	3.582806947	7.257349369
H	-4.011807311	4.760805392	6.121518581
C	-3.815496535	-0.107345771	2.247738734
C	-2.262635371	1.364471777	1.111700018
H	-1.912676182	3.284615095	2.030274199
C	-6.115112983	2.36409704	7.348575303
H	-6.485651507	0.446105284	6.443842805
C	-5.640320407	-0.572847226	4.360376889
H	-5.566708213	4.356148411	8.013459502
C	-2.952616197	0.140355035	1.18998306
H	-4.358392171	-1.049443835	2.304753582
H	-1.593264387	1.561874437	0.27203292
H	-6.803653117	2.185208282	8.176903484
C	-5.12497786	-1.686535909	5.029353028
C	-6.889699344	-0.620612753	3.735226218
H	-2.817663209	-0.617555862	0.415648205
C	-5.874110043	-2.865975978	5.072299526
H	-4.14612239	-1.621686922	5.509478574
C	-7.632344128	-1.803369425	3.782673393
H	-7.265290836	0.265295767	3.220756703
C	-7.125792394	-2.924340779	4.449906795
H	-5.477965377	-3.740702955	5.593640653

H	-8.609522517	-1.847623297	3.296335048
H	-7.709272998	-3.847628811	4.485003531

XYZ Coordinates of *o*-NPP-TP in T₁ optimized geometry

C	-1.064245361	5.774283193	4.444539392
C	-1.702240487	4.531894367	4.546860918
C	-2.953869863	4.335969671	3.968907541
C	-3.629919653	5.363602347	3.260600077
C	-2.961772059	6.616507622	3.17592954
C	-1.714550618	6.813558477	3.752966425
H	-1.236510266	3.699431172	5.079856334
H	-0.08262942	5.929135932	4.897202796
H	-3.465771467	7.421298432	2.638961074
H	-1.232993679	7.791660584	3.66666295
N	-5.648297282	4.062753701	2.61169757
N	-5.545440496	6.252004812	1.986756834
N	-6.74795476	4.391418662	1.930419047
C	-4.936673958	5.213409598	2.629371801
C	-6.689183928	5.738569504	1.544622558
C	-7.773697141	6.27353929	0.810389063
C	-8.846210628	5.443982573	0.501428326
C	-8.85707623	4.089794557	0.909960812
C	-7.796435202	3.566403281	1.628247631
H	-7.733378555	7.320520111	0.509543644
H	-9.692346989	5.840035176	-0.065260592
H	-9.698572091	3.440093002	0.663432204
H	-7.713354147	2.539073647	1.981632538
N	-3.578151855	3.045850593	4.11425813
C	-4.427543504	2.835710803	5.183657002

C	-3.392710121	2.098106516	3.127004509
C	-5.086049929	1.560901642	5.315177213
C	-4.665807607	3.832927698	6.155020563
C	-4.05538864	0.824516957	3.244681066
C	-2.577711472	2.345030328	2.000675227
C	-5.921361965	1.33001599	6.435086492
N	-4.885457916	0.601404053	4.333410124
C	-5.499781867	3.5899036	7.231947882
H	-4.180014141	4.80125303	6.040287379
C	-3.846141524	-0.154915622	2.244055378
C	-2.398700368	1.377127644	1.028486426
H	-2.09516415	3.317435175	1.908185874
C	-6.125955305	2.319664015	7.377740939
H	-6.408435466	0.361385463	6.544726443
C	-5.586915473	-0.650858222	4.431941915
H	-5.67657199	4.376474746	7.968245479
C	-3.034345254	0.110176317	1.157273451
H	-4.338225766	-1.122861366	2.336241521
H	-1.770434439	1.590438602	0.161332358
H	-6.773960254	2.12298351	8.234796822
C	-4.992012646	-1.727208702	5.09576264
C	-6.858186735	-0.768987459	3.863633978
H	-2.884969609	-0.657788674	0.395050495
C	-5.682956083	-2.940874789	5.19021172
H	-3.998251065	-1.605202318	5.531574485
C	-7.54379396	-1.984507975	3.961510091
H	-7.296361154	0.091315082	3.353418365
C	-6.955616395	-3.068477758	4.623739907
H	-5.224720443	-3.78710017	5.708056917

H	-8.538167644	-2.083957483	3.519544165
H	-7.492792981	-4.017492934	4.698550562

XYZ Coordinates of *m*-Cz-TP in S₀ optimized geometry

C	-1.447636	5.888076	5.109228
C	-1.951278	4.600246	4.864513
C	-3.078544	4.434603	4.052958
C	-3.698916	5.549693	3.468068
C	-3.196983	6.836888	3.72254
C	-2.080484	6.998269	4.544884
H	-3.479146	3.43626	3.873341
H	-0.55937	6.005978	5.733081
H	-3.693099	7.695472	3.267027
H	-1.68758	7.999778	4.738038
N	-5.39244	4.164932	2.344454
N	-5.514575	6.413255	2.004312
N	-6.424483	4.448545	1.534
C	-4.876035	5.376112	2.601568
C	-6.49784	5.829834	1.325456
C	-7.527123	6.327493	0.489748
C	-8.409816	5.432736	-0.078128
C	-8.292533	4.03423	0.167465
C	-7.292857	3.554502	0.977918
H	-7.588858	7.403255	0.322155
H	-9.211418	5.795422	-0.725766
H	-8.993549	3.330293	-0.283384
H	-7.123426	2.505837	1.22409
N	-1.31594	3.466274	5.432632
C	-0.83927	2.35915	4.724406

C	-1.056028	3.269735	6.791476
C	-0.261635	1.438089	5.640669
C	-0.846583	2.111658	3.345624
C	-0.399907	2.019728	6.960981
C	-1.377632	4.08088	7.887322
C	0.299100	0.244761	5.163622
C	-0.280467	0.917244	2.896604
H	-1.278293	2.82858	2.64542
C	-0.044544	1.592334	8.248122
C	-1.014716	3.631436	9.158252
H	-1.900109	5.029388	7.752473
H	0.743714	-0.470823	5.860294
C	0.283727	-0.011908	3.792735
H	-0.2754	0.701527	1.824753
C	-0.350502	2.402792	9.341399
H	0.461970	0.633787	8.388859
H	-1.255049	4.24762	10.028863
H	0.716021	-0.938766	3.407342
H	-0.078877	2.081885	10.350181

XYZ Coordinates of *m*-Cz-TP in S₁ optimized geometry

C	-1.213313305	5.826575999	4.893608327
C	-1.85515686	4.581882247	4.738468582
C	-3.022482353	4.40217722	4.017195562
C	-3.632865607	5.520156313	3.376243156
C	-2.98998738	6.787604129	3.52261253
C	-1.820827845	6.929315164	4.253649392
H	-3.492677092	3.420890352	3.934934802
H	-0.280973634	5.919334665	5.451156913

H	-3.452651656	7.646999776	3.033783404
H	-1.353337159	7.914727199	4.336068032
N	-5.458022498	4.174978469	2.458316491
N	-5.474969835	6.414161355	1.983232752
N	-6.515825781	4.47078296	1.704491815
C	-4.840829214	5.37535415	2.614607236
C	-6.53051696	5.847213197	1.408951293
C	-7.587675047	6.352743323	0.610060036
C	-8.569269223	5.462715826	0.150757569
C	-8.513758891	4.097571718	0.471612202
C	-7.474044259	3.59506284	1.258691648
H	-7.602640318	7.417102479	0.378942738
H	-9.390292536	5.837418604	-0.465962033
H	-9.279474471	3.4070045	0.113592396
H	-7.348755728	2.556691676	1.559521904
N	-1.25034571	3.41908789	5.366825986
C	-0.650114681	2.374356365	4.701634862
C	-1.178846857	3.199170037	6.72269978
C	-0.159567752	1.427551902	5.652132969
C	-0.500302636	2.199168927	3.314724292
C	-0.503156497	1.964679712	6.967940049
C	-1.680276569	4.005570739	7.759706112
C	0.489000634	0.288736379	5.202588457
C	0.15717502	1.044577902	2.885581519
H	-0.895786415	2.940222629	2.62049164
C	-0.322871899	1.538222313	8.273868224
C	-1.486061505	3.555625445	9.067054431
H	-2.193535816	4.939177169	7.53051291
H	0.875818799	-0.455292328	5.902223655

C	0.643103284	0.104654501	3.808694312
H	0.291643989	0.869490578	1.816692147
C	-0.819248938	2.346272865	9.323048835
H	0.187276665	0.598661598	8.496724625
H	-1.860310677	4.151247335	9.90170543
H	1.150855589	-0.790967855	3.444437675
H	-0.682509378	2.018401735	10.35577034

XYZ Coordinates of *m*-Cz-TP in T₁ optimized geometry

C	-1.601863327	5.858328723	5.289875898
C	-2.095244925	4.509684455	4.936333036
C	-3.133949667	4.350909805	4.054605275
C	-3.77422215	5.486463295	3.465175081
C	-3.262809458	6.839881851	3.812468836
C	-2.216597513	6.981054953	4.692611704
H	-3.51018661	3.356242839	3.814904025
H	-0.707453889	5.956076598	5.904369925
H	-3.747379184	7.698458926	3.346793459
H	-1.840202246	7.97992164	4.930704047
N	-5.396303504	4.127526017	2.243799084
N	-5.537811778	6.415675757	2.025031482
N	-6.399796239	4.452632611	1.430147359
C	-4.880772851	5.347631698	2.598846218
C	-6.484899563	5.857775871	1.296177821
C	-7.501867449	6.385929117	0.458173375
C	-8.359575939	5.513736196	-0.18459545
C	-8.232705897	4.108646809	-0.015765948
C	-7.244758969	3.590795887	0.797170625
H	-7.572435166	7.468553872	0.349604583

H	-9.147499577	5.905531162	-0.832350535
H	-8.911996405	3.422826545	-0.524178413
H	-7.073138341	2.530712589	0.985124857
N	-1.409107101	3.409774775	5.471423995
C	-0.95350636	2.282455787	4.763630794
C	-1.023319838	3.270365104	6.812595087
C	-0.251353247	1.430472019	5.65738948
C	-1.055623337	1.981835485	3.399868452
C	-0.295689534	2.060688102	6.965169294
C	-1.321609937	4.087836066	7.910923897
C	0.331421837	0.250499268	5.183102311
C	-0.463923096	0.799507874	2.948421265
H	-1.573308775	2.647641669	2.709556567
C	0.182801807	1.692000898	8.226282558
C	-0.825118712	3.704495947	9.159680922
H	-1.934093323	4.983258234	7.799825493
H	0.873906273	-0.409462311	5.86479091
C	0.216217025	-0.063407027	3.826673833
H	-0.533640185	0.543254401	1.888179552
C	-0.07608313	2.524847762	9.318955868
H	0.741670465	0.76155028	8.354687659
H	-1.038518779	4.328825548	10.03107186
H	0.663048059	-0.983387711	3.441704373
H	0.290891536	2.24903061	10.31063449

XYZ Coordinates of *m*-DPA-TP in S₀ optimized geometry

C	-0.95238	5.650434	4.245732
C	-1.70173	4.478128	4.460264
C	-2.98834	4.38095	3.910158

C	-3.530907	5.441435	3.169383
C	-2.773149	6.605066	2.954305
C	-1.487249	6.695446	3.490488
H	-3.579829	3.477913	4.064191
H	0.048479	5.732836	4.673941
H	-3.205054	7.419958	2.371536
H	-0.894527	7.600354	3.331763
N	-5.636133	4.23204	2.766288
N	-5.472511	6.32756	1.890529
N	-6.767662	4.544074	2.114816
C	-4.886244	5.333244	2.604961
C	-6.665613	5.832164	1.578008
C	-7.768502	6.343706	0.851557
C	-8.889566	5.553764	0.70405
C	-8.942418	4.247366	1.270056
C	-7.871334	3.754184	1.974788
H	-7.69558	7.347307	0.431241
H	-9.750961	5.929647	0.146927
H	-9.831008	3.625601	1.151429
H	-7.818553	2.770945	2.443326
N	-1.166164	3.409919	5.225339
C	-1.99125	2.714821	6.146254
C	0.190655	3.032341	5.06016
C	-1.910777	1.315001	6.263739
C	-2.904786	3.413412	6.957277
C	0.982413	2.701922	6.175686
C	0.768619	2.983933	3.777943
C	-2.718447	0.635758	7.177342
H	-1.208677	0.765307	5.633698

C	-3.721151	2.724086	7.855216
H	-2.972446	4.499899	6.873879
C	2.315776	2.324642	6.007546
H	0.541634	2.741456	7.173822
C	2.107966	2.623268	3.621028
H	0.159182	3.234279	2.907317
C	-3.631518	1.332976	7.976031
H	-2.641693	-0.452363	7.25475
H	-4.426146	3.283776	8.476118
C	2.889727	2.287199	4.73183
H	2.915589	2.070157	6.885779
H	2.54035	2.591696	2.617091
H	-4.267607	0.797368	8.68514
H	3.936083	1.99872	4.604478

XYZ Coordinates of *m*-DPA-TP in S₁ optimized geometry

C	-1.136385636	5.777973165	4.787490069
C	-1.803917989	4.543831046	4.702681168
C	-2.995636413	4.363616162	4.019204091
C	-3.603388386	5.468940579	3.361901195
C	-2.938321024	6.724797945	3.446419542
C	-1.745046277	6.872733738	4.141692705
H	-3.478839743	3.386301421	3.975059031
H	-0.205099556	5.877441736	5.346337807
H	-3.40382797	7.575256911	2.94444544
H	-1.268067863	7.855509647	4.191873721
N	-5.487967796	4.138661846	2.552852662
N	-5.467111109	6.354029103	1.989981574
N	-6.561280502	4.429467492	1.818461238

C	-4.843004392	5.325306067	2.640597447
C	-6.555616027	5.789839214	1.468236593
C	-7.622942495	6.292577171	0.681919166
C	-8.641244437	5.404572432	0.287969086
C	-8.605488398	4.054558025	0.661118052
C	-7.554288578	3.55296248	1.436483757
H	-7.619792327	7.346675191	0.408787595
H	-9.472661479	5.773237082	-0.318261309
H	-9.397841241	3.369709584	0.352551247
H	-7.440966975	2.524803052	1.772787215
N	-1.212383492	3.394575272	5.379263165
C	-1.913108099	2.810796744	6.432303905
C	0.020458593	2.930769768	4.941541336
C	-1.832024041	1.416765659	6.681907212
C	-2.75816339	3.616542209	7.236585825
C	0.935744574	2.313349583	5.835908339
C	0.392223688	3.118672212	3.583750228
C	-2.551856506	0.857628418	7.73131617
H	-1.247214723	0.781865276	6.015366782
C	-3.460319042	3.042301982	8.286321744
H	-2.828216006	4.683843893	7.028500885
C	2.165668024	1.866782108	5.370594458
H	0.687025988	2.236771474	6.894837329
C	1.620962974	2.655440685	3.13640935
H	-0.310967543	3.59964321	2.904678602
C	-3.360935265	1.664730025	8.542716435
H	-2.504110539	-0.219829401	7.903497246
H	-4.096052552	3.670093306	8.9140049
C	2.512438991	2.025746822	4.020490663

H	2.872112768	1.410612888	6.067583733
H	1.891366014	2.781013205	2.085951643
H	-3.928769284	1.219633942	9.362614418
H	3.481416483	1.673144633	3.660466542

XYZ Coordinates of *m*-DPA-TP in T₁ optimized geometry

C	-0.856270228	5.568121739	4.07654905
C	-1.71045898	4.403018421	4.404342457
C	-3.018183612	4.336080682	3.94225712
C	-3.562275664	5.362839629	3.143309599
C	-2.703912892	6.52662051	2.82087292
C	-1.407031541	6.594742281	3.292574806
H	-3.637932262	3.469477927	4.176383475
H	0.124039326	5.664872281	4.540848663
H	-3.133617801	7.319424292	2.207544345
H	-0.796948564	7.474051324	3.066182154
N	-5.727479593	4.248105772	2.882862509
N	-5.433628665	6.259156203	1.816259255
N	-6.834686861	4.580374816	2.213437949
C	-4.887673682	5.289705999	2.622944846
C	-6.653155337	5.815412651	1.559035052
C	-7.731263208	6.328362724	0.794913714
C	-8.907736498	5.602739571	0.722276957
C	-9.040628185	4.363918895	1.400490078
C	-7.990532873	3.863018573	2.145437779
H	-7.597266422	7.283228085	0.285720843
H	-9.746741467	5.985906544	0.136219206
H	-9.968255828	3.792349832	1.343492091
H	-8.000763048	2.922919081	2.697473209

N	-1.169212317	3.416646896	5.22768123
C	-2.000868451	2.679028557	6.117412585
C	0.197223197	3.066314763	5.109635206
C	-1.916862233	1.277445569	6.165788849
C	-2.906979717	3.354691099	6.953075152
C	0.954517562	2.744280149	6.253373407
C	0.812652878	3.058978877	3.841264547
C	-2.73054082	0.562235269	7.047048861
H	-1.219548367	0.758098859	5.505723097
C	-3.717478928	2.631233453	7.826448082
H	-2.965893664	4.443589123	6.906418903
C	2.304652895	2.428369945	6.126912826
H	0.476142869	2.757263732	7.234608309
C	2.171419647	2.752928142	3.730374489
H	0.213189026	3.269167522	2.95411107
C	-3.632997125	1.233318971	7.878321102
H	-2.665743951	-0.528567022	7.074415219
H	-4.415987734	3.163123775	8.477331502
C	2.921837227	2.436666938	4.86588959
H	2.88639129	2.184429324	7.019525991
H	2.641182707	2.747606202	2.743382467
H	-4.271018062	0.670226168	8.56398012
H	3.982886958	2.19217086	4.773049321

XYZ Coordinates of *m*-DMAc-TP in S₀ optimized geometry

C	-1.477796	5.87513	5.167525
C	-1.960018	4.587037	4.899363
C	-3.068959	4.411599	4.069724
C	-3.705474	5.524202	3.495335

C	-3.217783	6.813926	3.766232
C	-2.110096	6.984442	4.598928
H	-3.437813	3.40534	3.865844
H	-0.609278	5.991721	5.819503
H	-3.720337	7.670693	3.313849
H	-1.735282	7.990006	4.806338
N	-5.379329	4.135514	2.347428
N	-5.502982	6.383952	2.007728
N	-6.39926	4.417078	1.521087
C	-4.870054	5.347775	2.613152
C	-6.47381	5.798411	1.31309
C	-7.490767	6.293711	0.461017
C	-8.360386	5.396685	-0.123233
C	-8.242162	3.998216	0.122104
C	-7.254765	3.520863	0.948875
H	-7.553321	7.369471	0.293692
H	-9.151888	5.757515	-0.784202
H	-8.932425	3.292409	-0.34222
H	-7.085188	2.472379	1.195674
N	-1.312585	3.445451	5.474556
C	-0.263584	2.831043	4.77215
C	-1.738218	2.979223	6.728257
C	0.401412	1.704336	5.306896
C	0.135974	3.341298	3.516326
C	-1.121794	1.858584	7.330219
C	-2.794299	3.634955	7.400306
C	1.442736	1.136568	4.556317
C	0.021888	1.085439	6.659096
C	1.173989	2.752836	2.799722

H	-0.375344	4.208474	3.100248
C	-1.592042	1.4444	8.58598
C	-3.23484	3.196136	8.645465
H	-3.273383	4.497208	6.937997
C	1.839506	1.639342	3.317179
H	1.964024	0.264211	4.95699
C	-0.430045	-0.381328	6.430566
C	1.261583	1.106079	7.591526
H	1.460096	3.171442	1.830993
C	-2.633145	2.09136	9.25192
H	-1.126829	0.578618	9.0631
H	-4.05423	3.724548	9.140305
H	2.655732	1.166893	2.765587
H	-1.310394	-0.415895	5.770482
H	-0.696651	-0.867902	7.381488
H	0.370415	-0.976479	5.964618
H	2.098814	0.540154	7.155139
H	1.032215	0.655615	8.569275
H	1.599374	2.139838	7.761864
H	-2.968717	1.735051	10.228755

XYZ Coordinates of *m*-DMAc-TP in S₁ optimized geometry

C	-1.431568362	5.881274181	5.195507794
C	-1.955275357	4.610243414	4.894238692
C	-3.047763299	4.403519282	4.074358981
C	-3.70579118	5.521854499	3.480462702
C	-3.184147287	6.820038133	3.777216941
C	-2.086447334	6.986956709	4.60590495
H	-3.418386401	3.397940727	3.868635766

H	-0.566467519	5.998591728	5.848580253
H	-3.682448757	7.680132313	3.3263396
H	-1.714677345	7.995085028	4.810975042
N	-5.352489858	4.121959733	2.333169045
N	-5.508800004	6.384631725	2.018549561
N	-6.373982025	4.398350119	1.523598387
C	-4.84139582	5.348689131	2.621440844
C	-6.473678823	5.78951033	1.327261331
C	-7.508464903	6.276935039	0.488616657
C	-8.383699141	5.358125141	-0.104881853
C	-8.245497391	3.9788865	0.12058393
C	-7.227755827	3.494760951	0.945490184
H	-7.589436553	7.352176705	0.333579279
H	-9.186227971	5.719458281	-0.753174846
H	-8.928573591	3.264627358	-0.342590716
H	-7.043119655	2.447619263	1.178397959
N	-1.298476934	3.436467033	5.482731269
C	-0.265577803	2.834107769	4.78803373
C	-1.725775412	2.9820302	6.716723133
C	0.402703318	1.693724837	5.31953241
C	0.124072569	3.370009439	3.528029385
C	-1.11653388	1.84807541	7.327055966
C	-2.788264075	3.664785298	7.373449268
C	1.436990267	1.134054629	4.562698026
C	0.014190714	1.077622846	6.657471103
C	1.152397073	2.787653377	2.812205019
H	-0.401565647	4.239021555	3.140277531
C	-1.599395971	1.443101098	8.57543802
C	-3.235023868	3.232950606	8.607447755

H	-3.240732981	4.525474722	6.887180484
C	1.816785961	1.662056878	3.327677927
H	1.964116145	0.257576763	4.942655963
C	-0.456619736	-0.385368616	6.413281632
C	1.25431989	1.082128624	7.595459025
H	1.441792377	3.205292912	1.846047289
C	-2.640604547	2.115483029	9.217310231
H	-1.154620708	0.575414605	9.065161292
H	-4.051678812	3.762464773	9.10174744
H	2.628694469	1.196194481	2.765069583
H	-1.333996455	-0.406681184	5.749877747
H	-0.728875253	-0.871116747	7.361547076
H	0.342782743	-0.979868823	5.947644178
H	2.083144362	0.512053734	7.15174857
H	1.014659368	0.621080724	8.564397568
H	1.601102848	2.110170509	7.778424431
H	-2.991430619	1.768246234	10.19157146

XYZ Coordinates of *m*-DMAc-TP in T₁ optimized geometry

C	-1.444905585	5.893992623	5.197233068
C	-1.945382139	4.616489703	4.91561198
C	-3.044698226	4.404282674	4.096280053
C	-3.696289922	5.516371376	3.508724238
C	-3.199069711	6.814701284	3.785571649
C	-2.097832912	6.998483998	4.612281275
H	-3.403578734	3.393075291	3.900214584
H	-0.576977507	6.013393495	5.847570178
H	-3.705391531	7.667581762	3.329667057
H	-1.731037864	8.008608229	4.812204878

N	-5.345348815	4.107879294	2.363291083
N	-5.496793363	6.361165948	2.026374079
N	-6.365461565	4.378943266	1.537722903
C	-4.844331181	5.331271057	2.636656147
C	-6.457032483	5.763882255	1.331258081
C	-7.480051482	6.245546563	0.477211481
C	-8.340642016	5.335491796	-0.112275924
C	-8.206832685	3.943672336	0.129710098
C	-7.20996847	3.475877792	0.961696537
H	-7.556053022	7.320443623	0.31095065
H	-9.134846663	5.689636581	-0.774073171
H	-8.886676615	3.228542537	-0.335962809
H	-7.028931976	2.429082778	1.206277778
N	-1.283377325	3.469312006	5.500365206
C	-0.260367148	2.874033483	4.784596026
C	-1.721215791	3.022056168	6.733308676
C	0.387619716	1.693118012	5.303972003
C	0.145637847	3.413505696	3.527968579
C	-1.123573801	1.849181124	7.326466832
C	-2.770504281	3.707631786	7.41421291
C	1.402924769	1.120681251	4.524644723
C	-0.007531085	1.079699757	6.637784612
C	1.153608435	2.821806391	2.799171468
H	-0.353252728	4.30310591	3.146726874
C	-1.619459063	1.433954874	8.570343301
C	-3.222435632	3.267016622	8.638442642
H	-3.215083069	4.588309684	6.9531063
C	1.796199988	1.652086989	3.299547141
H	1.906672328	0.223022119	4.88989342

C	-0.487411395	-0.380530465	6.391844433
C	1.238472303	1.068017752	7.570256994
H	1.453703572	3.249533315	1.84041947
C	-2.641742123	2.108589344	9.23206896
H	-1.190723491	0.54656428	9.041499093
H	-4.024870795	3.804865686	9.147334806
H	2.592416126	1.172618414	2.725745296
H	-1.369306477	-0.392314404	5.733655687
H	-0.758170795	-0.870517084	7.33923948
H	0.304190827	-0.980695258	5.918445976
H	2.061525442	0.491521115	7.12171207
H	0.999383493	0.609428759	8.541523754
H	1.594652047	2.093321512	7.751679334
H	-2.99736243	1.748231896	10.19998304

XYZ Coordinates of *m*-PTZ-TP in S₀ optimized geometry

C	-0.947756	5.858135	4.432494
C	-1.618776	4.634623	4.548359
C	-2.876873	4.467702	3.961736
C	-3.474538	5.524304	3.255885
C	-2.79625	6.750209	3.14365
C	-1.540445	6.912164	3.730483
H	-3.397324	3.513057	4.053685
H	0.034438	5.967228	4.897327
H	-3.271038	7.564092	2.592766
H	-1.016991	7.867495	3.641491
N	-5.477475	4.200894	2.723702
N	-5.423276	6.33978	1.943835
N	-6.603443	4.467167	2.042447

C	-4.799224	5.355036	2.637209
C	-6.568894	5.78115	1.564155
C	-7.675708	6.250999	0.816024
C	-8.735104	5.396572	0.592348
C	-8.721237	4.066235	1.102172
C	-7.646265	3.61345	1.827452
H	-7.6546	7.2745	0.440332
H	-9.598525	5.739058	0.017236
H	-9.56122	3.393525	0.923006
H	-7.545164	2.616063	2.256455
N	-0.994489	3.565806	5.275405
C	-1.358379	3.375934	6.63136
C	-0.2765	2.587658	4.544399
C	-0.568909	2.570564	7.483765
C	-2.505439	3.981964	7.176971
C	0.61565	1.708221	5.199558
C	-0.419174	2.46025	3.150143
S	0.995167	1.934866	6.922886
C	-0.949411	2.350041	8.811409
C	-2.856138	3.788722	8.516289
H	-3.128119	4.620534	6.55161
C	1.293607	0.715832	4.484277
C	0.293136	1.491534	2.43727
H	-1.087356	3.131771	2.612312
C	-2.088205	2.964882	9.339712
H	-0.328181	1.704674	9.438234
H	-3.747813	4.284733	8.908426
C	1.145602	0.606857	3.098569
H	1.960172	0.03815	5.024393

H	0.165802	1.429435	1.353404
H	-2.365345	2.801774	10.383875
H	1.695213	-0.159352	2.546723

XYZ Coordinates of *m*-PTZ-TP in S₁ optimized geometry

C	-0.980215212	5.741657047	4.457433985
C	-1.70750961	4.539780355	4.536169214
C	-2.951697859	4.356688858	3.964187496
C	-3.564008029	5.427996593	3.246101938
C	-2.835131929	6.655880486	3.15855468
C	-1.58866862	6.801453693	3.745068162
H	-3.47894652	3.405258604	4.051693034
H	-0.000157677	5.843104903	4.924283222
H	-3.296523891	7.479640049	2.61084528
H	-1.060396406	7.755320256	3.657640622
N	-5.559866607	4.11713512	2.711737953
N	-5.490831518	6.271978967	1.939515613
N	-6.67392197	4.392938583	2.034788123
C	-4.854341083	5.277851147	2.639209417
C	-6.635293924	5.718061694	1.558098072
C	-7.741919044	6.194294289	0.809609375
C	-8.819813797	5.331432929	0.577328299
C	-8.81354188	4.016958508	1.073006499
C	-7.726195726	3.544479458	1.810475368
H	-7.716765335	7.218263119	0.438538227
H	-9.679148273	5.68498942	0.001649419
H	-9.65454746	3.345645867	0.890665851
H	-7.632131577	2.545707813	2.233078673
N	-1.108367526	3.417055037	5.27110304

C	-1.380460356	3.320044414	6.626289399
C	-0.308138862	2.537952853	4.559377711
C	-0.859142457	2.279715147	7.450992805
C	-2.216377976	4.28661809	7.247939976
C	0.33225349	1.412526714	5.157195593
C	-0.100798148	2.742450687	3.168489136
S	0.181405599	1.020419976	6.847353144
C	-1.168808325	2.218987416	8.82485261
C	-2.508569865	4.21131373	8.596397809
H	-2.627435889	5.087363845	6.638710552
C	1.134681663	0.542961615	4.391125342
C	0.689629998	1.879574635	2.433575967
H	-0.581732009	3.592034329	2.690629012
C	-1.987835695	3.175302832	9.398944752
H	-0.755864801	1.407422771	9.429336088
H	-3.156777595	4.96940748	9.04052836
C	1.315577388	0.769952695	3.038120214
H	1.609820062	-0.31231797	4.878320872
H	0.825161174	2.065297426	1.366206454
H	-2.227550404	3.124184351	10.46264596
H	1.936107481	0.093502168	2.447425678

XYZ Coordinates of *m*-PTZ-TP in T₁ optimized geometry

C	-1.006739614	5.732467102	4.444005251
C	-1.701934455	4.523334907	4.541151486
C	-2.95346379	4.348162667	3.960592105
C	-3.546104066	5.415115302	3.254240933
C	-2.851046154	6.637712826	3.152288109
C	-1.597585482	6.79331228	3.740421601

H	-3.473685819	3.39394897	4.052862822
H	-0.026109364	5.83198452	4.913027901
H	-3.319158231	7.457021679	2.603557537
H	-1.070038815	7.746581435	3.654978624
N	-5.555850993	4.110935704	2.715108629
N	-5.481854046	6.255347106	1.944802969
N	-6.677973163	4.391096026	2.035206342
C	-4.864005139	5.261249787	2.635798129
C	-6.631236841	5.708716221	1.562655303
C	-7.73439445	6.191542552	0.816697664
C	-8.803315115	5.346904217	0.588904585
C	-8.802179393	4.016279538	1.091546399
C	-7.729124952	3.549298448	1.815747669
H	-7.704038059	7.216471067	0.445784161
H	-9.6633246	5.700947357	0.015484522
H	-9.648206645	3.351829519	0.909896188
H	-7.637840592	2.549085303	2.239980173
N	-1.103009822	3.4268167	5.267640185
C	-1.388665939	3.345391639	6.625457628
C	-0.301778448	2.555632357	4.53940228
C	-0.863975687	2.27098292	7.452210594
C	-2.217665929	4.309665166	7.259825495
C	0.332223781	1.404032385	5.159982087
C	-0.076551702	2.753333077	3.150216806
S	0.158567087	1.028922536	6.833437163
C	-1.192822364	2.218119739	8.833852133
C	-2.518731626	4.237569005	8.605149127
H	-2.627217744	5.125110767	6.66581957
C	1.135335303	0.53249315	4.375818997

C	0.711025497	1.893067701	2.411686759
H	-0.540246289	3.606241733	2.656873346
C	-1.999426262	3.171031178	9.410760709
H	-0.78976554	1.398515169	9.436196253
H	-3.159135849	4.99961387	9.053819153
C	1.329721158	0.758487234	3.033252467
H	1.600786337	-0.329505783	4.862981624
H	0.859508969	2.08151488	1.346516857
H	-2.243234151	3.114238926	10.47378653
H	1.949471995	0.077669121	2.445814138

XYZ Coordinates of *m*-PXZ-TP in S₀ optimized geometry

C	-1.459841	5.867576	5.164531
C	-1.951643	4.582592	4.896806
C	-3.064073	4.413991	4.069387
C	-3.69492	5.531283	3.497779
C	-3.197572	6.817437	3.768172
C	-2.086524	6.981025	4.597628
H	-3.440779	3.410537	3.865583
H	-0.589012	5.978623	5.814427
H	-3.696229	7.677508	3.317645
H	-1.704725	7.984094	4.804276
N	-5.381476	4.154819	2.354285
N	-5.493386	6.404649	2.019765
N	-6.403787	4.444133	1.533411
C	-4.86408	5.363512	2.619793
C	-6.471162	5.826234	1.328597
C	-7.489622	6.329445	0.483105
C	-8.367786	5.438884	-0.098273

C	-8.256536	4.039247	0.143506
C	-7.267568	3.554166	0.963914
H	-7.54654	7.405968	0.318604
H	-9.160749	5.805894	-0.754063
H	-8.95346	3.338492	-0.318525
H	-7.103247	2.504072	1.207424
N	-1.311305	3.440646	5.470322
C	-1.733362	2.94372	6.715772
C	-0.268274	2.79557	4.782589
C	-2.788797	3.512484	7.442474
C	-1.070514	1.824425	7.266563
C	0.358321	1.679528	5.38056
C	0.182971	3.212544	3.522483
C	-3.17254	2.984183	8.682596
H	-3.312573	4.376146	7.031302
O	-0.025307	1.212923	6.615487
C	-1.453222	1.301216	8.496446
C	1.394596	1.012431	4.737196
C	1.228832	2.53964	2.876215
H	-0.289767	4.071833	3.045403
C	-2.50924	1.879826	9.214276
H	-3.998608	3.448094	9.227192
H	-0.906001	0.435201	8.874791
C	1.837967	1.44011	3.477966
H	1.843302	0.156049	5.245072
H	1.560607	2.887601	1.89482
H	-2.803494	1.462532	10.180017
H	2.653483	0.911017	2.97963

XYZ Coordinates of *m*-PXZ-TP in S₁ optimized geometry

C	-1.424087147	5.861577304	5.190736193
C	-1.959413478	4.596282965	4.883366997
C	-3.054197562	4.399556962	4.063933568
C	-3.705225805	5.52610858	3.476378257
C	-3.171999554	6.819398782	3.779223306
C	-2.072145996	6.974958178	4.606366199
H	-3.432937212	3.397650988	3.854878464
H	-0.557546792	5.969479948	5.843424509
H	-3.664690889	7.685502201	3.333662438
H	-1.693069934	7.979573975	4.815062146
N	-5.365695273	4.144396132	2.326811481
N	-5.506900154	6.41074896	2.026933141
N	-6.388800111	4.433655602	1.523393027
C	-4.84398002	5.366221609	2.620835061
C	-6.478754151	5.827255062	1.33672551
C	-7.51418573	6.327185818	0.506323239
C	-8.398341083	5.419811028	-0.088642934
C	-8.26919926	4.037373224	0.126840551
C	-7.251325964	3.541507404	0.943411632
H	-7.588175327	7.404084193	0.358967902
H	-9.201359326	5.791440223	-0.730456786
H	-8.95949274	3.331146154	-0.337772931
H	-7.073434795	2.491309091	1.168306507
N	-1.313187759	3.419044743	5.467778413
C	-1.725527093	2.943512877	6.694243564
C	-0.283564599	2.794050942	4.797142166
C	-2.781270378	3.540442806	7.421464644
C	-1.07360982	1.810377185	7.256105828

C	0.345723448	1.662764833	5.387940977
C	0.174533301	3.234384227	3.533758752
C	-3.153293147	3.015907154	8.64766237
H	-3.2853655	4.404780023	6.99338772
O	-0.055297783	1.200791392	6.598986982
C	-1.454731041	1.28739988	8.493814889
C	1.390390932	0.991424249	4.748752531
C	1.210590519	2.563330823	2.906686774
H	-0.30624012	4.097111183	3.07652533
C	-2.495074527	1.890403842	9.189594535
H	-3.971328456	3.48132701	9.20057664
H	-0.922542691	0.415607931	8.877195993
C	1.822584489	1.441791378	3.507616535
H	1.836159552	0.128245664	5.245196661
H	1.555722986	2.908636327	1.930330431
H	-2.80415346	1.489831999	10.15691495
H	2.636797449	0.92450915	2.996564836

XYZ Coordinates of *m*-PXZ-TP in T₁ optimized geometry

C	-1.445437983	5.866538352	5.178118353
C	-1.953082853	4.593324565	4.896964443
C	-3.058469341	4.400797189	4.076463255
C	-3.695949206	5.521082894	3.499509823
C	-3.190124262	6.81030061	3.776937708
C	-2.082963983	6.979651703	4.603287766
H	-3.429622169	3.39482698	3.876419328
H	-0.575146419	5.974817586	5.827803747
H	-3.689687901	7.669826139	3.326120557
H	-1.704901375	7.984530002	4.807469351

N	-5.369976518	4.139241731	2.35407236
N	-5.49501287	6.393345128	2.028315932
N	-6.392567123	4.426470543	1.535365536
C	-4.855415605	5.352949169	2.627676098
C	-6.468060331	5.811529799	1.335912614
C	-7.490235086	6.311111429	0.491790532
C	-8.365059566	5.41584902	-0.094648536
C	-8.246522811	4.019239217	0.140470193
C	-7.251812258	3.535451264	0.961442139
H	-7.55376724	7.387748565	0.331390703
H	-9.159770119	5.7821538	-0.748964201
H	-8.938906743	3.315585421	-0.324061114
H	-7.081890552	2.485378375	1.200228659
N	-1.30520381	3.443591537	5.476455057
C	-1.729909159	2.974690501	6.704175638
C	-0.280186514	2.826330223	4.786044203
C	-2.771901239	3.571761071	7.456634771
C	-1.084055139	1.798825316	7.247813336
C	0.330653351	1.652920819	5.373780403
C	0.198853744	3.26858177	3.527749138
C	-3.151368204	3.041564476	8.673953137
H	-3.269868607	4.455647561	7.056744333
O	-0.086505866	1.186411832	6.571843357
C	-1.48265859	1.268919512	8.484539763
C	1.365316399	0.975055205	4.711098903
C	1.220601677	2.594063689	2.888935114
H	-0.254193485	4.149399422	3.071536282
C	-2.501642566	1.873003056	9.199261129
H	-3.955275342	3.51527407	9.24081444

H	-0.966572024	0.378691926	8.85071571
C	1.814643835	1.429439483	3.484038212
H	1.791924445	0.093022621	5.193828776
H	1.578327479	2.950148735	1.92076928
H	-2.813311663	1.460516011	10.16097813
H	2.619071593	0.90229168	2.967154645

XYZ Coordinates of *m*-NPP-TP in S₀ optimized geometry

C	-1.002006	5.804107	4.438707
C	-1.685633	4.58447	4.536589
C	-2.939189	4.433383	3.939754
C	-3.522411	5.502394	3.239409
C	-2.832922	6.723295	3.145034
C	-1.579992	6.869797	3.743138
H	-3.465136	3.480995	4.020702
H	-0.022475	5.902587	4.911741
H	-3.296537	7.546666	2.598719
H	-1.048514	7.82193	3.667429
N	-5.535054	4.206031	2.674478
N	-5.451639	6.353843	1.922044
N	-6.652805	4.493411	1.988274
C	-4.843506	5.353586	2.608117
C	-6.600136	5.812915	1.526781
C	-7.696234	6.30437	0.776757
C	-8.763706	5.465014	0.535008
C	-8.768433	4.128488	1.028372
C	-7.703601	3.654584	1.755277
H	-7.660771	7.3322	0.414113
H	-9.619127	5.824478	-0.041727

H	-9.61467	3.467599	0.835163
H	-7.61695	2.650919	2.172624
N	-1.098617	3.492772	5.249465
C	-1.353718	3.353147	6.628253
C	-0.278852	2.579081	4.557882
C	-0.756991	2.278473	7.340335
C	-2.180534	4.248694	7.316347
C	0.317446	1.503721	5.269277
C	-0.033726	2.704944	3.185505
C	-1.011227	2.146153	8.710387
N	0.076018	1.37367	6.651932
C	-2.426073	4.103294	8.690052
H	-2.640293	5.072229	6.770222
C	1.132903	0.600115	4.578282
C	0.786863	1.791502	2.506663
H	-0.490303	3.529435	2.638002
C	-1.841658	3.052726	9.386661
H	-0.55365	1.322327	9.258192
C	0.679793	0.294512	7.368653
H	-3.076175	4.819498	9.198369
C	1.369742	0.739477	3.20235
H	1.591084	-0.224698	5.123933
H	0.959133	1.917739	1.435042
H	-2.020594	2.922228	10.456706
C	1.940753	0.461465	7.95522
C	0.012071	-0.931378	7.485152
H	2.011604	0.017563	2.691602
C	2.531747	-0.594725	8.654501
H	2.447481	1.423919	7.854433

C	0.604847	-1.986339	8.184684
H	-0.970911	-1.044504	7.022361
C	1.864587	-1.819186	8.77037
H	3.516146	-0.461222	9.110872
H	0.081339	-2.942044	8.27271
H	2.327234	-2.644746	9.31769

XYZ Coordinates of *m*-NPP-TP in S₁ optimized geometry

C	-0.961759793	5.837775509	4.455489852
C	-1.680596734	4.630983229	4.532587566
C	-2.923993148	4.445241788	3.956594366
C	-3.538039778	5.5126722	3.239371423
C	-2.817909526	6.743234377	3.155384751
C	-1.572315618	6.894589236	3.745733222
H	-3.447188944	3.491172651	4.039683108
H	0.017434896	5.943521015	4.923702852
H	-3.28299544	7.56465085	2.607287669
H	-1.048934276	7.851444391	3.661082486
N	-5.523988488	4.19292419	2.690062237
N	-5.463205704	6.347501204	1.92215318
N	-6.634968759	4.461935044	2.006273946
C	-4.82694564	5.356370283	2.623934979
C	-6.603190249	5.786335023	1.531383533
C	-7.706530373	6.257911614	0.775325174
C	-8.779352466	5.385112659	0.533760739
C	-8.767081263	4.07228622	1.027463273
C	-7.681774318	3.602899139	1.773738365
H	-7.68518512	7.282263423	0.405741605
H	-9.636849459	5.733300623	-0.047917609

H	-9.602425489	3.395610863	0.837790398
H	-7.583003215	2.604874908	2.195916437
N	-1.078960659	3.512494232	5.259988815
C	-1.319248979	3.375437495	6.612514343
C	-0.276284669	2.61664949	4.582336903
C	-0.734186091	2.287238229	7.331680005
C	-2.139133712	4.293016561	7.306710498
C	0.316723098	1.521604646	5.284327031
C	-0.028144351	2.758143702	3.198693718
C	-0.983088029	2.150072369	8.712319321
N	0.070678824	1.382947372	6.646442005
C	-2.369192639	4.13769765	8.663397875
H	-2.584747801	5.115070679	6.750941482
C	1.133282548	0.607579248	4.588096384
C	0.777991787	1.847688689	2.536230104
H	-0.487083952	3.591307031	2.671040449
C	-1.791326624	3.065684321	9.37016406
H	-0.537043241	1.319148943	9.25656795
C	0.658723171	0.277167952	7.361925247
H	-3.007335201	4.85437676	9.183767413
C	1.361085998	0.76963115	3.229364982
H	1.581784618	-0.226407168	5.125627655
H	0.957320455	1.970333954	1.466454201
H	-1.978432598	2.948513362	10.43938181
C	1.917931479	0.43006573	7.94933641
C	-0.040093004	-0.929839696	7.456761648
H	1.994090203	0.05451101	2.700318846
C	2.484457926	-0.643672828	8.641704085
H	2.442542781	1.383862731	7.860346446

C	0.53350172	-1.998703711	8.150935634
H	-1.022526627	-1.0230756	6.988799023
C	1.793346686	-1.856053695	8.742619617
H	3.468244371	-0.531485578	9.103347147
H	-0.006668607	-2.945051529	8.229075454
H	2.238612025	-2.693659937	9.284847888

XYZ Coordinates of *m*-NPP-TP in T₁ optimized geometry

C	-0.978935454	5.846542027	4.445150625
C	-1.663872577	4.629275508	4.53772939
C	-2.912195541	4.439159218	3.956837236
C	-3.519607387	5.500663446	3.249100187
C	-2.834451732	6.733254888	3.152657486
C	-1.585320435	6.902366411	3.741825576
H	-3.42100904	3.47847829	4.046315393
H	0.000392602	5.956620383	4.914220953
H	-3.310901247	7.548338566	2.604689715
H	-1.06977618	7.862562403	3.658195199
N	-5.508855385	4.171123824	2.700615498
N	-5.459430301	6.319191443	1.933870334
N	-6.630000512	4.437499791	2.015672
C	-4.828815207	5.331937456	2.627649106
C	-6.59852739	5.75768116	1.545023985
C	-7.704462584	6.225981125	0.79330854
C	-8.761821582	5.365816618	0.55721818
C	-8.745595962	4.036409452	1.056767663
C	-7.668619114	3.582343494	1.78805435
H	-7.686145716	7.251776053	0.424190406
H	-9.622885771	5.709610184	-0.021043307

H	-9.580941515	3.360146066	0.868995864
H	-7.56621472	2.582722454	2.210800539
N	-1.054184623	3.539830142	5.258864856
C	-1.305048597	3.41429559	6.614442905
C	-0.251030219	2.649085462	4.567960935
C	-0.728238145	2.294929307	7.332542854
C	-2.115582693	4.33435648	7.320505335
C	0.324660328	1.526484437	5.28202837
C	0.018456651	2.790235038	3.185962852
C	-0.997251588	2.158399898	8.717752709
N	0.063846003	1.39328976	6.637610958
C	-2.358040775	4.179209515	8.672283115
H	-2.550955888	5.172294568	6.776742761
C	1.132148704	0.603861509	4.570729565
C	0.814704545	1.878635496	2.518795805
H	-0.416334714	3.63423575	2.650974621
C	-1.790858122	3.07332145	9.379928825
H	-0.567766326	1.315755468	9.259582649
C	0.635976021	0.280828115	7.348768998
H	-2.985512777	4.902648952	9.196655269
C	1.377253016	0.767644394	3.222239396
H	1.561935189	-0.243325577	5.105065227
H	1.010750097	2.008963997	1.452662879
H	-1.985721942	2.94796573	10.44721368
C	1.895548699	0.417377765	7.938428067
C	-0.075796076	-0.918227566	7.440050736
H	2.002060464	0.044153708	2.694099596
C	2.450425459	-0.665261456	8.630068647
H	2.427655673	1.366791031	7.849447143

C	0.484559533	-1.997272372	8.133024822
H	-1.058033031	-0.99493605	6.969155086
C	1.745101061	-1.869850412	8.727120623
H	3.434975775	-0.565932753	9.093758309
H	-0.065912927	-2.938335767	8.207976832
H	2.180225974	-2.714047869	9.268318655

XYZ Coordinates of *p*-Cz-TP in S₀ optimized geometry

C	-1.421329	5.85961	5.106513
C	-2.248464	4.734837	5.260793
C	-3.365958	4.568753	4.446535
C	-3.670358	5.513722	3.450607
C	-2.833107	6.631284	3.292244
C	-1.723819	6.808223	4.116654
H	-2.000683	3.990158	6.019698
H	-4.009764	3.695412	4.566255
H	-3.077214	7.365106	2.522031
H	-1.087967	7.68905	4.008195
N	-5.681084	4.304747	2.713425
N	-5.174349	6.228958	1.605336
N	-6.595572	4.536097	1.757825
C	-4.846895	5.348121	2.584637
C	-6.282767	5.718181	1.078147
C	-7.137326	6.132749	0.027735
C	-8.236797	5.357888	-0.277598
C	-8.512186	4.162614	0.446951
C	-7.680745	3.762449	1.464443
H	-6.898543	7.052909	-0.50659
H	-8.908691	5.660024	-1.084324

H	-9.383175	3.552722	0.20282
H	-7.80841	2.86688	2.073237
N	-0.293353	6.034624	5.945344
C	1.021546	6.24438	5.516939
C	-0.307611	6.024916	7.344123
C	1.864107	6.370232	6.655186
C	1.538727	6.297802	4.216125
C	1.015448	6.230996	7.821757
C	-1.388655	5.886908	8.224237
C	3.240289	6.573525	6.480764
C	2.912335	6.499842	4.069648
H	0.891457	6.179725	3.345667
C	1.255564	6.276234	9.202429
C	-1.123133	5.93659	9.59395
H	-2.405469	5.751121	7.852621
H	3.895962	6.673157	7.349827
C	3.757881	6.641418	5.187308
H	3.338573	6.545972	3.06391
C	0.184538	6.124016	10.08296
H	2.269656	6.432991	9.579448
H	-1.951061	5.829829	10.300031
H	4.82863	6.800186	5.036721
H	0.357573	6.155365	11.161594

XYZ Coordinates of *p*-Cz-TP in S₁ optimized geometry

C	-1.410193704	5.865860046	5.11374542
C	-1.914155563	4.566505087	4.869668899
C	-3.021169547	4.402429722	4.05917354
C	-3.674303221	5.525601174	3.455979818

C	-3.138594607	6.826294392	3.721651573
C	-2.032766037	6.996131926	4.532445083
H	-1.426667701	3.698753332	5.323197601
H	-3.417786051	3.404362565	3.865519177
H	-3.630931791	7.686342627	3.264699153
H	-1.637209808	7.997009627	4.727336407
N	-5.369920576	4.150176566	2.346585179
N	-5.481298161	6.413981324	2.014499728
N	-6.39859407	4.443511748	1.552367894
C	-4.825227024	5.367302076	2.616650222
C	-6.469915332	5.835911296	1.345953349
C	-7.509027809	6.337246578	0.521220093
C	-8.413351915	5.435814119	-0.047310961
C	-8.301687124	4.053508309	0.188321504
C	-7.281151693	3.557141595	0.998134671
H	-7.56960379	7.412798693	0.357566944
H	-9.219314495	5.809332498	-0.684344762
H	-9.008316959	3.350371741	-0.255848208
H	-7.115330182	2.507827463	1.237484637
N	-0.259083793	6.040389671	5.970163915
C	1.052224879	6.065503843	5.553536579
C	-0.298812262	6.207798956	7.336076635
C	1.911412477	6.255260481	6.679038404
C	1.540738094	5.934044619	4.242305636
C	1.029202225	6.346987203	7.842984222
C	-1.432966375	6.244621603	8.164836385
C	3.28151306	6.31326859	6.483260474
C	2.924874226	5.995763289	4.068579861
H	0.84752851	5.791642629	3.413123171

C	1.219842003	6.525206961	9.203496231
C	-1.217214646	6.425576442	9.532683269
H	-2.428116828	6.134151071	7.733768221
H	3.968053917	6.457556487	7.320388015
C	3.781593784	6.181761664	5.165937167
H	3.346901774	5.898509523	3.066604293
C	0.082979384	6.56312892	10.04539872
H	2.221022901	6.63485228	9.626038986
H	-2.070515171	6.460470891	10.21256585
H	4.860320908	6.226615473	5.001167794
H	0.222819093	6.702997899	11.11950721

XYZ Coordinates of *p*-Cz-TP in T₁ optimized geometry

C	-1.419380062	5.867636885	5.118259603
C	-2.352219295	4.785986165	5.351422948
C	-3.434581084	4.610168265	4.54673046
C	-3.699291784	5.528180435	3.433409371
C	-2.75496169	6.623929076	3.215138251
C	-1.664243356	6.775968848	4.011870396
H	-2.139636756	4.075447198	6.152766826
H	-4.115440258	3.771182689	4.695748867
H	-2.96956691	7.324711397	2.407099067
H	-0.987881011	7.620922171	3.868404726
N	-5.730280571	4.348914381	2.779940826
N	-5.124997165	6.196634293	1.539919727
N	-6.610755329	4.560024308	1.804195777
C	-4.822512547	5.366826651	2.601548079
C	-6.236636079	5.695275999	1.044670642
C	-7.070147323	6.069168109	-0.044503717

C	-8.196341858	5.317056022	-0.313620266
C	-8.52760476	4.184298088	0.480063896
C	-7.722814001	3.816848152	1.538681556
H	-6.790060223	6.942393908	-0.634232493
H	-8.846086662	5.592401204	-1.147913481
H	-9.418681783	3.593519583	0.263213741
H	-7.896690207	2.967498414	2.199688958
N	-0.30800688	6.03713797	5.942146312
C	1.008365239	6.285451922	5.515092435
C	-0.304631692	5.984799865	7.34730094
C	1.855118384	6.395928866	6.650196264
C	1.520060055	6.352688293	4.212495128
C	1.017921021	6.196575185	7.820122452
C	-1.381086226	5.832796784	8.230956667
C	3.224002903	6.622654856	6.477147901
C	2.889519419	6.585692426	4.063733159
H	0.8777918	6.212951535	3.342573093
C	1.270905417	6.209700153	9.195375251
C	-1.104028374	5.843690171	9.60022882
H	-2.402888758	5.724723609	7.866487328
H	3.88408406	6.706316725	7.344270173
C	3.734264643	6.727269507	5.179880442
H	3.311954446	6.647884153	3.05759731
C	0.206119189	6.021478286	10.0813884
H	2.284726794	6.374416104	9.56903101
H	-1.926245344	5.720984229	10.30988031
H	4.801790519	6.905571324	5.028989768
H	0.3888751	6.026618792	11.15876107

XYZ Coordinates of *p*-DPA-TP in S₀ optimized geometry

C	-1.460071	5.898561	5.149087
C	-2.374809	4.85206	5.384243
C	-3.482851	4.680828	4.560987
C	-3.708602	5.537986	3.468394
C	-2.793466	6.578837	3.231603
C	-1.691063	6.762494	4.060297
H	-2.206028	4.171094	6.220378
H	-4.18243	3.863924	4.749032
H	-2.970645	7.251089	2.389945
H	-0.995237	7.581552	3.869766
N	-5.772646	4.386848	2.786194
N	-5.108964	6.153551	1.510229
N	-6.639114	4.573399	1.777295
C	-4.867763	5.359359	2.586264
C	-6.229672	5.659485	0.995227
C	-7.021542	6.013438	-0.124382
C	-8.156067	5.276598	-0.395244
C	-8.529132	4.179566	0.432819
C	-7.758854	3.838787	1.518638
H	-6.708098	6.858723	-0.737989
H	-8.779972	5.53361	-1.254528
H	-9.427006	3.599011	0.216038
H	-7.962431	3.018867	2.208067
N	-0.333006	6.075387	5.984213
C	-0.431768	5.847705	7.381916
C	0.911428	6.475196	5.428449
C	0.595051	5.174213	8.068216
C	-1.552609	6.296969	8.103899

C	1.696806	7.450759	6.068449
C	1.380521	5.896876	4.235118
C	0.502727	4.963532	9.44499
H	1.466073	4.820813	7.51287
C	-1.645035	6.065893	9.477435
H	-2.350214	6.825568	7.578066
C	2.926863	7.830401	5.528522
H	1.335731	7.904484	6.993649
C	2.603672	6.294847	3.692897
H	0.77636	5.135992	3.736887
C	-0.618226	5.402351	10.158272
H	1.310607	4.438897	9.962511
H	-2.523735	6.421278	10.022726
C	3.386698	7.259672	4.336527
H	3.525468	8.58988	6.038971
H	2.953574	5.83520	2.764483
H	-0.690725	5.229265	11.234856
H	4.346978	7.563868	3.912687

XYZ Coordinates of *p*-DPA-TP in S₁ optimized geometry

C	-1.423982725	5.898534241	5.163345458
C	-1.949884084	4.60636514	4.96576275
C	-3.050834524	4.431677933	4.142022906
C	-3.668446663	5.540946977	3.493476783
C	-3.116747097	6.836314055	3.716067234
C	-2.01135657	7.012887179	4.534018062
H	-1.487969942	3.749073346	5.463526311
H	-3.469475933	3.436573449	3.98270221
H	-3.584905073	7.685598749	3.215780266

H	-1.591846156	8.010535315	4.691854219
N	-5.369110468	4.162256161	2.398117108
N	-5.436540661	6.410698553	1.990525352
N	-6.37739198	4.4433616	1.574421877
C	-4.81493415	5.374395509	2.635053795
C	-6.424640949	5.82476812	1.318526893
C	-7.436129147	6.318588457	0.456522681
C	-8.345202432	5.406227809	-0.102658425
C	-8.258831306	4.034612147	0.18196514
C	-7.264597307	3.543100768	1.030667707
H	-7.47533021	7.388469637	0.256292067
H	-9.131779951	5.768636501	-0.769483334
H	-8.96764693	3.32855191	-0.254996796
H	-7.11929123	2.50110789	1.308522432
N	-0.264857223	6.082008987	6.024315925
C	-0.449182554	6.043251341	7.404751233
C	0.978559092	6.286055691	5.432906435
C	0.572448562	5.573153038	8.274147167
C	-1.706828956	6.408816114	7.952727012
C	1.985061286	7.059771622	6.07360111
C	1.22622483	5.775325726	4.130992811
C	0.351955953	5.519577248	9.64485325
H	1.509388298	5.203043789	7.856854419
C	-1.902053132	6.364196698	9.325376841
H	-2.501139379	6.736255554	7.283311877
C	3.208038106	7.268240868	5.448681456
H	1.773764656	7.534713647	7.032013722
C	2.459522957	5.980595097	3.530623086
H	0.443020304	5.212020029	3.625561355

C	-0.878150378	5.925181392	10.1811617
H	1.13621805	5.135528405	10.3010971
H	-2.865504437	6.66953953	9.739098705
C	3.459542139	6.721665617	4.18223193
H	3.965343918	7.882975814	5.94039766
H	2.64780277	5.564039046	2.538848939
H	-1.047445078	5.878940729	11.2591426
H	4.421921705	6.890535568	3.694239979

XYZ Coordinates of *p*-DPA-TP in T₁ optimized geometry

C	-1.438934088	5.907760962	5.168339459
C	-2.395365739	4.848352197	5.420319683
C	-3.473376196	4.670206601	4.608683438
C	-3.706909544	5.550620855	3.467108844
C	-2.749736806	6.622305114	3.228766585
C	-1.665360593	6.787210349	4.033697116
H	-2.217288308	4.168800712	6.256411395
H	-4.175983845	3.854116351	4.783026223
H	-2.940485904	7.296738464	2.392702605
H	-0.968060431	7.609257147	3.859468036
N	-5.742948634	4.378253137	2.805412135
N	-5.089245529	6.173686406	1.523403923
N	-6.601525573	4.566824923	1.803109566
C	-4.822822667	5.374875163	2.614569669
C	-6.197949074	5.670230703	1.017579324
C	-7.001118562	6.018435789	-0.101081941
C	-8.131259683	5.270374712	-0.372727897
C	-8.493291791	4.169038781	0.44825497
C	-7.715759435	3.827811305	1.536970465

H	-6.697192354	6.868927893	-0.711930946
H	-8.75822367	5.526429356	-1.230380141
H	-9.386042349	3.580910095	0.230769008
H	-7.91395437	3.002366023	2.220988392
N	-0.326467296	6.078910565	5.990268256
C	-0.432645357	5.864251671	7.387241969
C	0.918218268	6.460486258	5.429621133
C	0.598244325	5.210684211	8.092555564
C	-1.589385568	6.277316715	8.078164027
C	1.743209516	7.397343931	6.084743932
C	1.326467565	5.925355862	4.191393337
C	0.47244864	4.986699333	9.462074179
H	1.487207967	4.875323064	7.555243914
C	-1.706478448	6.03982438	9.447264559
H	-2.381450566	6.791073493	7.530379791
C	2.954818291	7.779049109	5.512518073
H	1.420115493	7.824700956	7.035831544
C	2.538066368	6.321520964	3.625724106
H	0.689276643	5.193359543	3.691855977
C	-0.679221996	5.39610807	10.14797723
H	1.276096446	4.475191719	9.998407345
H	-2.605288283	6.371152243	9.973947332
C	3.359730999	7.246925865	4.280372199
H	3.58498814	8.509559831	6.026677261
H	2.847926414	5.893991716	2.66855428
H	-0.77497238	5.212858686	11.2209289
H	4.308705961	7.553491776	3.833764173

XYZ Coordinates of *p*-DMAc-TP in S₀ optimized geometry

C	-1.432692	5.867811	5.125392
C	-1.930568	4.582916	4.871771
C	-3.045474	4.411686	4.052756
C	-3.676757	5.526344	3.47254
C	-3.171062	6.812758	3.727128
C	-2.057223	6.980733	4.548641
H	-1.433715	3.72339	5.327072
H	-3.43887	3.413194	3.853351
H	-3.66665	7.672346	3.27246
H	-1.659174	7.977033	4.75315
N	-5.388498	4.15655	2.354929
N	-5.481849	6.405141	2.006966
N	-6.417677	4.45115	1.544395
C	-4.855185	5.361757	2.606868
C	-6.473423	5.832689	1.33163
C	-7.497654	6.341523	0.496355
C	-8.39282	5.456931	-0.067759
C	-8.293038	4.057658	0.181251
C	-7.298395	3.567251	0.991564
H	-7.545575	7.417597	0.326194
H	-9.190732	5.828318	-0.715026
H	-9.00352	3.361623	-0.267044
H	-7.142262	2.517021	1.239712
N	-0.293023	6.044	5.974648
C	0.989326	6.060591	5.40331
C	-0.491422	6.208462	7.355059
C	2.135594	6.261354	6.205529
C	1.140734	5.87474	4.010758
C	0.605256	6.409414	8.223649

C	-1.800472	6.173483	7.886148
C	3.388444	6.271524	5.573092
C	2.055221	6.469726	7.723916
C	2.399676	5.890234	3.417305
H	0.259331	5.717521	3.390072
C	0.339798	6.565828	9.592955
C	-2.026371	6.331462	9.250417
H	-2.647576	6.02003	7.21863
C	3.540059	6.090811	4.198343
H	4.282564	6.428153	6.180912
C	2.879437	5.361088	8.429735
C	2.647647	7.860473	8.073362
H	2.484406	5.744701	2.336954
C	-0.951291	6.529727	10.119653
H	1.177534	6.723399	10.276063
H	-3.050746	6.298483	9.631141
H	4.534469	6.10671	3.746067
H	2.47051	4.366887	8.192804
H	2.862307	5.486298	9.523202
H	3.932561	5.382553	8.110142
H	3.695301	7.94252	7.744869
H	2.624323	8.041584	9.158982
H	2.071999	8.659356	7.581141
H	-1.112896	6.655436	11.192863

XYZ Coordinates of *p*-DMAc-TP in S₁ optimized geometry

C	-1.439170536	5.890037622	5.125871339
C	-1.926587719	4.589582009	4.871199638
C	-3.030764528	4.416945279	4.055952744

C	-3.695030201	5.535251558	3.458736323
C	-3.175384203	6.839023228	3.736056653
C	-2.072175715	7.014193357	4.551976541
H	-1.430239158	3.724255872	5.319788671
H	-3.414828048	3.415526531	3.854391199
H	-3.676297793	7.696927912	3.284464119
H	-1.688312467	8.018151676	4.754626759
N	-5.369466087	4.149258625	2.330808637
N	-5.50626316	6.413407396	2.016068082
N	-6.397674612	4.436138386	1.534006116
C	-4.841392162	5.369980291	2.612616658
C	-6.485334586	5.8286511	1.337822416
C	-7.526134549	6.324693516	0.51205526
C	-8.417285145	5.415726472	-0.068437167
C	-8.289818737	4.033941409	0.15690853
C	-7.267176459	3.542161373	0.968190173
H	-7.598778115	7.400641827	0.356700268
H	-9.224617526	5.784339826	-0.706593741
H	-8.98578304	3.325948307	-0.296461425
H	-7.089534989	2.493299989	1.20025981
N	-0.279172867	6.073436366	5.988481911
C	0.985887034	6.081417677	5.42422745
C	-0.472086746	6.235099692	7.350725172
C	2.149679961	6.259596479	6.227592974
C	1.110173552	5.908345217	4.016712062
C	0.631337492	6.418510317	8.234014083
C	-1.800231639	6.21486488	7.862707734
C	3.391604107	6.256659574	5.58508112
C	2.070635938	6.453356428	7.736459203

C	2.356687385	5.911821783	3.420121347
H	0.20725039	5.774858956	3.425799014
C	0.356893329	6.573307534	9.596309412
C	-2.0289885	6.371567298	9.216542625
H	-2.625106116	6.074175829	7.168452472
C	3.508888016	6.086691522	4.204248715
H	4.299634623	6.391683045	6.174954381
C	2.872667102	5.317730263	8.433470832
C	2.691672321	7.833383584	8.097278207
H	2.438749288	5.778696091	2.339660014
C	-0.947268919	6.552001154	10.09432483
H	1.182424039	6.715992917	10.29551003
H	-3.052098861	6.35419488	9.596997984
H	4.497062484	6.090707449	3.739117441
H	2.446310124	4.333188093	8.189781866
H	2.855906143	5.440228668	9.526047544
H	3.924313047	5.327307888	8.11262736
H	3.740116075	7.887481774	7.77015011
H	2.67012071	7.99961775	9.184074652
H	2.135970863	8.649707675	7.612121052
H	-1.12109384	6.676253655	11.1654178

XYZ Coordinates of *p*-DMAc-TP in T₁ optimized geometry

C	-1.427972589	5.859872022	5.135987623
C	-1.922299735	4.572097026	4.88363322
C	-3.035527189	4.394558676	4.065828083
C	-3.673742912	5.506395884	3.482661762
C	-3.171729875	6.796071606	3.737162516
C	-2.057947511	6.968591174	4.558000829

H	-1.422044606	3.714821878	5.339516159
H	-3.422949572	3.393080862	3.868807846
H	-3.667949713	7.655895809	3.283793816
H	-1.664274847	7.967067559	4.760412082
N	-5.388113177	4.154064561	2.344805474
N	-5.492683963	6.396281861	2.013218118
N	-6.421363237	4.462206645	1.530867999
C	-4.845758876	5.335104819	2.620299873
C	-6.480217928	5.823788103	1.332982963
C	-7.496109799	6.378367973	0.50308681
C	-8.454181256	5.435485605	-0.114413969
C	-8.34826416	4.098646808	0.117076939
C	-7.310744224	3.547069599	0.964066127
H	-7.539859637	7.454680214	0.34807323
H	-9.244306463	5.829047232	-0.756122282
H	-9.05249471	3.396894069	-0.335438125
H	-7.159165422	2.49647547	1.198335755
N	-0.287764042	6.041166949	5.982911803
C	0.994036001	6.056330403	5.409930638
C	-0.483904261	6.207045072	7.363572342
C	2.14118211	6.26148958	6.209775116
C	1.143754861	5.864685143	4.017992093
C	0.613747234	6.413133786	8.229730794
C	-1.791805872	6.168283222	7.897186267
C	3.3932009	6.269940874	5.575629374
C	2.062432459	6.478972279	7.726939062
C	2.401932183	5.878427369	3.422817357
H	0.261601781	5.704308102	3.399178855
C	0.35027866	6.571438961	9.599213818

C	-2.015723595	6.32802569	9.261609664
H	-2.639521214	6.010515696	7.23142753
C	3.543164537	6.083200037	4.201493678
H	4.287963145	6.430387279	6.181495161
C	2.895166713	5.380652797	8.438741644
C	2.646504073	7.875921099	8.065831614
H	2.485370119	5.728239577	2.342993782
C	-0.939717447	6.531890018	10.12838815
H	1.188697326	6.733555542	10.28041732
H	-3.039242978	6.292025096	9.644378134
H	4.536985583	6.097858571	3.747873519
H	2.492188125	4.382192959	8.20964728
H	2.879681188	5.513424193	9.531307221
H	3.947530183	5.406642374	8.11708209
H	3.693064843	7.962312952	7.734829308
H	2.623563421	8.064324549	9.150263000
H	2.064957278	8.667710115	7.569076037
H	-1.099734915	6.659302259	11.20164151

XYZ Coordinates of *p*-PTZ-TP in S₀ optimized geometry

C	-1.452968	6.056895	5.106106
C	-1.893606	4.748064	4.856361
C	-3.003763	4.523956	4.044735
C	-3.690151	5.607712	3.467647
C	-3.244176	6.915867	3.71899
C	-2.133166	7.137105	4.533005
H	-1.356061	3.910667	5.306977
H	-3.350941	3.50792	3.848187
H	-3.782322	7.751115	3.26734

H	-1.779193	8.149993	4.736525
N	-5.33978	4.154869	2.362858
N	-5.541472	6.395262	2.007717
N	-6.385483	4.397222	1.55617
C	-4.863737	5.385151	2.608284
C	-6.507673	5.77363	1.338726
C	-7.557949	6.229938	0.505513
C	-8.412423	5.301672	-0.051586
C	-8.245706	3.909728	0.202733
C	-7.225816	3.470317	1.010844
H	-7.657261	7.30182	0.331259
H	-9.229358	5.632175	-0.697263
H	-8.924411	3.178923	-0.239435
H	-7.019547	2.429647	1.262686
N	-0.316713	6.312236	5.944107
C	0.974995	6.220459	5.369737
C	-0.517129	6.352636	7.346099
C	1.181149	5.609405	4.118857
C	2.102115	6.749461	6.039331
C	0.469232	6.894356	8.201781
C	-1.699211	5.863922	7.933084
C	2.45974	5.519544	3.561025
H	0.331578	5.207015	3.56834
S	1.897609	7.709078	7.523089
C	3.38266	6.619929	5.492132
C	0.287952	6.895579	9.588611
C	-1.888687	5.905532	9.317419
H	-2.486919	5.455429	7.301169
C	3.569825	6.013376	4.246758

H	2.580028	5.047662	2.582433
H	4.235911	7.020621	6.045922
C	-0.894252	6.410722	10.155366
H	1.079323	7.302544	10.223704
H	-2.824601	5.52722	9.736676
H	4.572477	5.934379	3.820089
H	-1.033082	6.434134	11.238772

XYZ Coordinates of *p*-PTZ-TP in S₁ optimized geometry

C	-1.411948493	5.911366305	5.140557966
C	-1.869903756	4.598963317	4.893083292
C	-2.972530223	4.395078837	4.08266094
C	-3.665681064	5.494670363	3.482647584
C	-3.175928857	6.812040574	3.751682779
C	-2.074177542	7.016536648	4.562952716
H	-1.351797318	3.747714004	5.344255081
H	-3.333381557	3.383877293	3.887221505
H	-3.698781826	7.655493911	3.297809554
H	-1.71393972	8.030522126	4.759528632
N	-5.312669508	4.064607444	2.368977846
N	-5.503915783	6.323745986	2.045443544
N	-6.351544563	4.324105162	1.576669115
C	-4.811504205	5.298561421	2.642845582
C	-6.472646141	5.713368153	1.375077381
C	-7.529421139	6.181464788	0.553334383
C	-8.402802088	5.249508362	-0.01786325
C	-8.242055532	3.872135086	0.212616451
C	-7.203344207	3.407724529	1.019868939
H	-7.628007401	7.254729343	0.393862768

H	-9.222225532	5.596560888	-0.652670591
H	-8.924119048	3.146234448	-0.233465854
H	-7.000385081	2.364222359	1.255214968
N	-0.254292547	6.127068835	6.002366136
C	1.000638848	6.158213917	5.41010655
C	-0.479082142	6.290467858	7.362445139
C	1.115880497	5.98242517	4.00464553
C	2.208939065	6.361328068	6.141604207
C	0.565511161	6.506754032	8.310283434
C	-1.808437621	6.243981088	7.862684518
C	2.34934059	6.0091876	3.381604855
H	0.207154401	5.826612471	3.428598019
S	2.247877848	6.591643511	7.867525093
C	3.457797625	6.385479039	5.489411635
C	0.281338565	6.665661648	9.681273132
C	-2.068696986	6.402214401	9.210860707
H	-2.619411652	6.080630523	7.157406728
C	3.534040553	6.211307203	4.118281518
H	2.398984899	5.871042672	2.299564603
H	4.364528657	6.543438379	6.079031269
C	-1.025511705	6.614635784	10.13488933
H	1.104765202	6.829824269	10.38115493
H	-3.102918721	6.36065103	9.558685301
H	4.503259459	6.230925505	3.616466995
H	-1.241958413	6.73816265	11.19767904

XYZ Coordinates of *p*-PTZ-TP in T₁ optimized geometry

C	-1.413233003	5.852844881	5.165454492
C	-1.881366199	4.556061499	4.916567116

C	-2.995422984	4.372365918	4.097932797
C	-3.64589146	5.476982512	3.521068968
C	-3.161165931	6.775957576	3.780292487
C	-2.049699799	6.961109432	4.599880039
H	-1.367881061	3.704763663	5.368026022
H	-3.372240709	3.368175632	3.895208094
H	-3.671513354	7.627890234	3.32846282
H	-1.665714948	7.962264641	4.807213192
N	-5.32923523	4.078216343	2.397929621
N	-5.458999974	6.326282002	2.051876734
N	-6.358816591	4.356063173	1.583733763
C	-4.816660501	5.292916763	2.654239003
C	-6.43758661	5.737228648	1.371333724
C	-7.465464216	6.228892047	0.530703268
C	-8.343324355	5.32849962	-0.039687613
C	-8.221274314	3.93256913	0.20913555
C	-7.222046765	3.457555055	1.025486525
H	-7.530452495	7.304015082	0.360645207
H	-9.143482615	5.686913222	-0.691505617
H	-8.917273157	3.224552974	-0.243232276
H	-7.049711535	2.409997326	1.273656409
N	-0.261407604	6.044560311	6.013983109
C	0.978736071	6.09243379	5.386951749
C	-0.504519754	6.218808589	7.37213124
C	1.109161058	5.831989282	3.995219575
C	2.190101419	6.446894099	6.115506303
C	0.560052849	6.582755813	8.297862099
C	-1.814463615	6.08381662	7.908110566
C	2.326577591	5.91103296	3.351056015

H	0.221901448	5.564831313	3.42261707
S	2.197089707	6.791778467	7.803154207
C	3.427169209	6.53502909	5.423641044
C	0.258054871	6.797902196	9.668820831
C	-2.077166336	6.284040242	9.247754484
H	-2.63259531	5.815067016	7.241133687
C	3.511856161	6.275282563	4.075308909
H	2.384171677	5.696218516	2.28197386
H	4.322303994	6.814201391	5.987679206
C	-1.023012182	6.654138065	10.14949026
H	1.071000272	7.081244077	10.34423289
H	-3.096488457	6.161423503	9.619653632
H	4.472372944	6.347169051	3.560785382
H	-1.235401205	6.822152674	11.20739356

XYZ Coordinates of *p*-PXZ-TP in S₀ optimized geometry

C	-1.449023	5.867136	5.145615
C	-1.969019	4.585717	4.917834
C	-3.083242	4.417418	4.097037
C	-3.690107	5.530669	3.488932
C	-3.164004	6.813394	3.719652
C	-2.051947	6.979442	4.54399
H	-1.489104	3.726926	5.392408
H	-3.493072	3.422124	3.915578
H	-3.641812	7.67144	3.24354
H	-1.637222	7.972782	4.729133
N	-5.410769	4.166525	2.378453
N	-5.464149	6.409088	1.986097
N	-6.423947	4.461118	1.54794

C	-4.86233	5.368007	2.614161
C	-6.455184	5.838796	1.307833
C	-7.458547	6.346818	0.447142
C	-8.358108	5.464955	-0.114192
C	-8.283467	4.069361	0.162968
C	-7.309305	3.579837	0.998293
H	-7.487064	7.419967	0.255459
H	-9.139811	5.835637	-0.781332
H	-8.99711	3.375423	-0.283568
H	-7.172849	2.53228	1.268382
N	-0.307712	6.039445	5.987287
C	-0.469561	6.202981	7.374609
C	0.983362	6.069403	5.430914
C	-1.723387	6.176064	8.001359
C	0.674509	6.406486	8.178001
C	2.091409	6.278481	6.281817
C	1.224084	5.897101	4.060538
C	-1.835854	6.34331	9.388194
H	-2.617428	6.023037	7.3959
O	1.937525	6.451408	7.63687
C	0.560771	6.57247	9.553669
C	3.385117	6.316946	5.773968
C	2.528771	5.936531	3.550398
H	0.380504	5.732001	3.389356
C	-0.698438	6.541061	10.168914
H	-2.826015	6.317324	9.849806
H	1.477629	6.726928	10.126468
C	3.612493	6.146693	4.401233
H	4.204179	6.483381	6.476894

H	2.685959	5.800547	2.477544
H	-0.779182	6.671751	11.250469
H	4.631904	6.179523	4.010103

XYZ Coordinates of *p*-PXZ-TP in S₁ optimized geometry

C	-1.457625512	5.884217474	5.145369619
C	-1.949253439	4.584305866	4.888471677
C	-3.050065044	4.416331833	4.069114537
C	-3.706970776	5.538407977	3.467964725
C	-3.184101358	6.841354377	3.74861304
C	-2.084375552	7.012374696	4.568617736
H	-1.457969353	3.716532422	5.338070129
H	-3.437556607	3.41664907	3.865723823
H	-3.679934335	7.701021248	3.294850896
H	-1.697323673	8.015028401	4.771938721
N	-5.376699455	4.157505063	2.326510485
N	-5.503743089	6.422983542	2.011975691
N	-6.396967807	4.448522311	1.520622601
C	-4.846731559	5.377073184	2.614064875
C	-6.477952746	5.841963978	1.324957307
C	-7.509600796	6.341267032	0.48967702
C	-8.397320111	5.436726739	-0.099678651
C	-8.276525437	4.053487507	0.125751713
C	-7.263511857	3.559129042	0.946096262
H	-7.577370735	7.417612179	0.334317235
H	-9.197263076	5.808468353	-0.745271644
H	-8.97024656	3.348019947	-0.334773085
H	-7.091520251	2.509308917	1.178768724
N	-0.295278217	6.061690134	6.000389067

C	-0.449791851	6.226837482	7.362808374
C	0.974523599	6.068181872	5.457028664
C	-1.721753992	6.23081023	7.981081246
C	0.699322983	6.39889217	8.185236585
C	2.102674581	6.244246146	6.306995823
C	1.200355259	5.905782765	4.070396406
C	-1.821430281	6.398682989	9.352157226
H	-2.601825983	6.099770703	7.354046299
O	1.943979909	6.404015196	7.645076089
C	0.590999468	6.567364042	9.567169889
C	3.404215246	6.25931761	5.80143835
C	2.493960794	5.921708311	3.576127423
H	0.339127421	5.771398578	3.418421232
C	-0.670073252	6.567183476	10.15114347
H	-2.808181226	6.400176982	9.819134383
H	1.504655554	6.694874011	10.14971776
C	3.600146573	6.098037559	4.435072914
H	4.232244956	6.398213372	6.498178128
H	2.656882309	5.796020783	2.504015452
H	-0.7675847	6.69791723	11.23059194
H	4.612906976	6.108319205	4.027685843

XYZ Coordinates of *p*-PXZ-TP in T₁ optimized geometry

C	-1.448263205	5.795596564	5.159333808
C	-1.986875188	4.51850615	4.93492338
C	-3.100562324	4.379848837	4.10944139
C	-3.684760773	5.504824329	3.497736832
C	-3.127320256	6.783493343	3.733776546
C	-2.01675184	6.925881728	4.559222048

H	-1.526754842	3.649195521	5.409403904
H	-3.530620503	3.393544457	3.92527443
H	-3.584585948	7.651654842	3.256804639
H	-1.579572854	7.909624079	4.74502982
N	-5.422829326	4.172294352	2.380838388
N	-5.434194878	6.418634698	1.993063604
N	-6.425718486	4.486552606	1.54855525
C	-4.850280751	5.365039931	2.623185201
C	-6.432316673	5.866894157	1.310351086
C	-7.42388384	6.393120719	0.447101887
C	-8.338907951	5.526225662	-0.12048996
C	-8.289860405	4.132205367	0.153587778
C	-7.325208903	3.622440584	0.993276429
H	-7.433140813	7.466782732	0.257120919
H	-9.111314493	5.912673547	-0.789640431
H	-9.013585599	3.450991679	-0.296489989
H	-7.208261201	2.572270713	1.261448231
N	-0.295093712	5.937279608	6.00875461
C	-0.471541195	6.114122608	7.369069266
C	0.963769418	5.981826807	5.440335325
C	-1.730914527	6.036443349	8.015591968
C	0.686964479	6.448267317	8.172403144
C	2.088701833	6.334604657	6.286475252
C	1.213452115	5.752907988	4.061921364
C	-1.839332497	6.263555086	9.372964368
H	-2.613500525	5.795202522	7.422211917
O	1.911493679	6.551291149	7.608742003
C	0.557993112	6.693767394	9.546702226
C	3.375268108	6.46588815	5.748838029

C	2.489306616	5.867844251	3.550965658
H	0.377844836	5.487876803	3.413001183
C	-0.682830049	6.601562606	10.15439178
H	-2.816025872	6.188590895	9.855381171
H	1.458660544	6.95424985	10.10713538
C	3.590513075	6.237695052	4.399136064
H	4.186566364	6.746597929	6.424335074
H	2.663830024	5.677937729	2.489893321
H	-0.783186794	6.791050905	11.22495155
H	4.593079021	6.34087275	3.979610153

XYZ Coordinates of *p*-NPP-TP in S₀ optimized geometry

C	-1.444061	5.889801	5.131723
C	-1.935749	4.600799	4.885009
C	-3.049824	4.419339	4.066938
C	-3.686621	5.527613	3.480632
C	-3.188978	6.818287	3.729681
C	-2.076102	6.996606	4.550321
H	-1.433728	3.746195	5.343878
H	-3.437396	3.417709	3.871785
H	-3.689406	7.672665	3.270456
H	-1.683363	7.996085	4.749528
N	-5.385732	4.141886	2.363065
N	-5.491215	6.388146	2.003473
N	-6.412488	4.426124	1.545626
C	-4.861232	5.351663	2.61184
C	-6.475549	5.806188	1.325691
C	-7.497762	6.304277	0.481557
C	-8.383866	5.411316	-0.083834

C	-8.276852	4.014014	0.17286
C	-7.284181	3.534038	0.99196
H	-7.551093	7.379185	0.305624
H	-9.179827	5.774508	-0.738132
H	-8.979983	3.311126	-0.276366
H	-7.123094	2.485972	1.246062
N	-0.304128	6.075485	5.973206
C	-0.491444	6.244636	7.35984
C	0.98112	6.108232	5.396276
C	0.638951	6.46216	8.192332
C	-1.765375	6.205764	7.938395
C	2.111431	6.327811	6.228272
C	1.173469	5.929625	4.021421
C	0.446777	6.631977	9.568313
N	1.923617	6.503328	7.614252
C	-1.941998	6.376525	9.319726
H	-2.633178	6.039847	7.300022
C	3.385307	6.364654	5.649422
C	2.456785	5.968764	3.455657
H	0.307238	5.758901	3.38214
C	-0.836534	6.589583	10.134091
H	1.312938	6.800361	10.208271
C	3.061953	6.718596	8.451437
H	-2.949537	6.340325	9.740985
C	3.562058	6.187066	4.268894
H	4.252896	6.535525	6.286719
H	2.573355	5.827529	2.378403
H	-0.95315	6.725112	11.212095
C	3.514469	8.021054	8.698072

C	3.728616	5.627578	9.023751
H	4.569475	6.22245	3.847224
C	4.631008	8.23076	9.512466
H	2.982669	8.860192	8.243978
C	4.844962	5.839361	9.837814
H	3.362403	4.618488	8.821815
C	5.29739	7.140613	10.082942
H	4.981816	9.248648	9.70209
H	5.36351	4.985539	10.281913
H	6.170809	7.305272	10.719442

XYZ Coordinates of *p*-NPP-TP in S₁ optimized geometry

C	-1.462462766	5.91845961	5.129015943
C	-1.93619255	4.613935046	4.875547972
C	-3.03843593	4.426639071	4.059278161
C	-3.712666752	5.535521955	3.459591701
C	-3.209521493	6.844491644	3.735398624
C	-2.108131704	7.032262468	4.552677201
H	-1.430219362	3.754822081	5.325463471
H	-3.411849281	3.420985447	3.858767729
H	-3.720151392	7.695389904	3.281530591
H	-1.735117606	8.040775373	4.753392715
N	-5.368060274	4.13103204	2.325970232
N	-5.528788759	6.391914387	2.00810104
N	-6.395374425	4.404707258	1.524268202
C	-4.855622341	5.356681872	2.608352302
C	-6.498822589	5.794873425	1.325228118
C	-7.540655619	6.279112355	0.493828925
C	-8.419827103	5.356845106	-0.090758997

C	-8.277329917	3.978708473	0.137259823
C	-7.252627576	3.497242315	0.955026025
H	-7.624648385	7.353803869	0.336739653
H	-9.22817222	5.715039751	-0.733573018
H	-8.963067865	3.26229029	-0.318801416
H	-7.063761853	2.451230532	1.189572511
N	-0.30097632	6.11558203	5.982235767
C	-0.471420068	6.281855414	7.344147579
C	0.963213972	6.137435358	5.422714631
C	0.66418183	6.479343113	8.190813742
C	-1.759545175	6.260532873	7.92443333
C	2.111989984	6.333820772	6.25156329
C	1.14636005	5.96888527	4.03185131
C	0.48001383	6.648279552	9.577831375
N	1.932955455	6.500728737	7.620960421
C	-1.91615258	6.428123116	9.290424044
H	-2.616852809	6.109996965	7.27179699
C	3.396267496	6.355166203	5.671414507
C	2.418212061	5.99393424	3.483920391
H	0.266247396	5.820883102	3.40973889
C	-0.796436122	6.622594912	10.12125902
H	1.347459223	6.799140981	10.21857902
C	3.084810809	6.70205817	8.465238787
H	-2.919173917	6.408607813	9.720990529
C	3.547197832	6.187169873	4.302367624
H	4.268214772	6.50480896	6.306286295
H	2.540026643	5.862438677	2.407017562
H	-0.926442986	6.754382269	11.19728293
C	3.543770243	8.000794326	8.703753198

C	3.724737606	5.595605352	9.031313895
H	4.547109931	6.205960359	3.864341663
C	4.661155876	8.191828555	9.521278386
H	3.02552254	8.848125077	8.24950851
C	4.841368146	5.79519666	9.847858784
H	3.345923834	4.59137631	8.829188077
C	5.308869933	7.091059727	10.09261881
H	5.025634929	9.203950512	9.711747393
H	5.346721199	4.935140202	10.2933638
H	6.182118147	7.243733249	10.73133493

XYZ Coordinates of *p*-NPP-TP in T₁ optimized geometry

C	-1.439121505	5.759486166	5.155515463
C	-1.972650528	4.486628264	4.892548109
C	-3.087377117	4.364592113	4.067160638
C	-3.682688863	5.503485313	3.490468073
C	-3.131778352	6.778213247	3.764489551
C	-2.019761462	6.902285324	4.59077874
H	-1.506202387	3.606276124	5.340015558
H	-3.511839374	3.381317284	3.855548619
H	-3.596194494	7.657566215	3.315629685
H	-1.58947029	7.883325914	4.805340371
N	-5.415662295	4.19117797	2.343118311
N	-5.447360652	6.44826415	2.02232494
N	-6.425939979	4.521638001	1.527075498
C	-4.85012434	5.38117129	2.618399383
C	-6.44529916	5.90882766	1.329954114
C	-7.44770417	6.451995649	0.489879524
C	-8.360970969	5.594217215	-0.096787986

C	-8.298891662	4.194124319	0.135281342
C	-7.322896782	3.667084472	0.952723711
H	-7.467136357	7.530688076	0.332070728
H	-9.141645919	5.99431517	-0.748178831
H	-9.020640972	3.520431815	-0.329182717
H	-7.195626557	2.61050151	1.188816388
N	-0.285828553	5.882735269	6.008006114
C	-0.474642444	6.049813557	7.37050756
C	0.973037145	5.911087249	5.430625094
C	0.669964996	6.369463805	8.203852775
C	-1.753889053	5.962091236	7.971758608
C	2.119793951	6.239998495	6.258405734
C	1.174980696	5.674667539	4.048267505
C	0.466685405	6.592566811	9.586919877
N	1.92183209	6.457850717	7.613488022
C	-1.919675611	6.169217488	9.32702683
H	-2.613171892	5.728868123	7.343103998
C	3.39513655	6.336062719	5.653139254
C	2.434180471	5.757113793	3.488564848
H	0.313068819	5.429608037	3.427652365
C	-0.793080682	6.494644828	10.14643719
H	1.323074853	6.842559336	10.21328539
C	3.054541421	6.792148389	8.435137682
H	-2.914277822	6.086189525	9.769976512
C	3.561066602	6.101168631	4.301145558
H	4.254676115	6.597313018	6.270638923
H	2.566861364	5.562026985	2.422357212
H	-0.925575764	6.670395582	11.21608707
C	3.400938049	8.133108709	8.619355174

C	3.791230628	5.768083319	9.036577792
H	4.554670841	6.181853564	3.855439677
C	4.504001413	8.452923458	9.419782698
H	2.806185261	8.911173224	8.136369341
C	4.893654295	6.094249266	9.835673913
H	3.496243099	4.729489751	8.873349199
C	5.247960705	7.434216027	10.02623354
H	4.781063487	9.499406065	9.569020925
H	5.474966416	5.299139755	10.30905881
H	6.108887336	7.686455469	10.65081860