

Computational Insights into the Synergistic Modulation of ΔE_{ST} , Spin-Orbit Coupling, and Reorganization Energy in Phthalimide- Based TADF Emitters

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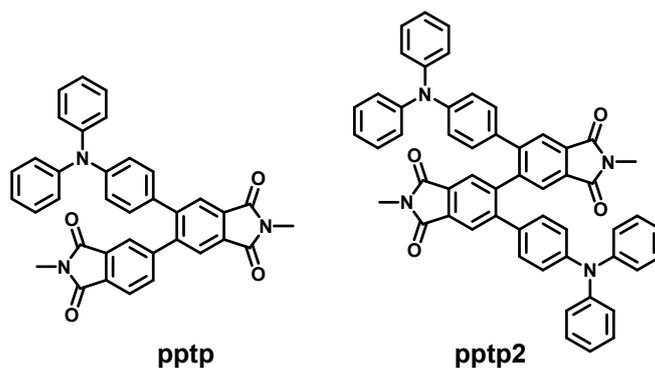


Figure S1. Structures of the reported molecules.

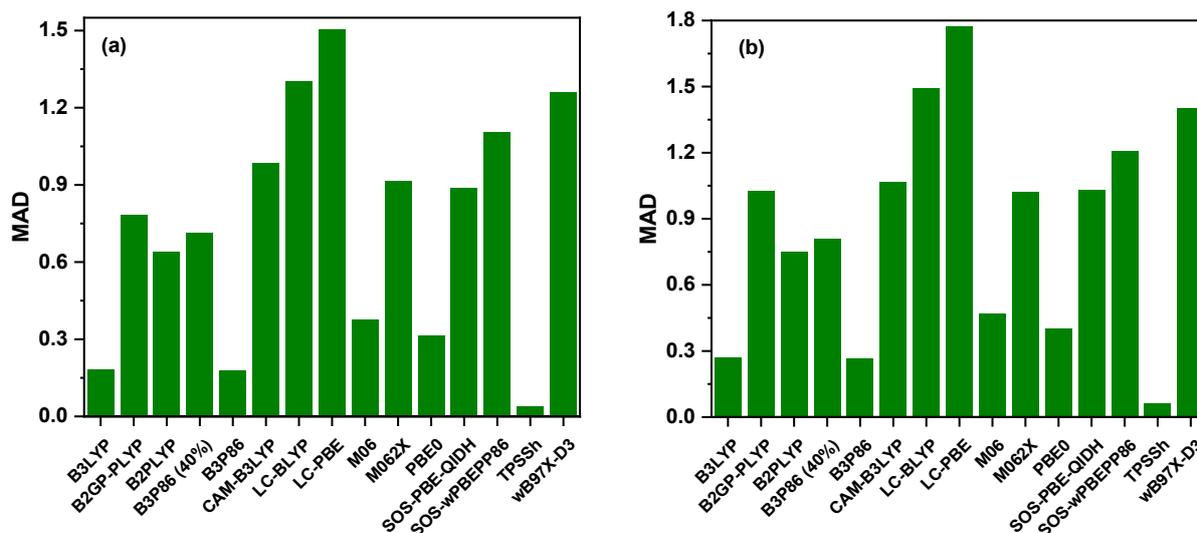


Figure S2. Calculated MAD from benchmarking results for (a) *pptp* and (b) *pptp2* reported molecules involving S_1 , T_1 and ΔE_{ST} parameters.

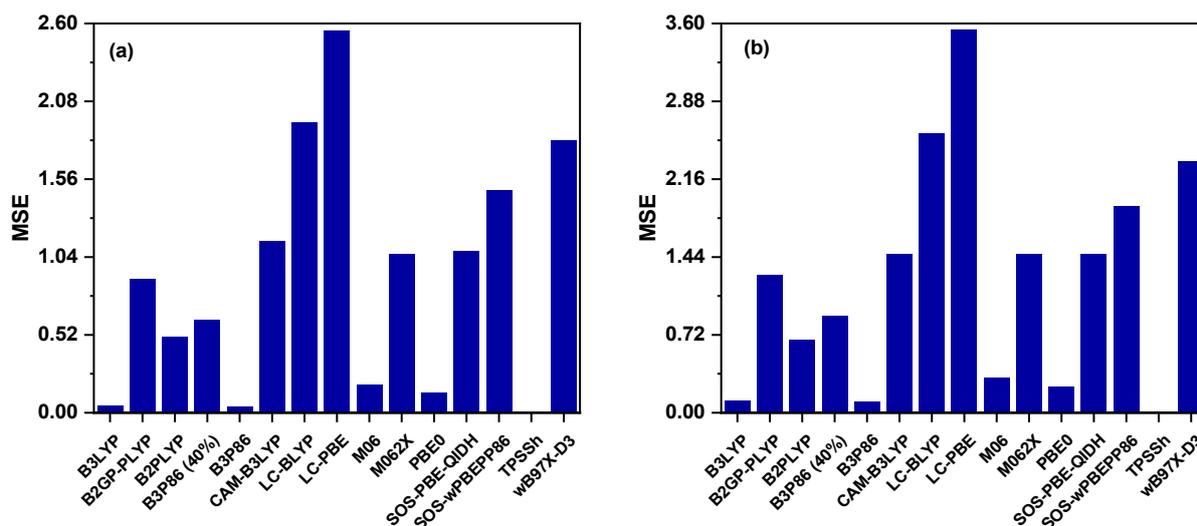


Figure S3. Calculated MSE from benchmarking results for (a) *pptp* and (b) *pptp2* reported molecules involving S_1 , T_1 and ΔE_{ST} parameters.

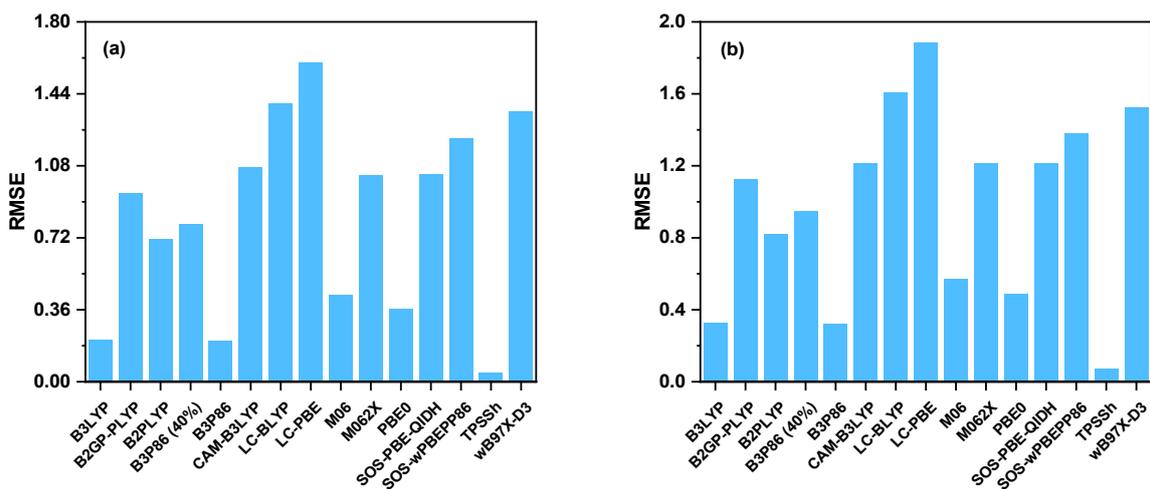


Figure S4. Calculated RMSE from benchmarking results for (a) *pptp* and (b) *pptp2* reported molecules involving S_1 , T_1 and ΔE_{ST} parameters.

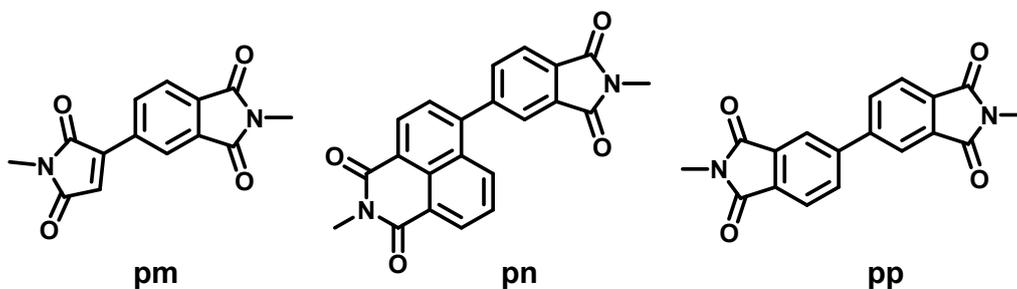


Figure S5. Structures of the proposed dimers.

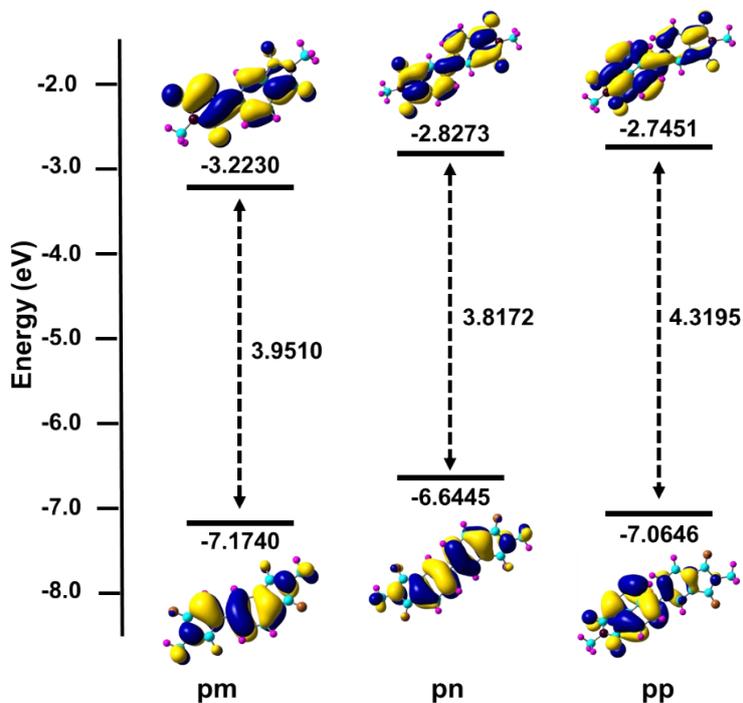


Figure S6. HOMO-LUMO distributions and levels of the dimers.

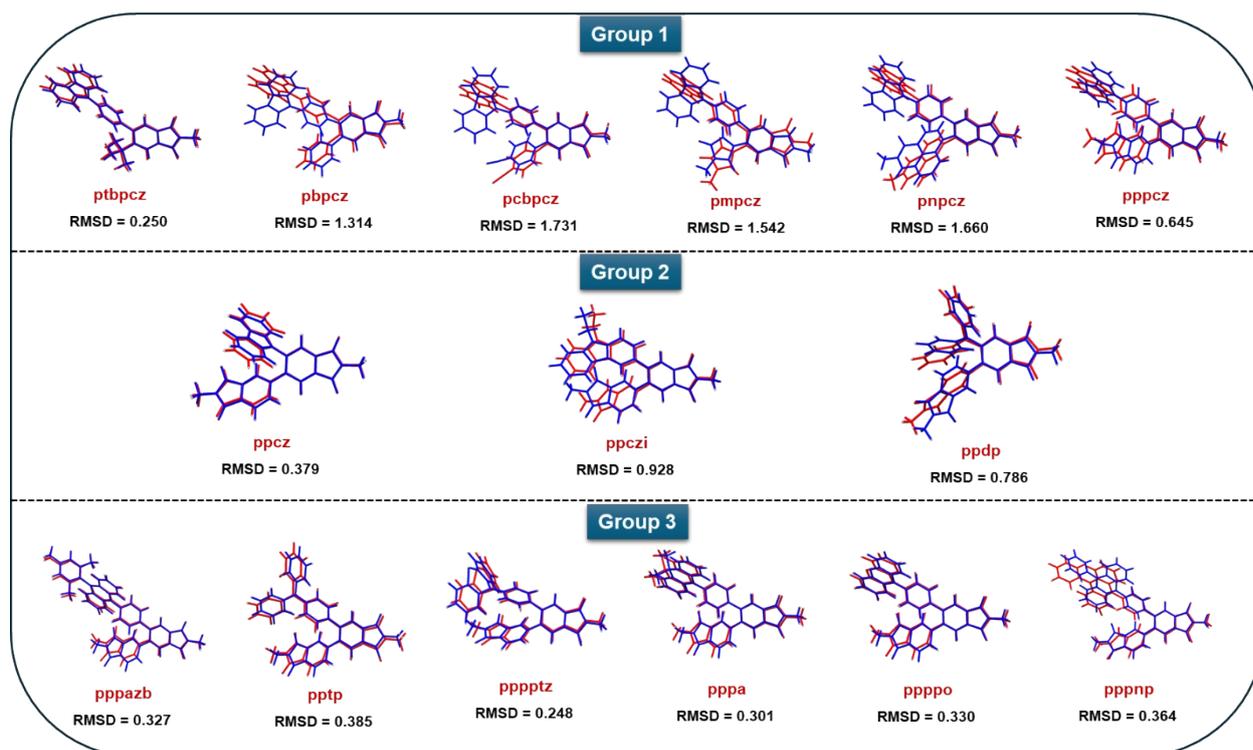


Figure S7. Structural variations between the S_0 and S_1 states for the molecules. (Color codes: Blue: S_1 and Red: S_0)

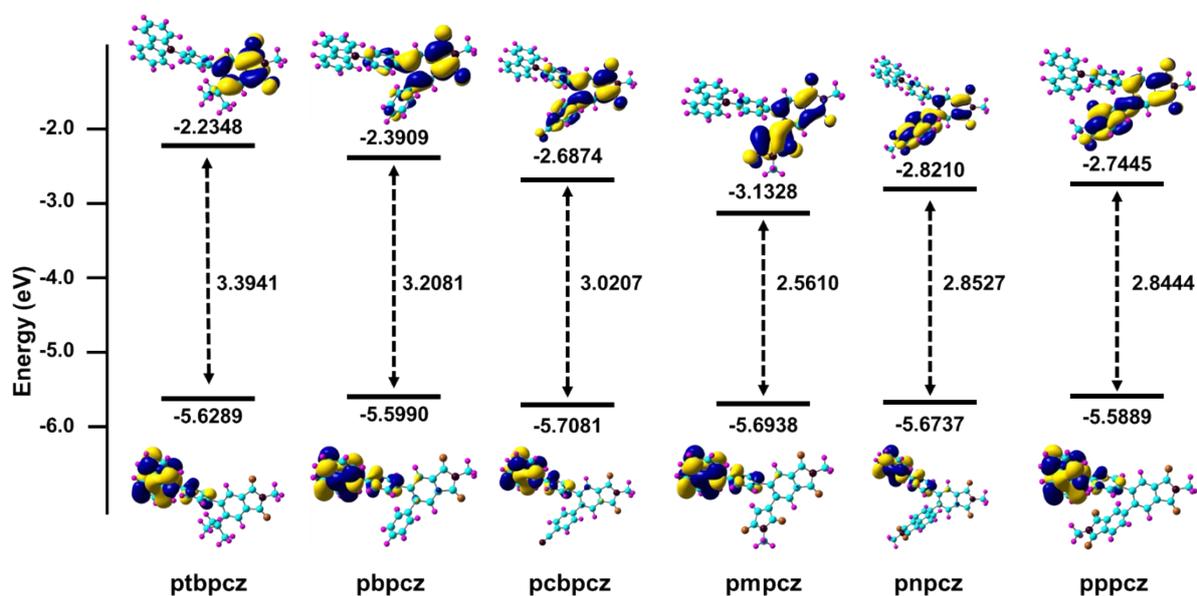


Figure S8. HOMO & LUMO levels of the **Group 1** molecules.

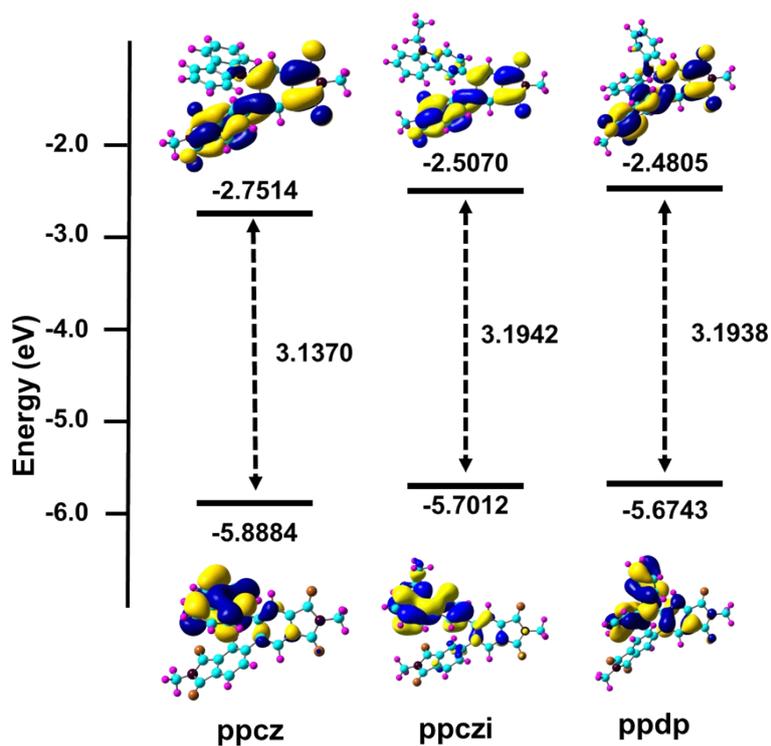


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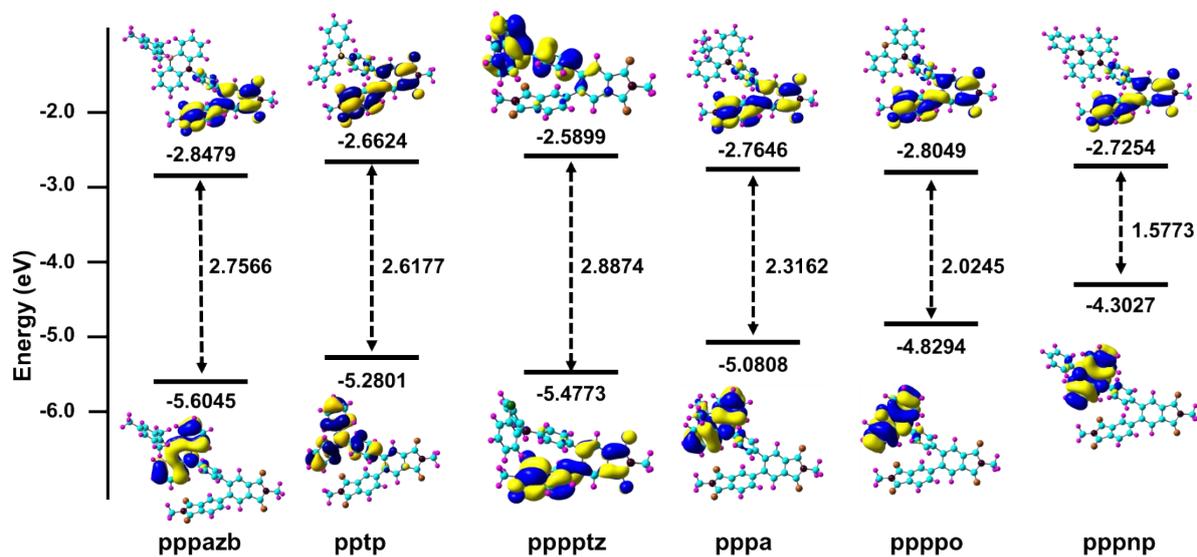


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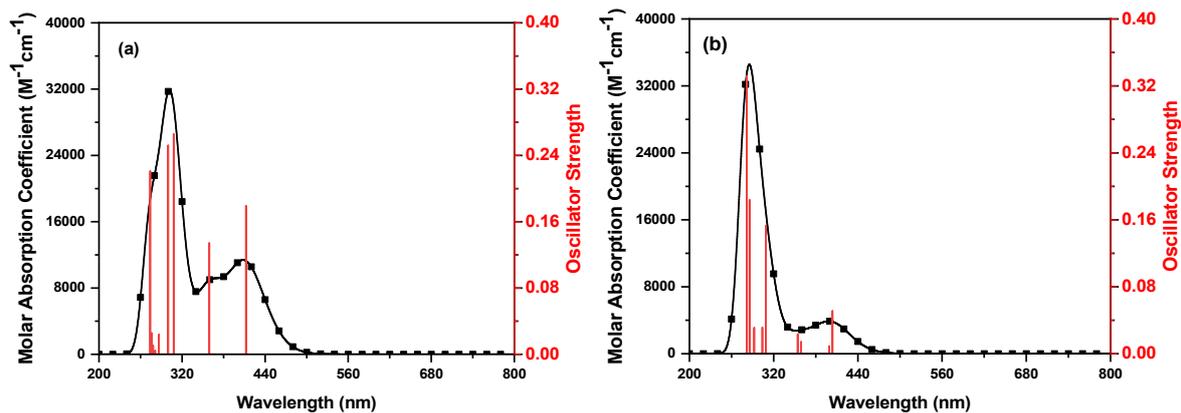


Figure S11. Simulated absorption spectra for (a) *pptp* and (b) *pptp2* using 0.45 eV FWHM.

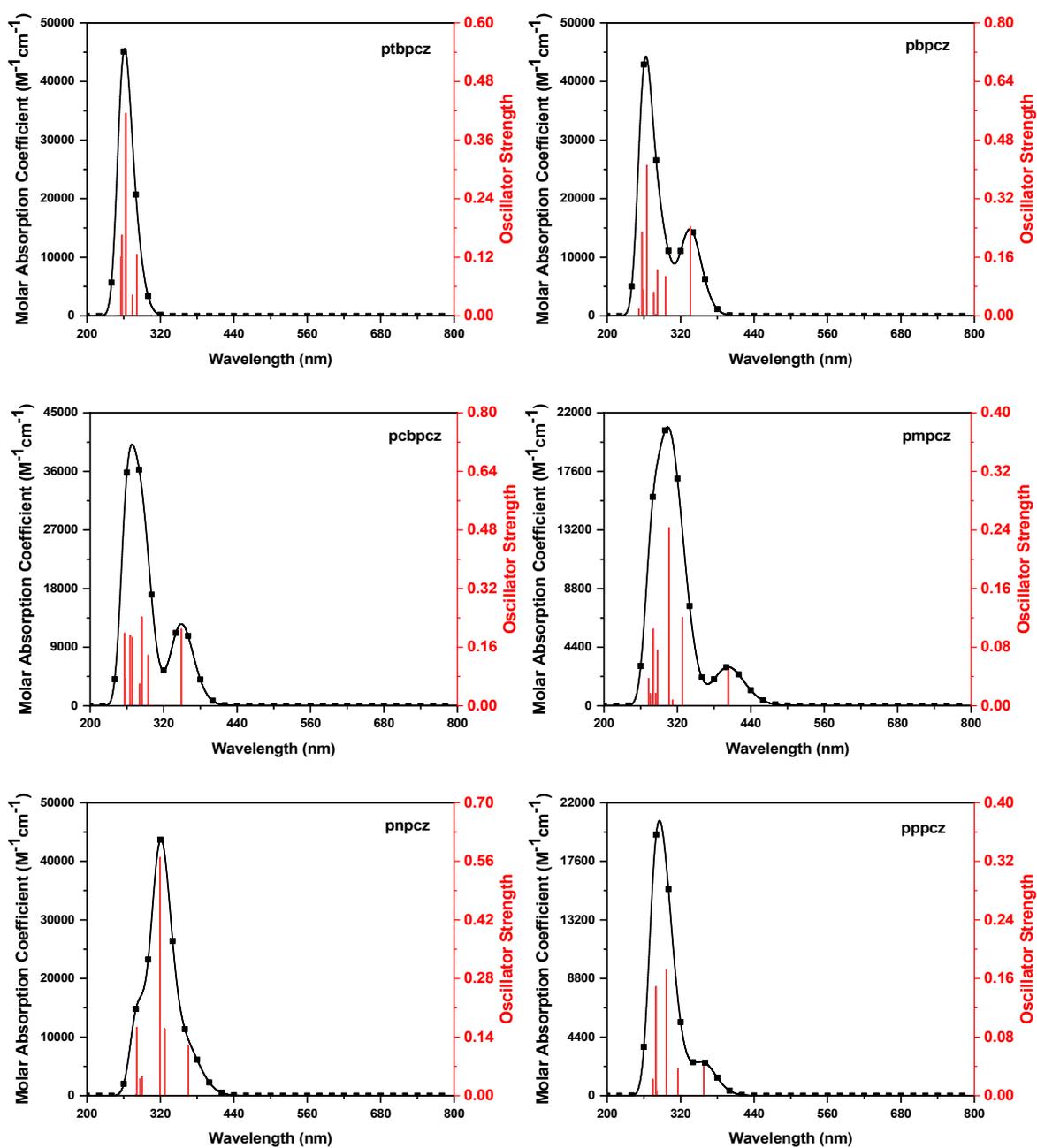


Figure S12. Simulated absorption spectra for the **Group 1** molecules using 0.45 eV FWHM.

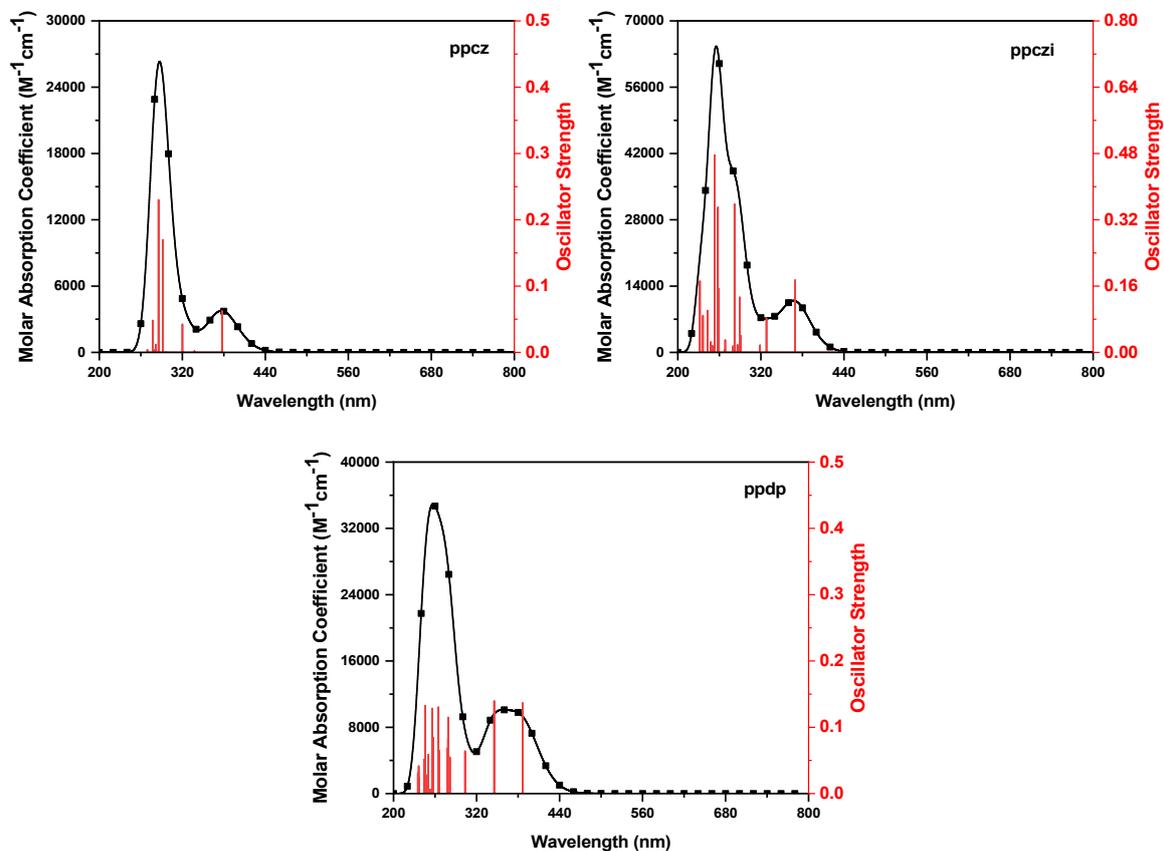


Figure S13. Simulated absorption spectra for the **Group 2** molecules using 0.45 eV FWHM.

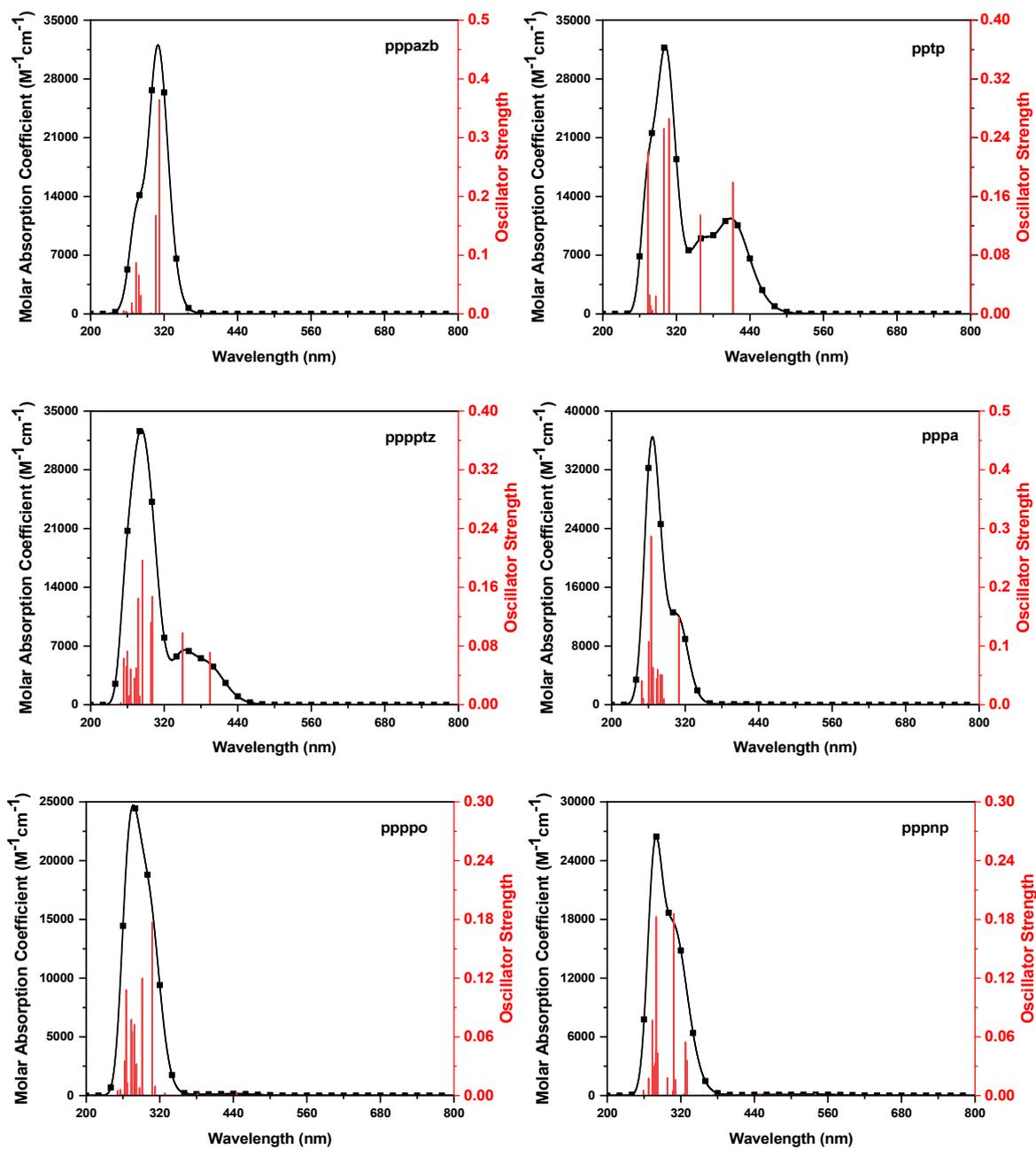


Figure S14. Simulated absorption spectra for the **Group 3** molecules using 0.45 eV FWHM.

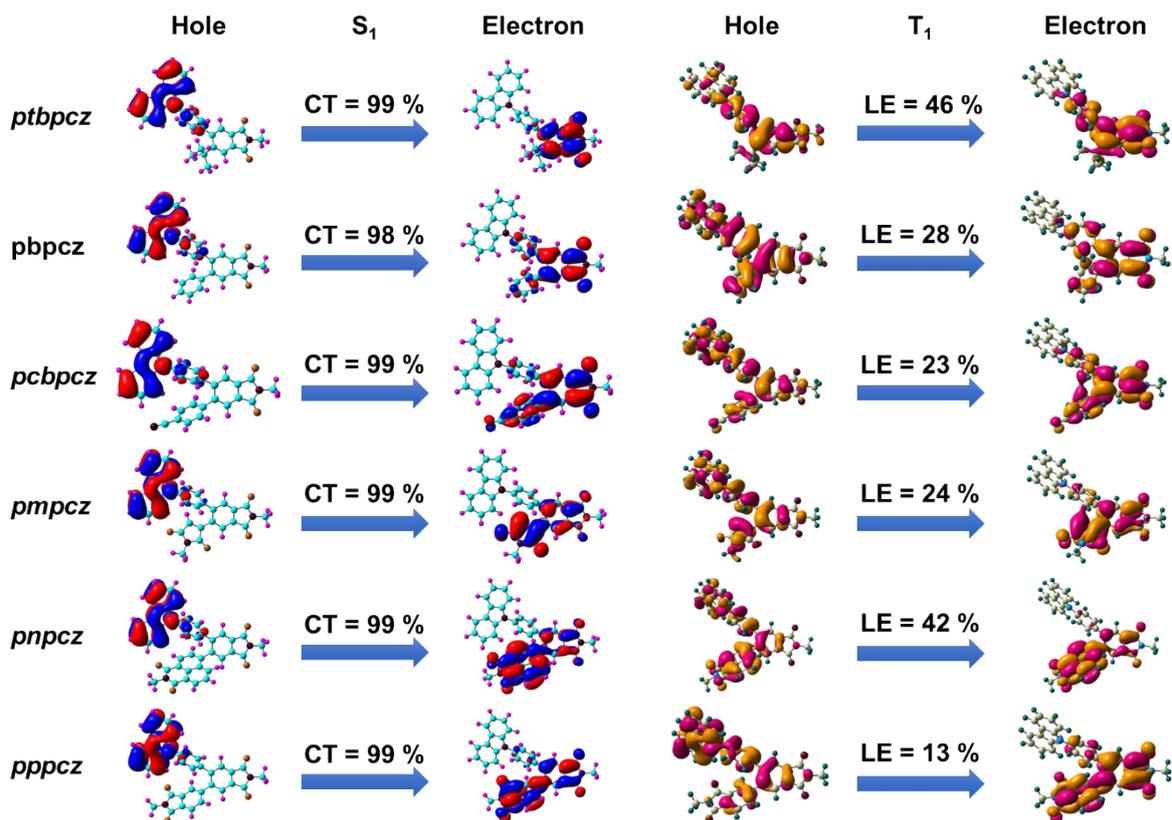


Figure 15. Natural transition orbital analysis of S_1 and T_1 states for **Group 1** molecules.

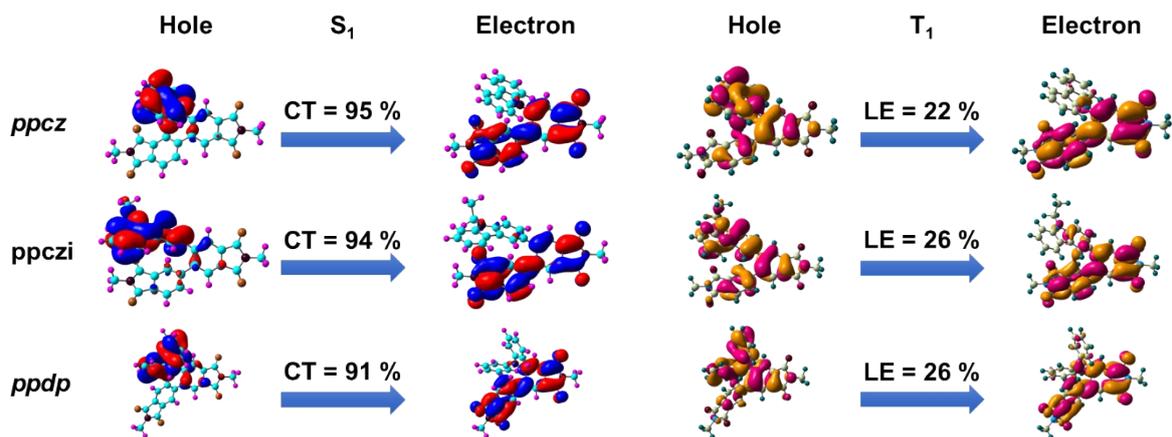


Figure 16. Natural transition orbital analysis of S_1 and T_1 states for **Group 2** molecules.

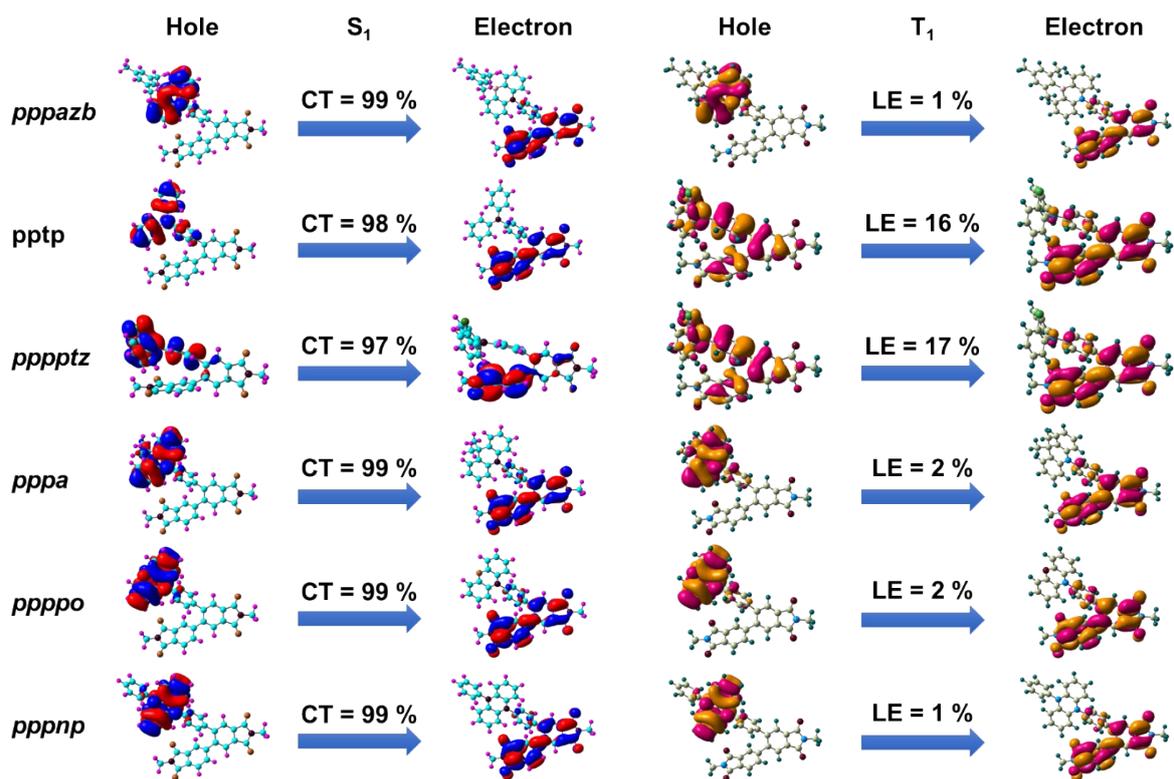


Figure 17. Natural transition orbital analysis of S_1 and T_1 states for **Group 3** molecules.

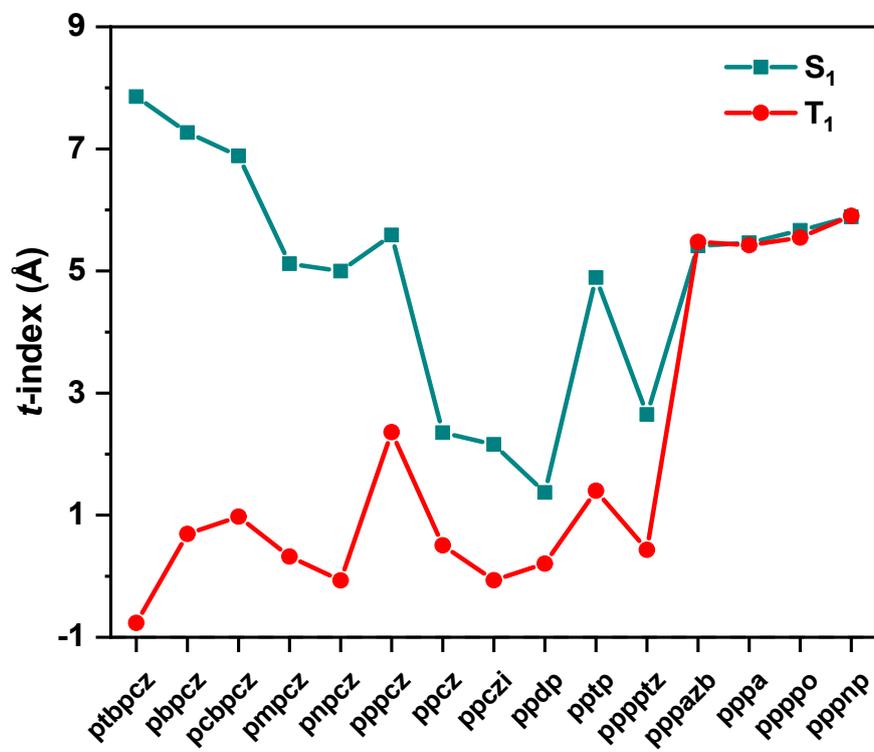


Figure S18. Plot of t -index of molecules at the S_1 state and T_1 state geometries.

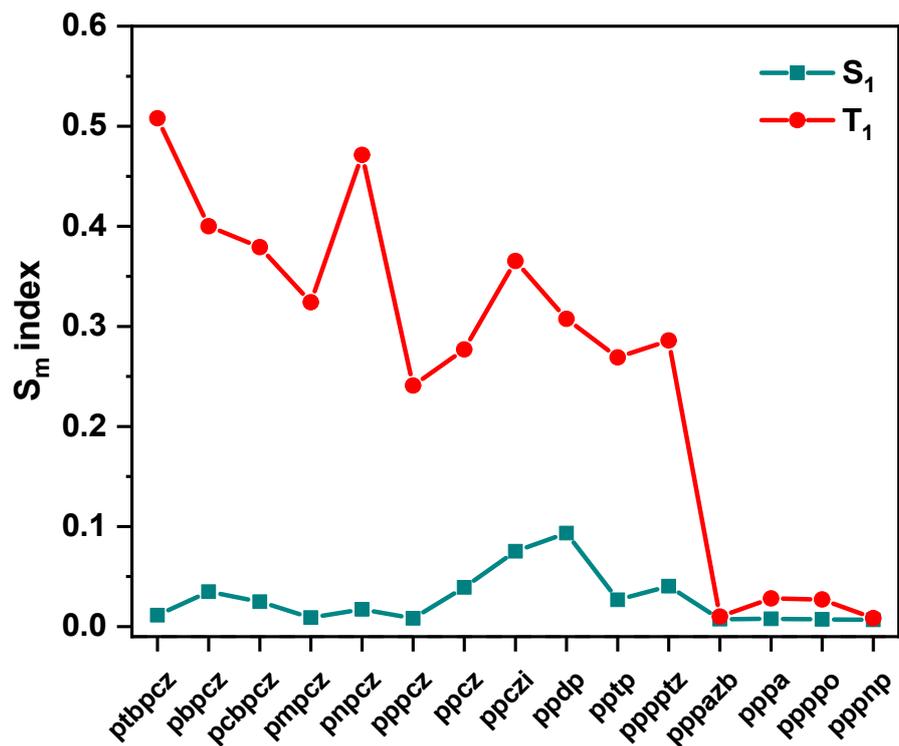


Figure S19. Plot of S_m index of molecules at the S_1 state and T_1 state geometries.

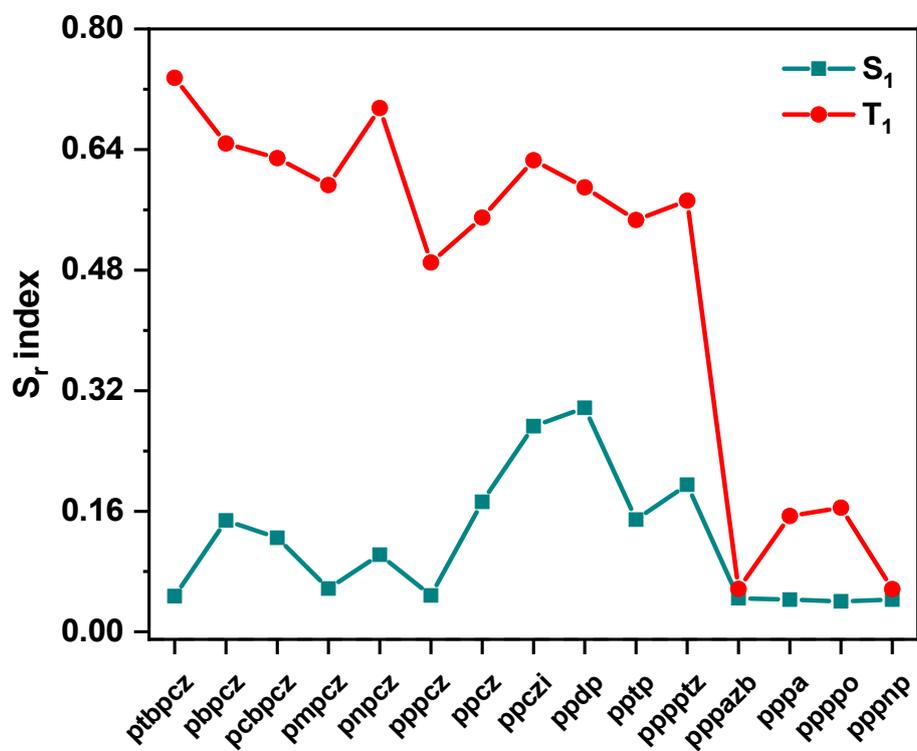


Figure S20. Plot of S_r index of molecules at the S_1 state and T_1 state geometries.

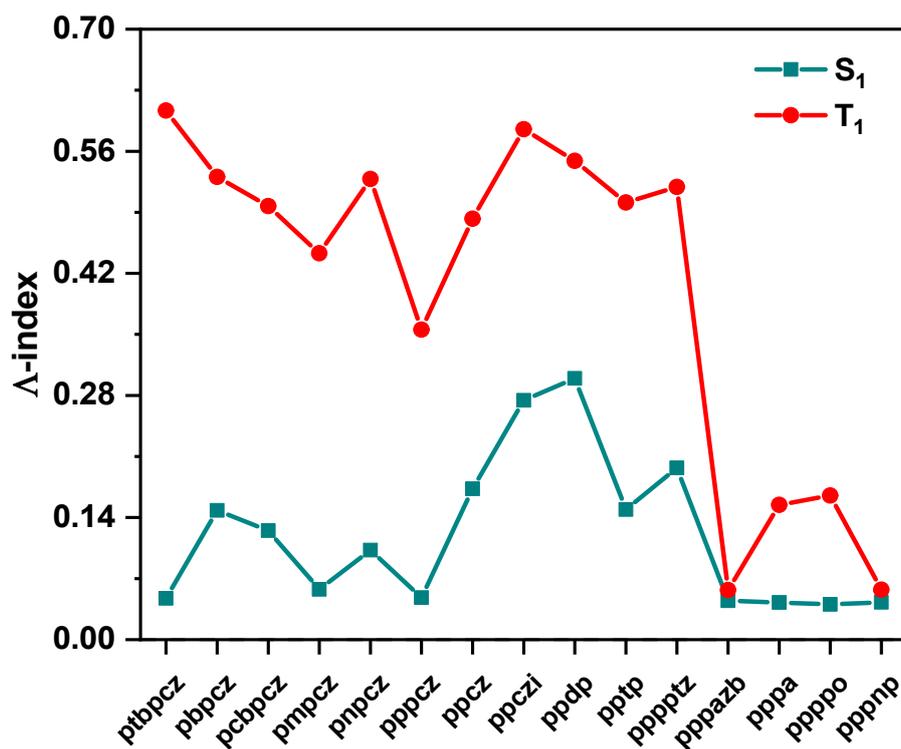


Figure S21. Plot of Λ index of molecules at the S₁ state and T₁ state geometries.

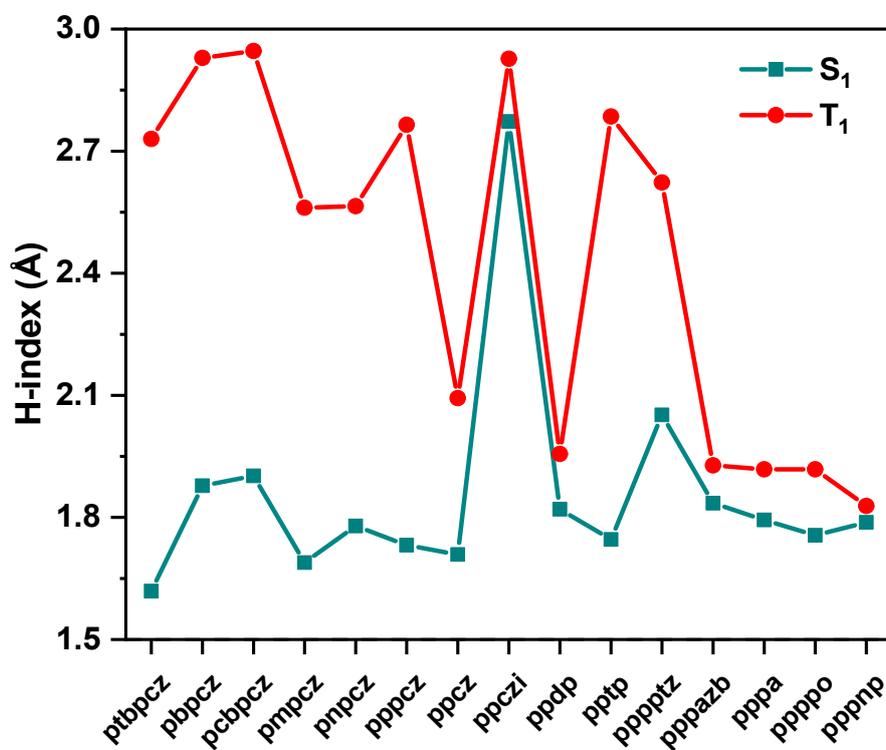


Figure S22. Plot of H-index of molecules at the S₁ state and T₁ state geometries.

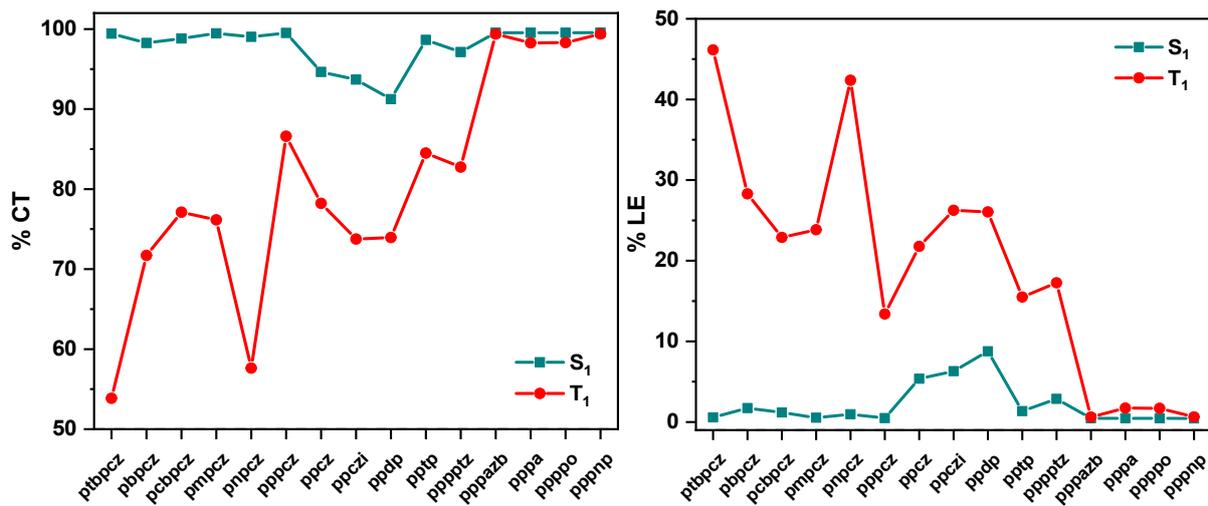


Figure S23. Plot of (a) % CT (b) %LE of molecules at the S_1 state and T_1 state geometries.

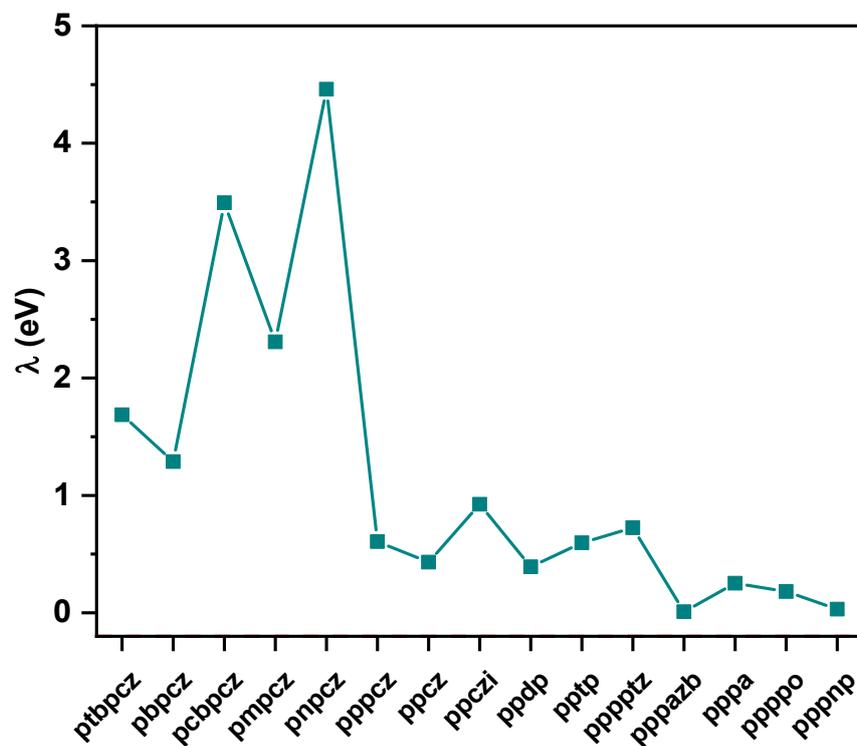


Figure S24. Calculated reorganization energy between the S_1 and T_1 states for the molecules

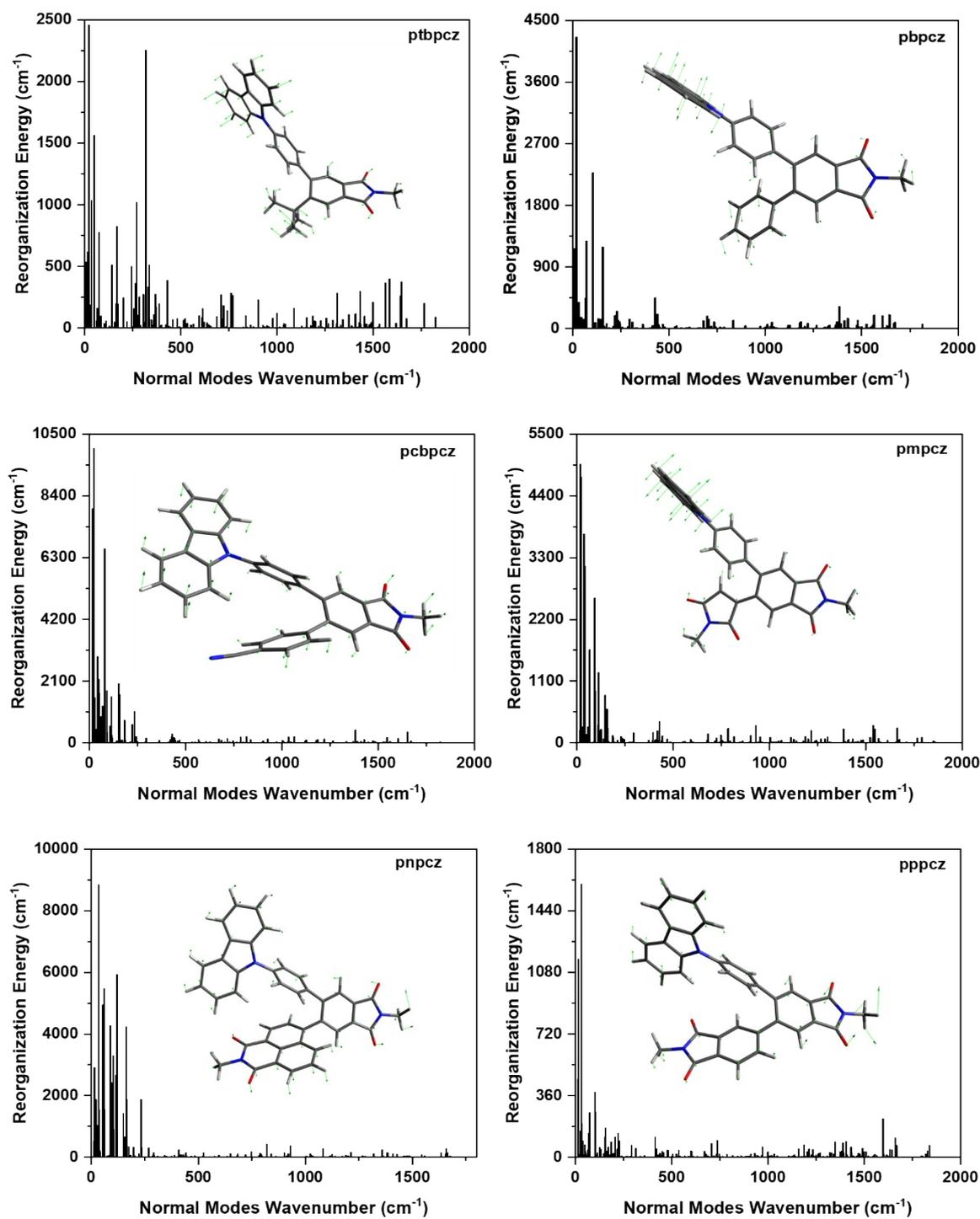


Figure S25. Reorganization energy vs the normal mode frequencies between the S_1 and T_1 states for **Group 1** molecules.

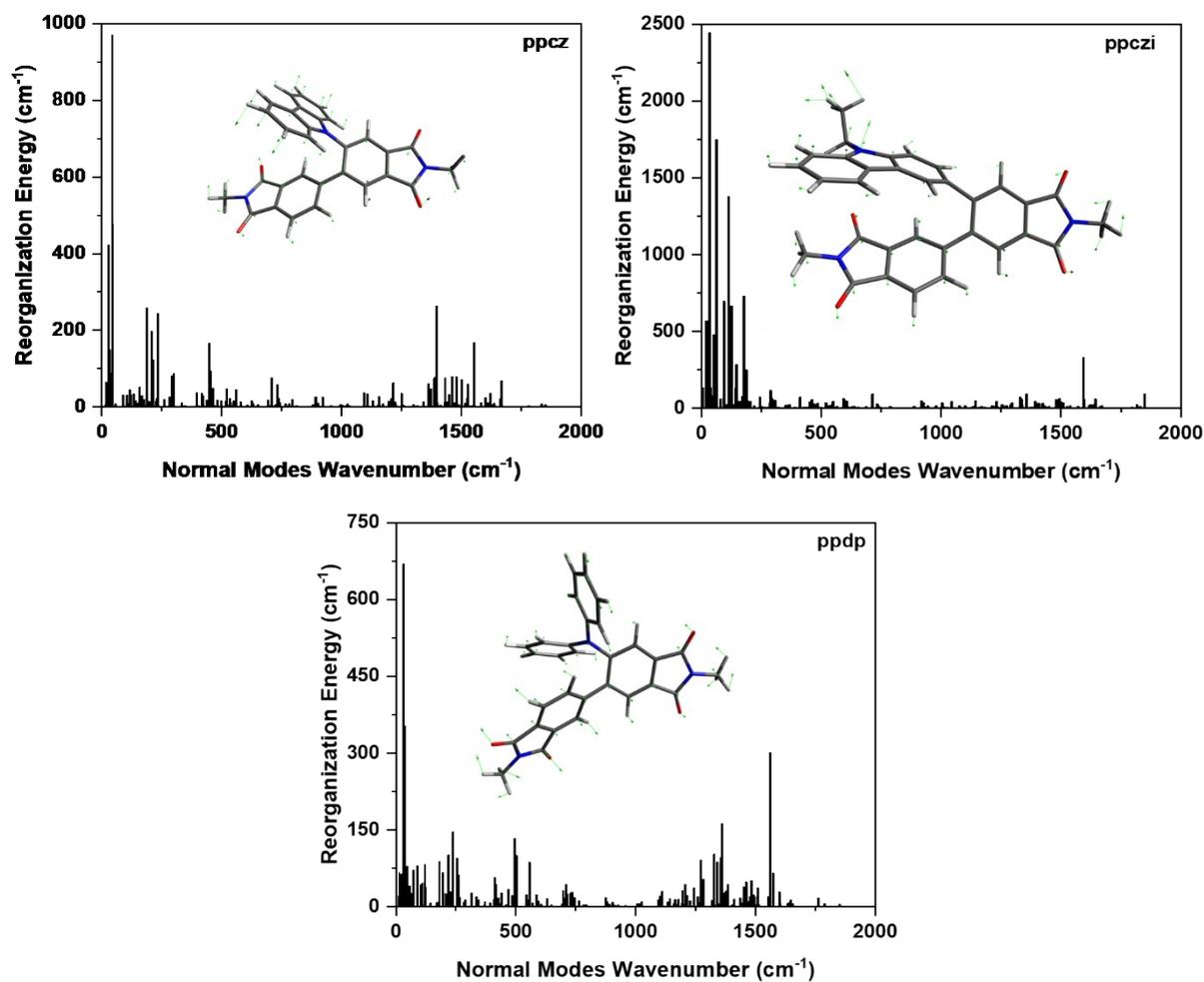


Figure S26. Reorganization energy vs the normal mode frequencies between the S_1 and T_1 states for **Group 2** molecules.

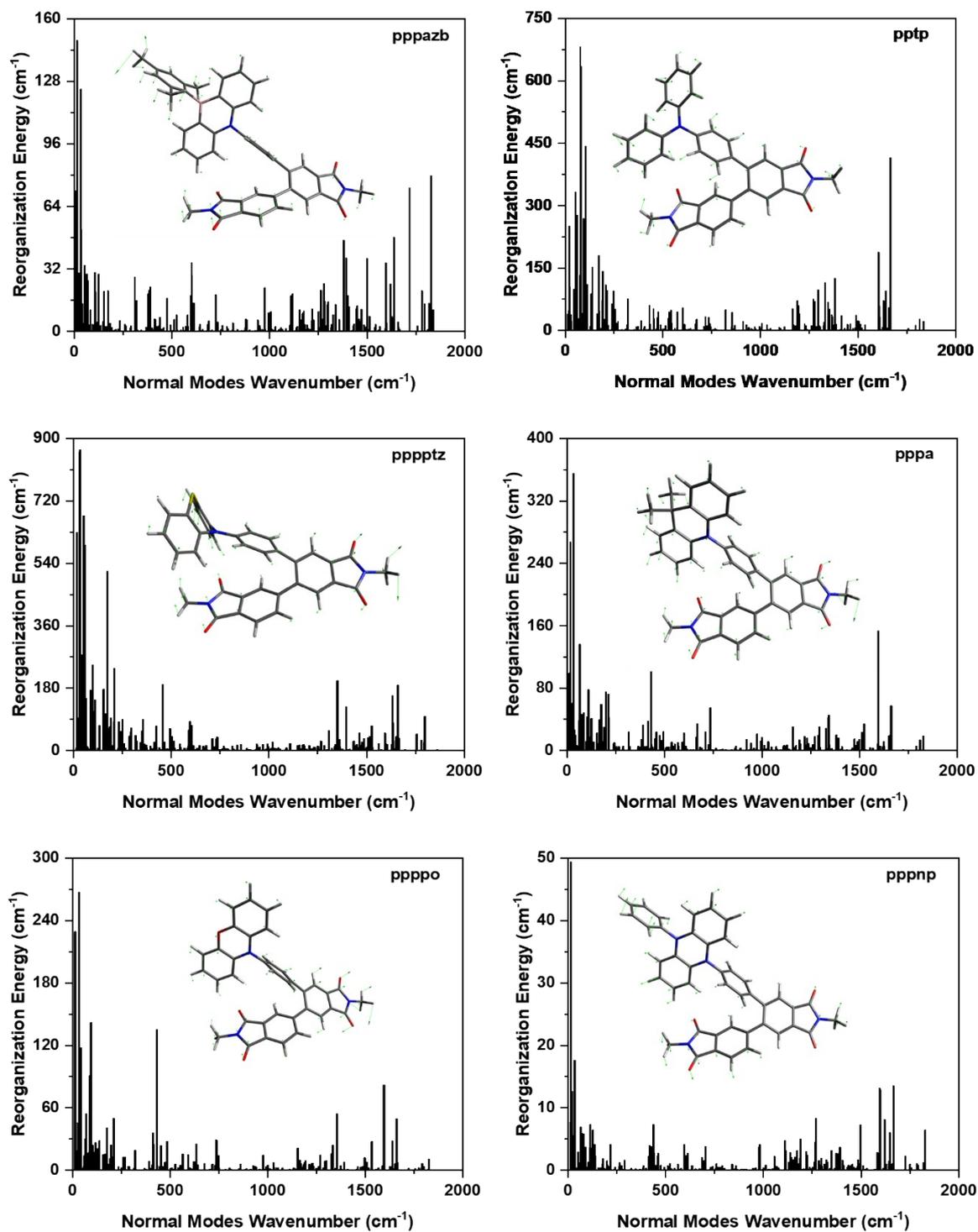


Figure S27. Reorganization energy vs the normal mode frequencies between the S_1 and T_1 states for **Group 3** molecules.

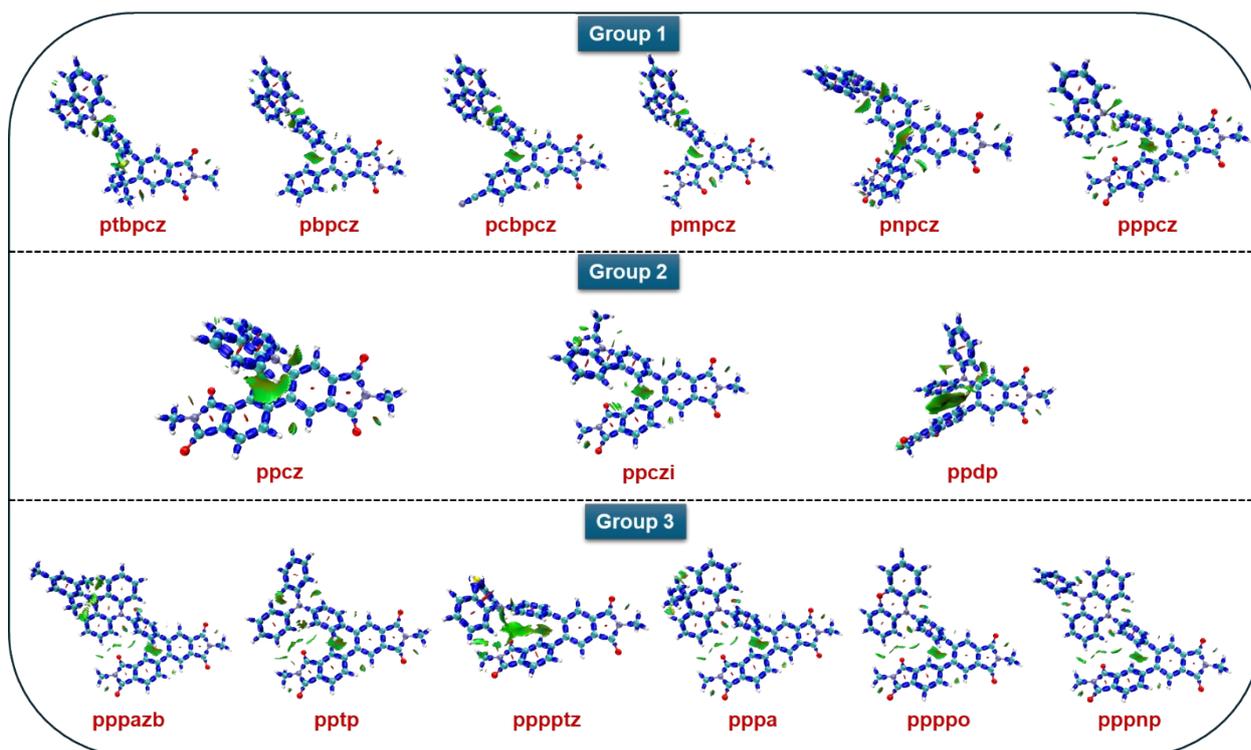


Figure S28. The IRI isosurface map of all the molecules.

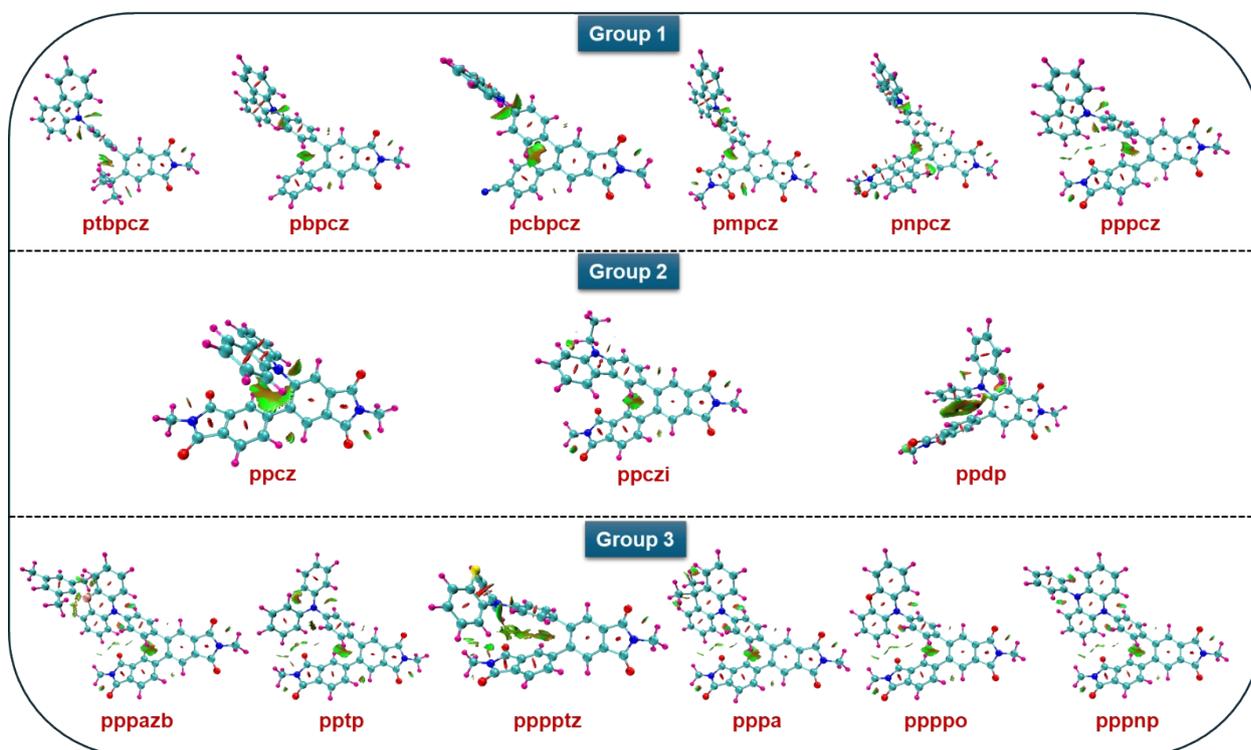


Figure S29. The NCI isosurface map of all the molecules.

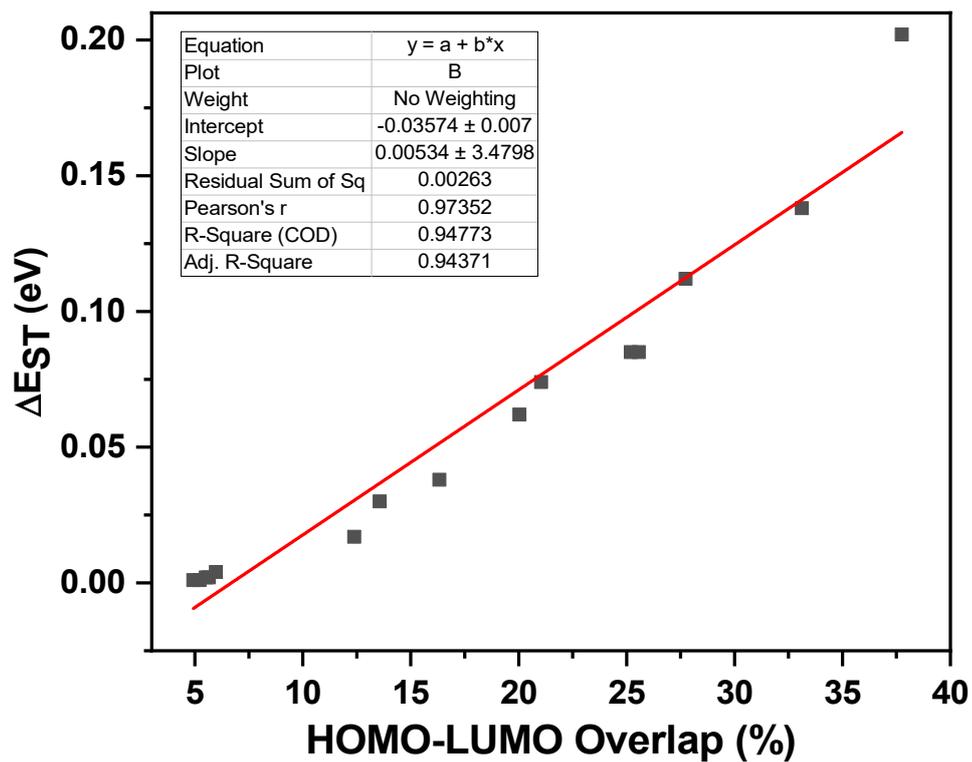


Figure S30. The relationship of the HOMO-LUMO overlap with the predicted energy gap between the S_1 and T_1 states at the S_0 geometry.

Table S1. Benchmarking data of ΔE_{ST} , S_1 and T_1 energies for *pptp* molecule.

Functionals	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV)	MAD	MSE	RMSE	MAPE
B3LYP	2.212	2.112	0.100	0.182	0.045	0.211	25.405
B2GP-PLYP	3.077	3.048	0.029	0.784	0.894	0.945	59.440
B2PLYP	2.692	2.828	-0.136	0.638	0.508	0.713	130.993
B3P86 (40%)	3.007	2.677	0.330	0.712	0.620	0.787	163.564
B3P86	2.207	2.102	0.105	0.179	0.042	0.205	27.629
CAM-B3LYP	3.418	2.894	0.524	0.986	1.147	1.071	271.011
LC-BLYP	3.891	3.072	0.819	1.302	1.939	1.392	429.078
LC-PBE	4.198	3.059	1.139	1.506	2.554	1.598	593.325
M06	2.503	2.370	0.133	0.376	0.190	0.436	51.422
M062X	3.311	2.983	0.328	0.915	1.062	1.031	173.247
PBE0	2.411	2.281	0.130	0.315	0.132	0.363	46.762
SOS-PBE-QIDH	3.270	3.077	0.193	0.888	1.081	1.039	107.054
SOS- ω PBEP86	3.594	3.112	0.482	1.104	1.484	1.218	257.026
TPSSH	1.895	1.811	0.084	0.040	0.002	0.044	10.283
ω B97X-D3	3.826	3.067	0.759	1.258	1.823	1.350	398.021
Reported	1.940	1.870	0.067	-	-	-	-

Table S2. Benchmarking data of ΔE_{ST} , S_1 and T_1 energies for *pptp2* molecule.

Functionals	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV)	MAD	MSE	RMSE	MAPE
B3LYP	2.262	2.225	0.037	0.269	0.109	0.329	15.499
B2GP-PLYP	2.990	3.360	-0.370	1.026	1.272	1.128	406.351
B2PLYP	2.665	2.944	-0.279	0.749	0.671	0.819	313.083
B3P86 (40%)	3.070	2.922	0.148	0.807	0.897	0.947	138.359
B3P86	2.256	2.218	0.038	0.265	0.105	0.324	14.386
CAM-B3LYP	3.461	3.153	0.308	1.068	1.471	1.213	289.948
LC-BLYP	4.094	3.299	0.795	1.490	2.584	1.607	731.159
LC-PBE	4.518	3.263	1.255	1.773	3.543	1.882	1141.607
M06	2.560	2.512	0.048	0.467	0.323	0.568	33.991
M062X	3.387	3.259	0.128	1.019	1.470	1.213	132.668
PBE0	2.460	2.416	0.044	0.401	0.238	0.488	26.932
SOS-PBE-QIDH	3.278	3.366	-0.088	1.030	1.472	1.213	164.254
SOS- ω PBEP86	3.668	3.366	0.302	1.206	1.910	1.382	292.295
TPSSH	1.945	1.913	0.032	0.061	0.005	0.073	8.490
ω B97X-D3	3.959	3.302	0.657	1.400	2.328	1.526	607.742
Reported	1.860	1.820	0.038	-	-	-	-

Table S3. Photophysical data of the dimers: *pm*, *pn* and *pp*.

Dimers	HOMO (eV)	LUMO (eV)	H-L gap (eV)	ΔE_{ST} (eV)
<i>pm</i>	-7.173	-3.222	3.951	0.823
<i>pn</i>	-6.644	-2.827	3.817	1.081
<i>pp</i>	-7.065	-2.745	4.320	0.746

Table S4. Dihedral angles of the molecules at S₀, S₁ and T₁ optimized geometries.

Molecules	Dihedral angle	S ₀	S ₁	T ₁	Δ S ₀ -S ₁	Δ S ₀ -T ₁	Δ S ₁ -T ₁
<i>ptbpcz</i>	α	-	-	-	-	-	-
	γ	89.49	85.91	46.3	3.58	43.19	39.61
	γ'	54.73	61.67	50.79	6.94	3.94	10.88
<i>pbpcz</i>	α	51.95	46.8	34.46	5.15	17.49	12.34
	γ	50.48	46.04	29.63	4.44	20.85	16.41
	γ'	54.52	66.06	50.25	11.54	4.27	15.81
<i>pcbpcz</i>	α	51.52	46.15	32.6	5.37	18.92	13.55
	γ	50.49	55.64	30.43	5.15	20.06	25.21
	γ'	53.53	63.21	49.48	9.68	4.05	13.73
<i>pmpcz</i>	α	36.17	24.44	18.67	11.73	17.5	5.77
	γ	56.97	65.35	40.38	8.38	16.59	24.97
	γ'	53.55	74.63	49.94	21.08	3.61	24.69
<i>pnpcz</i>	α	66.02	58.27	52.19	7.75	13.83	6.08
	γ	48.15	55.18	45.88	7.03	2.27	9.3
	γ'	53.56	67.08	52.06	13.52	1.5	15.02
<i>pppcz</i>	α	51.91	34.53	26.05	17.38	25.86	8.48
	γ	62.5	53.92	40.15	8.58	22.35	13.77
	γ'	65.82	88.9	58.05	23.08	7.77	30.85
<i>ppcz</i>	α	47.84	34.09	28.3	13.75	19.54	5.79
	β	62.1	75.74	50.82	13.64	11.28	24.92
<i>ppczi</i>	α	50.28	33.12	29.17	17.16	21.11	3.95
	β	48.91	57.87	28.99	8.96	19.92	28.88
<i>ppdp</i>	α	67.68	39.53	34.22	28.15	33.46	5.31
	β	-	-	-	-	-	-
	α	48.32	34.28	30.84	14.04	3.44	3.44
<i>pptp</i>	γ	47.42	57.58	29.01	10.16	28.57	28.57
	γ'	-	-	-	-	-	-
	α	55.25	58.3	27.45	3.05	27.8	30.85
<i>pppptz</i>	γ	63.03	70.35	39.51	7.32	23.52	30.84
	γ'	48.52	39.72	45.95	8.8	2.57	6.23
	α	49.93	34.2	43.25	15.73	6.68	9.05
<i>pppazb</i>	γ	52.64	52.96	50.48	0.32	2.16	2.48
	γ'	88.42	89.93	85.99	1.51	2.43	3.94
	α	50.4	34.44	29.5	15.96	20.9	4.94
<i>pppa</i>	γ	52.64	52.57	40.53	0.07	12.11	12.04
	γ'	88.34	89.83	75.28	1.49	13.06	14.55
	α	50.16	34.36	31.62	15.8	18.54	2.74
<i>ppppo</i>	γ	53.4	52.32	43.28	1.08	10.12	9.04
	γ'	86.71	89.36	73.94	2.65	12.77	15.42
	α	50.95	34.58	37.61	16.37	13.34	3.03
<i>ppnp</i>	γ	53.03	51.81	45.82	1.22	7.21	5.99
	γ'	87.2	88.94	89.39	1.74	2.19	0.45

Table S5. ΔE_{ST} , SOC using TPSSh functional of the molecules at S_0 , S_1 and T_1 optimized geometries and RMSD values.

Molecules	HOMO-LUMO overlap	ΔE_{ST} (S_0), eV	ΔE_{ST} (S_1), eV	ΔE_{ST} (T_1), eV	ΔE_{ST} (adia), eV	SOC (S_0), cm^{-1}	SOC (S_1), cm^{-1}	SOC (T_1), cm^{-1}	RMSD (S_0-S_1)	RMSD (S_0-T_1)	RMSD (S_1-T_1)
<i>ptbpcz</i>	5.98	0.004	0.002	0.665	0.649	0.017	0.000	0.506	0.251	1.386	1.495
<i>pbpcz</i>	21.04	0.074	0.034	0.414	0.339	0.153	0.094	0.343	1.314	0.471	1.632
<i>pcbpcz</i>	20.04	0.062	0.020	0.328	0.216	0.123	0.030	0.338	1.731	0.480	2.058
<i>pmpcz</i>	13.56	0.030	0.004	0.271	0.036	0.066	0.014	0.390	1.542	0.325	1.755
<i>pnpcz</i>	16.33	0.038	0.011	0.143	-0.047	0.070	0.030	0.202	1.660	0.259	1.681
<i>pppcz</i>	12.38	0.017	0.001	0.148	-0.005	0.047	0.000	0.254	0.645	0.529	0.821
<i>ppcz</i>	27.73	0.112	0.030	0.298	0.025	0.163	0.079	0.395	0.379	0.311	0.396
<i>ppczi</i>	33.12	0.138	0.087	0.431	0.254	0.068	0.059	0.128	0.928	0.342	0.931
<i>ppdp</i>	37.75	0.202	0.105	0.395	0.082	0.357	0.130	0.275	0.786	0.689	0.484
<i>pptp</i>	25.20	0.085	0.026	0.341	-0.088	0.066	0.014	0.114	0.385	0.238	0.403
<i>pppptz</i>	25.57	0.085	0.048	0.347	0.016	0.066	0.037	0.178	0.249	0.400	0.586
<i>pppazb</i>	4.93	0.001	0.000	0.001	-0.272	0.000	0.000	0.017	0.327	0.280	0.426
<i>pppa</i>	5.22	0.001	0.001	0.031	-0.069	0.000	0.000	0.066	0.301	0.469	0.475
<i>ppppo</i>	5.65	0.002	0.001	0.038	-0.138	0.000	0.000	0.035	0.330	0.389	0.466
<i>pppnp</i>	5.51	0.002	0.001	0.002	-0.079	0.000	0.000	0.000	0.364	0.298	0.193

Table S6. Benchmarking for λ_{abs} calculations for pptp and pptp2 and the calculated λ_{abs} in toluene solvent for all molecules using B3P86 (40%) functional.

Functionals	pptp	Pptp2		Molecules	λ_{abs} (nm)
B3LYP	560.4	548.1		<i>ptbpcz</i>	305.4
B2GP-PLYP	402.9	414.6		<i>pbpcz</i>	335.7
B2PLYP	460.6	465.2		<i>pcbpcz</i>	349.1
B3P86 (40%)	412.3	403.8		<i>pmpcz</i>	402.7
B3P86	561.8	549.5		<i>pnpcz</i>	365.4
CAM-B3LYP	362.8	358.2		<i>pppcz</i>	357.5
LC-BLYP	318.7	302.9		<i>ppcz</i>	377.1
LC-PBE	295.3	274.4		<i>ppczi</i>	369.6
M06	495.3	484.3		<i>ppdp</i>	386.5
M062X	374.4	366.1		<i>pptp</i>	412
PBE0	514.3	503.9		<i>pppptz</i>	403.5
SOS-PBE-QIDH	379.1	378.3		<i>pppazb</i>	358.7
SOS-ωPBEP86	345	338		<i>pppa</i>	394.7
TPSSh	654.2	637.5		<i>pppo</i>	413.1
ωB97X-D3	324	313.2		<i>pppnp</i>	445.2
Reported	413	410			

Table S7. Charge transfer indices for S₁ and T₁ excited states of the molecules.

Mol.	States	S _m (a.u.)	S _r (a.u.)	D (Å)	H (Å)	t (Å)	HDI	EDI	Λ	%CT	%LE
<i>ptbpcz</i>	S ₁	0.011	0.047	8.571	1.619	7.856	8.590	9.460	0.047	99.43	0.57
	T ₁	0.508	0.735	1.544	2.730	-0.765	6.040	7.000	0.607	53.85	46.15
<i>pbpcz</i>	S ₁	0.035	0.148	8.312	1.878	7.268	8.520	8.660	0.148	98.27	1.73
	T ₁	0.400	0.648	2.951	2.929	0.694	5.110	6.890	0.531	71.71	28.29
<i>pcbpcz</i>	S ₁	0.025	0.125	7.956	1.902	6.885	8.510	7.990	0.125	98.82	1.19
	T ₁	0.379	0.629	3.528	2.946	0.976	5.490	6.340	0.497	77.11	22.89
<i>pmpcz</i>	S ₁	0.009	0.057	6.205	1.689	5.120	8.680	8.550	0.058	99.47	0.53
	T ₁	0.324	0.593	2.573	2.561	0.323	5.580	7.390	0.443	76.15	23.85
<i>pnpcz</i>	S ₁	0.017	0.102	6.205	1.779	4.999	8.510	6.020	0.103	99.03	0.97
	T ₁	0.471	0.695	2.192	2.565	-0.068	4.990	5.850	0.528	57.62	42.38
<i>pppcz</i>	S ₁	0.008	0.048	6.731	1.732	5.589	8.760	6.370	0.048	99.51	0.49
	T ₁	0.241	0.490	4.716	2.765	2.359	6.350	6.040	0.356	86.61	13.39
<i>ppcz</i>	S ₁	0.039	0.172	3.806	1.709	2.350	8.500	6.970	0.173	94.64	5.36
	T ₁	0.277	0.550	2.462	2.093	0.507	7.240	6.340	0.483	78.22	21.78
<i>ppczi</i>	S ₁	0.075	0.273	3.621	2.773	2.160	8.390	6.340	0.274	93.69	6.31
	T ₁	0.365	0.626	2.359	2.927	-0.065	5.860	5.930	0.585	73.75	26.25
<i>ppdp</i>	S ₁	0.093	0.297	2.526	1.820	1.371	9.150	6.430	0.300	91.23	8.77
	T ₁	0.308	0.590	1.785	1.956	0.207	8.090	6.460	0.549	73.95	26.05
<i>pptp</i>	S ₁	0.027	0.149	6.202	1.746	4.892	9.430	6.600	0.149	98.65	1.35
	T ₁	0.269	0.547	3.863	2.785	1.401	7.180	5.710	0.501	84.50	15.50
<i>pppptz</i>	S ₁	0.040	0.195	3.012	2.052	2.648	8.470	8.730	0.197	97.13	2.87
	T ₁	0.286	0.572	2.670	2.623	0.433	6.980	5.910	0.519	82.74	17.26
<i>pppazb</i>	S ₁	0.007	0.045	6.370	1.835	5.412	8.170	6.400	0.045	99.54	0.47
	T ₁	0.010	0.057	6.664	1.928	5.476	8.430	6.200	0.057	99.38	0.62
<i>pppa</i>	S ₁	0.008	0.043	6.311	1.794	5.461	9.310	6.290	0.043	99.54	0.47
	T ₁	0.028	0.154	6.566	1.918	5.423	9.310	6.110	0.154	98.27	1.73
<i>ppppo</i>	S ₁	0.007	0.040	6.480	1.756	5.666	9.540	6.370	0.040	99.55	0.45
	T ₁	0.027	0.165	6.728	1.918	5.548	9.580	6.050	0.165	98.30	1.70
<i>pppnp</i>	S ₁	0.007	0.043	6.786	1.788	5.887	8.940	6.300	0.043	99.56	0.44
	T ₁	0.008	0.057	6.921	1.828	5.903	8.760	6.130	0.057	99.38	0.63

Table S8. Oscillator strength, rate of radiative processes, RISC rates, SOC, computed at the B3LYP/def2-svp level of theory.

Molecules	f ($S_1 \rightarrow S_0$)	k_r (s^{-1}) ($S_1 \rightarrow S_0$)	λ (eV) (S_1-T_1)	SOC (S_1-T_1 , cm^{-1})	k_{RISC} (s^{-1}) (T_1-S_1)
ptbpcz	0.00005	1.93×10^4	1.687	0.489	3.64
pbpcz	0.08885	3.16×10^7	1.288	0.348	6.03
pcbpcz	0.07966	2.47×10^7	3.493	0.389	6.25×10^{-9}
pmpcz	0.02006	4.09×10^6	2.309	0.411	2.29×10^{-3}
pnpcz	0.03534	9.55×10^6	4.460	0.221	1.64×10^{-13}
pppcz	0.01617	4.23×10^6	0.606	0.315	6.00×10^4
ppcz	0.03720	1.09×10^7	0.432	0.045	6.54×10^4
ppczi	0.08175	2.70×10^7	0.925	0.354	6.70×10^{-1}
ppdp	0.03332	1.02×10^7	0.391	0.045	6.46×10^2
pptp	0.07308	1.56×10^7	0.596	0.136	1.91×10^3
pppztz	0.03371	8.30×10^6	0.725	0.085	2.63×10^2
pppazb	0.00081	1.99×10^5	0.009	0.340	1.79×10^7
pppa	0.00097	1.57×10^5	0.252	0.299	3.86×10^6
ppppo	0.00174	2.05×10^5	0.181	0.032	9.93×10^4
pppnp	0.00172	1.09×10^5	0.032	0.000	0.00

XYZ Coordinates of *ptbpcz* in S_0 optimized geometry

C	8.123319	-4.243255	12.264458
H	8.409853	-3.686029	13.169812
H	7.692031	-5.213625	12.544372
H	9.028152	-4.400564	11.656490
N	7.124216	-3.512928	11.514131
C	5.853776	-4.021379	11.187641
O	5.437575	-5.115510	11.489103
C	5.181965	-2.930786	10.416423
C	3.926717	-2.858250	9.838354
H	3.234239	-3.700046	9.909631
C	3.540007	-1.685877	9.149967
C	4.430413	-0.571090	9.043377

C	5.702103	-0.693005	9.651732
H	6.432103	0.112418	9.613017
C	6.056041	-1.853070	10.319941
C	7.323639	-2.211524	11.028733
O	8.330277	-1.558860	11.180172
C	4.079534	0.752590	8.309559
C	2.882374	1.451404	8.995892
H	2.705140	2.433186	8.527029
H	1.955477	0.872957	8.905069
H	3.084436	1.618483	10.066247
C	3.749452	0.490711	6.821335
H	3.609991	1.450245	6.297375
H	2.827870	-0.088299	6.693044
H	4.570853	-0.050063	6.324086
C	5.259104	1.749050	8.338528
H	4.969644	2.666861	7.804082
H	6.155041	1.347807	7.839726
H	5.533313	2.042362	9.363731
C	2.155313	-1.760964	8.572681
C	1.034456	-1.393084	9.334063
H	1.178065	-0.988787	10.338888
C	-0.259312	-1.547846	8.833645
H	-1.123893	-1.271596	9.440294
C	-0.460249	-2.073727	7.548948
C	0.651232	-2.465706	6.787918
H	0.498268	-2.876163	5.787985
C	1.939485	-2.325432	7.304901
H	2.797253	-2.640138	6.705731
N	-1.769628	-2.212740	7.028392
C	-2.324128	-3.388667	6.511224

C	-1.775100	-4.674847	6.433207
H	-0.766743	-4.882298	6.795128
C	-2.564308	-5.687036	5.883582
H	-2.156908	-6.698966	5.811393
C	-3.871750	-5.432421	5.425846
H	-4.461884	-6.247552	4.999834
C	-4.418923	-4.152778	5.518652
H	-5.437375	-3.955339	5.174006
C	-3.646803	-3.118618	6.066503
C	-3.897307	-1.714640	6.325426
C	-4.993188	-0.870989	6.095535
H	-5.904593	-1.265512	5.638739
C	-4.900360	0.474453	6.451713
H	-5.747304	1.143184	6.279221
C	-3.719720	0.982832	7.027225
H	-3.663366	2.042482	7.290482
C	-2.614760	0.163518	7.267216
H	-1.700301	0.566406	7.705619
C	-2.717827	-1.189447	6.920032

XYZ Coordinates of *ptbpcz* in S_1 optimized geometry

C	8.00564798652965	-4.43497062421807	12.05912305384547
H	8.26071848998961	-3.97309633209122	13.02800669458434
H	7.57142271253440	-5.43149656383261	12.22255886787541
H	8.94241402413270	-4.52629666127179	11.48302314661283
N	7.03547612371994	-3.64501374466309	11.35035606098240
C	5.77225605947407	-4.13828410871868	10.94489316115892
O	5.36301425688747	-5.28883188644856	11.15057714318039
C	5.15089721375009	-3.00830992538342	10.27869285477094
C	3.90583345337242	-2.85707629301167	9.66265597270147
H	3.21705143870658	-3.70711878094846	9.64526930374510

C	3.53882321964630	-1.64019317712439	9.08532203357767
C	4.44307967193946	-0.49603153055041	9.09508270952233
C	5.67890594869745	-0.67812226521617	9.71871222961961
H	6.41337593948260	0.12422954754744	9.76899087615139
C	6.04367947930013	-1.89668214645677	10.30628587611028
C	7.26133220038196	-2.29647874626515	10.99334947764665
O	8.29827078261091	-1.67343270653170	11.24907502728300
C	4.10391759596754	0.86661270987835	8.43540679176010
C	2.88217620573451	1.53443040165594	9.10965082037967
H	2.71678172089583	2.54510408685911	8.69767872080994
H	1.95601209100784	0.96638362812199	8.95207318773942
H	3.04257895679402	1.63046593235438	10.19545322444643
C	3.82490351195649	0.69948684469519	6.92299469867996
H	3.67019434225004	1.68281995803289	6.44599776776742
H	2.92612662810948	0.09984756462225	6.72623501084178
H	4.67598552422297	0.20860617236479	6.42443023175553
C	5.27288021123984	1.86805633804850	8.55822362336418
H	4.99884366131802	2.81741380529444	8.06955477706253
H	6.18613432625278	1.49336255473534	8.07238184320895
H	5.51361644437574	2.09159072587849	9.60833612852120
C	2.15912082802752	-1.66932444153698	8.49608026145389
C	1.03106487301457	-1.32009396636629	9.26200936327703
H	1.18324118059092	-0.94004008691177	10.27352042152605
C	-0.26547638119923	-1.47882571425443	8.77285074563349
H	-1.13147036249457	-1.22987755520973	9.39057550427649
C	-0.44457589720168	-2.00915320104907	7.49054135919586
C	0.65063019620179	-2.37550233209911	6.70188784613908
H	0.49550244597622	-2.78204124162538	5.69984064429826
C	1.93739922093155	-2.19923060593432	7.21088640649470
H	2.80136495699853	-2.48392731821593	6.60799937053195

N	-1.77710982989933	-2.20101836515216	6.98378783639375
C	-2.32616167643936	-3.41682997607240	6.62669689878108
C	-1.74529288150729	-4.69574247258547	6.70388574386797
H	-0.73053507878934	-4.82786766235992	7.07899680705027
C	-2.52441737643222	-5.77668867325468	6.28931686766115
H	-2.10916476434782	-6.78486944200659	6.33278971745704
C	-3.83644081431478	-5.58506994797240	5.82564867899187
H	-4.42397957254577	-6.44942317475839	5.50986042750365
C	-4.41919495264466	-4.29845664736988	5.76743343328833
H	-5.44560160021720	-4.17403671693152	5.41647951530803
C	-3.66260689760055	-3.20956453624240	6.17035829287368
C	-3.91019617753576	-1.77274028431484	6.27355791705731
C	-4.98816446899421	-0.95037764828856	5.98385285269320
H	-5.92082859115055	-1.36000755906444	5.59069298654339
C	-4.85552384834238	0.43913593633036	6.20313288576752
H	-5.69873332709651	1.09573406619398	5.97959833426243
C	-3.66233831063858	0.99316226907236	6.69361062016388
H	-3.58985911539313	2.07181421771926	6.84268553344569
C	-2.56251626483690	0.18432778749527	6.98779588067755
H	-1.62502987270178	0.59870761879234	7.35853544569939
C	-2.70845886069839	-1.19765110338374	6.78178608598031

XYZ Coordinates of *ptbpcz* in T₁ optimized geometry

C	7.32722582543649	-4.20153584058813	12.63629544922625
H	8.21922815049991	-3.62726839991194	12.93619399790768
H	6.74772031844565	-4.47583636281855	13.52782988741048
H	7.66881313241548	-5.10505120220376	12.10812681694808
N	6.47630029831254	-3.41390041439755	11.77422463247179
C	5.19533237665817	-2.96336011834192	12.14455060555739
O	4.65166963120907	-3.18549329067925	13.20753672533819
C	4.70591564845866	-2.20449463386361	10.97184383937245

C	3.50155352598917	-1.61935685857523	10.74363512387679
H	2.70842476010727	-1.70613785567605	11.48974983205529
C	3.26175485046230	-1.10225888821216	9.40736631691149
C	4.47759023496727	-0.70699097323407	8.59403004645189
C	5.64358382797128	-1.45277335476390	8.80230135183143
H	6.53625195431143	-1.31695249661296	8.18871800908008
C	5.74170210499280	-2.23876497797231	9.94861622903072
C	6.87325565044132	-3.01038199676713	10.47764713535735
O	7.94811148421501	-3.27852174825520	9.97491785927927
C	4.56819234631071	0.69524763397619	7.95997072390691
C	4.83231157255786	1.65771765615420	9.15348238663074
H	4.93496019385128	2.69394261877957	8.78991350558627
H	4.00010897001798	1.63085294920635	9.87498945058975
H	5.75561661456817	1.38314642216362	9.68653863843311
C	3.29319046655760	1.18335375591175	7.24201954909122
H	3.42722258721805	2.23854806058594	6.95456969123417
H	2.40261877610798	1.12530515087148	7.88246729648945
H	3.09139502971023	0.61731919739253	6.32136780139836
C	5.74264384305206	0.79526447597624	6.96645731528295
H	5.74488925470233	1.79029115700753	6.49459494133692
H	5.65437312740827	0.04071014304013	6.16829974485110
H	6.71942629644782	0.66704601113867	7.45553885981948
C	1.97797387342252	-1.32740699594890	8.81010274852805
C	0.77769655372530	-1.40847657565061	9.58449227616984
H	0.81502871997936	-1.23798114030625	10.66142510005052
C	-0.44620758292277	-1.68340759716206	9.00099220845510
H	-1.34428053517001	-1.74380695021118	9.61843662850544
C	-0.54589305440289	-1.92293898062201	7.61318060586574
C	0.62677059470449	-1.86512599414721	6.82835411021373
H	0.55917968001287	-2.04202659290818	5.75338687464646

C	1.84720630455471	-1.56936537444121	7.40793780367921
H	2.74295174378878	-1.54543803769335	6.78574077932903
N	-1.78900046768848	-2.22258570710694	7.02580021784690
C	-2.05152736342749	-3.30386771539651	6.17031071250603
C	-1.19826225727923	-4.32560932239715	5.73507758562436
H	-0.15333024573223	-4.36443150521252	6.04514006919334
C	-1.73306294297901	-5.30876260238750	4.89975055480747
H	-1.08515719418107	-6.11500300451921	4.54605576288902
C	-3.08596768574477	-5.28640607560050	4.51241289559795
H	-3.47229358483097	-6.07119463689967	3.85749158599021
C	-3.93772849213955	-4.27921314513460	4.96778667019836
H	-4.99297907622607	-4.27019361266386	4.68308610938017
C	-3.42391124131614	-3.28060780663703	5.80539390204897
C	-4.01694470201137	-2.13540692445879	6.46929822837089
C	-5.30798208585088	-1.59168634140736	6.47902021934189
H	-6.11020122772197	-2.06854443259152	5.91000534877082
C	-5.55012506373113	-0.43287200269769	7.21794687746441
H	-6.55271042504228	0.00133051366613	7.23699736951815
C	-4.50967108940219	0.19029620196528	7.93234769125202
H	-4.71514706965525	1.10568396451776	8.49338291946228
C	-3.21461849334333	-0.33251767557536	7.93752550451419
H	-2.41233174992886	0.16733746511294	8.48183949964037
C	-2.98185969286448	-1.50794121481514	7.21257337738057

XYZ Coordinates of *pbpcz* in S_0 optimized geometry

C	8.115814	-3.571102	12.808536
H	8.454243	-2.794308	13.511907
H	7.651724	-4.397426	13.363140
H	8.992913	-3.939018	12.254115
N	7.125578	-3.037594	11.897303
C	5.804710	-3.509404	11.804321

O	5.332633	-4.411729	12.455861
C	5.156438	-2.663952	10.755028
C	3.865465	-2.686480	10.254318
H	3.145798	-3.423820	10.616662
C	3.504036	-1.767885	9.244382
C	4.461119	-0.822930	8.771477
C	5.773632	-0.835431	9.292297
H	6.512082	-0.108605	8.946903
C	6.100880	-1.755066	10.275232
C	7.383867	-1.981112	11.010099
O	8.442134	-1.406882	10.901665
C	4.119852	0.217353	7.759068
C	3.007827	1.061459	7.932399
H	2.376619	0.941831	8.815352
C	2.707602	2.046206	6.990477
H	1.841235	2.694984	7.143736
C	3.510340	2.203385	5.854805
H	3.270345	2.971123	5.114623
C	4.621747	1.374766	5.673855
H	5.254037	1.489728	4.789452
C	4.926827	0.392899	6.621193
H	5.790635	-0.260086	6.470313
C	2.123558	-1.849367	8.689341
C	1.894087	-1.934237	7.304048
H	2.741525	-1.916401	6.616166
C	0.601037	-2.022567	6.794327
H	0.435122	-2.067203	5.716309
C	-0.502185	-2.041591	7.662630
C	-0.285910	-1.974608	9.046660
H	-1.140816	-2.004588	9.724964

C	1.011875	-1.875319	9.549124
H	1.165012	-1.810608	10.629417
N	-1.817919	-2.125060	7.147075
C	-2.289722	-3.099108	6.260070
C	-1.627553	-4.207468	5.716866
H	-0.583080	-4.414835	5.954916
C	-2.351295	-5.045200	4.866141
H	-1.855385	-5.916546	4.430154
C	-3.703379	-4.793553	4.562342
H	-4.239952	-5.469034	3.891465
C	-4.361885	-3.695586	5.115915
H	-5.414050	-3.503918	4.889483
C	-3.657605	-2.839273	5.974054
C	-4.023668	-1.652214	6.721082
C	-5.207161	-0.909153	6.834308
H	-6.104305	-1.217950	6.291435
C	-5.220417	0.227708	7.642465
H	-6.136487	0.815389	7.740872
C	-4.059226	0.630363	8.330307
H	-4.087025	1.529798	8.951299
C	-2.868599	-0.092602	8.234991
H	-1.970678	0.231006	8.763743
C	-2.864146	-1.241178	7.433168

XYZ Coordinates of *pbpcz* in S_1 optimized geometry

C	8.45041554787521	-3.99591650393339	11.98166312437334
H	8.81420563475417	-3.37742865309655	12.81907665877161
H	8.08059386906528	-4.95879683296698	12.36100936733191
H	9.30199238479239	-4.16509271991043	11.30127256071984
N	7.36332514910636	-3.34652107965204	11.29717307724632
C	6.07628102403503	-3.91405729457468	11.15868421189738

O	5.74027246436571	-5.01527565772987	11.59780369615935
C	5.31896041243182	-2.91622597490046	10.41384433492922
C	3.99823084607297	-2.91767313000508	9.96810174836987
H	3.37915910522104	-3.80096628472527	10.14875543360342
C	3.50224873916535	-1.83028041758685	9.24144753049370
C	4.35260545884671	-0.67871259616855	8.98523329208792
C	5.68096304927401	-0.70341234430764	9.42413548079382
H	6.33053860035675	0.16080351894346	9.26155087487860
C	6.17191511940344	-1.80491977972314	10.12739450112583
C	7.48859076801066	-2.07373268332420	10.69835528452316
O	8.52265613508806	-1.40624439597611	10.70185980967217
C	3.82613371440675	0.55771250111793	8.35260897153688
C	2.60287191804138	1.13177305676790	8.76175229886009
H	2.04326628128605	0.65932538277849	9.57237355335959
C	2.11402581101893	2.29840762260171	8.17105706688737
H	1.17208630749135	2.72961894701302	8.52465837775030
C	2.83541627482361	2.93273531186242	7.15211504512675
H	2.45678735807152	3.84938250220229	6.69162897407786
C	4.05564249057713	2.38535770178936	6.74076342040033
H	4.63367479866407	2.87077600364517	5.94900722752350
C	4.54151372423275	1.21524752040172	7.33062411419924
H	5.48764610450974	0.78687241906521	6.98997053804047
C	2.14440817095979	-1.94256465377632	8.65555551429000
C	1.89610229954294	-1.61357753998053	7.30338052994983
H	2.72227250147974	-1.26608099323889	6.68245228153307
C	0.62561679338522	-1.72035021490925	6.74763370780599
H	0.45422476410309	-1.46487520926747	5.69919447610322
C	-0.43309159852650	-2.17084052539039	7.54458626665776
C	-0.22448446003103	-2.52557954523990	8.88089746222579
H	-1.06213609924394	-2.85807793190470	9.49894050481146

C	1.05521469236640	-2.40779115446301	9.42258893625145
H	1.21648690342443	-2.65373619750017	10.47388415744512
N	-1.76113303282680	-2.23536847220484	6.98744808265762
C	-2.49285832436229	-3.38438133933777	6.78610312890345
C	-2.11763295419259	-4.71485979042685	7.04833055453807
H	-1.13732519629999	-4.94353237013681	7.46676339132654
C	-3.04788388994187	-5.71065158235465	6.74906646615682
H	-2.79630465684032	-6.75563544717068	6.93832105789732
C	-4.30199259391692	-5.38658800050273	6.20404395576197
H	-5.01025419095707	-6.18660865467366	5.97915412969860
C	-4.66817651475411	-4.04780624653672	5.93442501647749
H	-5.64565679694043	-3.82059510989522	5.50397633483498
C	-3.76133247284383	-3.04103562942020	6.22514712350598
C	-3.76222273000847	-1.58574545604452	6.08613366237080
C	-4.67559717471256	-0.65273290875795	5.61911230978063
H	-5.65195901883754	-0.95957276608168	5.23822878832750
C	-4.31841665396363	0.71441326027336	5.64725455629582
H	-5.02981492027196	1.45724965186449	5.28068807869928
C	-3.07302340097773	1.13745780050460	6.13863716590425
H	-2.83100934314200	2.20158162796380	6.14986016711882
C	-2.13806985290475	0.21639445466473	6.61674919938157
H	-1.16680302096082	0.52558203412059	7.00454691552334
C	-2.49926631879281	-1.14084622978397	6.57663150302490

XYZ Coordinates of *pbpcz* in T₁ optimized geometry

C	7.96153795903585	-3.54707995616744	12.82413012137937
H	8.64553721488383	-2.75575030799870	13.17078465699639
H	7.41681466551087	-3.97253953312640	13.67737479209512
H	8.56780446846160	-4.32609445121194	12.33522806609528
N	6.99165028660670	-3.00837484876317	11.89916709448283
C	5.60001255212320	-3.02709622542060	12.12884514808114

O	5.05630925683252	-3.49890549159462	13.10937837321677
C	5.01412808892898	-2.36486194878681	10.94917059971297
C	3.70732771719280	-2.13469227067867	10.62233645763691
H	2.92607187072421	-2.51585204330777	11.28263317241373
C	3.39321710929845	-1.54099687536052	9.35940825694593
C	4.52536539630792	-0.93817105515337	8.55982506660220
C	5.85107507614287	-1.29010262779834	8.89363570728304
H	6.69678126183040	-0.90868018516002	8.31729670171009
C	6.09753816877998	-1.99428549161515	10.05405226787976
C	7.36328129762400	-2.40365631627597	10.67775117756111
O	8.51068028391454	-2.28478271063365	10.28913743390528
C	4.28465927231018	0.12184528464303	7.58816330334072
C	3.18835246629282	1.01781462523606	7.72536004389297
H	2.51900646287583	0.91662397263808	8.58028940952322
C	2.97966346723196	2.04839176992907	6.81167221767516
H	2.13720047663540	2.73039481966666	6.95418420579047
C	3.84036344692214	2.21510719716234	5.72098456378423
H	3.66885994876629	3.01758328126201	4.99921144907747
C	4.92751107112699	1.33977536535485	5.56198880345766
H	5.59955210141240	1.45454185067528	4.70734703053459
C	5.15219759215580	0.31972853602813	6.47874438217173
H	5.98841467533104	-0.36469188099643	6.32154650760386
C	2.07132751305843	-1.68072524992928	8.81277941364531
C	1.82856569232798	-1.69544501927286	7.39982276661828
H	2.66787474481086	-1.60760498470780	6.71176547133059
C	0.55560567625380	-1.85137488599001	6.87867320692796
H	0.40752531482450	-1.85043844695506	5.79740751257323
C	-0.56007051635420	-1.98160643435932	7.73007466940892
C	-0.34968910334012	-1.97636816416235	9.13058602905463
H	-1.20419851073998	-2.09835881511243	9.79857463207170

C	0.92168122350161	-1.84507874133039	9.65221354430744
H	1.03977870189909	-1.84031857177706	10.73667354131412
N	-1.85641421033708	-2.11822567816497	7.20452943378795
C	-2.24461297075774	-3.00821265785154	6.19028165634194
C	-1.49296936310317	-3.98168508355031	5.52025915992815
H	-0.43603568380703	-4.13591103892406	5.74062572954580
C	-2.14580030957679	-4.76560246689395	4.56626483774389
H	-1.57860390162984	-5.53041966875617	4.02953081585912
C	-3.51516006649832	-4.59598731842084	4.28943716334800
H	-3.99516129654763	-5.22590530941616	3.53655427570901
C	-4.26510513692950	-3.64021439364200	4.97688800941842
H	-5.33275364769485	-3.51892412615055	4.77686305545415
C	-3.63201022822310	-2.84140017715219	5.93709055127812
C	-4.10306882188937	-1.80361765796808	6.83488494562219
C	-5.34893216758545	-1.19486179351346	7.03006756530166
H	-6.21476903537821	-1.51225999236582	6.44349140338596
C	-5.46386885791153	-0.17389143814775	7.97510092342832
H	-6.43018837056507	0.30906529737737	8.13932036370942
C	-4.34166837744682	0.24930097779491	8.71129832348810
H	-4.44786861014770	1.06125953693432	9.43534584659386
C	-3.08858172039265	-0.34126038088632	8.53247769793660
H	-2.22171777657267	0.00878627167908	9.09416183697970
C	-2.98412383850708	-1.38190507093084	7.60096460703716

XYZ Coordinates of *pcbpcz* in S_0 optimized geometry

C	8.133668	-3.532221	12.784247
H	8.468237	-2.752649	13.486166
H	7.680440	-4.363411	13.340412
H	9.010684	-3.891333	12.224153
N	7.133170	-3.006578	11.878675
C	5.817669	-3.492434	11.790458

O	5.356290	-4.400694	12.440487
C	5.154915	-2.650797	10.745297
C	3.862112	-2.687595	10.250502
H	3.152625	-3.434120	10.613987
C	3.485306	-1.770426	9.244961
C	4.431637	-0.814717	8.772365
C	5.747111	-0.812675	9.285051
H	6.477282	-0.077252	8.939894
C	6.087682	-1.730883	10.264632
C	7.376414	-1.944979	10.993779
O	8.426522	-1.357641	10.880945
C	4.073120	0.226850	7.768080
C	2.947329	1.052485	7.947607
H	2.318397	0.918323	8.829310
C	2.624796	2.035432	7.017633
H	1.749934	2.670908	7.169045
C	3.426799	2.214278	5.873459
C	4.560384	1.401771	5.688881
H	5.185111	1.537564	4.803708
C	4.876863	0.424552	6.631032
H	5.751471	-0.211321	6.473917
C	3.089772	3.218175	4.903097
N	2.815592	4.028475	4.117722
C	2.104152	-1.862442	8.694769
C	1.869725	-1.943179	7.310008
H	2.714260	-1.923335	6.618286
C	0.575178	-2.033418	6.804323
H	0.405895	-2.073332	5.726753
C	-0.525277	-2.060438	7.676571
C	-0.302905	-2.000380	9.060670

H	-1.154630	-2.038769	9.742341
C	0.995887	-1.898187	9.558956
H	1.152483	-1.839019	10.639093
N	-1.841260	-2.145026	7.166643
C	-2.309288	-3.103974	6.259608
C	-1.641925	-4.195692	5.690019
H	-0.595243	-4.402234	5.918737
C	-2.363554	-5.020465	4.824733
H	-1.863220	-5.878398	4.367808
C	-3.718651	-4.772452	4.532779
H	-4.253398	-5.436954	3.849670
C	-4.382597	-3.691965	5.113577
H	-5.437295	-3.503474	4.896768
C	-3.680399	-2.849266	5.986541
C	-4.053283	-1.682293	6.761550
C	-5.242827	-0.952605	6.894968
H	-6.139027	-1.257418	6.348419
C	-5.263124	0.166580	7.727200
H	-6.183833	0.743994	7.841169
C	-4.102867	0.565325	8.418356
H	-4.135751	1.451645	9.057579
C	-2.906241	-0.144848	8.302837
H	-2.009560	0.177700	8.834215
C	-2.894859	-1.276515	7.477614

XYZ Coordinates of *pcbpcz* in S_1 optimized geometry

C	8.84704676049471	-3.60578137388284	11.86888751600724
H	9.13961117275740	-2.97533356480953	12.72507402112274
H	8.62334866695509	-4.62371002032026	12.21697139041835
H	9.69602459059636	-3.62775048259891	11.16586800561335
N	7.66373694010209	-3.09050686931200	11.22839756944533

C	6.44416979333483	-3.81358100104477	11.13231720872767
O	6.27178451425352	-4.94638842938516	11.57593410552429
C	5.53993797937678	-2.91891856882464	10.42425279004832
C	4.21201033390260	-3.08596306857640	10.01039340088927
H	3.70832432710107	-4.04222482454064	10.17789022767805
C	3.57413816271591	-2.05290637331362	9.33000508371109
C	4.25670172535253	-0.79098358488631	9.08324867072331
C	5.60708635702244	-0.66587910858841	9.45377335463383
H	6.14841354864785	0.26815139783108	9.27842648772277
C	6.23597227621929	-1.71003671233746	10.11684471135410
C	7.60596950270440	-1.81827948054513	10.64093077731477
O	8.53608074825075	-1.02006799205339	10.60599301019488
C	3.51867154935125	0.34829581749463	8.51617673135182
C	2.22263385434363	0.67619199169198	8.99309872229276
H	1.83828698881911	0.15601101533178	9.87142117768530
C	1.43404107606627	1.62859616903787	8.37123533125433
H	0.43633840268072	1.85329804486584	8.75678032343538
C	1.91061037619560	2.31183324788481	7.22733144879473
C	3.23557781691754	2.06938771487820	6.79666964931622
H	3.62708514981449	2.60781719671022	5.93046303891602
C	4.02139298141655	1.11941591899905	7.44045482682702
H	5.02721253243556	0.91167091708395	7.06678241859046
C	1.01330377432800	3.15328453520867	6.50121768651450
N	0.21513358736826	3.76721061084662	5.91514757571003
C	2.23451101625862	-2.27189525933519	8.71216643606109
C	2.07211339598423	-2.08031874801819	7.32493232279028
H	2.95033119131785	-1.85753316281912	6.71733960706782
C	0.81645683198804	-2.10648945179720	6.72890370462831
H	0.70159684402817	-1.92007983875189	5.65882596151987
C	-0.30788144585397	-2.34498863484037	7.52602666933923

C	-0.17603160975225	-2.62483524549880	8.88882282812788
H	-1.06274588408718	-2.80726033972083	9.50055484305686
C	1.09565680356870	-2.59692949234668	9.46924969552570
H	1.20338532583965	-2.76276462129358	10.54350752516397
N	-1.61597284235464	-2.22004566564409	6.93523644199069
C	-2.55927255292821	-3.22749273416360	6.81757783735383
C	-2.45912872445037	-4.56796420112084	7.21869282242212
H	-1.55326528911865	-4.94236901008454	7.69617231650895
C	-3.56264967146633	-5.39202297371533	6.97710273073731
H	-3.52427634190569	-6.44120576831237	7.27564103243922
C	-4.71452651800488	-4.88958414370398	6.35355016978038
H	-5.56176066965842	-5.55524288094830	6.17629664301915
C	-4.80148146719758	-3.54011165332758	5.94357159681939
H	-5.70388246996384	-3.17049819282330	5.45210141545739
C	-3.71937042459440	-2.70397085067661	6.17542691434213
C	-3.43117494847163	-1.29839392573788	5.89431676520272
C	-4.12869861505968	-0.26114986384132	5.29598605507579
H	-5.13743406311830	-0.41069571199061	4.90535018215810
C	-3.50691224737329	1.00638126948647	5.19952373127531
H	-4.04931929195023	1.82846159480375	4.72797915765103
C	-2.21190319104349	1.23758324867376	5.69880162313891
H	-1.75378617866542	2.22559691208693	5.61249710811501
C	-1.49525915166481	0.20977759967545	6.30982365029044
H	-0.49580243851561	0.37432433827365	6.71177968666680
C	-2.11426286131122	-1.05488271533287	6.39231726445548

XYZ Coordinates of *pcbpcz* in T₁ optimized geometry

C	7.97267258296154	-3.54493897157940	12.76148506159903
H	8.74186581843803	-2.78996525954192	12.98570595973554
H	7.45166802863254	-3.84531324313737	13.68022227912719
H	8.47542884833861	-4.42013869725970	12.31824040784524

N	6.99312614667778	-2.99964356294040	11.84943935510966
C	5.60132860027936	-3.02584722418418	12.09075048109238
O	5.07048065860116	-3.50745836617252	13.07193128648222
C	5.00099037989716	-2.35500445242226	10.92332905446866
C	3.68907528153661	-2.13233759889924	10.60404670052095
H	2.91330144754385	-2.52982075212512	11.26117379767373
C	3.36463985451572	-1.52498138501229	9.35279913630713
C	4.48271958299680	-0.90873732875103	8.55138192792953
C	5.81773879375809	-1.27028710680975	8.86931967918921
H	6.66069535947627	-0.89672199606452	8.28431072887623
C	6.06983138840033	-1.97225406417717	10.02334816164427
C	7.34874312391315	-2.38570002529851	10.63247538374298
O	8.48738404243556	-2.25628181419658	10.22756558039505
C	4.23684339782257	0.16160524130677	7.60604676051197
C	3.10965631525324	1.02729881075571	7.73480110853520
H	2.43032458759607	0.89909238071534	8.57728560285089
C	2.88272945132540	2.06350823259910	6.84231841948398
H	2.02281198281144	2.72277665201942	6.97842510184900
C	3.76103607041877	2.28013219763499	5.75935789593064
C	4.88804368112279	1.43395620122114	5.61189295577453
H	5.56863758248474	1.58902602585030	4.77208372540120
C	5.12193007717168	0.41344178138166	6.51552009441950
H	5.98397965066113	-0.23750878130811	6.36010622626637
C	3.51952374926638	3.33801889328659	4.82724383777412
N	3.32232685590077	4.19838364707850	4.06998282755107
C	2.03667708250236	-1.66806183690982	8.81503257967118
C	1.78589495544542	-1.68770797467875	7.40424619898530
H	2.62062449065180	-1.59144361698880	6.71128438520988
C	0.51264337005713	-1.85926005351064	6.89044598494779
H	0.35880044832204	-1.86156887297397	5.81012890979833

C	-0.59781824787342	-1.99481407359757	7.74942332744314
C	-0.37927992728000	-1.97832758230586	9.14902617430322
H	-1.22813156978065	-2.10476488884090	9.82315078386804
C	0.89432137270432	-1.83600696921321	9.66212483342191
H	1.01952356841156	-1.82664818588674	10.74579547527448
N	-1.89339494581122	-2.14689457515125	7.23281413305039
C	-2.27481992593248	-3.03562972389105	6.21297141945207
C	-1.51350275064037	-3.99408911610520	5.53258788208298
H	-0.45335990775511	-4.13612001694616	5.74503927040790
C	-2.16131580937972	-4.78163071287766	4.57781539222571
H	-1.58669358044030	-5.53436108468700	4.03219328154788
C	-3.53455170115295	-4.63048728907455	4.31218822951296
H	-4.01067393977911	-5.26236104101055	3.55857944444290
C	-4.29441600396312	-3.69089081673162	5.01207738747932
H	-5.36530820733811	-3.58540147371926	4.82125088166021
C	-3.66620819244780	-2.88916274519338	5.97202151348677
C	-4.14767524275556	-1.86555508870887	6.88163423629602
C	-5.40105213523196	-1.27752269337368	7.08698907734004
H	-6.26515967343944	-1.60350013561222	6.50277108136925
C	-5.52574992710403	-0.26346044730819	8.03898990374147
H	-6.49819951496463	0.20413453794892	8.21082501957476
C	-4.40618690158168	0.17358955532415	8.77017863712313
H	-4.52006285640994	0.98099340150050	9.49795034677743
C	-3.14506480539740	-0.39658686234083	8.58015192826422
H	-2.28025824811430	-0.03300993281457	9.13618056572610
C	-3.03123661375904	-1.43149611829058	7.64360417742702

XYZ Coordinates of *pmpez* in S_0 optimized geometry

C	8.145276	-3.589783	12.610865
H	8.477583	-2.832670	13.338174
H	7.706544	-4.445715	13.140524

H	9.020937	-3.917368	12.029943
N	7.131429	-3.043167	11.733010
C	5.815146	-3.523787	11.655210
O	5.359910	-4.446103	12.290027
C	5.137663	-2.656191	10.640391
C	3.837800	-2.684867	10.162110
H	3.130868	-3.436978	10.518977
C	3.448780	-1.746747	9.184523
C	4.386468	-0.774574	8.722348
C	5.715991	-0.788166	9.208841
H	6.449562	-0.067024	8.849061
C	6.063532	-1.726675	10.165318
C	7.363103	-1.958902	10.870529
O	8.411182	-1.368785	10.761858
C	4.006284	0.298662	7.790689
C	4.967951	0.844496	6.739545
O	6.101153	0.489703	6.508691
N	4.286880	1.849540	6.068324
C	2.991242	2.005837	6.584162
O	2.175844	2.809285	6.198344
C	2.856483	0.995328	7.676848
H	1.938922	0.896423	8.253126
C	4.843283	2.625483	4.979306
H	5.781841	3.107869	5.291608
H	4.104363	3.389344	4.702656
H	5.054184	1.984821	4.108749
C	2.061993	-1.839992	8.648016
C	0.957199	-1.770620	9.512419
H	1.120153	-1.627153	10.583709
C	-0.345515	-1.880303	9.023209

H	-1.196916	-1.838214	9.705029
C	-0.571100	-2.055780	7.649902
C	0.528554	-2.132955	6.778492
H	0.355493	-2.263300	5.708663
C	1.825655	-2.034558	7.275646
H	2.672955	-2.096781	6.588678
C	-2.926605	-1.246632	7.382303
N	-1.888949	-2.157820	7.148289
C	-2.377697	-3.188355	6.335412
C	-1.731863	-4.339616	5.867178
H	-0.688118	-4.543092	6.111423
C	-2.471260	-5.227162	5.082716
H	-1.987836	-6.132148	4.705251
C	-3.822880	-4.982810	4.772356
H	-4.371727	-5.697423	4.154069
C	-4.465650	-3.842107	5.253398
H	-5.517757	-3.655555	5.022746
C	-3.745475	-2.935847	6.044162
C	-4.095031	-1.696739	6.710459
C	-5.271982	-0.938291	6.781105
H	-6.176060	-1.277047	6.268548
C	-5.269446	0.252326	7.507732
H	-6.180024	0.853035	7.572029
C	-4.099150	0.693241	8.154968
H	-4.113681	1.635102	8.709769
C	-2.914847	-0.044416	8.100657
H	-2.010056	0.311304	8.595892

XYZ Coordinates of *pmocz* in S₁ optimized geometry

C	8.80754804757918	-3.49599394295484	11.89218278197930
H	8.57937875258093	-3.74445663953908	12.94105856547280

H	9.19858695696233	-4.40341044168625	11.40469555358084
H	9.56423720044088	-2.70052886220365	11.85570344555747
N	7.62828613586293	-3.01563916076806	11.21053518025440
C	6.45226524603894	-3.77801456246950	11.06908758868559
O	6.31045697656933	-4.90554946351399	11.49806778300910
C	5.51171383470266	-2.91478867663584	10.32239086209121
C	4.21320132959706	-3.14260987664895	9.88066641369153
H	3.73175527558517	-4.10783892330045	10.05786321779366
C	3.54791624866668	-2.13225081569533	9.17501690158825
C	4.16137030496617	-0.85025524706127	8.92960950277528
C	5.50819483720236	-0.67178575183335	9.36340445406296
H	6.01812814880079	0.26921549977750	9.15777070862260
C	6.14193070023014	-1.69177810623327	10.04483803241775
C	7.52119943808548	-1.74316249426075	10.62176349869276
O	8.39339054686610	-0.90353889971726	10.61453642964702
C	3.46363166515737	0.25017194926076	8.28487878378227
C	4.15121483306634	1.33058447441535	7.53799676332229
O	5.34770244068261	1.54531802505046	7.36139731489851
N	3.13731528554888	2.12942702065215	6.98863699893236
C	1.86255766573243	1.65142665560405	7.33626688994054
O	0.79501035358203	2.14869047969902	6.93488167372533
C	2.08745846874727	0.50138500151426	8.17046347753312
H	1.26862668847911	-0.02640846223182	8.64347981486216
C	3.39080134091326	3.27727587605408	6.15714554333311
H	3.92849029656380	4.06308380655501	6.71378994413479
H	2.41989085834958	3.66596705605078	5.81990127915186
H	4.00858711097411	3.00569818293260	5.28531608603912
C	2.19227061171418	-2.42413527341079	8.62143010652068
C	1.07762161064490	-2.58621525263910	9.45795112220345
H	1.21961343723505	-2.59226005242198	10.54087048767220

C	-0.21538647834455	-2.62728089302045	8.92918386480991
H	-1.08737034804877	-2.66762982461131	9.58599385477864
C	-0.38051212368903	-2.53103897627750	7.54595554147872
C	0.71821944976370	-2.48642229647459	6.68473174983118
H	0.56701774594136	-2.42628625936873	5.60479908443608
C	1.99804207139142	-2.44329455020759	7.22930555032032
H	2.86281747941675	-2.33808771371848	6.57229830251397
C	-2.18036895906099	-1.15448289596978	6.53592457233219
N	-1.70298033025893	-2.35560372516630	6.99578015408132
C	-2.67715122847097	-3.33412010114375	6.85089487934799
C	-2.60244814396391	-4.69082203369644	7.18625389954959
H	-1.69626617995613	-5.10858078199593	7.62652959425794
C	-3.73396142411667	-5.47466180864528	6.93185543887650
H	-3.71716936175829	-6.53772345355716	7.17931676643947
C	-4.88566988978146	-4.91317972759217	6.36257880056265
H	-5.75425677402642	-5.54761375420886	6.17414513840634
C	-4.94754050028826	-3.54325451868564	6.02460284325334
H	-5.85270743245384	-3.12565676193309	5.57859973327488
C	-3.83746881155313	-2.74714495659526	6.26959427802199
C	-3.51968194939536	-1.33385491931421	6.06194774565165
C	-4.19915242938828	-0.24218591463343	5.55043101784947
H	-5.22181895899916	-0.33486268795667	5.17893210591561
C	-3.53873802030646	1.01418847128531	5.51738465212603
H	-4.07222705374003	1.87792372709790	5.11470773868027
C	-2.22414355561469	1.17422379121150	5.99107037403103
H	-1.72001982821246	2.14134724385858	5.96950024901822
C	-1.52056181257913	0.09350490006548	6.51304923927237
H	-0.50626680063463	0.24455829891368	6.87901762490612

XYZ Coordinates of *pmocz* in T₁ optimized geometry

C	8.07786513369781	-3.54761421387614	12.67810018655124
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H	8.62015225377612	-2.74196012025142	13.19812835062315
H	7.56147937271779	-4.18091572384074	13.41153215854093
H	8.81038106721818	-4.14418409392842	12.11293293337615
N	7.08129893068332	-2.99775252974251	11.78418628144874
C	5.69534675310941	-3.20141422871908	11.93336677048325
O	5.17170073973395	-3.85443316239468	12.80891520406199
C	5.06826204526144	-2.45404293043140	10.81479623084357
C	3.74093910144682	-2.36166661765924	10.43813303398545
H	2.98384421905941	-2.93195256900458	10.98070926722740
C	3.40417274911407	-1.62188755102628	9.28723127176529
C	4.44498825777403	-0.84389946240944	8.59558494576456
C	5.82878234215578	-1.07802145431524	8.94861116716236
H	6.62023086783512	-0.59268758616495	8.37691079143982
C	6.09638952357351	-1.84509969256568	10.04631344025406
C	7.40637061848016	-2.19774573692902	10.67694244316892
O	8.52783707766184	-1.89112824960268	10.34788726078717
C	4.11916240363384	0.18625663202662	7.69827932070979
C	5.06745396328485	0.82287582235902	6.73444654406715
O	6.25969615322037	0.63548872082724	6.56549360126358
N	4.30360333613792	1.70533191252475	5.96924277235661
C	2.95038911713264	1.77419977136216	6.38365714721787
O	2.11528648310963	2.51231848670781	5.89258289758701
C	2.83669068032281	0.83169100579217	7.48623964923537
H	1.96158412277177	0.79304334442988	8.12826307008262
C	4.85562738283192	2.49307332280384	4.89169722862073
H	5.80652444153006	2.94586927804204	5.20987744017121
H	4.12263357958513	3.26708524267336	4.62782842986544
H	5.05696672331170	1.86482450555663	4.00758859923695
C	2.04564446582411	-1.73465980544672	8.74302189381195
C	0.91414442793632	-1.76105153222263	9.59152711502673

H	1.04713330432864	-1.65810764968966	10.67069836125462
C	-0.36889807088633	-1.88524090198095	9.07726392379115
H	-1.22898261390782	-1.90648111349543	9.74851015413177
C	-0.57515471993144	-2.00261238144445	7.68571701958071
C	0.53814228801341	-2.00392630175696	6.83019910736171
H	0.38988209396935	-2.08656258216015	5.75258258047376
C	1.82230435817706	-1.86997807697158	7.34843001860397
H	2.67640510361319	-1.89415435137489	6.67039747474340
C	-2.96993003182594	-1.30537223397643	7.50555196376649
N	-1.87893717038881	-2.12460983408297	7.17194484012952
C	-2.31282426948482	-3.08364501708785	6.24188679140012
C	-1.61030478162848	-4.14273206330183	5.65370939894561
H	-0.55751160355471	-4.32150162179593	5.87544117457385
C	-2.30590060712014	-4.97937643410390	4.77782101107088
H	-1.77665064367819	-5.81102288504891	4.30561548473591
C	-3.66958145193415	-4.77601953384442	4.49626135149009
H	-4.18350804154311	-5.44754204498583	3.80425353586928
C	-4.37028525620224	-3.73145309510382	5.10088367122537
H	-5.43320849749167	-3.58040633082353	4.89614552085272
C	-3.69408036729954	-2.87948536075583	5.98326837649528
C	-4.11187025242000	-1.74571150474121	6.78606712057623
C	-5.32945282876560	-1.06908768403619	6.93204111543971
H	-6.21305757158650	-1.40088276026250	6.38106744308205
C	-5.39295356720289	0.03653161579749	7.78133493740725
H	-6.33622681508115	0.57379447076884	7.90568491116848
C	-4.24726976736064	0.47636913748550	8.46992909737884
H	-4.31160444696787	1.35565707191914	9.11597223028591
C	-3.02206446053831	-0.18108216962664	8.33897113501250
H	-2.13647664523318	0.18428185190629	8.86030480241523

XYZ Coordinates of *pnpz* in S_0 optimized geometry

C	8.144463	-3.420592	12.880555
H	8.432568	-2.674512	13.637065
H	7.725843	-4.308551	13.372464
H	9.044807	-3.699995	12.311595
N	7.130236	-2.882029	11.998078
C	5.856161	-3.448227	11.823643
O	5.444730	-4.441692	12.375056
C	5.161126	-2.562052	10.837397
C	3.889539	-2.647513	10.296650
H	3.229036	-3.474013	10.567434
C	3.472642	-1.668516	9.366188
C	4.358373	-0.610064	9.019177
C	5.653705	-0.554976	9.576515
H	6.334588	0.258586	9.316356
C	6.035692	-1.534580	10.478104
C	7.318417	-1.727064	11.223404
O	8.327057	-1.061777	11.197461
C	3.932092	0.511164	8.129337
C	2.921004	1.366346	8.549117
H	2.430259	1.177726	9.506450
C	2.523841	2.472651	7.774115
H	1.736590	3.146967	8.116917
C	3.135880	2.732744	6.558715
C	2.706570	3.920110	5.768270
O	1.842415	4.681667	6.161579
N	3.354686	4.119309	4.538026
C	2.972921	5.270894	3.717809
H	3.845379	5.920659	3.556688
H	2.623651	4.928392	2.732987
H	2.179647	5.815750	4.238784

C	4.360506	3.297362	4.010986
O	4.860083	3.556023	2.931261
C	4.770881	2.121335	4.827072
C	5.752638	1.271545	4.343425
H	6.200807	1.493072	3.372606
C	6.146688	0.144494	5.096164
H	6.912122	-0.528030	4.701654
C	5.571094	-0.115563	6.326539
H	5.882699	-0.994589	6.893608
C	4.569399	0.741509	6.865310
C	4.158673	1.870756	6.084380
C	0.994855	-2.024188	9.584540
H	1.122840	-2.097412	10.667552
C	-0.281001	-2.159404	9.037708
H	-1.140173	-2.354243	9.682152
C	-0.470600	-2.050402	7.651774
C	0.641037	-1.818902	6.825447
H	0.497503	-1.726452	5.747339
C	1.913911	-1.697307	7.377798
H	2.766303	-1.524741	6.718197
C	2.114624	-1.787581	8.767612
N	-1.765118	-2.170378	7.095393
C	-2.135797	-3.037927	6.060495
C	-1.369089	-3.985642	5.370736
H	-0.312392	-4.134055	5.598540
C	-2.003861	-4.743660	4.384638
H	-1.424908	-5.488487	3.832161
C	-3.370392	-4.571504	4.091412
H	-3.835512	-5.180213	3.312077
C	-4.133297	-3.637205	4.791876

H	-5.196772	-3.509043	4.573831
C	-3.519482	-2.863807	5.786923
C	-4.002701	-1.844409	6.696994
C	-5.252345	-1.240002	6.892973
H	-6.110988	-1.544063	6.288738
C	-5.380412	-0.244776	7.861808
H	-6.348867	0.234115	8.025829
C	-4.268472	0.155956	8.627323
H	-4.386136	0.946081	9.373664
C	-3.013717	-0.430844	8.451726
H	-2.155246	-0.105663	9.041375
C	-2.893936	-1.440640	7.488638

XYZ Coordinates of *pnpcz* in S_1 optimized geometry

C	8.59922958730475	-3.75793812272990	12.52970735037848
H	8.25167083212459	-4.00842817935634	13.54458969367693
H	8.97550423686383	-4.68005293414104	12.05949907770516
H	9.40513718359206	-3.01399107442147	12.58718348889678
N	7.52553478388155	-3.18832841659232	11.74661081955615
C	6.33535890496380	-3.87672005738181	11.45249289500072
O	6.08113855515990	-5.00610052957410	11.81438364924591
C	5.52280849494022	-2.93308785015985	10.64256058600302
C	4.26567945729745	-3.07911810049971	10.07091032726894
H	3.72074900978217	-4.02141297863167	10.16850040669897
C	3.73489238929945	-2.00765702663128	9.33365070592330
C	4.44908565333300	-0.77201159569785	9.20115045848448
C	5.73534213380471	-0.66756408315222	9.77775861444628
H	6.30086429552582	0.26242875511792	9.69174754780764
C	6.24624241025770	-1.74251738093107	10.48602978490207
C	7.54936128710366	-1.89235332644272	11.20211184443191
O	8.45931790942971	-1.10169346069880	11.31269792872178

C	3.81798598554292	0.37092429779528	8.50251416430460
C	2.55470250594539	0.81607279474263	8.95100066804258
H	2.16220937146146	0.40999360069712	9.88646585293262
C	1.80239035759201	1.73529976727753	8.23968709613375
H	0.83361762750083	2.08327704902084	8.60146275202567
C	2.29085259203573	2.25704944540811	7.01938543316538
C	1.44540992220299	3.12743987955921	6.21998429510114
O	0.25378388149595	3.35980530372833	6.49023443853581
N	2.01939860305720	3.70287992257319	5.08264996700345
C	1.17830277284344	4.61925975085586	4.32133764144081
H	1.80648887488914	5.12073999098350	3.57775726445330
H	0.36910469766682	4.07209866453218	3.81004054394743
H	0.71102233677575	5.34475983734521	5.00139601753413
C	3.31350128706207	3.41799274166602	4.58729370193235
O	3.71309048332409	3.94822097629459	3.55412692618532
C	4.10304049089036	2.45172348908223	5.36007680630563
C	5.36815496621517	2.06610040328022	4.87618622596976
H	5.72796390679499	2.52170975259570	3.95251923189147
C	6.10951480165777	1.10891212208707	5.56494782637489
H	7.08183495603777	0.79139717896497	5.17832616514459
C	5.62338646900908	0.53759624101206	6.74611102115444
H	6.21818750960907	-0.22654458783203	7.24799566015560
C	4.37661618250682	0.92977962945408	7.29971947534507
C	3.59122055495967	1.89606986687458	6.56435522108570
C	1.25795715725248	-2.49123526216583	9.37730692146209
H	1.33444800647247	-2.69141169924611	10.44837078679285
C	0.00103748675125	-2.48514325625433	8.76570887436887
H	-0.90296043654959	-2.68422714109364	9.34557955084613
C	-0.09075729013993	-2.15308331824796	7.41310230397236
C	1.05415797783328	-1.89255503280316	6.65248880684033

H	0.96649222982375	-1.65162188583112	5.59111997830127
C	2.29780847424362	-1.91128088255726	7.27396824460266
H	3.18984992946206	-1.66858739351818	6.69533347001191
C	2.41459339418662	-2.16411151190052	8.65349487535458
N	-1.38406740429040	-2.02144754478756	6.79643420029691
C	-2.28247031133285	-3.06036817017080	6.56555800999807
C	-2.13490284215971	-4.42000603068555	6.85911007859771
H	-1.22919975565954	-4.79538554911203	7.33665303416887
C	-3.19432326668412	-5.26823073450294	6.51236171024554
H	-3.11783392412083	-6.33604788560343	6.72593861565750
C	-4.34615706657583	-4.76513013977503	5.89281057065381
H	-5.15691979218191	-5.44835521009141	5.63152945165406
C	-4.47919544941129	-3.39165779873711	5.59389312746771
H	-5.38087645629267	-3.01843550497411	5.10374200167106
C	-3.44153285301274	-2.53336977752417	5.93163420425224
C	-3.20843414573002	-1.09778780063841	5.78080313160196
C	-3.93552042895522	-0.04290738408889	5.25781868880024
H	-4.92568881609357	-0.19858074572453	4.82450674257664
C	-3.36842111216346	1.25538937323496	5.29878539129241
H	-3.93779398691200	2.09209871533076	4.88851950314507
C	-2.09924374917298	1.49898821546155	5.85774944154329
H	-1.66179891526255	2.49894275053791	5.88703069905098
C	-1.35099456234018	0.45468683338184	6.39263994527275
H	-0.37314515731563	0.64344083669944	6.83497578119709
C	-1.91443819541011	-0.84066282068642	6.34008228298612

XYZ Coordinates of *pnpcz* in T₁ optimized geometry

C	8.12906904916988	-3.37611581341340	12.81722885317310
H	8.42543034340989	-2.61367506088418	13.55467852630407
H	7.71375572094076	-4.25057496353813	13.33538282390269
H	9.02334959840688	-3.66788910905168	12.24560559535992

N	7.10851265156357	-2.85946736378766	11.92944495148683
C	5.80220257853187	-3.37599794340168	11.84620959587768
O	5.37138575689725	-4.30571802011067	12.48857981536718
C	5.11164368268167	-2.53693233450603	10.82295838592864
C	3.81625197507753	-2.59480552493790	10.33747971160424
H	3.13184016001526	-3.36936039934188	10.69049710758377
C	3.41232846915079	-1.67587816859533	9.34592110238616
C	4.33175543201979	-0.67895246371919	8.87582112564012
C	5.65973666410651	-0.66490753357214	9.38203919543555
H	6.36950568315655	0.09707773039214	9.05480567265645
C	6.02180578130098	-1.58550484461491	10.34429921087511
C	7.32005292886932	-1.77862929722510	11.06087995445534
O	8.35658110884572	-1.16674877280139	10.94682203219291
C	3.91126981183405	0.38401318527753	7.95608819979369
C	2.70381221540425	1.13810646699123	8.25762287379553
H	2.11494549091569	0.83872514067604	9.12566174886966
C	2.33473950336783	2.23161866490471	7.53443717656506
H	1.45229511217109	2.82110632102983	7.78507091391337
C	3.13050073653830	2.65641162548546	6.41104847895693
C	2.70956778235739	3.84137113593129	5.65570404433535
O	1.70917796589804	4.48354938549273	5.96149314292653
N	3.51291327264024	4.20868154090237	4.56315683758798
C	3.14776987056308	5.38969273745763	3.77983498964186
H	3.97861211078792	6.11011034936375	3.78214320023637
H	2.95801943183752	5.10275752094270	2.73507508178905
H	2.25129378633297	5.83292645596973	4.22464805654540
C	4.65247647323353	3.51804269885109	4.14200449551253
O	5.28737506593738	3.90117210920780	3.16780150173614
C	5.03910706158476	2.32162343469077	4.91746221246599
C	6.18055334911241	1.57428268104252	4.49464240070667

H	6.73089600793951	1.92760120610066	3.62174046954705
C	6.53247147387578	0.43765354925307	5.18414424157101
H	7.39000281063676	-0.15902641708101	4.86364554773739
C	5.78639718994070	0.01657430026976	6.32047467166679
H	6.06988567380699	-0.91209255949129	6.81731908086610
C	4.69001453351855	0.75671541896150	6.79873907340637
C	4.29254778354198	1.92171181503832	6.04379400047810
C	0.93190690433180	-1.99388135358680	9.60339165337660
H	1.06597374159383	-2.01716619170647	10.68768519991070
C	-0.34803831349310	-2.13326319512322	9.07220838277408
H	-1.20455761371821	-2.28575026756385	9.73122994327933
C	-0.54778420220131	-2.08573449178339	7.68192458288865
C	0.56133477406294	-1.91278123587158	6.83792157359449
H	0.41237066009991	-1.86877808313178	5.75770340436179
C	1.83927741458741	-1.78315437204476	7.37518759266979
H	2.69044133304347	-1.65854631939529	6.70327631137954
C	2.05083006539942	-1.80867170926006	8.76880097684754
N	-1.84722416861111	-2.21200805832146	7.14477469515762
C	-2.23656696623323	-3.10274228694469	6.13500053331288
C	-1.48513106763413	-4.07167852518907	5.45815062148805
H	-0.42591953762740	-4.22097345361575	5.67256167367766
C	-2.13892919460552	-4.85271162069783	4.50276880568676
H	-1.57180700129021	-5.61403991635549	3.96075907513191
C	-3.50916866376369	-4.68269110868768	4.22787155313496
H	-3.98940850391585	-5.30933851078003	3.47236342909306
C	-4.25730869169990	-3.72807354717541	4.91730015789135
H	-5.32413907805739	-3.60252237520337	4.71508084155029
C	-3.62403318019162	-2.93192069522104	5.88109847969376
C	-4.09093093710777	-1.89074334286352	6.77553494104105
C	-5.33606969556894	-1.27953381393703	6.97575985828903

H	-6.20436302859714	-1.59609039983158	6.39222116688766
C	-5.44730691740656	-0.26053995195019	7.92210684213976
H	-6.41232628092819	0.22394238408359	8.08957107195664
C	-4.32269606680816	0.15807191775402	8.65839201356829
H	-4.42652324664344	0.96789230928832	9.38529155046116
C	-3.07161432547609	-0.43492589946806	8.47684593664503
H	-2.20330747354183	-0.09230577881812	9.04142991316051
C	-2.96946583591909	-1.47066099075739	7.53959111806878

XYZ Coordinates of *pppcz* in S_0 optimized geometry

C	-0.591538	4.038340	6.135826
H	-0.384492	4.513858	5.168079
H	-0.755931	4.810381	6.903120
H	-1.499999	3.420181	6.062605
N	0.549841	3.214528	6.478998
C	1.687044	3.055969	5.662704
O	1.871958	3.607683	4.604450
C	2.561859	2.080169	6.385174
C	1.917621	1.712412	7.570349
C	0.619836	2.452239	7.647594
O	-0.227492	2.416473	8.512711
C	2.462014	0.784012	8.439368
H	1.936157	0.510838	9.354591
C	3.696937	0.189504	8.096224
C	4.353408	0.591179	6.915494
H	5.308744	0.124964	6.661314
C	3.794392	1.539382	6.043695
H	4.298442	1.831968	5.119900
C	4.287074	-0.863627	8.973036
C	5.612728	-0.717671	9.431124
H	6.214298	0.145384	9.136800

C	6.126206	-1.673095	10.294399
C	5.356670	-2.759017	10.715498
C	4.056726	-2.938435	10.266214
H	3.472049	-3.806617	10.578774
C	3.516207	-1.995012	9.370689
C	7.473109	-1.774299	10.939655
O	8.427751	-1.040380	10.836516
N	7.426170	-2.936511	11.723328
C	6.185091	-3.591009	11.644320
O	5.888525	-4.610148	12.221777
C	8.540156	-3.400403	12.524229
H	8.817304	-2.644337	13.275108
H	8.231899	-4.327217	13.025884
H	9.418332	-3.593846	11.889075
C	2.145964	-2.199332	8.817424
C	1.961177	-2.353496	7.432341
H	2.832942	-2.385110	6.774792
C	0.682223	-2.415396	6.884625
H	0.541376	-2.501952	5.805111
C	-0.442120	-2.318147	7.717721
C	-0.269319	-2.219965	9.105015
H	-1.149727	-2.159168	9.747888
C	1.015702	-2.168212	9.649070
H	1.143540	-2.057533	10.729156
N	-1.740852	-2.258142	7.154134
C	-2.344111	-3.226341	6.350742
C	-1.904020	-4.517609	6.037716
H	-0.957075	-4.898701	6.425616
C	-2.718755	-5.298695	5.215580
H	-2.399086	-6.311242	4.954948

C	-3.943168	-4.809756	4.719512
H	-4.557449	-5.447675	4.079126
C	-4.378112	-3.522767	5.038944
H	-5.329471	-3.145339	4.654650
C	-3.578033	-2.715621	5.860009
C	-3.706807	-1.365136	6.375688
C	-4.659800	-0.347710	6.217769
H	-5.555603	-0.520696	5.615451
C	-4.440532	0.889009	6.826947
H	-5.174355	1.690101	6.706372
C	-3.278463	1.119342	7.590458
H	-3.105262	2.094854	8.051605
C	-2.320699	0.120012	7.773295
H	-1.423900	0.315351	8.361286
C	-2.551362	-1.117883	7.164768

XYZ Coordinates of *pppcz* in S₁ optimized geometry

C	-0.21259218949600	4.55707750938836	6.13638547239773
H	0.23064317814719	5.35578608134743	5.52545212095500
H	-0.70941118428313	4.99303042271090	7.01798181745348
H	-0.97606833934459	4.02805967600083	5.54005581162361
N	0.85175107600848	3.67148578128929	6.53335667046771
C	2.20079178589543	3.79182442561312	6.04449035025233
O	2.55307442701375	4.66353931294619	5.26393310230142
C	2.92099018983950	2.69772927762127	6.67437885078533
C	2.01890332814134	1.97323745070139	7.50290606400944
C	0.68570704535921	2.59407610126831	7.38527213107443
O	-0.39432103235637	2.25185587383498	7.88001788414260
C	2.42753558647345	0.88120628318875	8.24650271991599
H	1.71122298969867	0.39548023632962	8.90891024684142
C	3.77074069339679	0.43542338861704	8.16712887076924

C	4.66722994230496	1.17561653864346	7.31944961227183
H	5.69919149001782	0.83235387735973	7.22086535947606
C	4.26063183602914	2.28554952608084	6.59240386553745
H	4.96350723491764	2.82421494323216	5.95200360661846
C	4.25745349121952	-0.71969940775810	8.93333770200395
C	5.58174870234960	-0.68761497656222	9.45237900728228
H	6.21885926032304	0.18241497343892	9.28347380031911
C	6.05009326485965	-1.72740081401993	10.22791648322329
C	5.25104705803710	-2.84763058543566	10.52635038409716
C	3.95750925914817	-2.92727833697237	10.01962866328962
H	3.35093305954034	-3.81473785872166	10.21708282908669
C	3.46070140334877	-1.89169085727542	9.21533605226677
C	7.37056277336540	-1.91015485506653	10.89598475402682
O	8.34595309293042	-1.18670417397025	10.90154528106716
N	7.28180435076084	-3.14468526453863	11.55083656495312
C	6.02482406595771	-3.77281365320084	11.37040882690849
O	5.71609765708143	-4.85077180459881	11.84378799871453
C	8.36073110511223	-3.70901398502180	12.32706295364116
H	8.62939488770472	-3.04558737292676	13.16493089910462
H	8.02278507070303	-4.67922869642854	12.71581219882333
H	9.25878950776107	-3.84899787096235	11.70412844376268
C	2.10419642586349	-2.08786450988407	8.62774746018738
C	1.88738240854846	-1.99583269530629	7.23957549150591
H	2.73036844309042	-1.77763720093334	6.58259656543536
C	0.61064370242346	-2.12411923705511	6.69983326277166
H	0.44546744530169	-2.01623027066018	5.62559430666057
C	-0.46861908431635	-2.36118042500248	7.55705715652802
C	-0.28219785479488	-2.50475220384424	8.93136847021492
H	-1.13729439932282	-2.68475577578151	9.58680513686923
C	1.00450925883604	-2.37087235678522	9.45634614893955

H	1.15481720222501	-2.44247120792214	10.53545173490728
N	-1.80857592770664	-2.38682025569890	7.01952916392428
C	-2.49178304176858	-3.51128751003865	6.57702190634353
C	-2.05019091026176	-4.83891241347808	6.54981536247656
H	-1.05361622553669	-5.10305385650427	6.90544916831703
C	-2.93987242110348	-5.79674399650106	6.04957401556557
H	-2.63492614168011	-6.84407084290723	6.01036332992509
C	-4.21531511312893	-5.42841888432829	5.59869010582602
H	-4.88945311628886	-6.19597309967218	5.21309044698457
C	-4.64947995776030	-4.08446030041554	5.63122634678834
H	-5.64678826752039	-3.81852823462748	5.27459980815403
C	-3.78337536503847	-3.11837122535501	6.12326506941976
C	-3.85751722464857	-1.66885172176458	6.31201309797921
C	-4.81026047023193	-0.69504186206943	6.07225306621324
H	-5.78366271148263	-0.94621185431348	5.64604738351132
C	-4.49576042025505	0.65337584111833	6.38837785263330
H	-5.24346637723629	1.42575570610519	6.19625359931652
C	-3.25224461115813	1.01805696422758	6.93432260054833
H	-3.01315648212950	2.05727718111584	7.16224084312901
C	-2.27851815604107	0.05730024633424	7.19255529564111
H	-1.31756344337608	0.35803866851003	7.61329744943883
C	-2.59862423146745	-1.27840883271510	6.87252195437959

XYZ Coordinates of *pppcz* in T_1 optimized geometry

C	-0.28807805793055	4.04895794377214	5.74315800855577
H	-0.01324706959208	4.53776448119471	4.79898238478614
H	-0.51098591696048	4.81727200061218	6.50124269318275
H	-1.18847823659833	3.43150594427546	5.60412985265344
N	0.82428265931055	3.22135841802516	6.15713647553805
C	2.09352229268416	3.22648636671280	5.52138740891653
O	2.38768400306386	3.92278571644258	4.57523327623035

C	2.90331954406674	2.22666004200229	6.25534152318917
C	2.10689131085238	1.67964386050112	7.27656105006166
C	0.75762512527005	2.31761939600448	7.21619811132614
O	-0.22133220037248	2.10634828956148	7.90342930880292
C	2.56779709121517	0.70675902190950	8.12849879711361
H	1.92535943862507	0.36144178194913	8.93564925752283
C	3.90202879179161	0.19703766195724	7.95944982302501
C	4.71517905897873	0.81023764439083	6.93988514602565
H	5.73362725229038	0.44782121380983	6.78974947348497
C	4.22978258446143	1.79866039837110	6.09359409589617
H	4.85730912849823	2.22488601577259	5.30751585106350
C	4.38176550046238	-0.89139232783671	8.76776534434400
C	5.76981996951295	-1.02867173455570	9.07880346930547
H	6.52918161948182	-0.42641123208947	8.57592875590372
C	6.13899210038581	-1.83450797625621	10.12110369269823
C	5.17192055969853	-2.57381585864916	10.90106456055790
C	3.83413474995718	-2.56832800453706	10.56053773491628
H	3.13769537814140	-3.22484350283092	11.08823804995653
C	3.41902736915705	-1.82881029503377	9.43368680727606
C	7.47995705908793	-2.09328835076308	10.69603102812508
O	8.56751985111791	-1.67451232170066	10.35375293163673
N	7.25478181234237	-2.96949081814143	11.76953138885639
C	5.89174699906284	-3.31251269187450	11.94919216409150
O	5.47092810023777	-4.06217509916126	12.80828545637597
C	8.32195817453268	-3.47143907806852	12.60479049293936
H	8.84412010708520	-2.64018518685402	13.10503924371197
H	7.87913114510013	-4.14128477152509	13.35379819717031
H	9.06077405207102	-4.01928503066033	11.99856622147914
C	2.10182310646090	-2.05252853299024	8.85867125318186
C	1.91617534327285	-2.10340671939535	7.44750001890014

H	2.78920108362944	-2.04015206032545	6.79607570338377
C	0.65509987947199	-2.21807770604725	6.88642605473254
H	0.53116518637734	-2.24206093391066	5.80208719122512
C	-0.48377274642638	-2.22294545761693	7.71349411913192
C	-0.32170145120520	-2.21003703016024	9.11576058151292
H	-1.20833984676899	-2.23306225408263	9.75238495091192
C	0.94500274197894	-2.16767521292949	9.67572384700101
H	1.05006644360915	-2.14342758465157	10.76262973681184
N	-1.77311574075507	-2.20825206043176	7.15441545123919
C	-2.29338565048619	-3.13416412665429	6.24218662941871
C	-1.69210543334146	-4.27214570915670	5.69242586160743
H	-0.66533797166661	-4.54616015983359	5.94066875228383
C	-2.45633832111197	-5.05092412453394	4.81996016809906
H	-2.01060847527446	-5.94297106637942	4.37261631010351
C	-3.78658468850743	-4.71144069641512	4.51166303127623
H	-4.35776326427401	-5.34220058659658	3.82616327011518
C	-4.38615804063616	-3.58329698841468	5.07861936485458
H	-5.42356730651639	-3.32863519286630	4.84750370202649
C	-3.63978643361629	-2.78378758998719	5.95141413745045
C	-3.93428757336342	-1.57749733776617	6.70717515979751
C	-5.05173354366059	-0.73941249067533	6.79471088853297
H	-5.96651333647447	-0.97708385976087	6.24588899844035
C	-4.97024851241201	0.41560659635449	7.57834933924481
H	-5.83413932060795	1.08079146167663	7.65279728534567
C	-3.77965631737482	0.74772003639926	8.25135154188054
H	-3.72160970694979	1.67617680116143	8.82451129561300
C	-2.65162404417380	-0.07323893589268	8.18384547210292
H	-1.71545965268724	0.22349278839581	8.65833096442407
C	-2.75649875359942	-1.24661018323992	7.42777184263054

XYZ Coordinates of *ppcz* in S_0 optimized geometry

C	0.290810	3.799562	4.748923
H	0.722239	4.803579	4.610732
H	-0.574924	3.859191	5.421804
H	-0.023597	3.421281	3.764263
N	1.258314	2.904963	5.348233
C	2.459191	2.539103	4.722777
O	2.818976	2.914047	3.631366
C	3.146672	1.620840	5.682992
C	2.337999	1.486566	6.815257
C	1.106644	2.314365	6.614444
O	0.162844	2.466277	7.353021
C	2.699519	0.682249	7.882436
H	2.046747	0.598834	8.752901
C	3.920966	-0.021997	7.797288
C	4.736292	0.133835	6.657110
H	5.672153	-0.427524	6.598482
C	4.361057	0.956214	5.585753
H	4.989606	1.063315	4.699051
C	4.348663	-0.937169	8.890196
C	5.662628	-0.849416	9.396921
H	6.366767	-0.118816	8.992939
C	6.031206	-1.670284	10.450646
C	5.135350	-2.582691	11.012046
C	3.848912	-2.721734	10.517306
H	3.154605	-3.456152	10.929575
C	3.456826	-1.898282	9.444914
C	7.328689	-1.768926	11.189093
O	8.351758	-1.151161	11.011293
N	7.125779	-2.756590	12.167571

C	5.831215	-3.295300	12.130208
O	5.409853	-4.151631	12.870899
C	8.133839	-3.178107	13.118416
H	7.779367	-3.023514	14.149066
H	8.365188	-4.246873	12.989627
H	9.036548	-2.578949	12.940295
N	2.147988	-2.046898	8.925948
C	1.814893	-2.356794	7.602228
C	2.648537	-2.731083	6.543618
H	3.727624	-2.818848	6.679898
C	2.052450	-2.980063	5.306111
H	2.681326	-3.268796	4.459965
C	0.659936	-2.866955	5.127950
H	0.225342	-3.068035	4.145734
C	-0.166932	-2.505943	6.192143
H	-1.248251	-2.423914	6.055845
C	0.408520	-2.246620	7.443995
C	-0.130598	-1.854400	8.732819
C	-1.422422	-1.571484	9.196816
H	-2.278950	-1.648927	8.522416
C	-1.595397	-1.180964	10.525123
H	-2.596939	-0.954939	10.898885
C	-0.490508	-1.063915	11.389572
H	-0.647592	-0.747933	12.424091
C	0.807145	-1.339805	10.952219
H	1.662082	-1.240972	11.623661
C	0.970482	-1.743800	9.622828

XYZ Coordinates of *ppcz* in S_1 optimized geometry

C	0.19232441590178	3.71923801619319	4.64689008427479
H	0.44083877153600	4.79149032144711	4.69976785297714

H	-0.77034078392112	3.54033819780318	5.14466735228095
H	0.12428750038429	3.43900122283139	3.58411968747897
N	1.19499038892287	2.92395385367740	5.31772025867163
C	2.54185257320906	2.84242376929981	4.87440177580188
O	2.96874821367504	3.42532025214166	3.89987789714908
C	3.21403285491742	1.93494895954113	5.82582627746058
C	2.27086362850026	1.52077643581832	6.78001114395331
C	0.95731847441912	2.14836819035374	6.45356834625455
O	-0.11144705026610	2.01372743544563	7.01799060556036
C	2.58653263178803	0.66302909776807	7.81184065074277
H	1.81793447339696	0.44295198672216	8.54862688902269
C	3.90581572199019	0.13923262960644	7.90839519708947
C	4.85633183790357	0.58302562491466	6.93535085692192
H	5.87161182249517	0.18325584321868	6.97502326482118
C	4.52961947076840	1.47047618503212	5.91134942670882
H	5.27817291799760	1.78101748540325	5.17841053076497
C	4.30238007986019	-0.81593275792909	8.94674375756701
C	5.62309962584271	-0.79425034968644	9.46693330204703
H	6.32910052782033	-0.02882847728369	9.13780876371682
C	6.02204476134923	-1.70234744487601	10.42592092912506
C	5.14826906486025	-2.70807024824564	10.92588201253124
C	3.84604190064322	-2.78649661037961	10.42554781149627
H	3.16246727907047	-3.56618803697198	10.77018766163454
C	3.44117333618553	-1.85509171675086	9.47937996866163
C	7.32683981415623	-1.84076835317591	11.11433297047299
O	8.34838613083596	-1.18677474605387	10.98025633270643
N	7.15540932922393	-2.92487825317127	11.98591881856507
C	5.85815486149264	-3.49618970372873	11.92711733899249
O	5.49481028030002	-4.44685551967241	12.60648013698851
C	8.18548568943128	-3.41745886658019	12.86903315365220

H	7.85127804700508	-3.37586603568830	13.91804842763183
H	8.43240376681610	-4.46582860850226	12.63590046743621
H	9.07514179719540	-2.78730688364108	12.73458995693057
N	2.09345663141646	-2.00278107188941	8.95972839766989
C	1.78273312886144	-2.50682985545891	7.73264136705448
C	2.66362840587667	-3.02019795072722	6.75566539414357
H	3.73466393356842	-3.06282358820102	6.95041269094251
C	2.10334716533472	-3.44244998102379	5.55641123237895
H	2.74570675862495	-3.84350902820299	4.77048658263330
C	0.71348649348377	-3.35018702570788	5.33556766334263
H	0.30352993534763	-3.68272679691229	4.37943970883353
C	-0.16451494195988	-2.83052304971264	6.31455647699123
H	-1.23482934804772	-2.75840967169591	6.11152049419396
C	0.36689702913772	-2.40826475223818	7.52059007390893
C	-0.17866332291865	-1.80795843353687	8.73494858910154
C	-1.44694457945085	-1.42620943679382	9.14661323560333
H	-2.31633973857572	-1.56849700719030	8.50142764666090
C	-1.59410437209652	-0.83327537007766	10.42184599755108
H	-2.58772565377818	-0.52563538349898	10.75412029778734
C	-0.49202220920857	-0.62786245388388	11.26046227645748
H	-0.63630241695370	-0.16591397145941	12.23899020093239
C	0.79816120880309	-1.00144975812202	10.86019316345106
H	1.67095614333789	-0.84594419054797	11.49466551340870
C	0.93034259348975	-1.58397711799944	9.59550208886188

XYZ Coordinates of *ppcz* in T₁ optimized geometry

C	0.34321970538539	3.90702312661880	4.78770599545498
H	0.70274062508637	4.94826078746718	4.80203576459148
H	-0.57847171324188	3.82631676162403	5.37922877095695
H	0.14480150196532	3.62836688886176	3.74126911945248
N	1.32485053074486	3.01795552329438	5.36937280618779

C	2.60675957284230	2.81681946287832	4.81332184428608
O	3.01216434946682	3.35642994074391	3.80740914463665
C	3.27868255515835	1.84539021450114	5.71003887086935
C	2.38905956552704	1.50910006998028	6.74395105104202
C	1.11666372336234	2.26800201682633	6.53384396350059
O	0.10455794984887	2.25358025693952	7.19828952671658
C	2.71759685362225	0.62231843773465	7.74288097215390
H	2.00368125450694	0.43963952310317	8.54426958714737
C	4.01107957510582	0.00336717031152	7.72170382457570
C	4.91741236512191	0.39268041785488	6.67556884676564
H	5.90408028364017	-0.07154645496845	6.63319475785851
C	4.56278815579405	1.28988098312462	5.67649551573089
H	5.26008942065157	1.55014369874062	4.87692692241976
C	4.39718646869476	-0.97422361020434	8.70711995570814
C	5.75994341812515	-1.11718911677687	9.10830174972746
H	6.56197581044879	-0.61206162117115	8.56685824548188
C	6.06187650407203	-1.79275609233562	10.25929780954296
C	5.04324912450052	-2.41117753765349	11.08491469053740
C	3.72048504026464	-2.41092968017472	10.67704902378567
H	2.97080251331783	-2.98197920955649	11.22885557090416
C	3.38617404222153	-1.77138854273725	9.47597648691695
C	7.37328701307414	-2.01709237454367	10.90798367036026
O	8.48108541487721	-1.66334933129263	10.55389392039287
N	7.07920770840102	-2.75815505848528	12.06520981761424
C	5.69944488482425	-3.03673184779074	12.23396600876036
O	5.23571724312102	-3.66263897343562	13.16933964560740
C	8.07989176344417	-3.19945241219322	13.00930169230006
H	7.86606409061229	-2.79671904096387	14.01211642498351
H	8.08400048354906	-4.29883703454355	13.08142751704296
H	9.05764604090790	-2.84199253861405	12.66003035801672

N	2.09512171110350	-1.93194310427728	8.95935206285694
C	1.77729916241616	-2.35365783194392	7.65357962627130
C	2.63630188541666	-2.75082851553379	6.62464914264810
H	3.71749726368696	-2.75892545923287	6.76175368684014
C	2.05626610953584	-3.13256334435162	5.41236443689721
H	2.70194386377512	-3.43579236173990	4.58477566502231
C	0.66050369945609	-3.14298389408855	5.24354021938395
H	0.23721761733875	-3.45027534100765	4.28429097376058
C	-0.19245473532810	-2.78334424181679	6.29369992393162
H	-1.27718196783957	-2.81649532181257	6.16763133022825
C	0.36809019183138	-2.38968606811020	7.51066078804809
C	-0.19710972194661	-1.99245999954899	8.79228141451596
C	-1.50277423312197	-1.80862067920828	9.24921677143625
H	-2.35264424445184	-1.99376084060981	8.58817917863767
C	-1.70281389545794	-1.36790824827064	10.56331960496492
H	-2.71962967272081	-1.22045943091606	10.93477951911148
C	-0.61196909500689	-1.09478596626340	11.40658912478555
H	-0.79192329060482	-0.73531283629588	12.42245181792382
C	0.70367012996691	-1.26505639612419	10.96790658924639
H	1.54763892507577	-1.03124621530616	11.61736735104320
C	0.89459345783051	-1.73293170670551	9.66216990041619

XYZ Coordinates of *ppczi* in S_0 optimized geometry

C	-2.88246566642660	-1.11880798350178	14.27939104196271
H	-3.19833053086172	-0.19370895366711	14.77963591520825
H	-2.81356382948698	-1.93593284767807	15.01414645666381
H	-3.62521540699861	-1.40216957150975	13.51732538313056
N	-1.59350161039063	-0.87506424971341	13.66811967817920
C	-0.91947590328856	0.35771415302357	13.71489971695760
O	-1.31876232985666	1.35586610677787	14.26807045463354
C	0.34697779732655	0.14650740732638	12.95054558526815

C	0.36934635807566	-1.17455707434524	12.49233822406251
C	-0.88427797307738	-1.84965797047121	12.95205497901705
O	-1.25376918622216	-2.98604518010842	12.76864351393406
C	1.41346207415649	-1.66554807800167	11.72872978617897
H	1.40362880144078	-2.69671360212429	11.37315727954931
C	2.47599962708393	-0.79064779176849	11.40949292438450
C	2.45176881276323	0.53295012541059	11.89433252153230
H	3.27544088669242	1.20267295884290	11.63476638509668
C	1.38763480147153	1.01984065708823	12.66831763089815
H	1.36825146464284	2.05070519926215	13.02881399649021
C	3.61962719623475	-1.25753349301911	10.57381342018702
C	4.92704778606684	-1.04214019579993	11.05903685246611
H	5.09011526138493	-0.53812109562803	12.01418272863198
C	6.00245232908359	-1.51655432878524	10.32629932355002
C	5.80794062714407	-2.20081696234304	9.12570589049430
C	4.53813493697800	-2.41223600558459	8.61608649276227
H	4.40468122100205	-2.91939800814492	7.65834638563334
C	3.41924756734003	-1.92997077256063	9.33085212302422
C	7.47058853937948	-1.44596622820710	10.59449978915054
O	8.05856545871564	-0.94245314997717	11.52331098869566
N	8.07997101304594	-2.10307975796414	9.51424556757292
C	7.14686434223776	-2.58751301865882	8.58228372182424
O	7.41283322531424	-3.18788234650442	7.56724913768472
C	9.51328198326602	-2.25722157902403	9.38431162464220
H	9.92112537944585	-2.82190074716932	10.23712253571362
H	9.71040524272892	-2.80032935459925	8.45051890582872
H	10.00708469184471	-1.27348161862247	9.35525300949669
C	2.06372128597816	-2.12720203792321	8.74970107941060
C	1.15642830667463	-1.06089021249705	8.65414639573001
C	1.67155242544006	-3.40837519844661	8.29221465672000

C	-0.12257681966851	-1.28008591905718	8.14180761861289
H	1.44674667854354	-0.06254220805679	8.98635845927561
C	0.40081121317386	-3.65340999267885	7.77436127480164
H	2.37894211121325	-4.23758504156941	8.37214621647239
C	-0.50200621142243	-2.58397159065284	7.71253181423754
C	-1.27391785250720	-0.42694415296835	7.93481852161772
H	0.12562028514677	-4.65501665561956	7.43896757800940
N	-1.81579902232486	-2.55629931324169	7.27749944947183
C	-2.29427540819253	-1.25514406755271	7.39015791704886
C	-1.52863319359942	0.93130901119685	8.16627227537002
C	-3.55378742471663	-0.73777781670715	7.06039120634101
H	-0.75283284954019	1.57319552899686	8.59192951934902
C	-2.78408766413950	1.44831916974696	7.84632986180562
H	-4.33532791421819	-1.36732916714509	6.63045130656369
C	-3.78170340582514	0.61917110348620	7.29728554964042
H	-2.99795439984049	2.50566324522131	8.02008951972293
H	-4.75718064713821	1.04606655457176	7.04941313981599
C	-2.53842076220960	-3.67494262415089	6.70020151484085
C	-2.35306108921099	-3.79422294403064	5.18603666648877
H	-3.60415625101626	-3.55868931539429	6.95362123907618
H	-2.20441282710284	-4.59437721263634	7.20698631073798
H	-2.91903545995795	-4.65381783515899	4.79256185262139
H	-2.70670336184632	-2.88430650814598	4.67607359206329
H	-1.29043797995000	-3.93462864183630	4.93247838364768

XYZ Coordinates of *ppczi* in S_1 optimized geometry

C	-3.39127475841553	-0.63816980995528	12.37458278624748
H	-3.68775240350988	0.15536561890355	13.07451008114976
H	-3.81314783817681	-1.60076563647668	12.70608401506901
H	-3.79576135702722	-0.41679545029547	11.37246933639063
N	-1.95110442866272	-0.68456200758677	12.35245311940759

C	-1.11842114825901	0.25484461172348	13.05963626204189
O	-1.56725810963767	1.13661440094290	13.77590839256478
C	0.24364920483352	-0.09158949296511	12.67779187185491
C	0.19437108298309	-1.20850495571258	11.80841433473878
C	-1.22020367709359	-1.55628453289661	11.56428553590213
O	-1.69869501976954	-2.36272336759517	10.76415769936155
C	1.32758982487191	-1.72933304751567	11.21972386479876
H	1.22956783427608	-2.63074451211655	10.61941458073763
C	2.57593759406597	-1.07791624990352	11.37919617388104
C	2.62106169171641	0.02815387932829	12.29960274252165
H	3.56986319536683	0.54706095043510	12.45272145317125
C	1.49026771518165	0.50720157091187	12.94700060377190
H	1.55503956794782	1.36591545308676	13.61974354678727
C	3.74324547389798	-1.42842102629978	10.56075621220231
C	5.04876799400174	-1.27879508140704	11.10278485511427
H	5.18239160969434	-0.96090968453851	12.13859463900510
C	6.15671510412977	-1.58367996875212	10.34028263278559
C	6.04801131499579	-2.03975150196573	9.01509070608134
C	4.78604633873739	-2.19129574303997	8.43820408279232
H	4.69600568950791	-2.52473456706169	7.40122597157754
C	3.64640779718889	-1.88690387501474	9.18675809209192
C	7.60695281438809	-1.53063373841466	10.69494679711912
O	8.13589919024269	-1.19556542805908	11.73525664117482
N	8.27901200189804	-1.95538504111898	9.54656756936434
C	7.39757960818028	-2.28314649235268	8.48407321066738
O	7.75290836636200	-2.67838322685737	7.38957400776910
C	9.71712273268786	-2.05763552826839	9.45949777384327
H	10.10533736291524	-2.76304526368802	10.21168146846106
H	9.96755349440116	-2.41480001675344	8.45138907791231
H	10.18996212656498	-1.07821400936563	9.63601437078312

C	2.31219139506018	-2.05820544067121	8.53324550190121
C	1.40219305547265	-0.96819714956117	8.45866871692338
C	1.89023417166526	-3.33324424888984	8.11305461206050
C	0.07897324126667	-1.21179852876038	8.14292625352946
H	1.73096815872408	0.02333925999663	8.77184579607312
C	0.56188497608250	-3.59226309540146	7.76043862399776
H	2.60453379938998	-4.15775350206872	8.14901403290313
C	-0.34560493959852	-2.53021958164216	7.84161932236727
C	-1.13128264928787	-0.40068992487656	8.21896443060916
H	0.24527292194321	-4.60231359867671	7.49600071581893
N	-1.73117869506592	-2.54842044717115	7.74229933475031
C	-2.22154599799409	-1.28970386439587	7.97317666719418
C	-1.38470964387409	0.91902785570733	8.54677925881329
C	-3.56027140222850	-0.86042596567881	8.03380378924673
H	-0.56935723390651	1.60735592344492	8.77573373257041
C	-2.72640823731936	1.35401182511615	8.60878305109577
H	-4.38777845475915	-1.54705503906213	7.85232821563545
C	-3.79412165307511	0.47622585410564	8.35168368899875
H	-2.93857985262726	2.39122540270759	8.87588502230640
H	-4.82009470640420	0.84374087378944	8.41455017989273
C	-2.54529701271169	-3.74879349916161	7.59668373440510
C	-2.92369451628054	-4.03129050091448	6.14195482068504
H	-3.43407797926978	-3.61884073541671	8.23029156871825
H	-1.97878019697849	-4.58277473639486	8.03259202129329
H	-3.53284667926486	-4.94629092850154	6.08822029697791
H	-3.50781093061663	-3.20145663065181	5.71496591357855
H	-2.02656892882760	-4.17562680632500	5.52049618850951

XYZ Coordinates of *ppczi* in T₁ optimized geometry

C	-2.96782215588765	-0.97172145590438	14.02250397197460
H	-3.25734714159902	-0.07413776330297	14.58514966749512

H	-2.98582790506385	-1.84997705748027	14.68668530176506
H	-3.68423016666077	-1.14525937839573	13.20390704936560
N	-1.63723222950190	-0.75596939668275	13.49888559721230
C	-0.89771535676495	0.43396975933665	13.68762571191104
O	-1.28265387972860	1.39950692038652	14.31016194364049
C	0.38299368810441	0.21878295016220	12.97264862538610
C	0.36029652412829	-1.05908342781002	12.39609650714080
C	-0.94823385176724	-1.70085929310279	12.73312018055052
O	-1.36928247134814	-2.79207358030355	12.41906381018247
C	1.40393544375537	-1.54491365911513	11.63906390966660
H	1.36039924632634	-2.56023255067214	11.24737420943644
C	2.54727448110077	-0.70816597738709	11.41548755633643
C	2.56502322482504	0.57770570900960	12.05455760935404
H	3.42033703964718	1.23517581499341	11.88950135133065
C	1.50174178486578	1.04707834974945	12.81526935568930
H	1.52372197218056	2.04193202475445	13.26578968640678
C	3.62122483371493	-1.12770755286574	10.54573349704444
C	4.95369132390173	-0.70299924368235	10.80664324193216
H	5.16774292990501	0.04903827291604	11.56870155946566
C	5.99927004402865	-1.34368341131340	10.19309998790328
C	5.78504059387369	-2.43111755669121	9.26602587668101
C	4.51507000141310	-2.80451874969819	8.89946936854277
H	4.39290497124698	-3.55556976419844	8.11656118636814
C	3.39450151112724	-2.11488933621957	9.43535585037020
C	7.45754185688815	-1.15423189209220	10.34528941144518
O	8.07519428912012	-0.35913030892673	11.02706777705669
N	8.03942756235060	-2.11489157513265	9.50188266366834
C	7.09614790501709	-2.91770014787414	8.81470852160419
O	7.37788256160841	-3.80623110832076	8.03328539070226
C	9.46927377304568	-2.26177634449270	9.35682340499634

H	9.93327794332029	-2.50809800186879	10.32532321532708
H	9.65469156115347	-3.06922935735561	8.63605784669613
H	9.91891129377432	-1.32303988070851	8.99575238512307
C	2.09687726594056	-2.26900161108796	8.81378997361758
C	1.13605605958997	-1.20829091184260	8.80787339301410
C	1.72475601747158	-3.50283725081884	8.17870791111759
C	-0.11888183581444	-1.40197705807207	8.25343746222202
H	1.39906375177572	-0.23344016375500	9.21516368909445
C	0.47743340444218	-3.70937917964245	7.62246422859077
H	2.43293198811598	-4.33230158081566	8.18277600247813
C	-0.46211601744999	-2.65634365702316	7.66988370141392
C	-1.29439225069773	-0.55954983471145	8.13517804685532
H	0.22759687647449	-4.67470857625041	7.17853234180815
N	-1.76150314936397	-2.61350632453974	7.22686090599287
C	-2.28553450486752	-1.34479870369547	7.48863536946450
C	-1.59223583087833	0.74795324892453	8.53219979188301
C	-3.55978876036078	-0.83806933760834	7.21438530072247
H	-0.84170928120945	1.35562328227172	9.04388408260709
C	-2.86556495253491	1.25833521549240	8.26688450503368
H	-4.31923432524717	-1.43740493681112	6.70879711033003
C	-3.83329433662875	0.47347111773922	7.61313966844134
H	-3.11479236322258	2.27804459067820	8.56964202084095
H	-4.82139982572967	0.89563858542678	7.41333799243055
C	-2.45870922007052	-3.67475616007256	6.51733725482614
C	-2.32777028310747	-3.56056370725774	4.99741625059684
H	-3.51646495114233	-3.64549447787151	6.82285698067400
H	-2.06284195770058	-4.63779102279298	6.87379306243602
H	-2.87448544904701	-4.37919711311573	4.50341375954269
H	-2.73911381333021	-2.60414106345413	4.63885560855625
H	-1.27142870750826	-3.61452459900425	4.69081324563715

XYZ Coordinates of *ppdp* in S_0 optimized geometry

C	0.318838	5.144794	6.449406
H	0.105919	5.222502	5.374933
H	0.851165	6.047814	6.787481
H	-0.623266	5.069248	7.013960
N	1.129253	3.963853	6.657333
C	1.594501	3.134560	5.621903
O	1.379749	3.295701	4.443070
C	2.369374	2.049895	6.298754
C	2.339452	2.283264	7.675738
C	1.531360	3.517162	7.924680
O	1.247113	4.047674	8.973108
C	2.944448	1.418444	8.574492
H	2.886346	1.598223	9.649425
C	3.572555	0.267491	8.061344
C	3.606341	0.044966	6.670303
H	4.090370	-0.859839	6.295326
C	3.012262	0.938289	5.769174
H	3.032673	0.762791	4.691342
C	4.144202	-0.753885	8.984260
C	5.286499	-0.454797	9.747474
H	5.747030	0.534247	9.691411
C	5.841332	-1.453661	10.535390
C	5.279109	-2.733547	10.577770
C	4.133260	-3.048941	9.869918
H	3.684196	-4.041710	9.932353
C	3.542252	-2.042185	9.074902
C	7.042119	-1.436321	11.420538
O	7.803634	-0.528057	11.659266
N	7.130795	-2.736298	11.954535

C	6.107771	-3.577240	11.497427
O	5.966707	-4.737865	11.805390
C	8.158473	-3.164979	12.879368
H	7.727615	-3.389794	13.868169
H	8.652744	-4.073837	12.504272
H	8.888787	-2.350381	12.974343
N	2.330537	-2.306683	8.392797
C	2.189036	-3.486123	7.621465
C	3.280408	-3.988961	6.888054
H	4.237729	-3.464421	6.918045
C	3.144640	-5.153396	6.130380
H	4.003958	-5.530231	5.569234
C	1.919923	-5.826752	6.074121
H	1.814973	-6.734296	5.474917
C	0.831520	-5.325132	6.796355
H	-0.129974	-5.844933	6.769185
C	0.961294	-4.171764	7.571457
H	0.111081	-3.795330	8.142926
C	1.237311	-1.411133	8.570639
C	0.473887	-0.987001	7.470109
H	0.701921	-1.380254	6.478062
C	-0.541348	-0.046579	7.643338
H	-1.116004	0.287745	6.775477
C	-0.806742	0.488819	8.910052
H	-1.588878	1.240686	9.038680
C	-0.060059	0.054289	10.009024
H	-0.262194	0.459540	11.003752
C	0.948866	-0.898074	9.845520
H	1.535627	-1.232798	10.703554

XYZ Coordinates of *ppdp* in S_1 optimized geometry

C	1.39467900298398	5.72603849229095	6.26571859638607
H	0.86918883778518	5.75908757210527	5.30172369812638
H	2.26819271601799	6.39698554132215	6.23629931733543
H	0.72555835602518	6.07520932432708	7.06840874974032
N	1.80439808431280	4.36054223146430	6.49859774024058
C	1.55596431208870	3.29682089434171	5.59598433287138
O	0.96907136533578	3.41252746069864	4.53627159102736
C	2.14133425177502	2.10496505853980	6.23360460188029
C	2.70862084581353	2.48678107946127	7.46938796019731
C	2.48576582650237	3.94915012383109	7.64938039877775
O	2.79991036731789	4.67341778809259	8.57278771649721
C	3.32003842204043	1.57763603218141	8.30821253300871
H	3.71509748674735	1.91332727565270	9.26974696808156
C	3.36479974525985	0.20666123442012	7.93118686824746
C	2.81975873802526	-0.15431780019872	6.65891868523498
H	2.91619779530981	-1.18031496861950	6.30847454783636
C	2.21077070039216	0.77513518650899	5.81774228576165
H	1.80920382403431	0.47802653751515	4.84550021067740
C	3.94682470987440	-0.77240221373434	8.85181969445557
C	5.09841060678939	-0.43175743513507	9.61583124986433
H	5.57210536604327	0.54373496537923	9.48745446049933
C	5.65439866632685	-1.34540117742302	10.48559091305404
C	5.11461920489988	-2.64012682906125	10.67376008301152
C	3.96032446524897	-3.00454284187528	9.97108696668896
H	3.49654477027202	-3.98169616361281	10.12458393407536
C	3.41804102740038	-2.09583315637248	9.07409081073671
C	6.86225691910726	-1.21775724903266	11.35222558857381
O	7.61418038149817	-0.27083855246015	11.48582043619344
N	6.96015404170674	-2.44694593528175	12.01022580844052
C	5.93671996947626	-3.36087796238975	11.64475513425742

O	5.83089863854971	-4.48915225741418	12.09827213850624
C	8.00041577350804	-2.77545957738773	12.95722995263713
H	7.55960348945103	-3.13624102119823	13.89930140110505
H	8.65590662662133	-3.56960200181022	12.56367123192799
H	8.59222679666191	-1.86821116076086	13.13913548578564
N	2.17501094389181	-2.48997663098928	8.41274767236845
C	2.20570147234280	-3.53595879593751	7.48670169776551
C	3.38360825583334	-3.77764241159259	6.73672056688282
H	4.25399745761546	-3.13902755504124	6.88406252656077
C	3.41700280411709	-4.81260604591552	5.81306414981826
H	4.32259875824767	-4.97605937325463	5.22482644154007
C	2.30252505028385	-5.64896355010505	5.63420132752913
H	2.34257101413172	-6.46859280915578	4.91342168141109
C	1.15151626392547	-5.44473971308872	6.40452025015377
H	0.29637246176621	-6.11679365994885	6.30252813125843
C	1.09682265307903	-4.40487091177935	7.32735931518276
H	0.21939480405939	-4.28621344254918	7.96362989828608
C	1.00984437454163	-1.84096356123196	8.79687375429561
C	-0.08049940557752	-1.69223790141411	7.89440942456423
H	0.01433793568755	-2.05903830107191	6.87263426234658
C	-1.21525159080305	-1.00011908459767	8.28351932378827
H	-2.03248691513037	-0.86296026777561	7.57223526362676
C	-1.29759681940645	-0.43512880520260	9.56785680473688
H	-2.19083309590634	0.11884881487653	9.86445094142662
C	-0.21732529883148	-0.55454510164610	10.45518550251450
H	-0.27385200690163	-0.10473621140828	11.44856238835308
C	0.93277299639478	-1.23389205543160	10.07916819766538
H	1.77407575543560	-1.32355212010334	10.76421938618279

XYZ Coordinates of *ppdp* in T₁ optimized geometry

C	1.23767648324713	5.73192179019795	6.26544845006886
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H	0.76496593501144	5.73476411488043	5.27414013818475
H	2.07199372965876	6.45174609794390	6.27705046803506
H	0.51017682565813	6.03875718690623	7.03251392854973
N	1.70960785665198	4.39025371886009	6.52919347492244
C	1.67346679664630	3.34126857420879	5.58461151191900
O	1.24178541485566	3.43510711975285	4.45587990812830
C	2.24994730034429	2.16595342234044	6.28153292680420
C	2.60069678538721	2.54947978885362	7.58933666741238
C	2.24672953310998	3.99197342027911	7.75979498789932
O	2.37171596037631	4.70326922303440	8.73170946685369
C	3.14571298817560	1.66422735288303	8.49340109812244
H	3.36967010969302	1.99552540212657	9.50935552726463
C	3.33766963321038	0.30861013605602	8.09520622044488
C	2.99951797676403	-0.05430355671371	6.75487315447412
H	3.18932253792191	-1.07408938136457	6.42001740693473
C	2.46047964103431	0.85902572792881	5.84942692964634
H	2.21362285741189	0.56437956389503	4.82667936983262
C	3.85798956730548	-0.66841730698350	9.03544684435825
C	4.85644724099687	-0.31270328450325	9.97382729206064
H	5.14981518657264	0.73078332462023	10.10927376399517
C	5.55463005615713	-1.29910175453377	10.63424539722312
C	5.29530994468291	-2.70766547738194	10.41062547080525
C	4.25984308155500	-3.10375779731901	9.59170764649184
H	3.99052780609941	-4.15907634737292	9.50802965116288
C	3.48916764745312	-2.11257409976825	8.94887344044902
C	6.66383839356361	-1.19144899464917	11.60460744968540
O	7.20313610416621	-0.20390332710287	12.06848879036713
N	7.00091525147560	-2.51718178920000	11.91878260082303
C	6.21582811824519	-3.48608011221795	11.24137716641006
O	6.33687784823490	-4.69122430890143	11.37096181587014

C	8.05545819334670	-2.85324736445435	12.84693344362408
H	8.09336523452008	-3.94730707048648	12.93345240058920
H	9.02476899895799	-2.47071361328897	12.48841500273063
H	7.85867824614240	-2.40189587124424	13.83247051086256
N	2.27834834357880	-2.46916718620976	8.33669554988134
C	2.19528384961217	-3.64804982969949	7.55776954745379
C	3.25234963981682	-3.98500052648980	6.68832313728663
H	4.12366434790296	-3.33083617423382	6.62247754074972
C	3.17745064326930	-5.14384878473201	5.91881120403593
H	3.99759608955021	-5.39300997359236	5.24113760071806
C	2.05640348056171	-5.97981600043908	6.00366871448843
H	2.00205810181283	-6.88804786460680	5.39883246156855
C	1.00887396805308	-5.64924462561512	6.87178348350865
H	0.13856953618883	-6.30486274124459	6.95523557340352
C	1.07267458009692	-4.49418529084522	7.64986446439703
H	0.26598335728577	-4.24821244209816	8.34194529799081
C	1.10808031622003	-1.72624379818086	8.64280386086371
C	0.12734843607649	-1.49533162704493	7.65892223217185
H	0.26482961266953	-1.90065343774804	6.65536282769741
C	-0.98479985840011	-0.71705426578409	7.96149041101391
H	-1.73500028322529	-0.52705295742806	7.19008403024473
C	-1.13133642410557	-0.15426524006498	9.23909263187252
H	-2.00207129810143	0.46503003871219	9.46737845276353
C	-0.16070847178713	-0.38789377152452	10.21697124147214
H	-0.27363674740205	0.03864530758313	11.21653394882691
C	0.95488945973868	-1.17610297203843	9.92860906829587
H	1.70428403595346	-1.38235134395615	10.69421739628791

XYZ Coordinates of *pppazb* in S_0 optimized geometry

C	-1.56150101262412	3.14097716125512	2.00837465210723
H	-1.36020624780264	4.01476189521317	1.37479605187058

H	-1.83583044460972	3.46642249107996	3.02301157492827
H	-2.40081925143347	2.56479764502718	1.58747800206421
N	-0.35924696617673	2.33349022557299	2.04721552341477
C	0.78851354523927	2.58720736975623	1.27035121311157
O	0.92793645967693	3.51498765874283	0.51013117860632
C	1.73974841613215	1.47945901952049	1.59409625343590
C	1.12777707506490	0.63907116752068	2.52804024105832
C	-0.22890861055599	1.18522711034909	2.83132266685114
O	-1.07360895947578	0.74299516749043	3.57884010550325
C	1.74564564863375	-0.50425436056048	3.00041960543038
H	1.24301620127745	-1.14572300512587	3.72536147134703
C	3.02574413310735	-0.82534288450032	2.49865645364391
C	3.64623639315760	0.04289849902278	1.57721939806439
H	4.63571879340533	-0.21783125544360	1.19330725001304
C	3.01222606145667	1.20531971130135	1.11197559134080
H	3.49093211509061	1.86385298262614	0.38389257143563
C	3.70914937125795	-2.07733477849529	2.93063849322593
C	5.03469601186392	-1.99378575327420	3.40570246110823
H	5.55263921130021	-1.03304990175468	3.44600987409804
C	5.65656154597613	-3.14603206342010	3.85763384806385
C	4.99435802958076	-4.37372138023051	3.85227781923716
C	3.69777084030570	-4.48951675052130	3.37798259513816
H	3.20145091538543	-5.46203651967811	3.35176596142120
C	3.04219354585015	-3.33721078414952	2.89648526502127
C	7.02815190805536	-3.35489779720664	4.41770845378269
O	7.91314094648508	-2.55087478006605	4.59305280688627
N	7.10551035714627	-4.72302282399573	4.71592119912559
C	5.92100299336819	-5.41110724299276	4.40432350532258
O	5.72928302480460	-6.59329712896062	4.56425721162036
C	8.28245404879252	-5.34724324315861	5.28382742681515

H	8.52779722942481	-4.89477136187111	6.25704119256961
H	8.06740351315322	-6.41612274457239	5.41379860283899
H	9.14810234900538	-5.21923810042327	4.61567155044256
C	1.66657204770891	-3.48065295365647	2.33983203411293
C	1.35082947485154	-2.99480427408686	1.05800270966135
H	2.12846703930040	-2.52388436476438	0.45363415404978
C	0.05560358968948	-3.09638110950227	0.55612028838836
H	-0.19024402566572	-2.71610112299455	-0.43750491300648
C	-0.95021061643538	-3.69043435899676	1.32642548196526
C	-0.64709644137178	-4.19946031255485	2.59214825346694
H	-1.43901764717540	-4.66319576108056	3.18374354624447
C	0.65305205288554	-4.09823421090059	3.09202075257646
H	0.87900598412469	-4.47791261147869	4.09161904744551
N	-2.28606188178788	-3.77947304944437	0.80791255914439
C	-2.61454674072699	-4.89441085008526	0.02615278599171
C	-3.17498639934820	-2.73056919385823	1.08549458696069
C	-3.90818188107585	-5.01500459521601	-0.55669788724230
C	-1.65378679092083	-5.91496892222481	-0.18848092242903
C	-4.49664059292951	-2.74542237061272	0.55420741324225
C	-2.76135964632821	-1.64772732834199	1.90088725511657
C	-4.18365356420750	-6.16325940097889	-1.33852929923224
B	-4.95480023680406	-3.91521968021675	-0.32667521658749
C	-1.97194804975236	-7.02263332425857	-0.96240069295168
H	-0.65998848643654	-5.84281147876633	0.25136177910181
C	-5.35386413293615	-1.66196067620066	0.86749816252187
C	-3.64055085009885	-0.61075326916012	2.18622853402555
H	-1.75993103749984	-1.61122340490299	2.32732661644288
C	-3.24284501366241	-7.15992165396371	-1.54826640401611
H	-5.17966257370941	-6.24625712637933	-1.78309136303225
C	-6.40177823358246	-3.98437529326770	-0.95482585948018

H	-1.21486478507088	-7.79762630684678	-1.11320370870936
C	-4.94833767420150	-0.60590927329328	1.66890049656309
H	-6.36663209231313	-1.68200843179502	0.45458627010130
H	-3.28855121689129	0.19944307813847	2.82855953539087
H	-3.47968942470632	-8.03686318781582	-2.15561424545432
C	-6.66113817312859	-3.41342328949317	-2.22117086879865
C	-7.45595571489237	-4.62242813122617	-0.26331043150099
H	-5.63101829285138	0.21539002391780	1.90123772970559
C	-7.94915848774733	-3.48642569371127	-2.76876103128830
C	-5.54418988645313	-2.72949575760211	-2.97821097159086
C	-8.73350740841924	-4.67834625755452	-0.83681236086467
C	-7.19616723085272	-5.24583885650376	1.09023637320830
C	-9.00242975969146	-4.11331348667828	-2.09030299342499
H	-8.13645923533625	-3.04376752268236	-3.75298386569222
H	-5.13522301815262	-1.88260509028712	-2.40100390547468
H	-4.70423982571367	-3.42196593228055	-3.15849389232304
H	-5.88159792245143	-2.34437613302885	-3.95233832765736
H	-9.54128728865219	-5.17848244223731	-0.29181128838451
H	-6.42664428050365	-6.03385600616826	1.02345956297815
H	-6.81754669701443	-4.49717345563621	1.80700209237106
H	-8.10495034281910	-5.69526474019451	1.51829364414674
C	-10.39350399998588	-4.15033688471472	-2.67736575452991
H	-10.98288202623564	-3.27206984742588	-2.35773604380223
H	-10.37005501671655	-4.14182549585556	-3.77865674629856
H	-10.94694323662349	-5.04646543520719	-2.35440876209605

XYZ Coordinates of *pppazb* in S_1 optimized geometry

C	-1.31872842646709	3.42146880895718	2.12799384385616
H	-0.98729246848857	4.40265921806729	1.76058465238672
H	-1.77473751496205	3.53003852035984	3.12509518070827
H	-2.08536362614332	3.02071134852567	1.44237856708436

N	-0.16251990736526	2.56420667714212	2.18427083844259
C	1.12818006062234	2.94710420488796	1.67292814099892
O	1.34689737962417	4.03556281874435	1.16301839891050
C	1.97875927140362	1.79141157987261	1.90944223179943
C	1.20445296547274	0.78087609811988	2.54112090171157
C	-0.17415393893277	1.27776369635715	2.69290297768978
O	-1.17203892658318	0.69769794730405	3.13199395086843
C	1.74337171823188	-0.43833602844866	2.90073019180812
H	1.11864082763664	-1.15517255132185	3.43283398718310
C	3.09901562235488	-0.72370361772953	2.60566914438866
C	3.87147385064008	0.30797332705839	1.96795357423478
H	4.91256256186964	0.10087163583342	1.71111419986230
C	3.33218236362539	1.54195901821534	1.62985160078714
H	3.94226520391509	2.30373936148185	1.13818909235994
C	3.70315206610054	-2.01472694931137	2.95160768517818
C	5.05972689191248	-2.05163776577916	3.37570085455788
H	5.64464679380668	-1.13175701583016	3.43255372481184
C	5.62690861549264	-3.24098425687533	3.78285051024218
C	4.89765087883816	-4.44582956732495	3.78716888080693
C	3.57631697432743	-4.45586753505724	3.35029494639545
H	3.02721808123503	-5.39983146067711	3.30801732593860
C	2.97904075486124	-3.26507060238955	2.91375987176941
C	6.99912044563954	-3.52954465955051	4.28801939138149
O	7.94384550506230	-2.78247693191420	4.44585597810206
N	7.00819232401446	-4.90314052082150	4.55844387724113
C	5.76769767420179	-5.52624455100539	4.27732131971943
O	5.53880716235385	-6.71178606915774	4.43348529925904
C	8.16246340928297	-5.60153092814111	5.07281431193018
H	8.46465335088192	-5.19247959794903	6.05041232865680
H	7.89292073793287	-6.66086461493279	5.18133829969664

H	9.01768154718525	-5.50259243377674	4.38513064367792
C	1.60476833919586	-3.37294829414665	2.34322899104640
C	1.30695089504069	-2.88544629008613	1.05585680417118
H	2.09195217516487	-2.39637314501246	0.47764774875768
C	0.02484992714507	-2.98849719837164	0.52264646128983
H	-0.19668957243357	-2.59936761701484	-0.47358705813769
C	-0.98187811933406	-3.59294641024837	1.27952953825166
C	-0.71857890299557	-4.10061502893959	2.54923618525518
H	-1.51679516739856	-4.56863442183441	3.12978676944110
C	0.57175324107799	-3.98775845487860	3.07203548011621
H	0.77723397890227	-4.35922289810643	4.07797173665957
N	-2.32684593515050	-3.71064450431706	0.72560117040601
C	-2.62493183312858	-4.85647152502936	-0.01114592181741
C	-3.22723943733815	-2.68686415553494	0.96592638754985
C	-3.92235645535491	-5.04575262293633	-0.57735530165955
C	-1.61903681213353	-5.84465506980331	-0.19417336599582
C	-4.56533866322114	-2.75628380374647	0.45610526335957
C	-2.80880451053951	-1.55267671888287	1.72464023816923
C	-4.16031330966579	-6.22083712379520	-1.30199630091464
B	-5.02041384412813	-3.97397170978210	-0.37679217631387
C	-1.89863760284655	-6.99377903843486	-0.92322143443030
H	-0.62915700160917	-5.70679002378819	0.23418293086029
C	-5.42432760900563	-1.68889700736311	0.73137296560722
C	-3.69743372336176	-0.51421833463538	1.97324451852828
H	-1.79961245372523	-1.46056325007820	2.11945700770539
C	-3.16805853961388	-7.19353802277938	-1.48268460879056
H	-5.15417613983785	-6.36722224331135	-1.73297805444972
C	-6.46505138069583	-4.11336389545754	-0.96945017693671
H	-1.11572489349323	-7.74339774743952	-1.05591614013277
C	-5.00841363052623	-0.57399170458086	1.48328863119436

H	-6.44540458282567	-1.73509820197689	0.34366297567674
H	-3.32289189743048	0.33585945238095	2.54514477557236
H	-3.38114383709565	-8.09939344915940	-2.05422843129250
C	-6.73381779256592	-3.70696689485142	-2.29673583530706
C	-7.50976075189765	-4.65019881259894	-0.18365068202195
H	-5.70592785029387	0.24312640304378	1.67986425635560
C	-8.02970693212085	-3.83973445248212	-2.81051063670071
C	-5.62614290593761	-3.12724133759725	-3.14881081339344
C	-8.79378418534936	-4.77120396950435	-0.73071750779076
C	-7.23499068591212	-5.09980182740725	1.23470453051960
C	-9.07637167998501	-4.36834300525169	-2.04253372867139
H	-8.22931549425074	-3.52230710316619	-3.83896302991661
H	-5.19777800885313	-2.21996782837744	-2.68848329984182
H	-4.79532812912193	-3.84323655952876	-3.27205211519242
H	-5.98039562785212	-2.85328176665421	-4.15308888447592
H	-9.59569582838548	-5.19355660457921	-0.11701602068893
H	-6.45487360864994	-5.88031447265570	1.26574488525065
H	-6.87340193341433	-4.26461433806204	1.85887398790394
H	-8.13373932023956	-5.51023988796936	1.71738815299798
C	-10.47340627970609	-4.47000585968626	-2.60445633015535
H	-11.02257981274411	-3.52227811949740	-2.46354024689412
H	-10.46112038851520	-4.67937874284666	-3.68557353972289
H	-11.05502571542565	-5.26165096416967	-2.10758747544709

XYZ Coordinates of *ppazb* in T_1 optimized geometry

C	-1.35007956690448	3.29240849552516	1.78482731497284
H	-1.09684281156830	4.15466099452709	1.15349778176557
H	-1.65180617522794	3.63942773229546	2.78540257501067
H	-2.19566703111095	2.74316846951498	1.34014025406653
N	-0.18002281335751	2.44691246782892	1.86924163040384
C	1.03457680057754	2.70602865083716	1.18483743044822

O	1.23652732492670	3.67045049263364	0.47954037297140
C	1.92289987007157	1.56852696871548	1.52502385434880
C	1.22070417791436	0.70143869245230	2.37870135293150
C	-0.13998948747733	1.25867451048183	2.59465864571504
O	-1.06616179634425	0.79182742931641	3.23493752693842
C	1.78165571253239	-0.46625697213845	2.86039537036498
H	1.21379624944305	-1.10531245775304	3.53741043809627
C	3.09175257477472	-0.80809808454006	2.45453746086466
C	3.79621182764167	0.08109436265130	1.60282279863893
H	4.80423871648579	-0.18909294633313	1.27916677543480
C	3.22633484668917	1.27080107759206	1.13593723922246
H	3.77701806262615	1.94023854972160	0.47102649978860
C	3.71720934094360	-2.07170658506148	2.91261453166987
C	5.05284030063388	-2.04073403900782	3.37286601323447
H	5.61858527799601	-1.10653805270045	3.37265308623445
C	5.62332620045949	-3.19566881777319	3.87793493392214
C	4.90048164269556	-4.39498281346603	3.94239846126351
C	3.59579882368017	-4.46455253431003	3.47981101707264
H	3.05669033849831	-5.41458526950099	3.49976394224684
C	2.99495023796626	-3.31030937022633	2.93945620970668
C	6.98277292729964	-3.43939317185531	4.44023476280685
O	7.91272805486153	-2.67406382601351	4.57130871714346
N	6.99436839056426	-4.79348877172627	4.80784974808833
C	5.77403709987050	-5.44124493834952	4.53803714401521
O	5.53316056672400	-6.60759129878109	4.76343671331402
C	8.14210738762325	-5.44332583732391	5.40191541364389
H	8.40919354656880	-4.96338405297641	6.35655620337222
H	7.88078718125260	-6.49576256007150	5.57545590972662
H	9.01324527239294	-5.38006668560268	4.73119925148654
C	1.62625423438195	-3.43689051067779	2.36984948715210

C	1.32932577795231	-2.97303137978715	1.07283476307714
H	2.11849719837287	-2.51800297292744	0.47194961060841
C	0.04305488122431	-3.07134202794394	0.55087455964800
H	-0.18176979968245	-2.71061860329952	-0.45487300075895
C	-0.97326478829314	-3.63978709636737	1.32609988097454
C	-0.70395660111907	-4.12395452618800	2.60705640547803
H	-1.50830496635940	-4.56489446407550	3.19945554966358
C	0.59103072906468	-4.02715573605148	3.11846000223122
H	0.79719549504919	-4.38650739823306	4.12925449217887
N	-2.31188846933532	-3.73706932924120	0.78652158638180
C	-2.61098827275459	-4.86458110897653	0.00343359726204
C	-3.20698176573168	-2.70294754940518	1.07570258666939
C	-3.90963539313971	-4.99567555163339	-0.59107243232258
C	-1.62075161064053	-5.85595746307900	-0.18465861111672
C	-4.55124562092229	-2.76281687659916	0.57007568478450
C	-2.77184366079589	-1.60757154945525	1.86359964957159
C	-4.12330217048559	-6.12787507971691	-1.39959534061247
B	-4.99383153328854	-3.93310093752176	-0.32790840440232
C	-1.88352803209361	-6.97325249831633	-0.98817018578124
H	-0.64566507927470	-5.76128762817760	0.28967189989434
C	-5.40828760479007	-1.71151497809163	0.93543119387224
C	-3.66163757055341	-0.57748304911195	2.19675457441304
H	-1.74876082337600	-1.53973467774787	2.22950065546024
C	-3.13278403449410	-7.10338895208363	-1.60082326035522
H	-5.09946767974101	-6.23992568241861	-1.87857313349594
C	-6.44852999338425	-4.03766820792755	-0.92979528193098
H	-1.11064981097683	-7.73189972002053	-1.12665516063843
C	-4.97846641005902	-0.63439386212989	1.73552101420062
H	-6.44118787008633	-1.74283639626460	0.57882029369385
H	-3.29394605446433	0.24938365636382	2.80437772964292

H	-3.34400103922072	-7.97003536710548	-2.23335449853532
C	-6.82362654460084	-3.26103882761795	-2.05197351030384
C	-7.40508276503300	-4.91376887904764	-0.36138671869990
H	-5.68176514728445	0.16314487083240	1.99154374873459
C	-8.11905845160334	-3.36783507987458	-2.57704227091865
C	-5.82134138471266	-2.32899609931408	-2.69728966429322
C	-8.69249486136898	-4.99526010348375	-0.90779341845778
C	-7.03974959019296	-5.75465268327044	0.84237686661919
C	-9.07207788302787	-4.22774399439121	-2.01705886840620
H	-8.39134842832047	-2.76690637588804	-3.45121236393300
H	-5.49825142075081	-1.54041885218648	-1.99675697047972
H	-4.90950680356854	-2.87158171243841	-2.99982677645049
H	-6.23460012464769	-1.83723173586451	-3.59088681939615
H	-9.42189964393018	-5.67550677126744	-0.45510895958554
H	-6.21759757609214	-6.45183728692697	0.60844718726180
H	-6.68862901303388	-5.12460114362983	1.67734243961483
H	-7.89359517208538	-6.34821929237414	1.20243331565517
C	-10.47530148560204	-4.30529759337547	-2.56900820892952
H	-11.15873714268649	-3.64252828614206	-2.00833457105355
H	-10.51497606653127	-3.99652474941826	-3.62533003877872
H	-10.88402972763236	-5.32591149869091	-2.49567570603928

XYZ Coordinates of *pptp* in S_0 optimized geometry

C	0.296652	4.103881	4.976491
H	0.809931	4.903412	4.424694
H	-0.316957	4.526665	5.783486
H	-0.358754	3.559249	4.276823
N	1.286224	3.221663	5.558334
C	2.514510	2.921608	4.941495
O	2.894531	3.379538	3.890009
C	3.191147	1.951975	5.854882

C	2.356129	1.728258	6.955308
C	1.110770	2.535216	6.766177
O	0.126312	2.596455	7.469726
C	2.703378	0.853781	7.970632
H	2.034085	0.692660	8.816562
C	3.928747	0.156766	7.862381
C	4.767951	0.404193	6.755890
H	5.708064	-0.147100	6.676248
C	4.413194	1.305137	5.740599
H	5.062778	1.481216	4.880376
C	4.340201	-0.840668	8.893392
C	5.642879	-0.739806	9.428096
H	6.322465	0.047198	9.093694
C	6.037079	-1.627533	10.415675
C	5.167389	-2.612843	10.885837
C	3.889252	-2.746506	10.371276
H	3.232350	-3.542555	10.728057
C	3.456586	-1.864094	9.355547
C	7.328252	-1.742165	11.159830
O	8.332844	-1.078625	11.050962
N	7.149816	-2.816244	12.049741
C	5.876614	-3.396004	11.946221
O	5.481323	-4.331192	12.602190
C	8.159830	-3.278155	12.978523
H	7.798679	-3.195752	14.015491
H	8.411282	-4.332333	12.784263
H	9.051999	-2.652120	12.844837
C	2.084858	-2.034294	8.808220
C	0.986800	-2.174012	9.677585
C	1.828424	-2.030215	7.423215

C	-0.317208	-2.245762	9.192643
H	1.151845	-2.171965	10.758197
C	0.530871	-2.104330	6.930943
H	2.661523	-1.965207	6.720741
C	-0.566188	-2.186228	7.809836
H	-1.157372	-2.318056	9.885791
H	0.349350	-2.088103	5.854556
N	-1.883621	-2.178581	7.301402
C	-2.866606	-3.047092	7.835259
C	-2.231991	-1.200933	6.328117
C	-4.190947	-2.609899	8.025168
C	-2.530306	-4.369232	8.183146
C	-3.007854	-1.551149	5.209429
C	-1.805991	0.129976	6.480624
C	-5.151520	-3.479970	8.544001
H	-4.461691	-1.585325	7.763395
C	-3.493922	-5.225296	8.717923
H	-1.507707	-4.719593	8.028844
C	-3.356221	-0.582334	4.266146
H	-3.337475	-2.585634	5.090998
C	-2.150693	1.089965	5.527345
H	-1.208303	0.422067	7.345860
C	-4.811530	-4.789957	8.898356
H	-6.175481	-3.122986	8.684748
H	-3.213675	-6.248629	8.982472
C	-2.928091	0.742102	4.417205
H	-3.960379	-0.868023	3.400694
H	-1.818585	2.118733	5.680861
H	-5.565795	-5.465195	9.309609
H	-3.203587	1.497300	3.676487

XYZ Coordinates of *pptp* in S₁ optimized geometry

C	0.61514289817627	4.22226505865939	4.72723712754542
H	1.18549995677750	4.85652986687726	4.03430978207492
H	0.09925881716623	4.84480885731004	5.47486525727840
H	-0.15072327504274	3.67168228896269	4.15212966076774
N	1.54385641177382	3.32749116593383	5.36820440963568
C	2.90164495271191	3.15834440970737	4.92839289004229
O	3.38087257592316	3.76597215726315	3.98086424946813
C	3.46056407628629	2.16650735216841	5.83226898695343
C	2.45837209191941	1.78438898691645	6.76783008176630
C	1.22262163922164	2.51918018252033	6.44822009779925
O	0.10093894284036	2.44682345257621	6.96288685125452
C	2.70841359250751	0.85878105915762	7.76634218042358
H	1.92504625347112	0.64677907638430	8.49348785696454
C	3.97686732621758	0.23868149331797	7.85049083803607
C	4.97624152663530	0.62899190834929	6.89042998963495
H	5.95202086741883	0.13964657293355	6.91862525963962
C	4.73265252397827	1.57565443779854	5.90624419975221
H	5.50844464298561	1.84954054324600	5.18693641911181
C	4.29778434414250	-0.75851615959532	8.88298022667651
C	5.61458406373700	-0.78438764782344	9.42123115969566
H	6.35858069189770	-0.05767958645987	9.09059278960503
C	5.94608447838952	-1.69313360249592	10.40476605871173
C	5.01487205489404	-2.61722784049793	10.90556316669275
C	3.71844076063065	-2.63247770157914	10.39677518094955
H	2.99892240911577	-3.36933941668074	10.76240383811433
C	3.35686831843305	-1.72511756546184	9.39179919739496
C	7.23853655167620	-1.89678104948916	11.12530085244962
O	8.29260401617190	-1.31069837066166	10.99432940729520
N	6.99474914961708	-2.94861318731226	12.01982720282346

C	5.66935386440331	-3.43391715283928	11.94422699900789
O	5.23208314153287	-4.33929200279086	12.62849323890286
C	7.98018948847825	-3.48194627604715	12.93129954765918
H	7.64863461362166	-3.36807238910628	13.97579001827244
H	8.14593547660530	-4.55450588007915	12.74231045102409
H	8.91635156448368	-2.92848513830336	12.77695347172403
C	1.96610494450134	-1.84889427766092	8.85435886923519
C	0.86438519561775	-1.73169077558062	9.71738192699326
C	1.72859601978785	-2.10370438593747	7.49186963223895
C	-0.44232210407285	-1.84501071939324	9.23895332970516
H	1.03659825423761	-1.52418804228036	10.77540765196000
C	0.43001800199360	-2.19957186382594	6.99693442044863
H	2.57570029310785	-2.19429957288477	6.81060963610270
C	-0.64968668830874	-2.06302268391950	7.87645435955008
H	-1.29599283094865	-1.73728818496015	9.91149576649863
H	0.24872812735295	-2.37525316396245	5.93442108867946
N	-2.00020886457091	-2.14088177791956	7.36806702170779
C	-2.83225287682983	-3.15887159243890	7.85464635674454
C	-2.42710793044776	-1.19082764005507	6.44513352212568
C	-4.21396908399360	-2.92955989216595	8.05899838142957
C	-2.27659374210836	-4.41742146896049	8.18454965552522
C	-3.42902352757932	-1.51029205288956	5.48594456345086
C	-1.83523734354714	0.09922236645153	6.43967562644966
C	-5.01978392483990	-3.95026040335215	8.55270948558561
H	-4.63147245888818	-1.94065506690994	7.86527980197666
C	-3.09716267157666	-5.42799416047783	8.67035541004913
H	-1.21051200163064	-4.58937547198203	8.03431177156932
C	-3.84294365280912	-0.54736655402309	4.57812871603211
H	-3.83406760132541	-2.52181845321422	5.44061257041473
C	-2.27072875555354	1.05175781652147	5.53017003149800

H	-1.05713021342508	0.37665064071256	7.15060752475986
C	-4.46998399415380	-5.20345070379260	8.85415274354069
H	-6.08188200572473	-3.76186628202404	8.72392841165452
H	-2.66622083377173	-6.40346988029168	8.90553914710476
C	-3.27477949342902	0.73858348258889	4.60003110096509
H	-4.59678326350287	-0.80088843599784	3.82956807388566
H	-1.80558896292401	2.03744168223267	5.57476926188819
H	-5.10663137623061	-6.00064523594689	9.24381875113135
H	-3.60591144320513	1.49035385148119	3.88026744395004

XYZ Coordinates of *pptp* in T₁ optimized geometry

C	0.33332816017335	4.16618263326917	5.02471039849800
H	0.84156641511020	4.93970787959622	4.43299104635253
H	-0.25553286891483	4.62420150188836	5.83200802614167
H	-0.35154626889939	3.61118815453242	4.36043115786042
N	1.33508941662504	3.29424259425177	5.59501895819168
C	2.62733749741568	3.11550512085863	5.03508386727451
O	3.03069641415688	3.69499640320874	4.05058970112727
C	3.29294666364438	2.11790308064726	5.90009502326420
C	2.40506415003121	1.75407302645821	6.92628034189743
C	1.12734801751848	2.50035505434483	6.72078357598328
O	0.08807334183774	2.43581033913973	7.35102264831414
C	2.73716017300618	0.82828018557985	7.89346304595758
H	2.03714847049794	0.61241623653430	8.70003640964335
C	4.01206336250063	0.18525518424250	7.83033933780745
C	4.90721958870479	0.58777955144668	6.78753970281208
H	5.87794926284967	0.09456276049856	6.70991020909555
C	4.56504067120966	1.53987591337255	5.83255601765627
H	5.25880935617890	1.81462888653713	5.03475502747909
C	4.38246021316209	-0.85461975170048	8.78031543435694
C	5.73413376824062	-0.95823332096183	9.19295076000926

H	6.50978798390615	-0.34510834367340	8.72965640238319
C	6.06667805127055	-1.74947986558207	10.27018195040748
C	5.06875092346384	-2.48123537519901	10.99468004619251
C	3.75778841408421	-2.46659344446967	10.59460421619994
H	3.04089820257776	-3.09874157676028	11.12208438933056
C	3.37324220875978	-1.73248239793365	9.43168689497075
C	7.37321643080685	-1.97762034280741	10.92291249497470
O	8.47305275202282	-1.54756089882178	10.63364848319783
N	7.09463385800775	-2.84248700330288	12.00070813678925
C	5.73274108445235	-3.19247920049722	12.10376834884678
O	5.27254526028086	-3.92768208210851	12.95602546111203
C	8.09822868792189	-3.32747157449699	12.92009921503027
H	7.87300335225620	-3.00119927048683	13.94818148480143
H	8.12844753604822	-4.42858468465321	12.91348177847342
H	9.06940839004372	-2.92309649553112	12.60480467607829
C	2.06404849474532	-1.96082892935381	8.87397624633749
C	0.94639765035319	-2.31280695929333	9.70412890022421
C	1.78819652067676	-1.84872731805140	7.46647123662624
C	-0.32848497309067	-2.43289460092203	9.20120485523924
H	1.08798057623314	-2.40031130161001	10.78217250362086
C	0.51449999082823	-1.96709622273263	6.96014149647417
H	2.61574164328449	-1.69280670556267	6.77571996431064
C	-0.58776492928564	-2.22262251461740	7.81614833232392
H	-1.16345194609800	-2.62425557469009	9.87741453870876
H	0.34404525006419	-1.87338335733657	5.88615243477193
N	-1.88994663035310	-2.21755229924697	7.31929442417843
C	-2.87696576237949	-3.08250312211524	7.85779439071826
C	-2.25027743362750	-1.27815929710318	6.31108576710849
C	-4.18262461196185	-2.61320997047403	8.09484931154871
C	-2.55352665063007	-4.41929031205748	8.15691423371771

C	-3.04917126708190	-1.67488779001371	5.22381934140205
C	-1.81321298436934	0.05444189124448	6.41237870273519
C	-5.14448559313300	-3.47302853733568	8.62384950186498
H	-4.43056624199739	-1.57425182646861	7.87018021055622
C	-3.52168533828665	-5.26733650319727	8.69482870971354
H	-1.54501907757056	-4.78522854643678	7.95427146186302
C	-3.40495719701473	-0.74154651636314	4.24995438758641
H	-3.38080718787741	-2.71253044543039	5.14886793101551
C	-2.17251105737790	0.97755260319046	5.43061128191072
H	-1.20095014358368	0.38006985565379	7.25489503049806
C	-4.82035737516606	-4.80081628925751	8.92897115771557
H	-6.15426703505892	-3.09891510319704	8.81089610537861
H	-3.26235539713642	-6.30488739742348	8.92003125509312
C	-2.96813133437619	0.58620427829478	4.34757893918569
H	-4.02111649203593	-1.05551515005869	3.40352593888596
H	-1.82997905120575	2.00838727229314	5.54042827782309
H	-5.57762473411874	-5.46909644898325	9.34579936541932
H	-3.25098462232068	1.31286326123525	3.58180009693201

XYZ Coordinates of *pppztz* in S_0 optimized geometry

C	-0.44053184530418	-0.07906058473687	-0.39280547669151
H	-0.27732637689246	0.84475171671321	-0.96578578028194
H	-1.05993423097602	0.12300293823867	0.49078315932787
H	-0.95779901215430	-0.80777036997374	-1.03828516458134
N	0.82925860387087	-0.60778352191119	0.06050214095659
C	1.94150736319323	-0.77691437559668	-0.78443272480448
O	1.97329287130346	-0.46720501375079	-1.95300876239130
C	2.98577675426788	-1.43725525467389	0.05518912853040
C	2.45182133540742	-1.63669690545430	1.33272021472620
C	1.05559757759539	-1.10784484969477	1.35010265293369
O	0.24475196730819	-1.12225808735280	2.24991377667643

C	3.14321407621183	-2.32237794027408	2.31275395794711
H	2.68980976630910	-2.49271195152886	3.28881706635283
C	4.40152708585159	-2.87299345963555	1.98244208644843
C	4.95873254956081	-2.61258222113048	0.71608513793860
H	5.93509868255802	-3.04068063258546	0.47471937556960
C	4.25843727981239	-1.89046892035306	-0.26452316064021
H	4.67837972752712	-1.72657701262082	-1.25939363958871
C	5.05984040447641	-3.82418562396519	2.92711885171644
C	6.37277210296515	-3.59088701757778	3.37656728145380
H	6.93495836730945	-2.71697465100259	3.03926756301020
C	6.92448952886500	-4.48032793843676	4.28709670622088
C	6.20447404875824	-5.58192459841094	4.75330874247257
C	4.91699790858901	-5.84755079982824	4.30946852729544
H	4.37324932878383	-6.72756853890061	4.65998666408683
C	4.33592854253843	-4.97400793142778	3.37091669861796
C	8.26825029123032	-4.48641757824357	4.94204950294445
O	9.18730385054940	-3.71139622664186	4.81282864786257
N	8.27382368704598	-5.61394294269587	5.77629260856883
C	7.06653070825705	-6.33061640374533	5.72047685988880
O	6.81727256878916	-7.33742098199126	6.34100489703159
C	9.40486500955504	-5.98936600770168	6.59790563052098
H	9.63104951987753	-5.19993882260630	7.33168371133187
H	9.14703543571321	-6.91931935196754	7.12183088456213
H	10.29891018909176	-6.14648706999126	5.97493661286220
C	2.97042405468016	-5.20748210009469	2.82579289798220
C	2.76821327080096	-5.33502190815269	1.44141171706762
H	3.62961265950715	-5.47914758011850	0.78496767539117
C	1.50627282855454	-5.21699399755126	0.87462813319611
H	1.40372328714182	-5.31633825185884	-0.20468570963809
C	0.37809169353160	-4.92515811499757	1.67593443417733

C	0.55693091955562	-4.96051278930767	3.07702991431516
H	-0.29520123423784	-4.83653557792221	3.74280014519727
C	1.82778862609543	-5.09891836444461	3.63230562972165
H	1.93813314706023	-5.04108994762725	4.71901379747816
N	-0.86275937807967	-4.62855443864940	1.09370757370546
C	-1.05448654649372	-4.59523515785149	-0.31713855302670
C	-2.05786894589827	-4.45991232114308	1.85524093179149
C	-0.32954276515275	-3.72521173894713	-1.14335417865626
C	-2.04859620951725	-5.41470482068491	-0.88123382181329
C	-3.15848326874808	-5.28503993155010	1.55892295130784
C	-2.18512519028026	-3.45468650790804	2.82444365164656
C	-0.54187906798939	-3.71679408415501	-2.52231067513022
H	0.41429733852370	-3.07172186279845	-0.69016673119911
S	-3.01752544024094	-6.44677924399901	0.20797607544571
C	-2.27388160890073	-5.39402113195869	-2.26426445045880
C	-4.34849707525432	-5.15896926035982	2.28619212333759
C	-3.36690053904770	-3.34663653135812	3.56111775980351
H	-1.35442918595099	-2.76515216088907	2.98741965235533
C	-1.50893038425356	-4.56026224263739	-3.08389104525680
H	0.04175674334341	-3.03922802073546	-3.15057742035467
H	-3.05693539737664	-6.02544648137038	-2.69112002043853
C	-4.44084404714220	-4.20728483736973	3.30457195198021
H	-5.20108094307969	-5.79711281165634	2.04134289633390
H	-3.45425480427647	-2.57311149045454	4.32810473757995
H	-1.68454467567026	-4.55312453853322	-4.16248165886840
H	-5.36698352904926	-4.11704282145907	3.87785523615073

XYZ Coordinates of *ppptz* in S₁ optimized geometry

C	-0.64916964233958	-0.30290538149971	-0.30835501777889
H	-0.53531245116016	0.61361342233453	-0.90694505695103
H	-1.25386467790177	-0.10121304553629	0.58654354569459

H	-1.16884838187559	-1.04745358572007	-0.93689769756937
N	0.63863932434303	-0.78310804208759	0.12124868579979
C	1.71968397494474	-0.98924840549753	-0.77618077708973
O	1.63607833265403	-0.79994322460346	-1.99577280498497
C	2.78305997474362	-1.54100289447515	0.04727792275307
C	2.29399143460323	-1.66867318931256	1.38459427789368
C	0.91625491009381	-1.21279640639452	1.43015113815586
O	0.08417908735645	-1.25034681322354	2.35421937212038
C	3.05411819505563	-2.31046888707573	2.36377988608493
H	2.63813115982716	-2.42844490880332	3.36548954985835
C	4.29675259739226	-2.85115150196372	2.03235007006068
C	4.81108511777388	-2.66598083742056	0.70520023098130
H	5.79110043989681	-3.08313928571468	0.45800400137452
C	4.06607667431207	-2.02242716743808	-0.27487587091939
H	4.45052131707943	-1.91406009682899	-1.29237567492492
C	4.98254378181377	-3.78240698708033	2.97151960325211
C	6.30831756298474	-3.54738312857607	3.38904863308185
H	6.84251164834036	-2.65974346690317	3.04342818284984
C	6.90982108555008	-4.44408119810794	4.26011320571908
C	6.23517417973170	-5.57172811018579	4.73107935033448
C	4.93482111482413	-5.84855793502129	4.32774923713217
H	4.42296761316196	-6.74710244672509	4.68010101189088
C	4.31115413764223	-4.96032224306445	3.43738463690626
C	8.27910497465370	-4.43565699888138	4.86588931971923
O	9.17752706881996	-3.63945524590258	4.72250451672183
N	8.33871937265490	-5.58099033457024	5.67316484143596
C	7.14318683401943	-6.32059083660849	5.64679869232206
O	6.93889050811294	-7.34566200846733	6.25679425911745
C	9.50576498933368	-5.94989505039764	6.44468628911733
H	9.76700153167412	-5.15220571734766	7.15736111510358

H	9.27084567567927	-6.87385864700328	6.98968953237585
H	10.37103164581192	-6.11732206356313	5.78424161823765
C	2.93369745706891	-5.23020755276165	2.92760664526392
C	2.74037972174144	-5.52073257676136	1.56573293973580
H	3.60223158719030	-5.75669877816771	0.93942388076544
C	1.49012170801406	-5.41221015276938	0.98187872728636
H	1.38459078934292	-5.62178397212222	-0.08031345065061
C	0.37809631661126	-4.98024855786154	1.74805567669281
C	0.53248172258300	-4.90651463594379	3.15202436395656
H	-0.31554443502051	-4.69698462511137	3.79821529920661
C	1.79464764873360	-5.02909473768303	3.72184373751062
H	1.90949531748161	-4.86862702517011	4.79608568521252
N	-0.83606003537316	-4.67201374914492	1.10727573522726
C	-0.92927625328418	-4.59233929092625	-0.30509344056382
C	-2.04072180847248	-4.40810940824530	1.80879699098921
C	-0.00831984563912	-3.82900134731661	-1.04272813438744
C	-2.00324142591337	-5.23154651795130	-0.96539365006071
C	-3.21697866207713	-5.08806760945709	1.40966263620879
C	-2.09595413066636	-3.44770396421609	2.83602865687856
C	-0.13159903918757	-3.72379701704821	-2.42064371896161
H	0.77763053648259	-3.29454525072938	-0.51687685399652
S	-3.22401820883756	-6.10628541575268	-0.03454450786095
C	-2.09300316919270	-5.16055619407814	-2.36481113641034
C	-4.39834644512716	-4.91890940952950	2.14821331306917
C	-3.28429715469150	-3.27137905223091	3.53697149979319
H	-1.22932508091979	-2.80449605128636	3.01190275497164
C	-1.16231311086984	-4.41283338472879	-3.08361875849797
H	0.55718332978940	-3.06582781109288	-2.95432253427399
H	-2.92002275990762	-5.65743819851979	-2.87693870686503
C	-4.42190849479111	-4.03166089250045	3.22100464466897

H	-5.30311320097753	-5.45222138517837	1.84802058448959
H	-3.33184428085716	-2.51355305983083	4.32180743105052
H	-1.26214662717309	-4.33282401525336	-4.16853784682428
H	-5.34852307766849	-3.89106569096272	3.78235171049878

XYZ Coordinates of *ppp*tz in T₁ optimized geometry

C	-0.19581216091885	0.01643455720500	-0.67477779657323
H	0.04202227242278	0.58492254393259	-1.58397769175115
H	-0.67373061513476	0.67670612506451	0.06527148232644
H	-0.90459329861406	-0.79159424892245	-0.92065319853312
N	1.04175463922614	-0.51957306058382	-0.15425566823017
C	2.30309956007728	-0.38604469662436	-0.81372727802510
O	2.45760508701839	0.19099013508823	-1.87072957407901
C	3.26494336945154	-1.09476977100043	0.04452952164122
C	2.57109118066190	-1.59079075687348	1.16706590060215
C	1.13542076577357	-1.23146739214674	1.03759508594353
O	0.19501531883706	-1.53341876158618	1.75419083986037
C	3.18074520644462	-2.36642640040280	2.12090649053773
H	2.61018070859637	-2.68426832898079	2.99183217567806
C	4.54815073229192	-2.75437234481627	1.94651777429723
C	5.26611436737625	-2.16146655350218	0.84719913425398
H	6.31845394210407	-2.41801226714196	0.70714110970179
C	4.64087148416533	-1.35560709689461	-0.09462043019642
H	5.19426958827605	-0.95858700580166	-0.94884700341585
C	5.12015869870168	-3.77810943772517	2.78909840454756
C	6.49690635867382	-3.77039951540485	3.14540682467591
H	7.19471883562321	-3.06209148551739	2.69300686177563
C	6.92305517223572	-4.58667794658098	4.16419137834290
C	6.03102661200381	-5.46185690186970	4.86632892167645
C	4.70798688420214	-5.57250563253207	4.48852470188131
H	4.06406602266077	-6.31322932020499	4.96944249157876

C	4.24502954008187	-4.81207135585437	3.39144989811404
C	8.27003477775513	-4.72134301958741	4.77405944729331
O	9.31000521711508	-4.16142724592294	4.48945124806367
N	8.11785666175737	-5.67113228695292	5.79297638745325
C	6.79585633746596	-6.16701251303778	5.90721126473923
O	6.43432912332829	-6.99685846612801	6.71865275304107
C	9.20855970153503	-6.09340477496207	6.64145658720656
H	9.60849908279499	-5.24106158677591	7.21386639647518
H	8.82423655979019	-6.85736035758011	7.33041591859826
H	10.02922725987264	-6.51037022405220	6.03648779951377
C	2.94364468206395	-5.07970325827288	2.80529213609310
C	2.74487828943852	-5.06294007297026	1.38904368016622
H	3.61993788153894	-5.02868018619021	0.73811386766095
C	1.49239532431764	-5.06883183753542	0.82236892594595
H	1.40132488032926	-5.06582167004108	-0.26185361694075
C	0.33284838608907	-5.01333045101668	1.64518028690414
C	0.51709204020114	-5.23279623765985	3.04478030296380
H	-0.35139574152200	-5.31907447464332	3.69613748538958
C	1.77959050059297	-5.29597954647556	3.59707186204191
H	1.87900841071890	-5.40639347965872	4.67920310887373
N	-0.91991128685285	-4.77443336173835	1.11899982325560
C	-1.19014059919839	-4.70455358969794	-0.28194586522503
C	-2.07810037607621	-4.62643096792242	1.94242843467676
C	-0.55274539909623	-3.78297755404661	-1.12421474451406
C	-2.18867748936313	-5.55432442750274	-0.79533340185283
C	-3.17629478667103	-5.46814444282984	1.69414635868626
C	-2.14880009740495	-3.63066678522705	2.92578703142163
C	-0.84097219310574	-3.77586358360658	-2.48947324917875
H	0.16763012229894	-3.08194089175609	-0.70387893853152
S	-3.09291557912743	-6.60913388506787	0.32466157871569

C	-2.47717085785016	-5.53713819340487	-2.16608503282136
C	-4.31767319658489	-5.37058179128114	2.49996926685955
C	-3.28706819445056	-3.54597683287385	3.72837444169333
H	-1.31169519329713	-2.93706145333692	3.03040229115149
C	-1.78887642625567	-4.66451253314008	-3.01180884953990
H	-0.33094910736513	-3.06420751986448	-3.14294237426606
H	-3.25490368983656	-6.19493288476339	-2.56115599972902
C	-4.35930980848149	-4.42561899317638	3.52808987045983
H	-5.17426095444848	-6.02053504666004	2.30660291779289
H	-3.34413859495350	-2.77877072648068	4.50405046791092
H	-2.01673283936887	-4.65698425066274	-4.08042912406799
H	-5.25057309993275	-4.35373167581873	4.15635889898823

XYZ Coordinates of *pppa* in S_0 optimized geometry

C	-2.97947232270259	1.68748905002956	1.74489617148227
H	-2.76357333307694	2.54184456684535	1.08988609148402
H	-3.28242290138906	2.04344986800370	2.74098089018443
H	-3.80514891029392	1.09479087660660	1.31992478905704
N	-1.77680076758601	0.88587664598794	1.84260063401712
C	-0.61113671311762	1.11333836892092	1.08544863014248
O	-0.45378207913857	2.01356251428189	0.29576785162936
C	0.33266326160629	0.01921603196275	1.47117506678890
C	-0.30183640701876	-0.78955232997689	2.41804022879996
C	-1.66473122278396	-0.23334834574728	2.67123148420254
O	-2.52553809502955	-0.64668538447508	3.41646048500785
C	0.30335051254489	-1.91724718910971	2.94137804175226
H	-0.21722830718548	-2.53635651043639	3.67307333802047
C	1.59437746064781	-2.25500638088410	2.48031642064821
C	2.23836552415634	-1.41673588687316	1.54766127004513
H	3.23654884387546	-1.69017108262277	1.19640702093274
C	1.61642275790496	-0.27022182164738	1.02949315493861

H	2.11273050190077	0.36407014012529	0.29171417705345
C	2.26209190263284	-3.49571109471714	2.96603848910339
C	3.57214275874442	-3.40213374437094	3.48016830554655
H	4.09175758290276	-2.44188055173979	3.50969691583087
C	4.17468760201222	-4.54283215672551	3.98481033609142
C	3.50791287400361	-5.76821248011300	3.99309872872653
C	2.22711164686349	-5.89403294522833	3.47994553936462
H	1.72781372932682	-6.86525135242288	3.46537776395195
C	1.59170371415892	-4.75409154029628	2.94489380465305
C	5.52587576562861	-4.73940611109110	4.59595108684641
O	6.40827837401207	-3.93368665633033	4.77729977327820
N	5.58769379002258	-6.09843752549942	4.93673249183898
C	4.41138655922924	-6.79173074127278	4.60572834763658
O	4.21010487332598	-7.96822356992751	4.79402165848955
C	6.74236378510341	-6.70944700475278	5.56139971625571
H	6.95938390954196	-6.22733216716918	6.52712322446026
H	6.51731576074357	-7.77266256292091	5.71830977777048
H	7.62973510891318	-6.60695069109513	4.91771866408303
C	0.23356960202827	-4.90629267500793	2.34941684408219
C	-0.03964719732745	-4.45293481279482	1.04609026075214
H	0.75982179764498	-4.00465816275534	0.45291686870278
C	-1.32070005606744	-4.55653292965739	0.50976350065405
H	-1.53345555455092	-4.20084660399632	-0.50050290694982
C	-2.35833103011335	-5.11869391877666	1.26411505051335
C	-2.09322935299679	-5.59673984482017	2.55172247991653
H	-2.90655813561101	-6.03682483311099	3.13231890726834
C	-0.80731100131505	-5.49498980641567	3.08715572588520
H	-0.61403162679651	-5.84943260572294	4.10285783452435
N	-3.67453713431729	-5.20509681764003	0.71334750124440
C	-4.01199474696471	-6.32296843291385	-0.06654111654716

C	-4.57301387450394	-4.14242702916891	0.91904089520357
C	-5.27722218133404	-6.41319745059188	-0.68886170255629
C	-3.08069995176800	-7.37269711531791	-0.23124110154221
C	-5.85616109891170	-4.16228694349226	0.32788819839173
C	-4.19547549228821	-3.04533996239267	1.72418207219362
C	-5.55276520025229	-7.55601050172185	-1.45520711817324
C	-6.34329160340546	-5.31760975422466	-0.55667538036216
C	-3.38840967963021	-8.49200399687441	-0.99906689885439
H	-2.10552111659007	-7.30945469918166	0.25016066023108
C	-6.70785689336097	-3.07312976422588	0.56926571380269
C	-5.06865913823435	-1.98387935500813	1.94871710270709
H	-3.21287640953938	-3.01938629444280	2.19348774314547
C	-4.63426021310380	-8.59235388650510	-1.62135211181954
H	-6.52636899149173	-7.63907900828765	-1.94344483286165
C	-6.67641394245397	-4.76633085180136	-1.96790438653407
C	-7.61992661311905	-5.93324105578431	0.07468045107176
H	-2.64675839238233	-9.28798455683406	-1.10759934733202
C	-6.33778394364664	-1.98999473651983	1.36608006362075
H	-7.70207692965147	-3.07396672242316	0.11680183866627
H	-4.73799854592409	-1.16382401163495	2.58893692665764
H	-4.89025518164253	-9.46444803121636	-2.22750712052205
H	-5.78078703163049	-4.32500808646835	-2.43152756645606
H	-7.45385667279943	-3.98878242437140	-1.91732505243520
H	-7.04601266719922	-5.56422343889131	-2.63014097289173
H	-8.01088160104676	-6.75745900211245	-0.54126290180826
H	-8.41978020240565	-5.18320762084706	0.17132180673253
H	-7.40089722423592	-6.33003692003050	1.07781670784222
H	-7.03527634154061	-1.16545316133473	1.53270777372143

XYZ Coordinates of *pppa* in S_1 optimized geometry

C	-2.76600276329442	1.95991418093441	1.75332246027876
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H	-2.42815714289398	2.92037032426230	1.33985200200447
H	-3.24185422916586	2.12158143963184	2.73383142037515
H	-3.51847811085035	1.52058802760324	1.07582607877628
N	-1.61036303102040	1.10918187356944	1.87903216688066
C	-0.31000121110093	1.46684553780945	1.37637155728804
O	-0.08090040527956	2.52660503985164	0.81383740034754
C	0.53745720569460	0.32707119527975	1.69196875352448
C	-0.24888177229731	-0.65116355898553	2.35734435430102
C	-1.63206277428251	-0.14946425449925	2.45430211874346
O	-2.63728624315588	-0.70658185957814	2.90263445064310
C	0.28267798596197	-1.84951381150165	2.78936506767431
H	-0.35314510193550	-2.54084994883673	3.34176813915162
C	1.64546270762316	-2.14629192710053	2.53907047742454
C	2.43058420512907	-1.14592180326395	1.86882312762481
H	3.47759943452583	-1.36312079439370	1.64663485555294
C	1.89714467747902	0.06796316634217	1.45610394510627
H	2.51692045721132	0.80546579448852	0.94011556333997
C	2.24210064170210	-3.41815262352334	2.95956917714748
C	3.58756708156351	-3.43216798655592	3.41831626601796
H	4.17010361911082	-2.50937098930620	3.44596037906948
C	4.14534813206770	-4.59937598372628	3.89630775179589
C	3.41677215659431	-5.80453206101282	3.93988332514311
C	2.10692302345221	-5.83781419575004	3.46933540913738
H	1.56049040715742	-6.78419625771856	3.45698151013236
C	1.51996035649598	-4.67081730390435	2.96211165861210
C	5.50385296626699	-4.86021478060237	4.44971702050246
O	6.44424698604555	-4.10451920909597	4.59518950695637
N	5.50651450894618	-6.21894530212999	4.78655212538784
C	4.27365721171683	-6.85763466910814	4.50395364794386
O	4.04208996391007	-8.03513491106422	4.71206154406442

C	6.64675645644907	-6.88957681944474	5.36448355154525
H	6.91721261465870	-6.44003483951728	6.33367630331375
H	6.37801283217968	-7.94498599622935	5.50794122645188
H	7.52249362520100	-6.81397448687684	4.70006586414614
C	0.16137783885638	-4.80783919198639	2.36031233828988
C	-0.10329684418705	-4.37532874833721	1.04644173280945
H	0.69591244675781	-3.90930129444690	0.46879516675412
C	-1.37123648056440	-4.50183230153966	0.48534303534335
H	-1.56730894611038	-4.15253813197345	-0.53073250647066
C	-2.39646013398617	-5.07717124046030	1.23979156972900
C	-2.16523613644838	-5.53284112282149	2.53514687282209
H	-2.97761185353423	-5.97765664770765	3.11417080947502
C	-0.88933459939398	-5.39490962324251	3.08646325416986
H	-0.70990074897816	-5.72368424335287	4.11199440372302
N	-3.72533635851993	-5.21467993860721	0.65905529379661
C	-4.02437624667552	-6.37819207138794	-0.03885653300683
C	-4.63876195225862	-4.18700246055950	0.82867997783238
C	-5.30970146616781	-6.56195017026570	-0.61981304239230
C	-3.03084775034161	-7.38663434019336	-0.16844628904839
C	-5.95303742588004	-4.29585529935495	0.28257313450958
C	-4.25338500696169	-3.02299751312085	1.55086002119486
C	-5.54569422685012	-7.75532879628318	-1.31048587959551
C	-6.40731708924283	-5.51208861064088	-0.51339715398401
C	-3.30402855697833	-8.55278546743500	-0.85909647562509
H	-2.05182247360612	-7.23460058881950	0.27914709322948
C	-6.82966066494852	-3.23010274896320	0.49454415273052
C	-5.14909067077054	-1.98742085651164	1.73433520322084
H	-3.25394482377768	-2.91831148363465	1.96608023585957
C	-4.56921512450288	-8.74360987759933	-1.43625346076459
H	-6.52216032395670	-7.92281424435060	-1.76697192469004

C	-6.79785450282177	-5.05229414825931	-1.94768768519895
C	-7.64141728444178	-6.14461889508198	0.19042378795832
H	-2.53231873339203	-9.31916654095495	-0.95179693981618
C	-6.44732678823210	-2.09027771228364	1.20755805146715
H	-7.84208303676094	-3.28177110338505	0.09139462333775
H	-4.80403568649241	-1.10895938628648	2.28038614852065
H	-4.79253800184558	-9.66170456124519	-1.98344071876742
H	-5.93582681131413	-4.60163503046700	-2.46176435834819
H	-7.60499699998195	-4.30687707374498	-1.91116882235290
H	-7.15293354056669	-5.90204895014150	-2.54836783736567
H	-8.01299980630815	-7.01247735328211	-0.37305743410337
H	-8.46331284508007	-5.41843463461973	0.26355554136612
H	-7.38365914484007	-6.47693360430634	1.20709907594572
H	-7.16298767076116	-1.27757419839241	1.34897533103954

XYZ Coordinates of *pppa* in T₁ optimized geometry

C	-2.71359972772030	1.84557634186785	1.48026541442962
H	-2.43025836811856	2.71416041577602	0.87066327953344
H	-3.06097428500849	2.18443484874095	2.46922363602019
H	-3.53897322062297	1.30185480036230	0.99331389889000
N	-1.55038814171142	0.99727052715905	1.60889089971256
C	-0.28686296697278	1.28890891924363	1.01951820244640
O	-0.05119542040229	2.28269461698118	0.36646768018818
C	0.58231201175647	0.15339571678144	1.38210034082190
C	-0.17100688214526	-0.75339032821606	2.15200569399895
C	-1.55114078417161	-0.21070518823949	2.29593600283419
O	-2.51125826680392	-0.70172067697435	2.86235818271404
C	0.35748575620615	-1.92302604332214	2.64196169212134
H	-0.25581900184044	-2.56292892461505	3.27436572566962
C	1.72162247781267	-2.25291490917533	2.34936747916266
C	2.48142266082992	-1.29736290051056	1.58824640831894

H	3.51925564602947	-1.52852823451538	1.34161295996516
C	1.92942161280940	-0.11807596583426	1.10424441693179
H	2.52362274124217	0.57847064442482	0.50816474705440
C	2.29962305904784	-3.49283472543758	2.81473207059530
C	3.68437140856318	-3.55916054207069	3.14601932726556
H	4.35953310660162	-2.73157901726376	2.91981135580347
C	4.15471901551944	-4.62392755882319	3.87117403202124
C	3.29186022043471	-5.69229998832168	4.29271412695602
C	1.96497487957444	-5.71907183462656	3.91102659103605
H	1.35335579585986	-6.59145372705308	4.15385646186435
C	1.45600959199136	-4.68313619609739	3.09978133363051
C	5.51228233458788	-4.89891993330227	4.39378620756819
O	6.53881380230092	-4.25852706619938	4.27778426774374
N	5.39771353040639	-6.11557875390087	5.08615838861625
C	4.08994115373371	-6.65735983234483	5.06372921747143
O	3.76117576304991	-7.70199201462930	5.59320864214469
C	6.51400582685767	-6.74636877630501	5.75124791955441
H	6.91814917461080	-6.09019265324796	6.53881891118669
H	6.15613623564126	-7.68538991350225	6.19412201214772
H	7.32466440962141	-6.95258750104558	5.03421885462814
C	0.15807274901935	-4.86115068495522	2.45577570492919
C	-0.05271559924260	-4.46910150188670	1.10448927700922
H	0.77844137764506	-4.04697934615893	0.53820315825804
C	-1.28805854837497	-4.61788109017747	0.49288989368074
H	-1.43201448652508	-4.32151842177736	-0.54832462894522
C	-2.37778009718999	-5.11650897069073	1.22460048732962
C	-2.19619200869676	-5.51483091938173	2.56040069218785
H	-3.05046866776262	-5.89648858069301	3.12372773412083
C	-0.94446110524471	-5.42158948490172	3.15244312081996
H	-0.82177772446933	-5.72858101613436	4.19321942068527

N	-3.67455549438268	-5.19768657959863	0.62977882081222
C	-3.94752132717385	-6.20406721577573	-0.30824475797906
C	-4.64149545813383	-4.25328302485944	1.00576477407774
C	-5.24692550086071	-6.34294858387737	-0.85396465067573
C	-2.92826841818615	-7.11243623771207	-0.68195588934923
C	-5.97602770625229	-4.36536423982855	0.54482087710945
C	-4.26268304547393	-3.15333043702215	1.81295568632392
C	-5.45587280361539	-7.36511384568673	-1.79070843421293
C	-6.42584476809384	-5.47677456287400	-0.40459808541860
C	-3.17103979294973	-8.10831446609636	-1.61855445231754
H	-1.94291990070376	-7.03723229467195	-0.22545594231647
C	-6.89677882320427	-3.40308722783300	0.97972078399314
C	-5.19963033264246	-2.21045624052053	2.21437558326584
H	-3.22646813034695	-3.01193390065806	2.11458623510861
C	-4.44210191439965	-8.23620395793882	-2.18825523342669
H	-6.45169963846216	-7.49329824862548	-2.21880350671012
C	-7.09792652908766	-4.83898716383348	-1.64964805773799
C	-7.44886102398859	-6.38228701995378	0.33462364987090
H	-2.36644124937488	-8.79388811068782	-1.89520600930718
C	-6.53265147114227	-2.34209469790510	1.81115162209233
H	-7.93551938919051	-3.47820221935298	0.65204352811132
H	-4.85923592463859	-1.36783656826745	2.81815189036525
H	-4.64767088045176	-9.01813375789881	-2.92282805389993
H	-6.38886493186213	-4.18710815464187	-2.18194959924786
H	-7.97175646962724	-4.23546825244944	-1.36497271797145
H	-7.44964878176210	-5.60994584330458	-2.35052724270088
H	-7.81902646169311	-7.18205766305268	-0.32513418837633
H	-8.31511733170758	-5.79470972802921	0.67510280354787
H	-6.98617484094759	-6.85202797541169	1.21602316807919
H	-7.28285672837303	-1.61136298063738	2.12278893776716

XYZ Coordinates of *ppppo* in S_0 optimized geometry

C	-2.17775305552767	1.01930680933085	1.35748921117632
H	-1.95756730135738	1.83804771851563	0.65978676045074
H	-2.48561781247964	1.42738610823705	2.33180701013843
H	-3.00157934986954	0.40552384329646	0.95978358567794
N	-0.97643203562175	0.22310213291067	1.50465679059824
C	0.19146799913108	0.40422325984012	0.73846922214314
O	0.35252260662081	1.25670622313682	-0.10164079400950
C	1.13224149565977	-0.66732044563126	1.18955656040930
C	0.49439811482528	-1.41839690138566	2.18072859586178
C	-0.86918328443333	-0.84672784797244	2.39620282786611
O	-1.73482111169951	-1.21625832243479	3.15900928898178
C	1.09844375618099	-2.51321021114050	2.77154521116317
H	0.57673890518169	-3.08673564851115	3.53870499396651
C	2.39048242084134	-2.87867736700234	2.33430708720119
C	3.03655071946963	-2.09781479433995	1.35442496177448
H	4.03522214153113	-2.39192626645570	1.02178219266195
C	2.41653595765006	-0.98346355905816	0.76835005252267
H	2.91490719492407	-0.39396052539565	-0.00434733703998
C	3.05850459378723	-4.08757412077914	2.89500226284750
C	4.36939167594950	-3.96355396414548	3.40060775261121
H	4.88981858835164	-3.00375234311154	3.37076062767574
C	4.97215799707819	-5.07167289211376	3.97314809033149
C	4.30515949802555	-6.29394962139169	4.05816985964980
C	3.02343693860712	-6.45038472535617	3.55574487755007
H	2.52277963959702	-7.41995053066183	3.60218269655610
C	2.38856372790599	-5.34502411051373	2.95262990533252
C	6.32480849358313	-5.23109173216492	4.59230104749805
O	7.20798974950414	-4.41620181370104	4.72062360317376
N	6.38647727344615	-6.56629958394574	5.01675278290072

C	5.20925902602772	-7.27805681681373	4.73153592324259
O	5.00741734618005	-8.44043470006658	4.99253334865795
C	7.54253164285769	-7.13866249331976	5.67474736565826
H	7.76219741923544	-6.59878890033607	6.60879770195052
H	7.31746238465164	-8.19019958082201	5.89683237717767
H	8.42826216820195	-7.07609728124516	5.02374863587189
C	1.02831599166217	-5.52960493203153	2.37149027171473
C	0.75661159519852	-5.16571146068905	1.04007708635337
H	1.56011562475837	-4.77148198839589	0.41481085874973
C	-0.52934252437064	-5.28129136706431	0.51879248346067
H	-0.74205318772000	-4.98851203571619	-0.51155739433386
C	-1.57325801322369	-5.76632036312437	1.31823913334075
C	-1.30804698981521	-6.16404705471653	2.63295977089789
H	-2.12593191981850	-6.54573929200946	3.24753012733893
C	-0.01644605398194	-6.05017695051747	3.15295512326180
H	0.17748639802703	-6.33668165227968	4.18972919174890
N	-2.89685942378005	-5.84124083187517	0.79284148389992
C	-3.76823723192304	-4.74127860808261	0.92567213772367
C	-3.28511085084701	-6.94355865841488	0.01035016548926
C	-3.44157556813389	-3.59683420604040	1.66513149453931
C	-5.02727136519267	-4.78806229027281	0.28847560727681
C	-4.55789528967064	-6.93370472493325	-0.60178333398558
C	-2.46372116940139	-8.06248224966057	-0.18548405785126
C	-4.34325714675510	-2.52892322001675	1.77255052491417
H	-2.48014638656568	-3.53082667556200	2.17432786081088
O	-5.42251731135825	-5.87713921596690	-0.45256640479073
C	-5.91917985394161	-3.72623979528140	0.39042568922016
C	-4.98297772927727	-8.00457694165440	-1.38022062677780
C	-2.89391523603046	-9.14055749787970	-0.97051261581901
H	-1.47893357005016	-8.08788867572567	0.28260790462314

C	-5.58190540631712	-2.58835580455720	1.13603588022478
H	-4.04919707842429	-1.66334146757878	2.36864623934025
H	-6.87835246608661	-3.81479877447766	-0.12413867362776
C	-4.15175546019868	-9.11677675116640	-1.57006073706292
H	-5.97558182727657	-7.94444090848489	-1.83147057038889
H	-2.23240852638717	-9.99970114079181	-1.10600207436054
H	-6.29137901573046	-1.76131638019326	1.21587788054655
H	-4.49390909138516	-9.95342662029018	-2.18332903670763

XYZ Coordinates of *ppppo* in S_1 optimized geometry

C	-1.97899012523425	1.29166348874254	1.35868725805358
H	-1.63645872234615	2.23428747501108	0.90962123265410
H	-2.46714744700779	1.49362163194467	2.32549221333280
H	-2.72240234167342	0.82407172459021	0.69012079621755
N	-0.82444825389324	0.44832666335180	1.53468603560133
C	0.47994743135639	0.78295209199602	1.02669941598315
O	0.71332965457379	1.81544860007666	0.41769246397006
C	1.32492634412059	-0.33991737928651	1.40260740940527
C	0.53428866088211	-1.28650824162990	2.10791128582890
C	-0.85064066843219	-0.78157412630102	2.16784366471087
O	-1.86160642314118	-1.31641429794573	2.63135234017852
C	1.06600581005184	-2.46020465546343	2.60415442464163
H	0.42795006688763	-3.12533225075658	3.18561324590480
C	2.43274690493983	-2.76383801525997	2.38228865266266
C	3.21994010341638	-1.79632894915198	1.66749435087490
H	4.26920557931876	-2.02100002846007	1.46452424564829
C	2.68683298234719	-0.60636433584263	1.19046882192333
H	3.30865157922813	0.10654480974928	0.64334650259252
C	3.03566951324764	-4.00604542879874	2.87712805268115
C	4.37803212997962	-3.98160515769293	3.34491485305845
H	4.95198094408505	-3.05330016503835	3.32524848579634

C	4.94349181883825	-5.11454319968996	3.89095904585413
C	4.22637671320365	-6.32249109173764	3.99762808163702
C	2.92025919309095	-6.39488998387777	3.52226834832186
H	2.38265031063728	-7.34563525720389	3.56046302334258
C	2.32587886093095	-5.26395972732352	2.94636582847536
C	6.30037222707009	-5.33016831044742	4.46692819778356
O	7.23215193814145	-4.55781067252566	4.57472030605593
N	6.31361986878997	-6.66760898251680	4.88039007647779
C	5.08920090942905	-7.33357929412160	4.62596136950624
O	4.86670496322185	-8.49956925959644	4.89826445152092
C	7.45592307337178	-7.29292889783262	5.50339659751846
H	7.70812575493714	-6.79363287537053	6.45300409782209
H	7.20027924503649	-8.34398087526588	5.69478673386139
H	8.33833759722194	-7.23615225473223	4.84611185671378
C	0.97146494720855	-5.44628251165378	2.34965020496440
C	0.70586430605414	-5.08492591896419	1.01446840195888
H	1.50431712087234	-4.64896471587755	0.41285444967487
C	-0.56349574368579	-5.23786867439144	0.46388457596801
H	-0.76320300529344	-4.93558894021090	-0.56651650826088
C	-1.58761802730249	-5.77044364602512	1.25143925452774
C	-1.35272966270311	-6.16546008617863	2.56648418790560
H	-2.16488796675766	-6.57555804544372	3.17098578487666
C	-0.07546422097004	-6.00147956311561	3.10629447959764
H	0.10708927171519	-6.27760722595977	4.14664529429824
N	-2.92403011646622	-5.89905606474415	0.69680322243865
C	-3.81978510033777	-4.84753100156026	0.81159567060966
C	-3.29944729286337	-7.06716426622356	0.06175004699675
C	-3.48703118495631	-3.63034653244818	1.44270098596147
C	-5.12766350991327	-4.99854352227863	0.27030072291342
C	-4.61692834120316	-7.17310424700194	-0.46523987737247

C	-2.42614053209944	-8.16794533378427	-0.08927402505118
C	-4.42811978622778	-2.61746324825036	1.52087954383687
H	-2.49903156369764	-3.46273700519626	1.86743720463233
O	-5.49511941683932	-6.15000460225103	-0.35052246154907
C	-6.07401769700270	-3.97627807046181	0.35675529913245
C	-5.04942993236980	-8.33126511813703	-1.11658195294330
C	-2.86302551523573	-9.31219342758116	-0.73666632923087
H	-1.41502779935393	-8.09913127920586	0.30801061562789
C	-5.72275349419051	-2.78640252539028	0.98282773984200
H	-4.12115406012706	-1.68872817524096	2.00311987890417
H	-7.06248073197730	-4.14307057991342	-0.07358287374724
C	-4.17350656441640	-9.40024406420273	-1.25222453534197
H	-6.06974529902151	-8.35954554686987	-1.50152596613407
H	-2.17980833971599	-10.15606132199002	-0.84796173512570
H	-6.45295067679105	-1.97815960864409	1.05473269136216
H	-4.50118682095901	-10.30930744239503	-1.75953128788481

XYZ Coordinates of *ppppo* in T₁ optimized geometry

C	-2.00151168081188	1.10100424917895	1.15588325613768
H	-1.72949688764224	1.94647480007100	0.50948723526275
H	-2.34536055889699	1.47634715718870	2.13290469156311
H	-2.82735008340408	0.53405990730756	0.69579914613125
N	-0.83070492835324	0.26946275559251	1.30995078472171
C	0.41897131477161	0.53320413972760	0.67048695074073
O	0.62339344800775	1.48868399037683	-0.04981956476447
C	1.30284619940418	-0.56722144629318	1.08339227616618
C	0.57503476322797	-1.42911992214366	1.93084902462897
C	-0.80451608266225	-0.89109672054878	2.07040423564767
O	-1.75347090781277	-1.35269288578741	2.68642350103472
C	1.13034936422758	-2.55759586869299	2.48628604685897
H	0.53862587870574	-3.16143069609513	3.17304768278028

C	2.48754758802285	-2.89329724970024	2.18706051187840
C	3.21854307236287	-1.99074780945544	1.34188885402168
H	4.25245969764983	-2.23239449129568	1.08740529059657
C	2.64491494507659	-0.84937667057734	0.79344531470155
H	3.21988904421483	-0.19072507822553	0.13813093496358
C	3.09471513212530	-4.09238102257819	2.73795632167518
C	4.47336019276306	-4.09515235119730	3.08743817649584
H	5.11771635139489	-3.24968005359106	2.83769213002252
C	4.97990671993355	-5.12286131425505	3.84751964741261
C	4.15666471792300	-6.20303677027747	4.29116244537593
C	2.83024933047030	-6.27929669452538	3.91019979874459
H	2.23923056001983	-7.15688310893719	4.18449536408783
C	2.29105784103918	-5.28040388271950	3.07316845566805
C	6.34402201559430	-5.33480473333802	4.38422096610833
O	7.34893541294480	-4.66286099123528	4.25542658145547
N	6.26949423369741	-6.53495798771781	5.11062117798766
C	4.98154596742964	-7.11943879609472	5.09540251079785
O	4.68330863568094	-8.15933323652434	5.65257000431317
C	7.40266034094871	-7.10833310348744	5.79812097418631
H	7.78449404693139	-6.41535135979024	6.56506961042402
H	7.07233854382402	-8.04297887738312	6.27091836041967
H	8.22207136270074	-7.31426609365562	5.09084417073223
C	0.97877216408131	-5.50419842396931	2.46587505447794
C	0.74798185126407	-5.21934909020793	1.09241637904240
H	1.57416574379878	-4.85103017168881	0.48263618692254
C	-0.50123116588713	-5.38943830136240	0.51725067521441
H	-0.66165290679010	-5.16444492617961	-0.53961005149387
C	-1.58234515943315	-5.80759803301757	1.31204810698126
C	-1.38116594041018	-6.11257479124915	2.66852320411791
H	-2.22804635465439	-6.43480641024641	3.27871623739973

C	-0.11416678113405	-5.99614757137445	3.22456526116297
H	0.02895432089762	-6.22517103834536	4.28277100232535
N	-2.89872074391336	-5.87615085555041	0.75809981391599
C	-3.84089738545722	-4.89997666489552	1.10020192724425
C	-3.25181069454181	-6.89014689714269	-0.13571792461555
C	-3.50809214306461	-3.76388579897937	1.86294850117879
C	-5.16764833780151	-5.02557093326285	0.61694306224840
C	-4.58717481124034	-6.95372710620829	-0.60647686356087
C	-2.34587270510941	-7.88267559753944	-0.55896798138295
C	-4.47803788874794	-2.81303266786065	2.16341704753856
H	-2.48630666302626	-3.60054490977099	2.20278887848200
O	-5.52975453082692	-6.06241911194383	-0.19309350151548
C	-6.14052900754129	-4.07902117636716	0.932257944444295
C	-4.99114567811082	-7.95232827558175	-1.49293243522351
C	-2.75380693059910	-8.87506277611969	-1.44532305143792
H	-1.32431499908808	-7.86742650155567	-0.18038665271696
C	-5.79813770350044	-2.97473835880274	1.71365550387580
H	-4.16990485392220	-1.93196974997635	2.72834129143127
H	-7.14920482079818	-4.22435812519644	0.54133427565705
C	-4.07406362928887	-8.91119129525850	-1.91974738373615
H	-6.03057569898841	-7.95492871740540	-1.82589972167182
H	-2.03628614807712	-9.63439325814407	-1.76366881940029
H	-6.55732152098173	-2.22705156889413	1.95418276096739
H	-4.38945502861656	-9.69308821922223	-2.61386512685047

XYZ Coordinates of *ppnp* in S_0 optimized geometry

C	-1.66061028513895	1.06728365934180	1.62721841215817
H	-1.46722049850873	1.88418681064653	0.91950386929927
H	-1.92268733527660	1.47823895620389	2.61373254488719
H	-2.50390696476026	0.45633854857684	1.26798273220114
N	-0.45804115858075	0.26483788328950	1.72076945939065

C	0.68108724788150	0.44943245813603	0.91389783052916
O	0.81546489670442	1.31121119938992	0.07822710767826
C	1.63210484020187	-0.63282357648304	1.31565226409465
C	1.02613284050624	-1.39468768197552	2.31839689828449
C	-0.32268676041787	-0.81576917369359	2.59617874711860
O	-1.15721530742951	-1.18599183266521	3.39193675144244
C	1.64131034211623	-2.50493060444380	2.86676152316816
H	1.14221680529786	-3.08925114032459	3.64082095090592
C	2.91232208211418	-2.87339794159330	2.37470192215283
C	3.52992350276693	-2.07984647339769	1.38696039465615
H	4.51321053598670	-2.37650524947655	1.01316957791444
C	2.89777921222419	-0.95110656779658	0.84258655446039
H	3.37188941427816	-0.35272384594962	0.06148138632343
C	3.58343704137939	-4.10248074609708	2.88488815994621
C	4.90736830906406	-4.00512068415663	3.36065256925192
H	5.43725604401036	-3.05019248313765	3.34210623973167
C	5.51103612121100	-5.13418406025184	3.88988409966751
C	4.83192652366512	-6.35089928852208	3.95988068941686
C	3.53703149463389	-6.48086186478917	3.48411039835812
H	3.02702413815334	-7.44608515305131	3.51703152203285
C	2.90039832062888	-5.35360315531543	2.92475685667506
C	6.87571333716981	-5.32400215861803	4.47230914340675
O	7.77127121939693	-4.52254239552592	4.60063275485880
N	6.93212747638564	-6.67025596702132	4.86128161331964
C	5.74026472880869	-7.36160194656483	4.58637985215161
O	5.53167127088072	-8.52802113884215	4.82324656539128
C	8.09621244659904	-7.27117979143989	5.47809882250793
H	8.34364432957472	-6.75634777341519	6.41932505228031
H	7.86401222031172	-8.32519922568824	5.68021755528791
H	8.96744256990944	-7.20282857967983	4.80834421818085

C	1.52636021847823	-5.50770084126482	2.36763956628380
C	1.23106825173040	-5.09971119012129	1.05414503580885
H	2.02502753754989	-4.69183974199792	0.42545198007073
C	-0.06527420096187	-5.19163462396141	0.55426272852588
H	-0.29548036050227	-4.86752729265700	-0.46277452616343
C	-1.09731845953191	-5.69628871683001	1.35645447855760
C	-0.80924287438254	-6.13493567737643	2.65348947192789
H	-1.61762309210958	-6.53146571477072	3.27120197332816
C	0.49245342346915	-6.04499601948567	3.15247004941159
H	0.70381580471552	-6.36495870155324	4.17603080279812
N	-2.42855512617668	-5.75627146408231	0.84808979840662
C	-3.29349719593099	-4.65856547924071	1.05020898629482
C	-2.82091803440478	-6.86991557105304	0.07821479436660
C	-4.58030476480913	-4.67281595142091	0.45006034326751
C	-2.91638940861342	-3.55665396915655	1.82533039016021
C	-4.10844911056623	-6.88065545993670	-0.52089260102251
C	-1.97381762379294	-7.96803845518707	-0.10872464814479
C	-5.43514718016718	-3.58259476132295	0.64945641419240
N	-4.96648537957187	-5.78038851231054	-0.33177349132974
C	-3.78584885127998	-2.47268012684156	2.02196927295921
H	-1.93475652719337	-3.53425145234427	2.29773170923798
C	-4.49128815963122	-7.98807514854992	-1.28663550919206
C	-2.37148389715428	-9.07076237777052	-0.87937273498413
H	-0.98709684072477	-7.96277307047227	0.35458402050504
C	-5.04390251020576	-2.48610217394288	1.43192426789356
H	-6.42241671736264	-3.59193217393492	0.18776172524757
C	-6.26665637914992	-5.79772964978240	-0.92537790256226
H	-3.45154132927542	-1.64265614163089	2.64613625415224
C	-3.62965858850481	-9.07986986852388	-1.46853416849333
H	-5.47799799906955	-7.99683710171762	-1.74948348138478

H	-1.68661706076957	-9.91239164341044	-1.00763477905932
H	-5.73746694504320	-1.65348553315484	1.57367271372851
C	-7.34977588912287	-6.34324486826173	-0.22466998115164
C	-6.45884437293776	-5.26916314186043	-2.20791871718143
H	-3.95840837023347	-9.92860995741029	-2.07301516352544
C	-8.62067994197585	-6.36004215248030	-0.80575926254063
H	-7.18164738295687	-6.75112860134606	0.77453305891505
C	-7.73073435672283	-5.28640485407652	-2.78716133985263
H	-5.60319954192302	-4.84723813128980	-2.73981796113677
C	-8.81243201639484	-5.83179584170403	-2.08715807065580
H	-9.46405958307987	-6.78661935081246	-0.25645010795620
H	-7.87773356421709	-4.87288959485188	-3.78836343352424
H	-9.80681643124107	-5.84509976576867	-2.54108621530964

XYZ Coordinates of *ppnp* in S_1 optimized geometry

C	-1.34621489822268	1.43095613995554	1.65272897840417
H	-0.99192066110847	2.38016367883914	1.22722926063187
H	-1.81330424771209	1.61184472078440	2.63404671949427
H	-2.11093979074479	0.99963806045885	0.98385341789153
N	-0.20687450422640	0.55901259770201	1.78159972143553
C	1.09502045094047	0.88121912322595	1.26175885398535
O	1.34079342834515	1.92652340227256	0.67997894929986
C	1.92276404884284	-0.27031855844910	1.58871725980338
C	1.12408552121122	-1.22181537533594	2.27692169134122
C	-0.24883917909616	-0.68952565177094	2.37860052393122
O	-1.26071796742512	-1.21576465955642	2.84604633249322
C	1.63579957073991	-2.42349877483253	2.72308386448280
H	0.99177749832678	-3.09497532178884	3.29042729627306
C	2.99140031382152	-2.75029034169387	2.46600483754276
C	3.78848915067952	-1.77605009603963	1.77276901913635
H	4.82893607119181	-2.01704687873450	1.54445385333213

C	3.27464791615485	-0.55887766478733	1.34475139314250
H	3.90335543661552	0.15801651252182	0.81082857813047
C	3.57040990807579	-4.02494835162321	2.90252759867920
C	4.91917633621377	-4.05128406943294	3.35072428301471
H	5.51552088012293	-3.13693265667843	3.35827449896981
C	5.46409663348344	-5.21776965864115	3.84492539107092
C	4.71787866642260	-6.41165572000635	3.91511296734865
C	3.40367592749007	-6.43296376501938	3.45518797025818
H	2.84335016224630	-7.37120982969096	3.46307828021869
C	2.82897724446411	-5.26681386680885	2.93274246903349
C	6.82212933879904	-5.48820493810255	4.39263082580767
O	7.77510224238038	-4.74399786612865	4.51862877778193
N	6.80760783862843	-6.84075810136197	4.75302857044167
C	5.56286245108779	-7.46653358671261	4.49120547709482
O	5.31674621794050	-8.63708916396449	4.72327132951287
C	7.94218147853950	-7.51783971684570	5.33380647953611
H	8.22818836061690	-7.05460973809123	6.29209820393395
H	7.65846088520361	-8.56612140531277	5.49929628692902
H	8.81345246401631	-7.46841584855807	4.66096392331443
C	1.46259734400503	-5.39238294211311	2.34731105079722
C	1.18643308633729	-4.96385326850361	1.03428796446829
H	1.98526026231183	-4.51480261408375	0.44274531949025
C	-0.09199891708261	-5.07080269017866	0.49356981194339
H	-0.29775841749273	-4.71996421875390	-0.52012707664895
C	-1.11801690723992	-5.62458358951166	1.26416014140461
C	-0.87159746970912	-6.08127886569539	2.55714208692496
H	-1.68311043999272	-6.50836925703608	3.15066270592983
C	0.41352677418756	-5.96163328419504	3.09035530594450
H	0.60227773258564	-6.28762823871231	4.11512778875043
N	-2.45776186627467	-5.72259898451393	0.71362675003648

C	-3.33808614716494	-4.66075893413886	0.87443893546368
C	-2.83125581376582	-6.87266179984884	0.04209438577883
C	-4.66032701416357	-4.76040802609731	0.34175307067491
C	-2.95677245365457	-3.48590296421522	1.55319230134153
C	-4.15207515356086	-6.97945973895906	-0.49457590104591
C	-1.93389876996036	-7.94880022041560	-0.13085508100620
C	-5.55813157222617	-3.68721390164219	0.50630789934063
N	-5.03484711482827	-5.92096855502270	-0.33102780482831
C	-3.85372004669286	-2.44021440864446	1.69932495115032
H	-1.95721136044213	-3.37511083275571	1.96795111721222
C	-4.53045369523130	-8.15334030388997	-1.17838180556642
C	-2.32889230245098	-9.09201307329603	-0.80729237078865
H	-0.92762685239198	-7.86567872702315	0.27413662764549
C	-5.15750382689718	-2.54154979723760	1.17808056386311
H	-6.56534610198171	-3.76518400480723	0.10027916882126
C	-6.36849834547519	-6.02401318872773	-0.87267211757272
H	-3.50358363888633	-1.54767271723063	2.21880265811577
C	-3.63000533816187	-9.19675859608542	-1.33208906962535
H	-5.53723868167263	-8.23214531340785	-1.58501542405193
H	-1.62057335860960	-9.91313683338354	-0.93141349921998
H	-5.86138736290399	-1.71560899675600	1.29767347674395
C	-7.39169225294257	-6.55477900573101	-0.08237441289363
C	-6.61433439945301	-5.59127842229954	-2.17865540396116
H	-3.93679656104192	-10.09920208206730	-1.86402790937395
C	-8.68143329234123	-6.65360558337180	-0.61126965534513
H	-7.17312779760651	-6.88386766289081	0.93580419188733
C	-7.90688954384157	-5.69379966405177	-2.69981470510235
H	-5.79730810555313	-5.17851868889939	-2.77426553434084
C	-8.93858654099438	-6.22423352642332	-1.91772270338633
H	-9.48686237735168	-7.06655861677174	0.00029471753224

H	-8.10726501148453	-5.35705056002232	-3.71947981259175
H	-9.94812537196789	-6.30232178037909	-2.32802580760993

XYZ Coordinates of *ppnp* in T₁ optimized geometry

C	-1.40583555087759	1.30873522919224	1.52744535353304
H	-1.09778060336611	2.20354261918749	0.96911588564331
H	-1.79769269704767	1.60238876947091	2.51449861088092
H	-2.21259105795578	0.79396630537189	0.97823059235332
N	-0.24866532055504	0.45928266135697	1.66668606814463
C	1.01844450108279	0.74442159958306	1.06930755175111
O	1.24417139152158	1.74127187027901	0.40791796405834
C	1.87390744701122	-0.38916868622711	1.43481189395606
C	1.11550483540720	-1.28997628155158	2.21824425422186
C	-0.25510865747911	-0.74843414762024	2.35175935736398
O	-1.23638555924446	-1.23889602980901	2.90205886129535
C	1.65022610410130	-2.46399949542595	2.71042038953621
H	1.03874295379498	-3.11214702838300	3.33902141791997
C	2.99089226899578	-2.80259061287114	2.39750303917882
C	3.74816140534359	-1.87841812249877	1.61335476793018
H	4.77648491374677	-2.13539266088421	1.34889923999877
C	3.20838035644440	-0.68405073552486	1.13925789266899
H	3.80521281292795	0.00084020146720	0.53168591561844
C	3.58511942329218	-4.06195197150654	2.87406252480791
C	4.92640547009159	-4.05688964972397	3.33044114341521
H	5.52030683041445	-3.14115583345607	3.29188217809762
C	5.46583875597791	-5.19472403735007	3.89813984876797
C	4.70523657758470	-6.37657828502365	4.03226786961890
C	3.40169342751128	-6.42943546864193	3.56596594487033
H	2.84286353641825	-7.36674884505995	3.62681883437814
C	2.83332587427013	-5.29554543049338	2.95146057938847
C	6.81084508025769	-5.44131334322789	4.47498762100396

O	7.77057985280073	-4.70149385934556	4.56958961650628
N	6.78216740278651	-6.77394608754105	4.91878086354189
C	5.54183709270572	-7.40521266052756	4.68261129740502
O	5.27832249635773	-8.55549753104378	4.97971909283035
C	7.90796557509499	-7.41954888299291	5.55170182811950
H	8.20575250545087	-6.87810236713998	6.46394931502188
H	7.60704901166204	-8.44441983686118	5.80829333783986
H	8.77684006461250	-7.44525483941681	4.87424221485003
C	1.49298672621005	-5.43974001813939	2.34308159907890
C	1.21978267079753	-4.96008215310469	1.04157578864532
H	2.01946878450271	-4.48572227697725	0.47091519030130
C	-0.04848748971498	-5.05878755761121	0.48371451402676
H	-0.24795957659900	-4.67433819213785	-0.51915071908032
C	-1.08298427041585	-5.65265790419879	1.22283371860510
C	-0.83876603096363	-6.16944901893047	2.49742089256392
H	-1.65323350398290	-6.62727343646239	3.06399881186467
C	0.43773968213005	-6.06500922558630	3.04688114337849
H	0.61555669037697	-6.43286117617679	4.05956166209221
N	-2.41401127431906	-5.71043131557745	0.66465915395435
C	-3.29961877684832	-4.67086359664644	0.91334446215699
C	-2.78541542197088	-6.81097485224288	-0.09204300059586
C	-4.64155761761542	-4.75976889803320	0.41715337339995
C	-2.91131024441461	-3.53349664539601	1.65401348048958
C	-4.12311786356237	-6.90401190376882	-0.59153263651993
C	-1.87292497196464	-7.85339570006377	-0.36943005507645
C	-5.54785894880073	-3.71364211548819	0.68905128716021
N	-5.01813737920416	-5.87635742461256	-0.32086600964005
C	-3.81644565121794	-2.51510209074474	1.90236875250871
H	-1.89597347331592	-3.43930597975418	2.03675588770517
C	-4.50132584698344	-8.03697424801424	-1.34349092986190

C	-2.26565379048494	-8.95207782979312	-1.11537369403873
H	-0.85670886394071	-7.77754294310356	0.01522618825522
C	-5.14043295263297	-2.60892368770222	1.42125931762903
H	-6.56922903789223	-3.78094797235493	0.31678205931654
C	-6.36748363800539	-5.96757632232036	-0.82138448808616
H	-3.46454974693038	-1.64879651100018	2.46439838502800
C	-3.58696787296061	-9.04605306428321	-1.60208096309419
H	-5.52071062626694	-8.11054306256607	-1.72003769443476
H	-1.54631301183308	-9.74682544116031	-1.32348795589394
H	-5.85388905907204	-1.80680066727978	1.62352412653288
C	-7.35296259772207	-6.57392752876248	-0.03733329649538
C	-6.66800987199946	-5.44633630396471	-2.08312114159190
H	-3.89602125147178	-9.91603704801360	-2.18539078570884
C	-8.65965534108577	-6.65867296236305	-0.52677258651694
H	-7.09161340624585	-6.97177212667817	0.94565257351859
C	-7.97702199341931	-5.53521743164056	-2.56538572631074
H	-5.87909292639335	-4.97652604840311	-2.67445752647108
C	-8.97106390549438	-6.14032006025529	-1.78857650412398
H	-9.43571331121376	-7.13052452754780	0.08053937584157
H	-8.21991337154234	-5.12974256670025	-3.55045784860440
H	-9.99354798665699	-6.20779854019911	-2.16813056842492