

# Unravelling the promising di-substitution pattern boosting radiative and reverse intersystem crossing rates in 1,8- naphthalimide D-A-D emitters: A computational study

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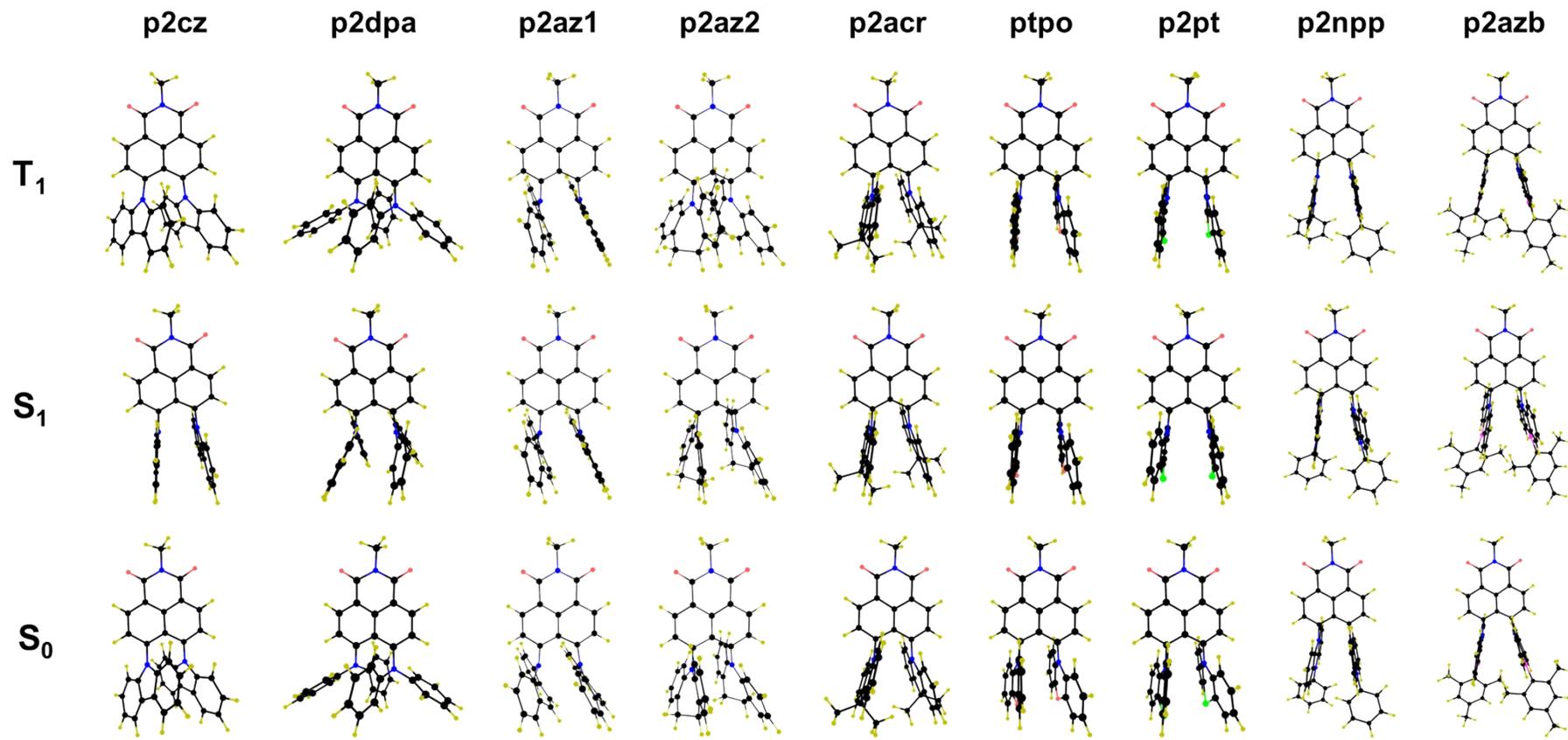


Figure S1. Optimized structures of 4,5-disubstituted derivatives at S<sub>0</sub>, S<sub>1</sub> and T<sub>1</sub> states.

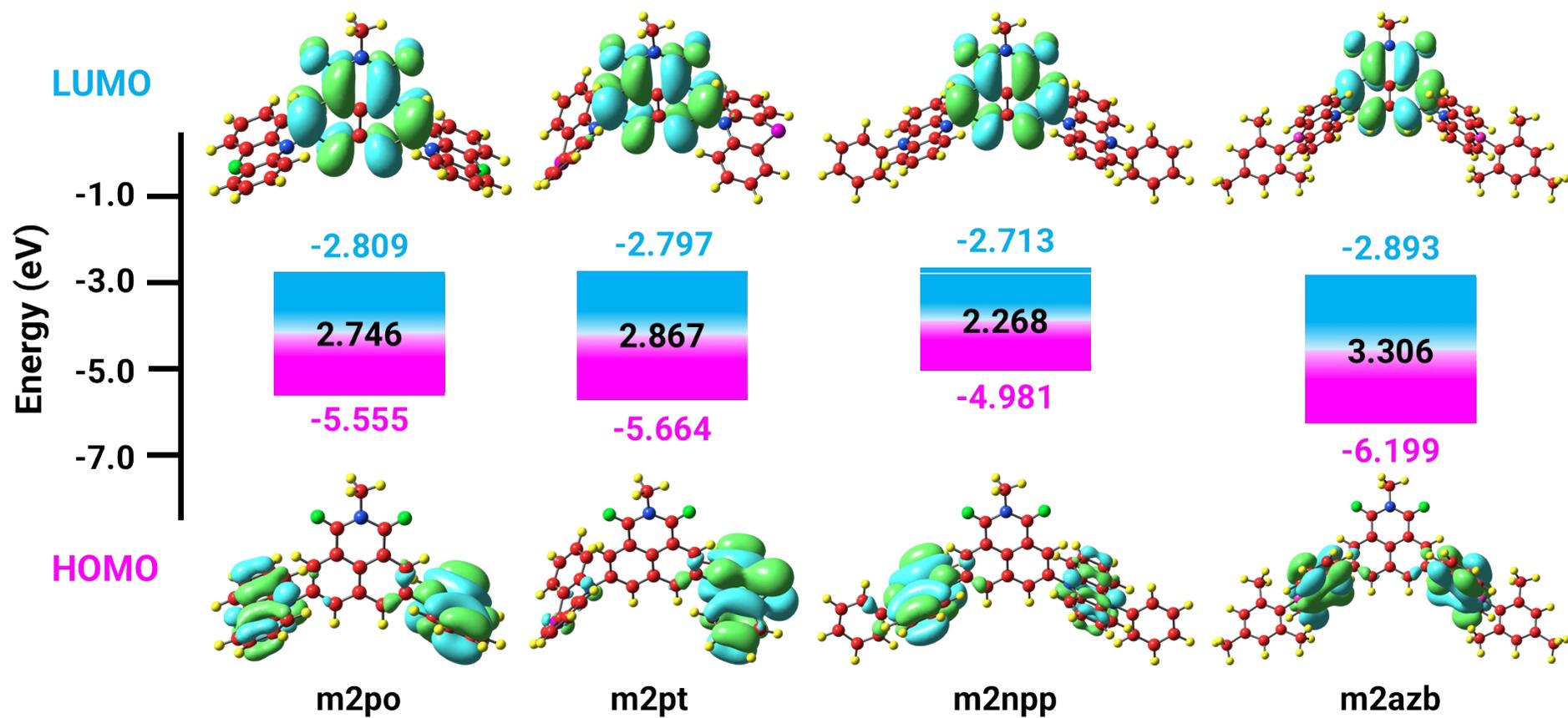


Figure S2. Energies and electronic distributions of the frontier molecular orbitals of **m2po**, **m2pt**, **m2npp** and **m2azb** at the M06/def2-TZVP level.

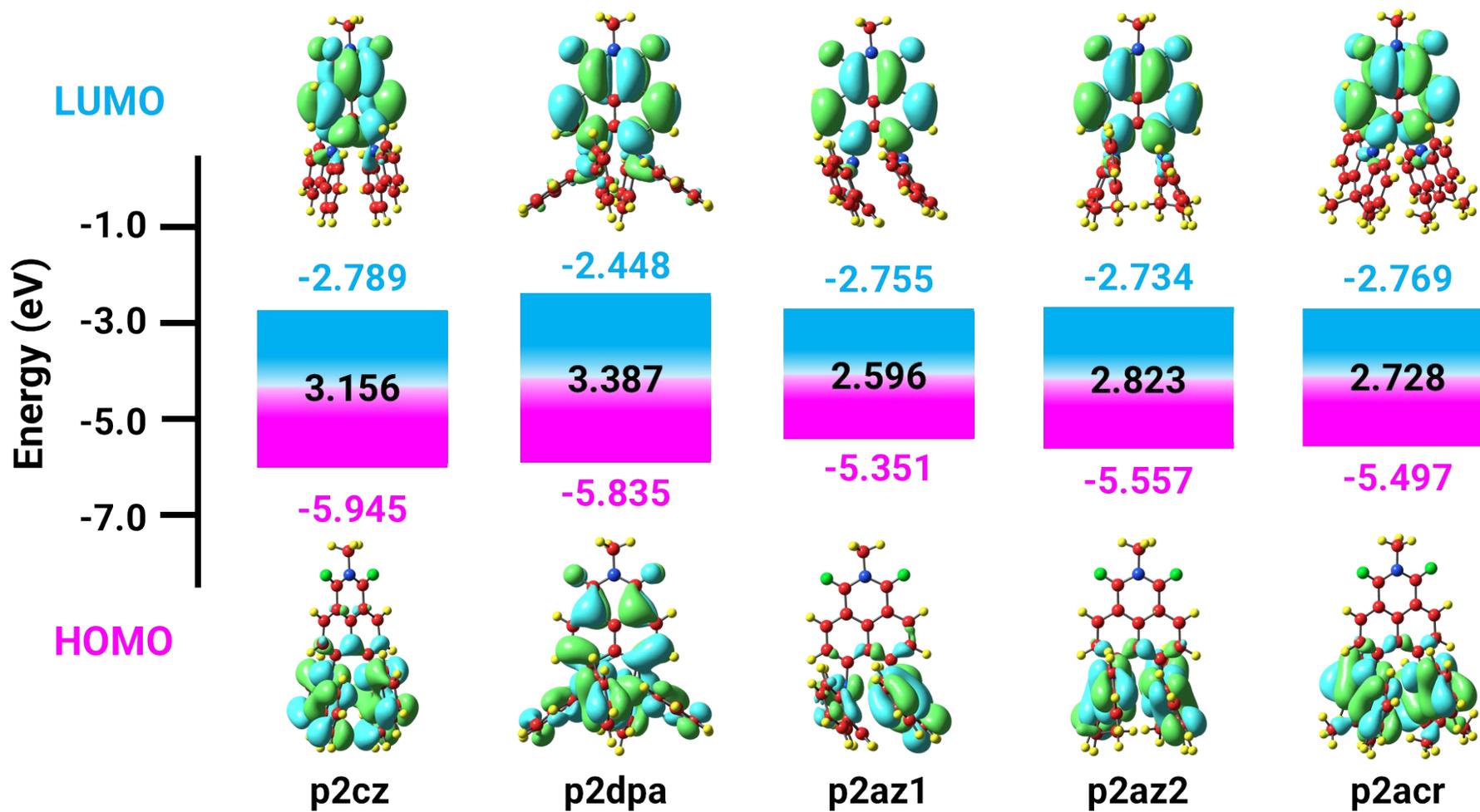


Figure S3. Energies and electronic distributions of the frontier molecular orbitals of p2cz, p2dpa, p2az1, p2az2 and p2acr at the M06/def2-TZVP level.

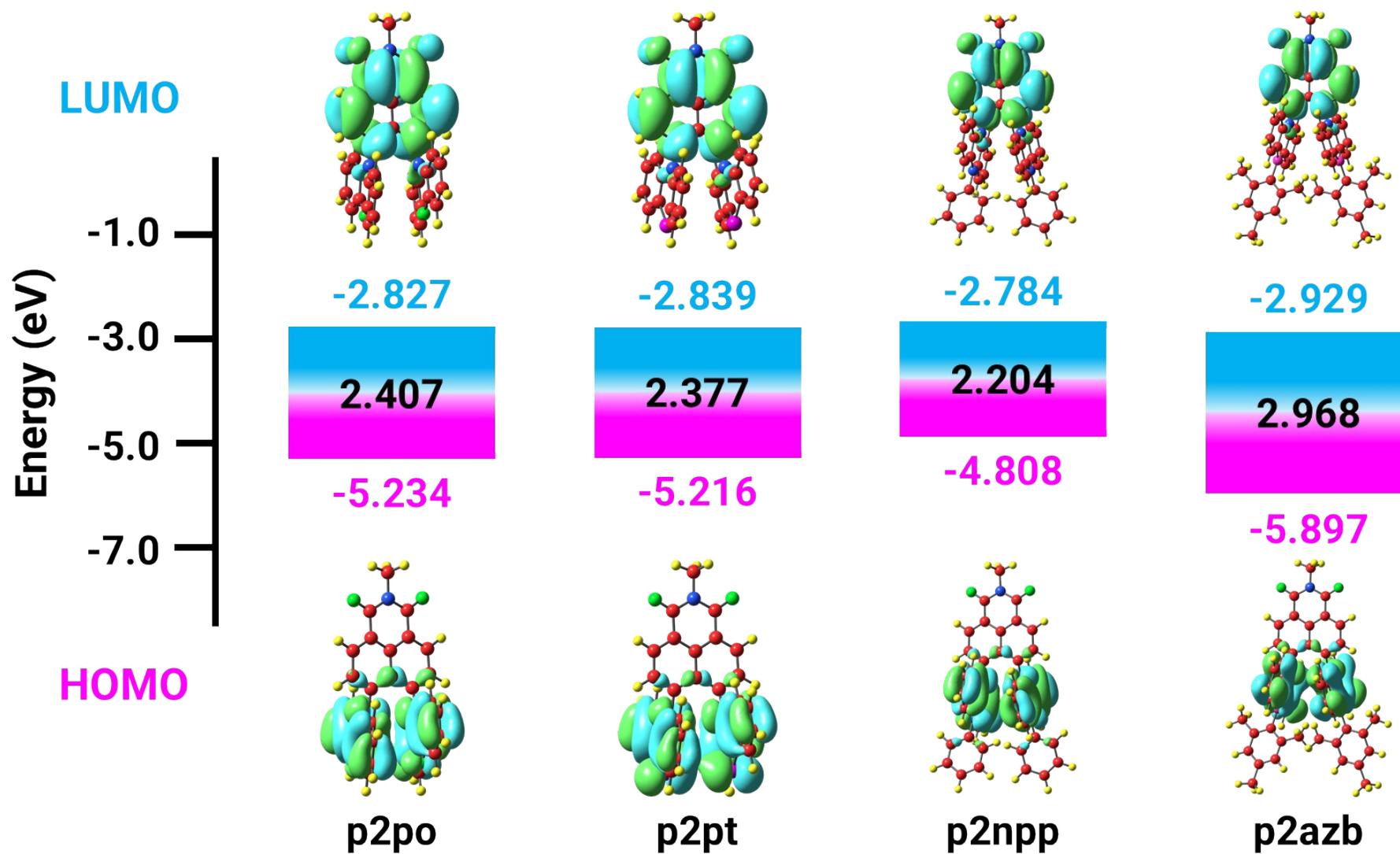


Figure S4. Energies and electronic distributions of the frontier molecular orbitals of **p2po**, **p2pt**, **p2npp** and **p2azb** at the M06/def2-TZVP level.

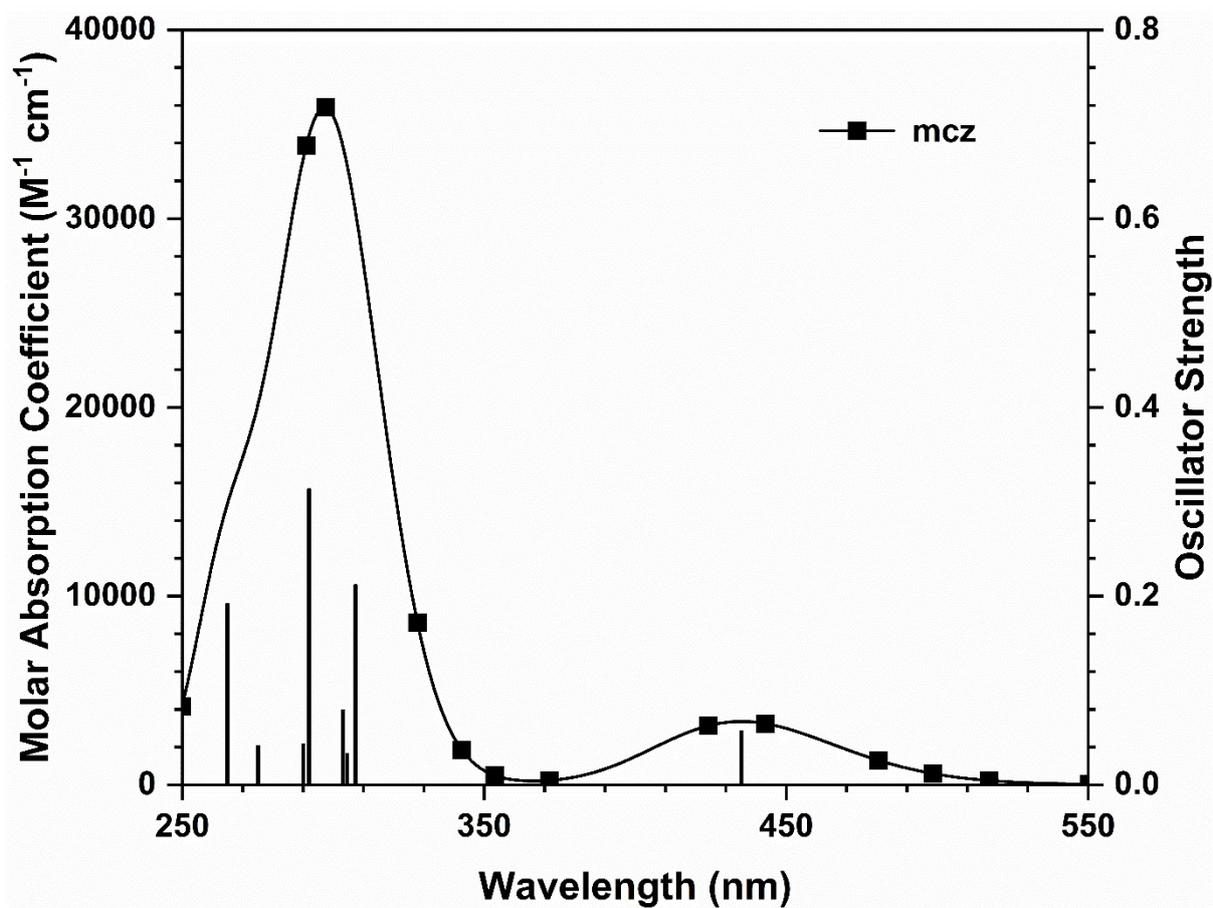


Figure S5. Simulated absorption spectrum of **mCz** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

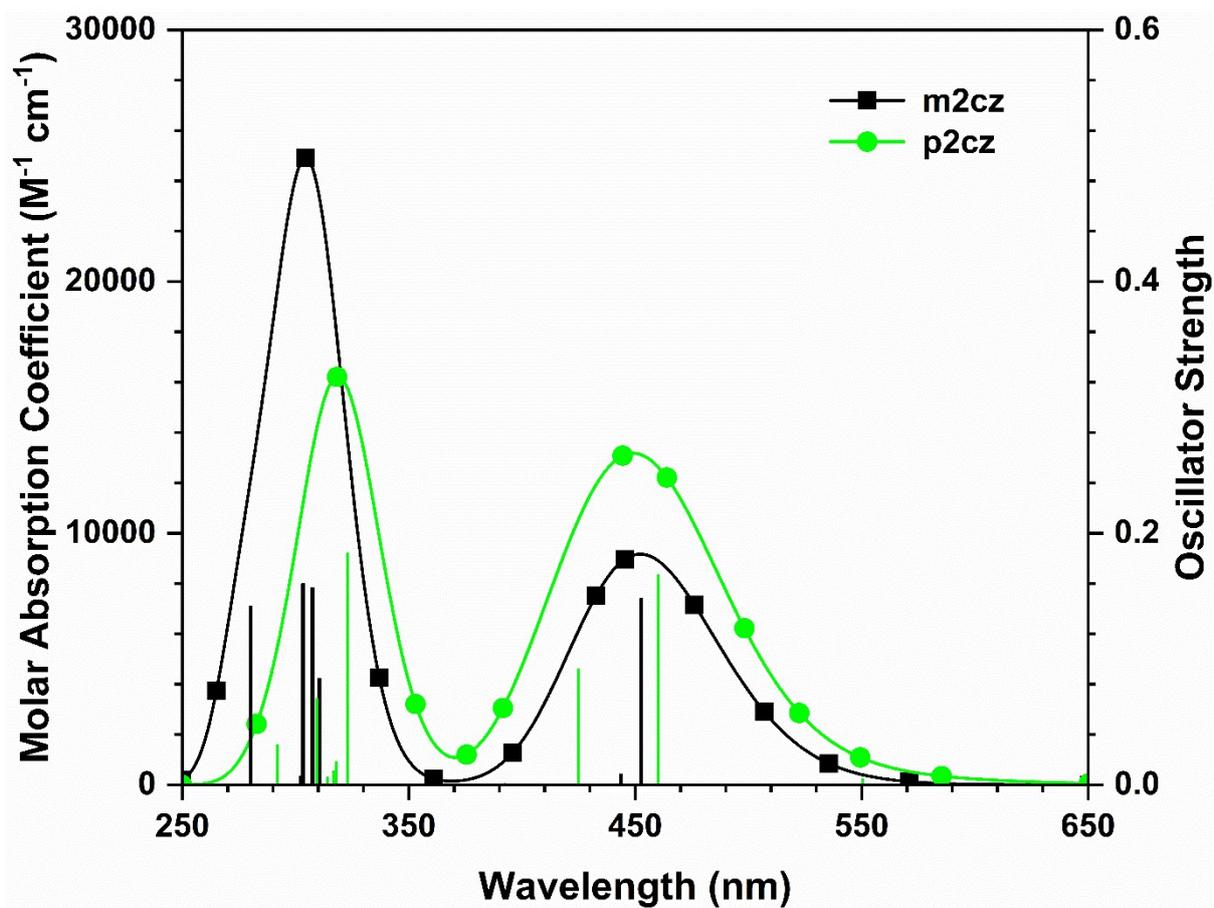


Figure S6. Simulated absorption spectra of **m2cz** and **p2cz** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

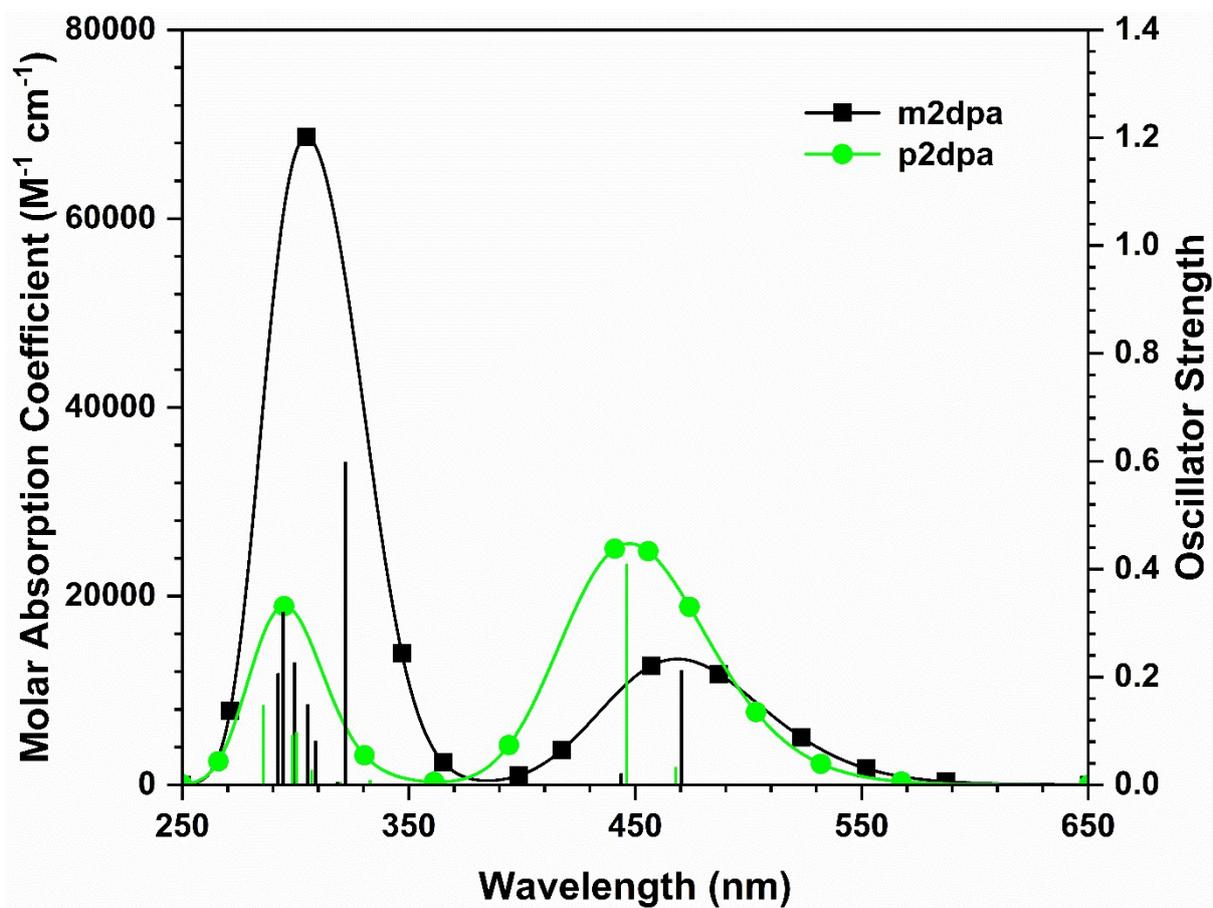


Figure S7. Simulated absorption spectra of **m2dpa** and **p2dpa** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

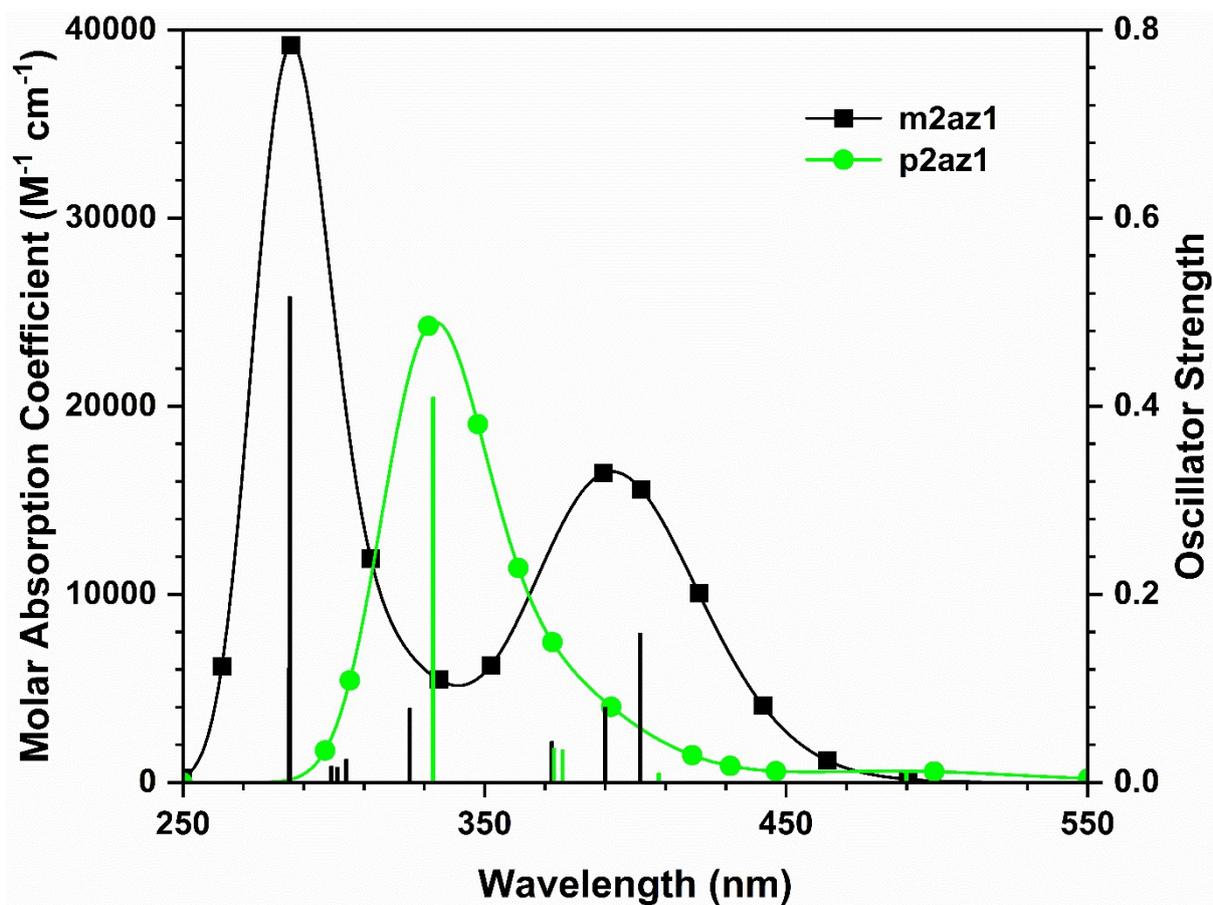


Figure S8. Simulated absorption spectra of **m2az1** and **p2az1** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

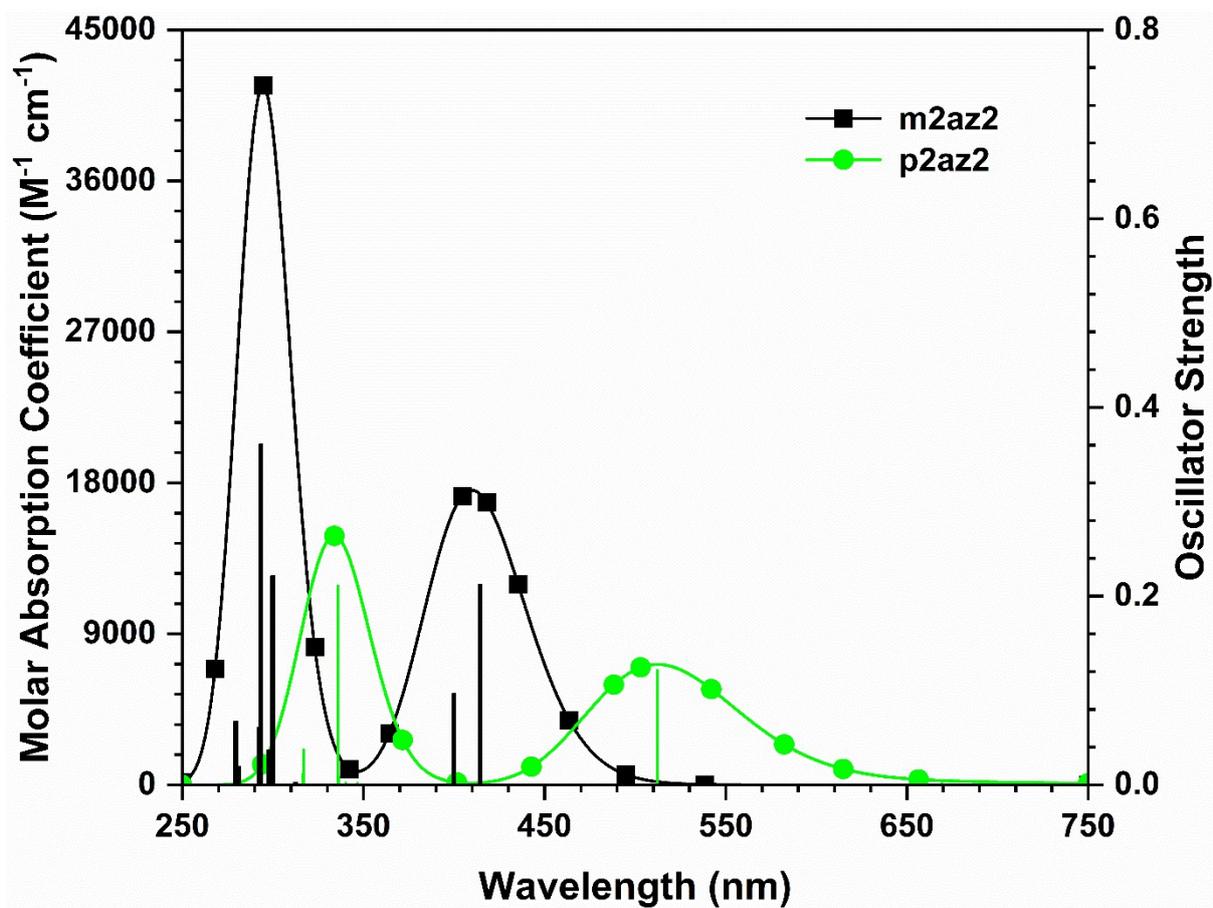


Figure S9. Simulated absorption spectra of **m2az2** and **p2az2** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

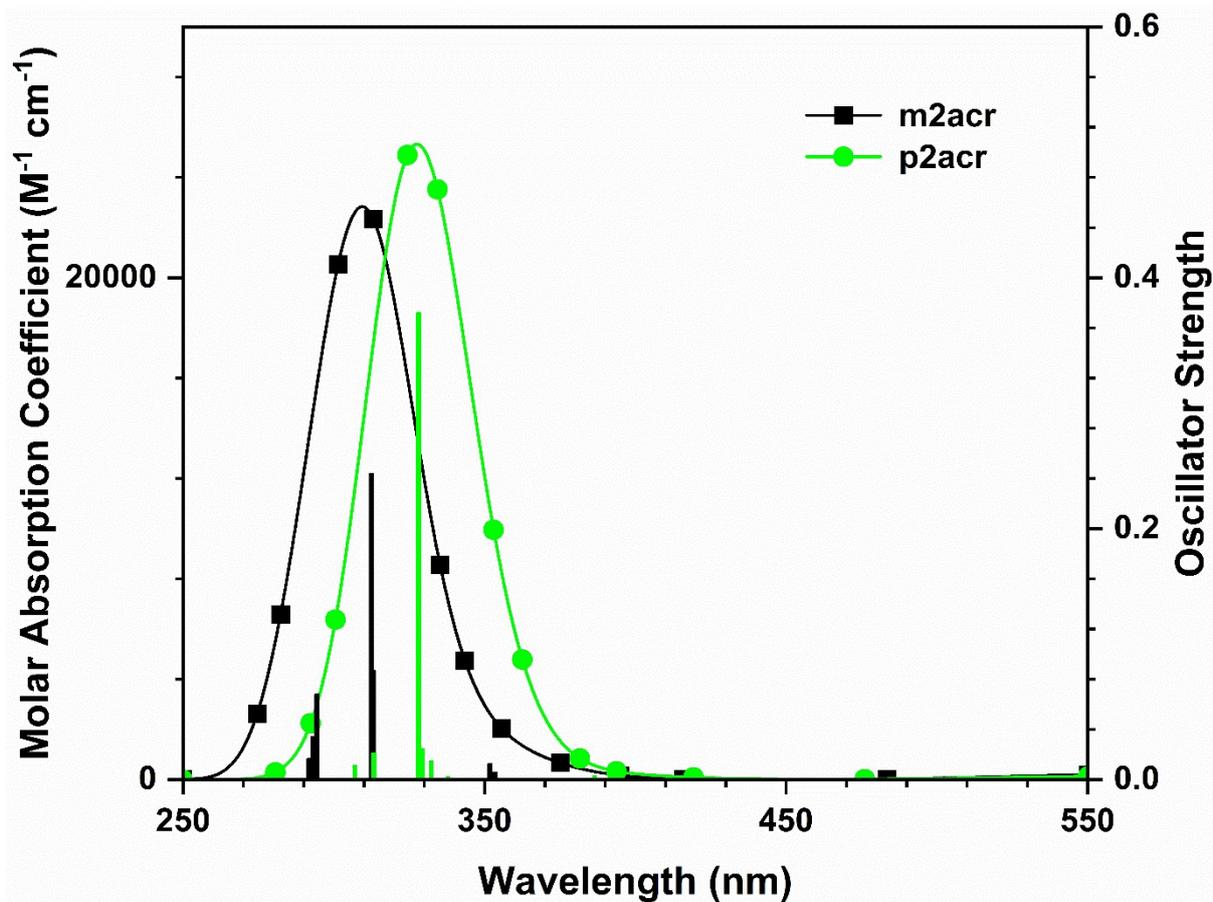


Figure S10. Simulated absorption spectra of **m2acr** and **p2acr** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

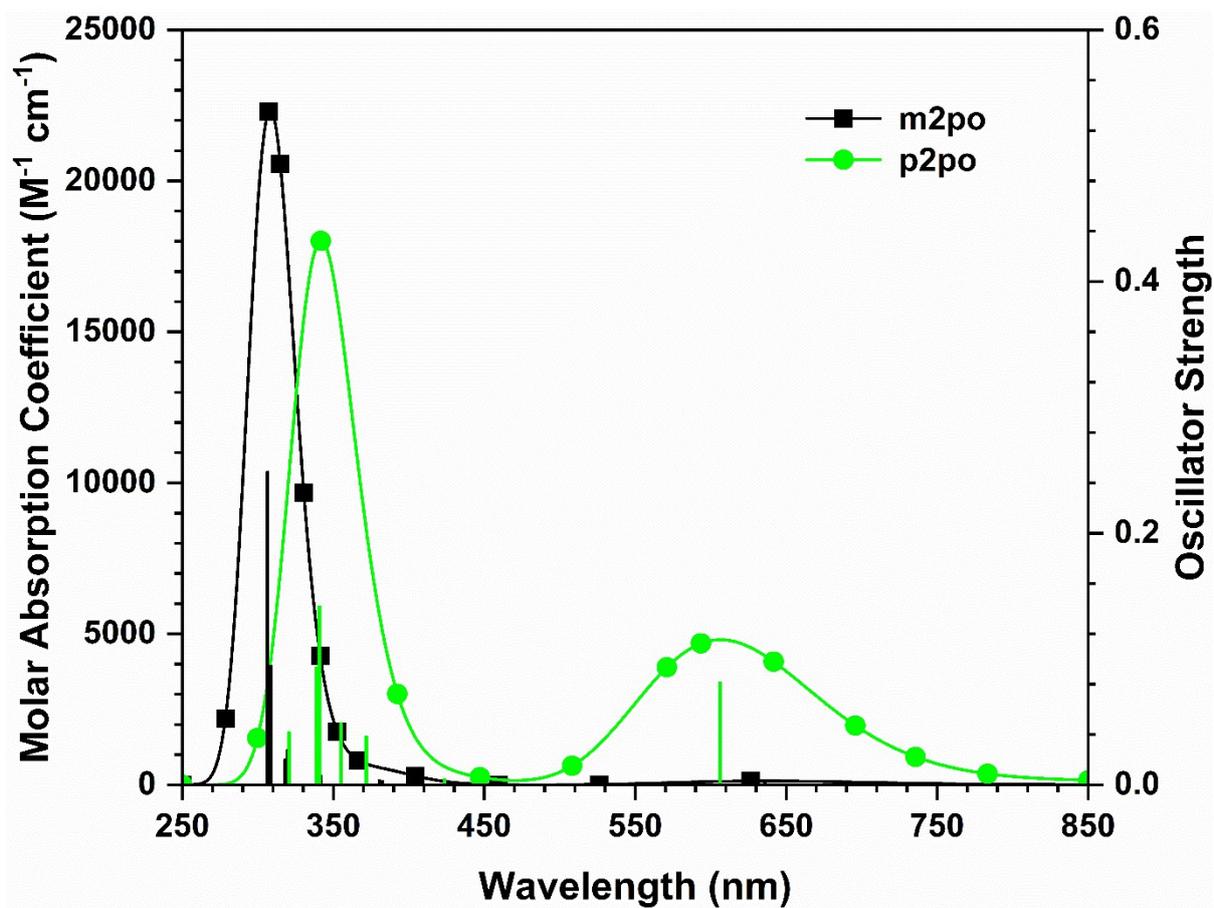


Figure S11. Simulated absorption spectra of **m2po** and **p2po** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

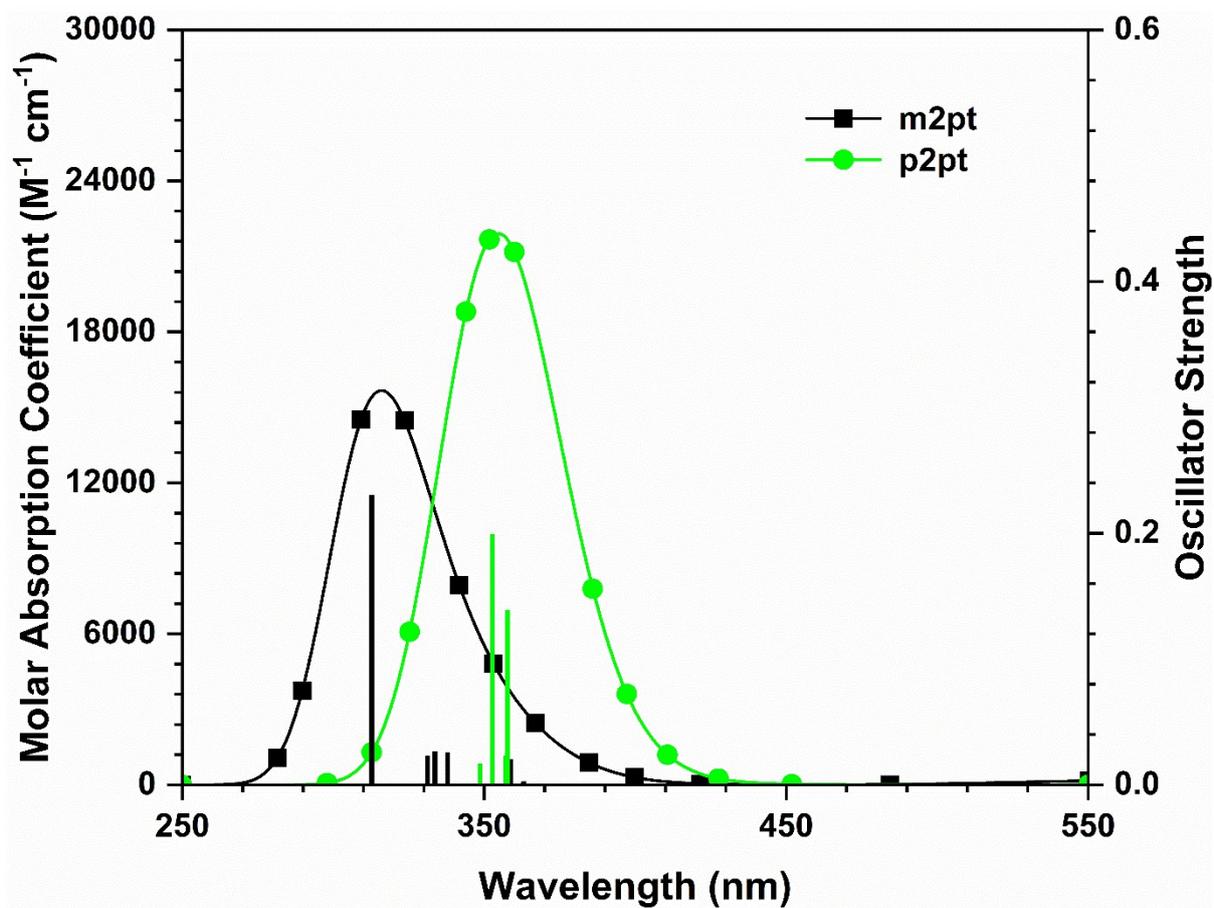


Figure S12. Simulated absorption spectra of **m2pt** and **p2pt** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

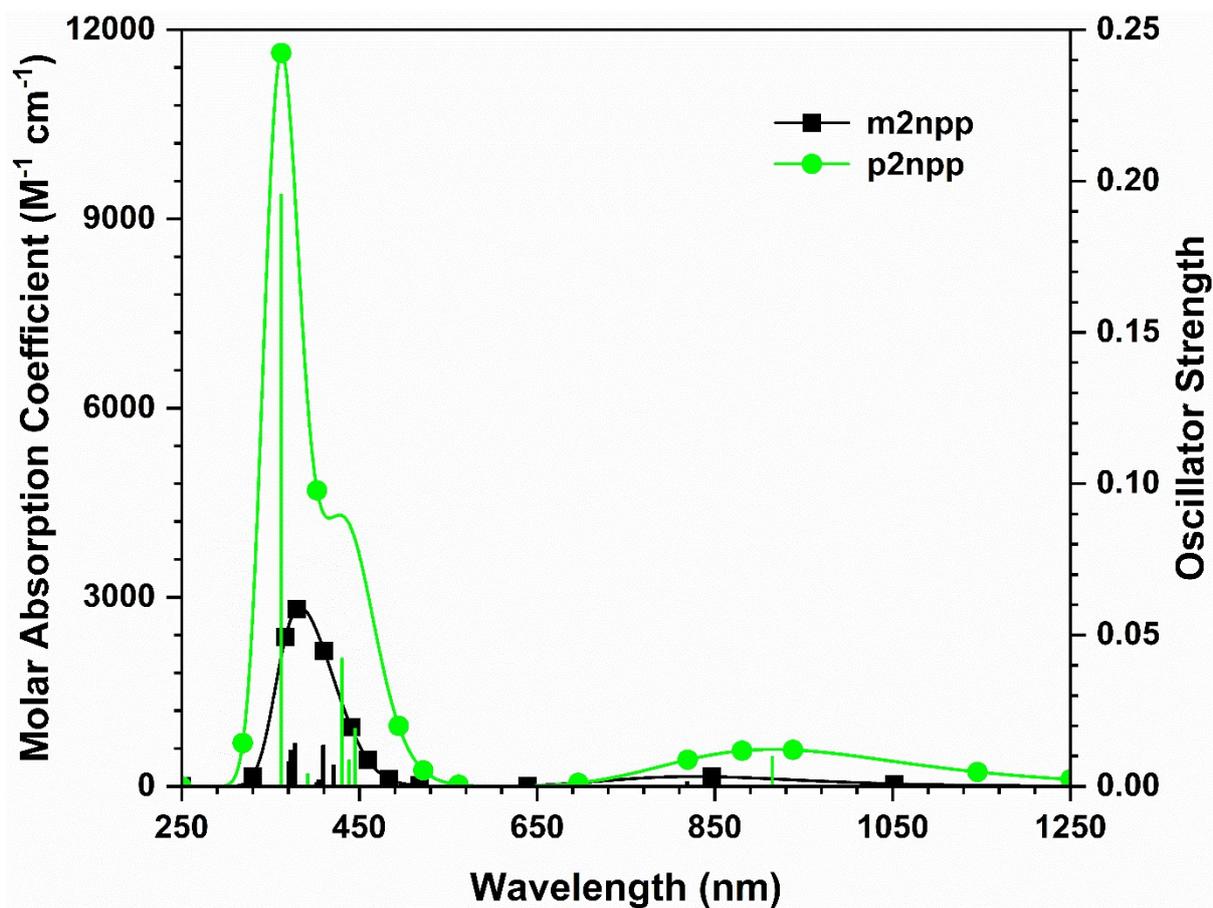


Figure S13. Simulated absorption spectra of **m2npp** and **p2npp** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.

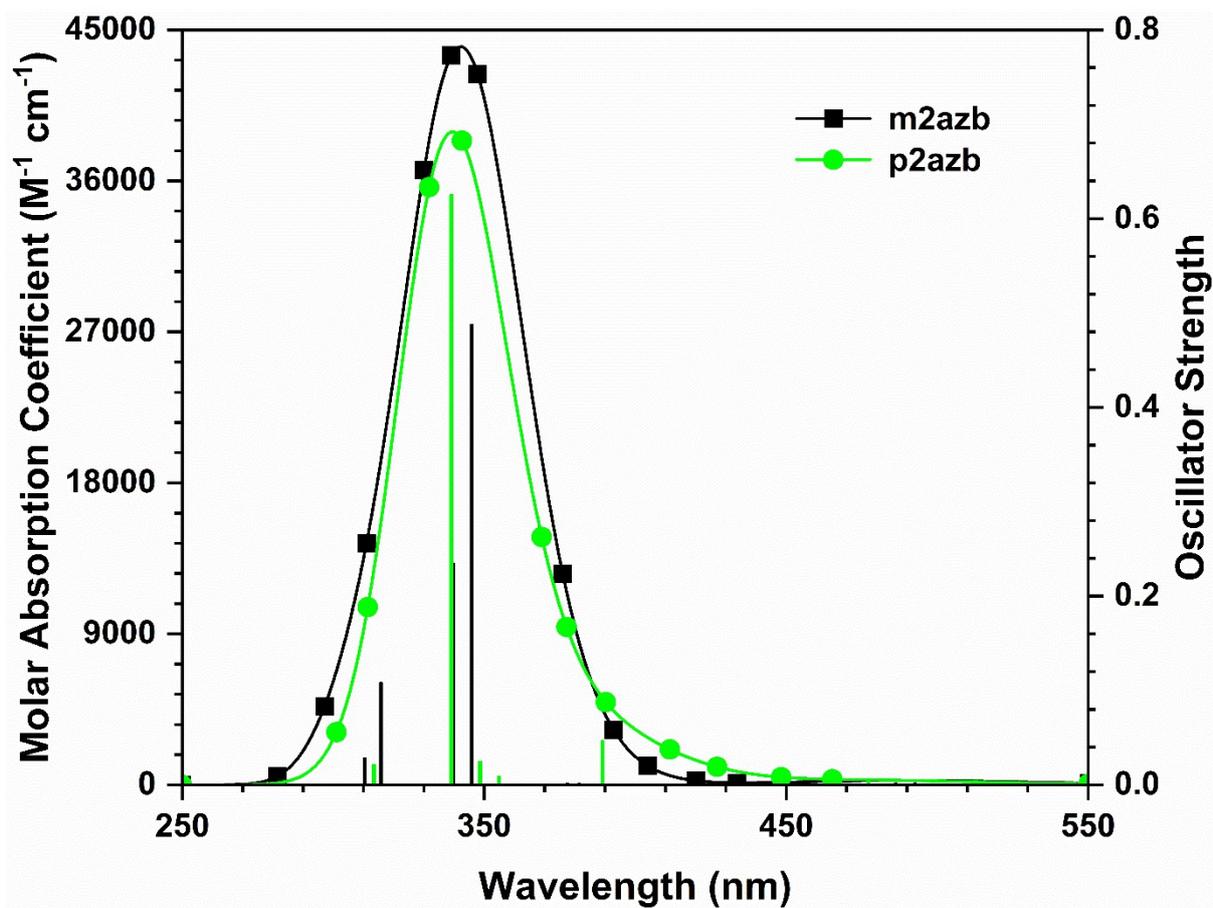


Figure S14. Simulated absorption spectra of **m2azb** and **p2azb** with FWHM of 0.46 eV at B2PLYP/def2-TZVP level.



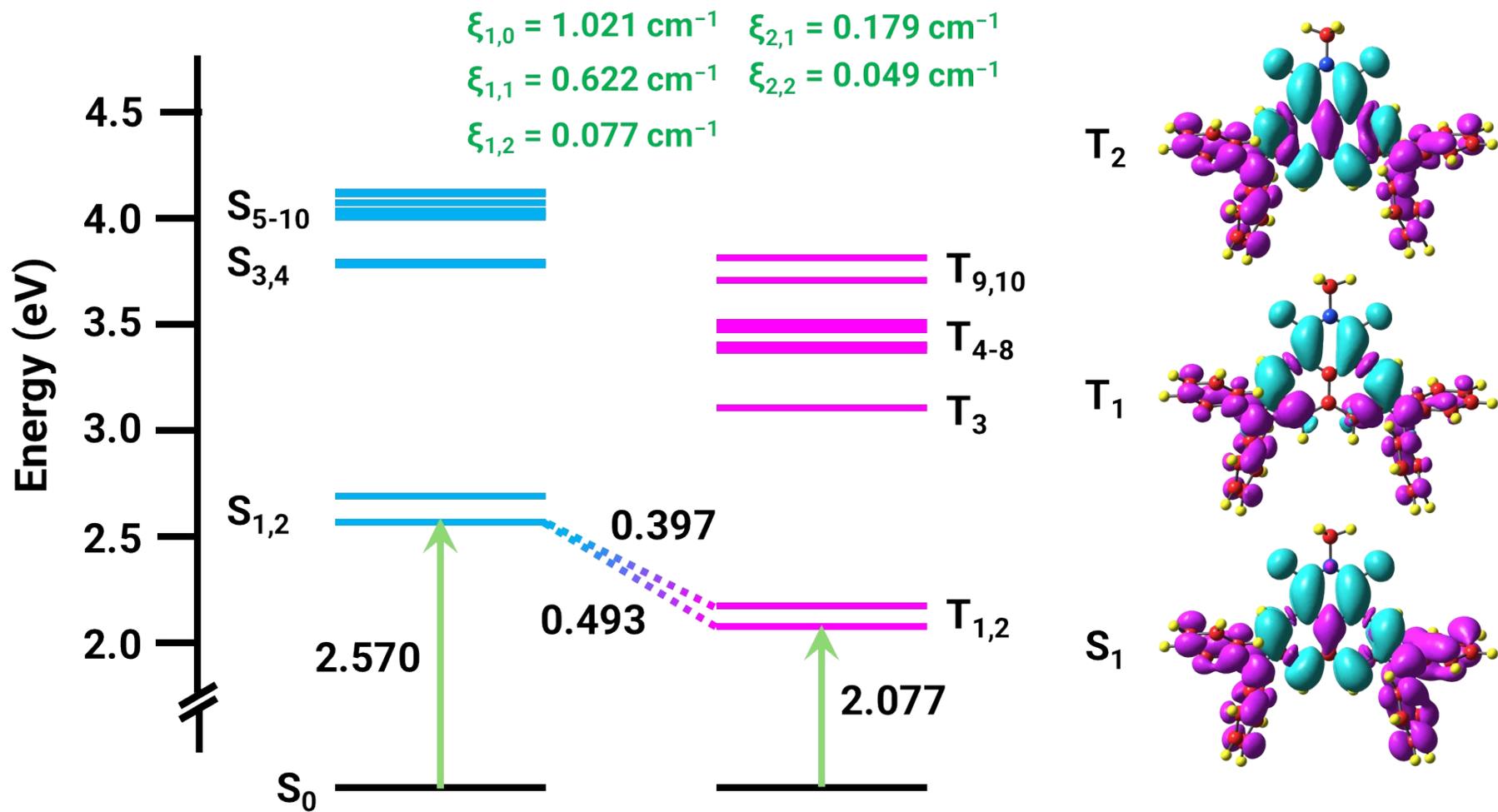


Figure S16. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of  $m2dpa$ .

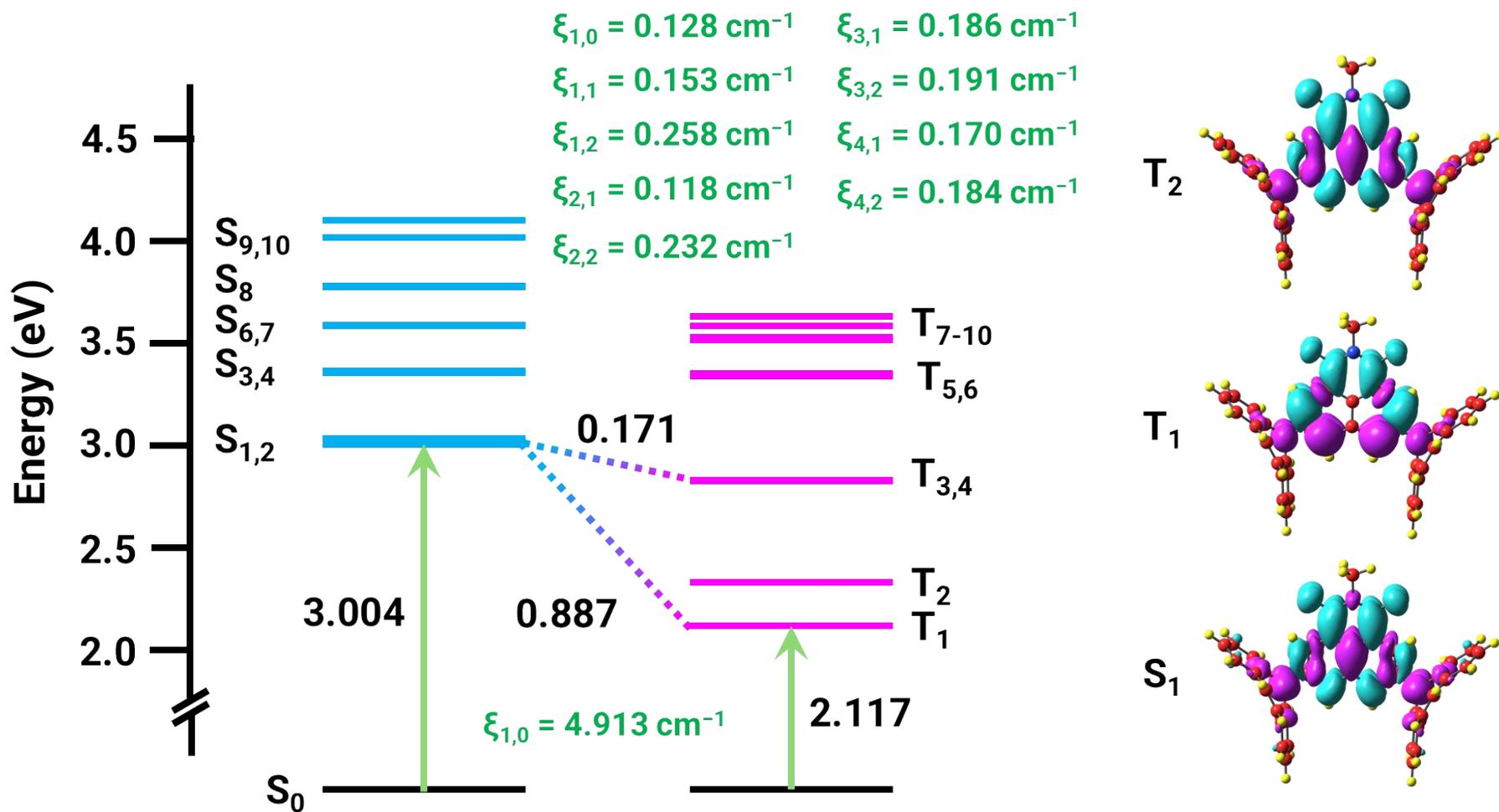


Figure S17. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **m2az1**.

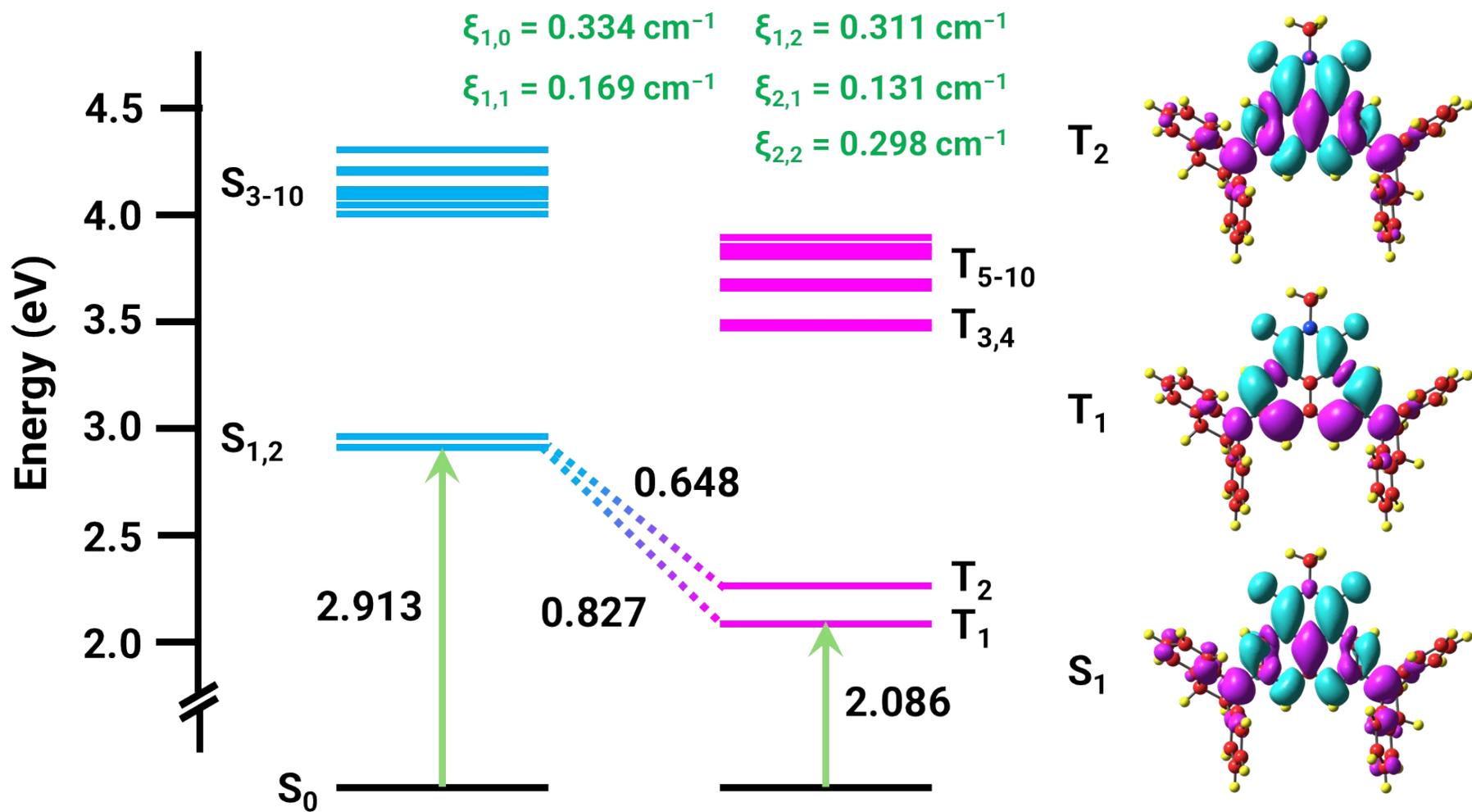


Figure S18. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **m2az2**.

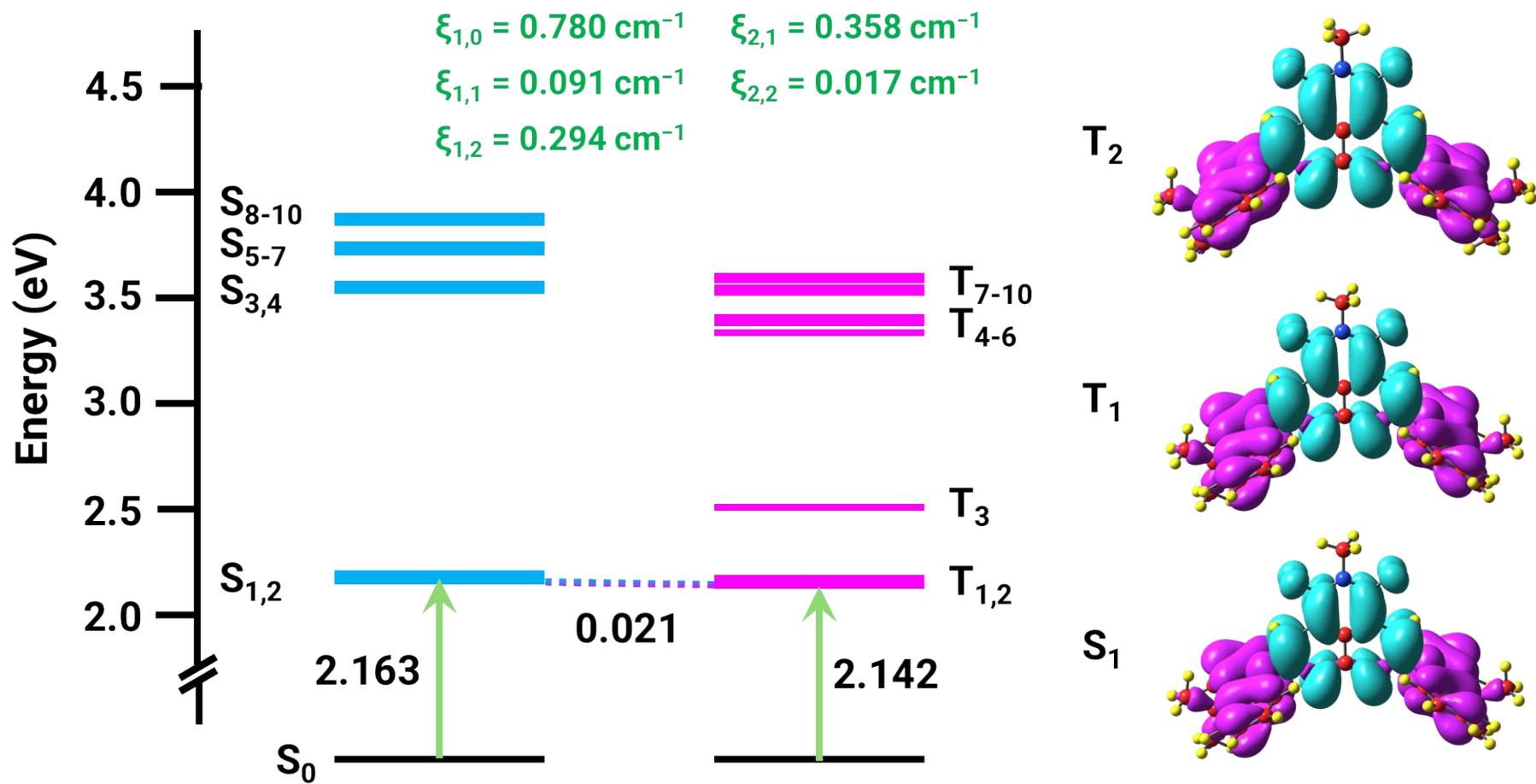


Figure S19. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **m2acr**.

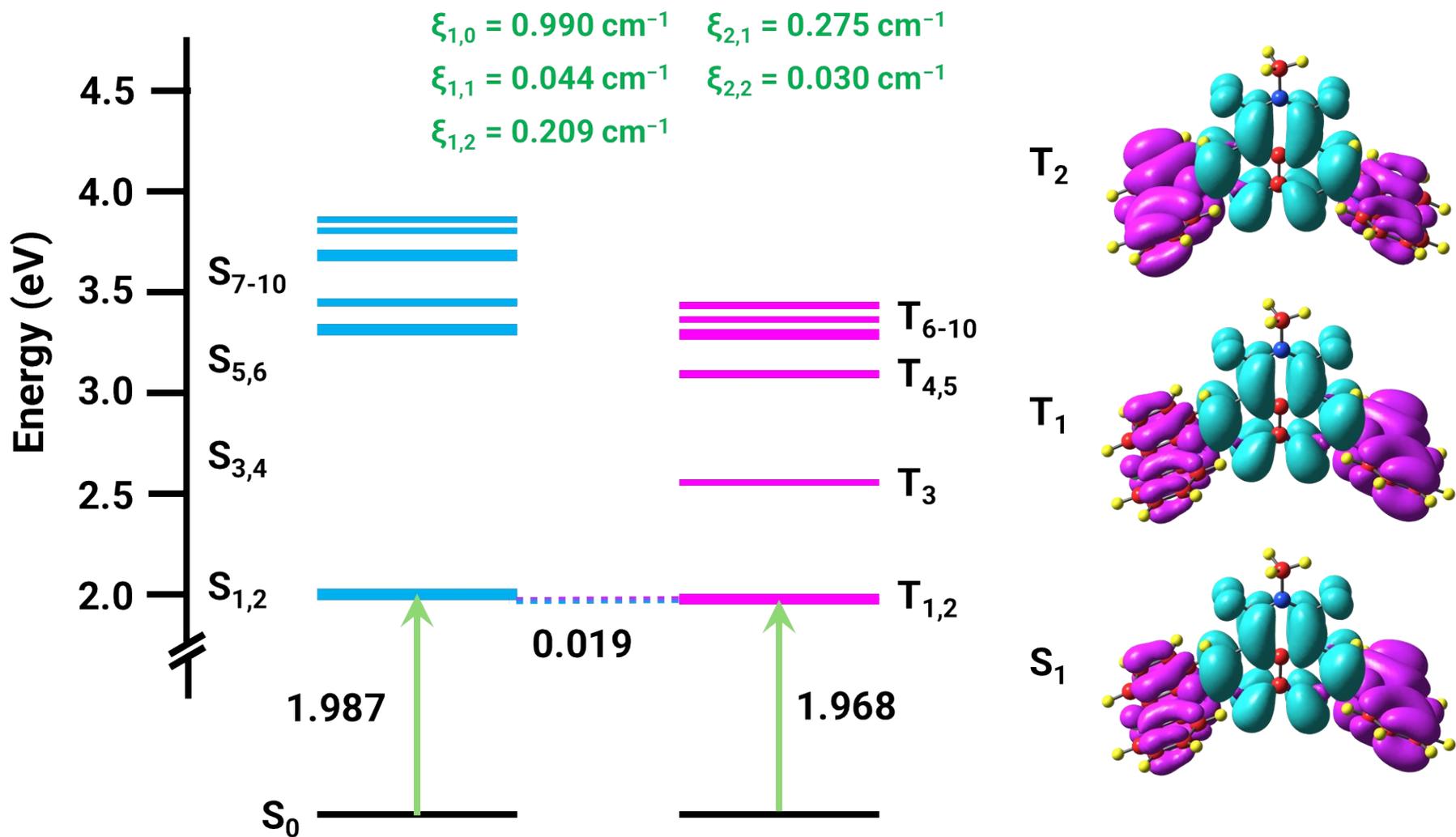


Figure S20. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **m2po**.

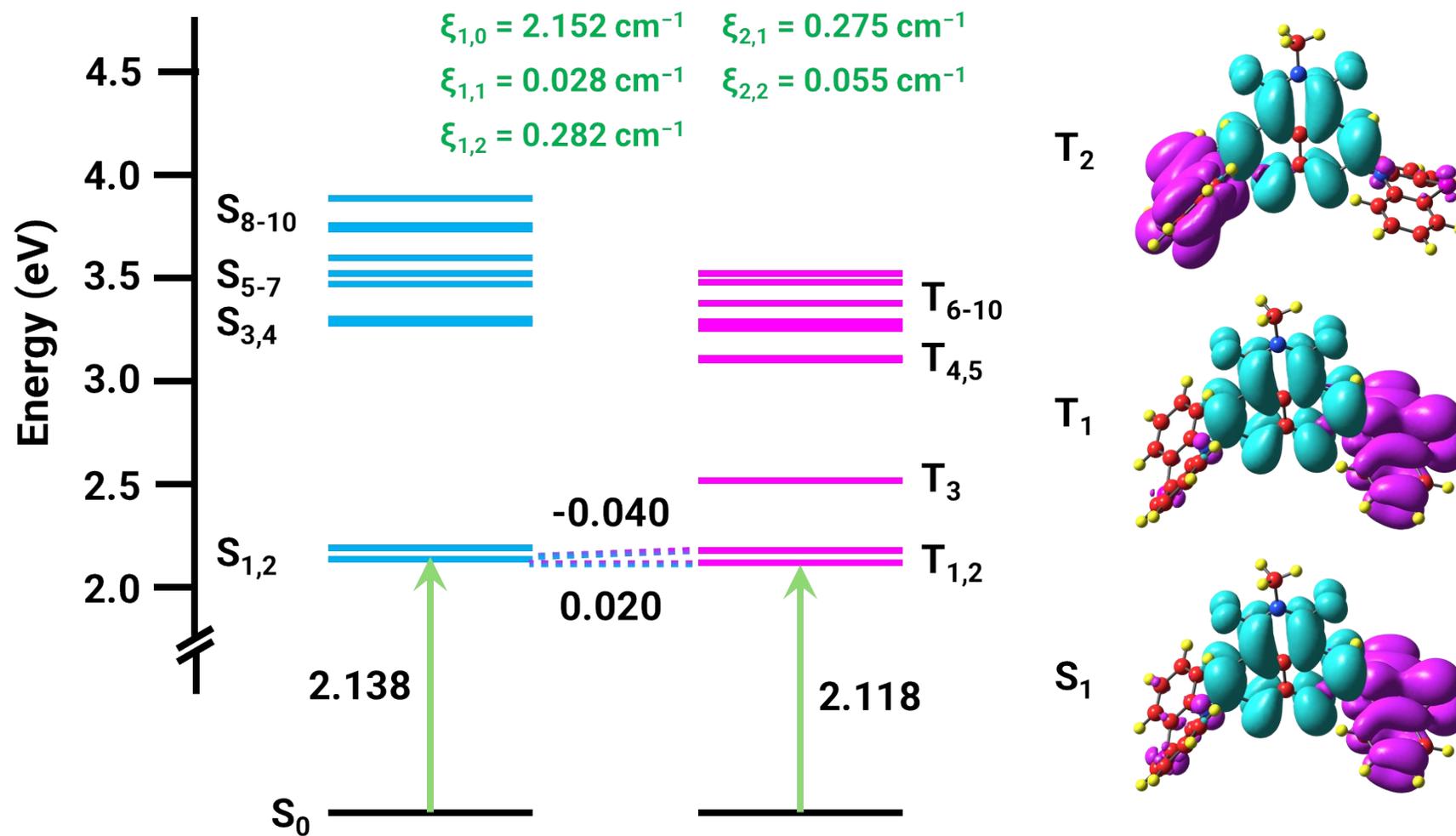


Figure S21. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **m2pt**.

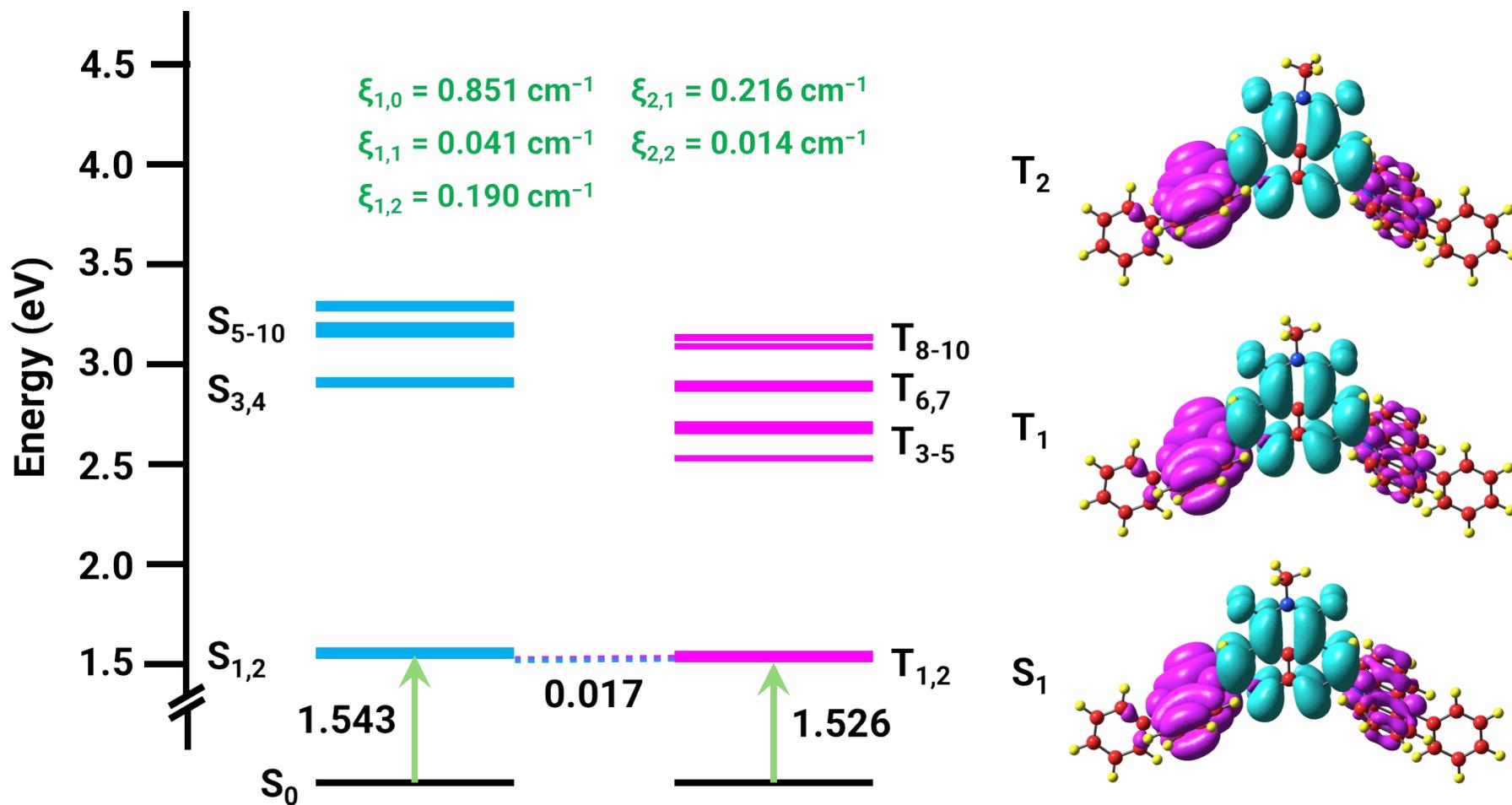


Figure S22. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of  $m2npp$ .

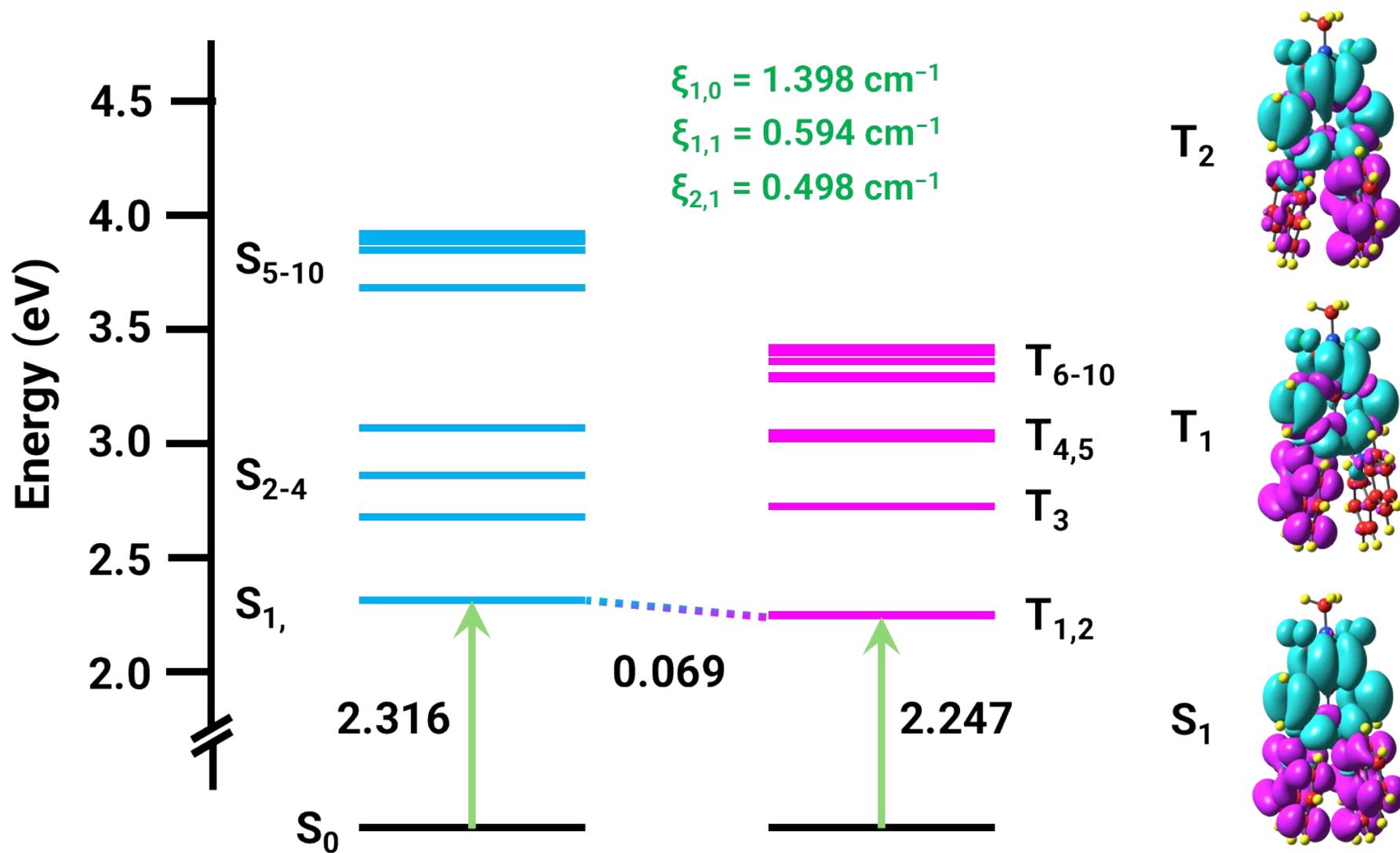


Figure S23. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2cz**.

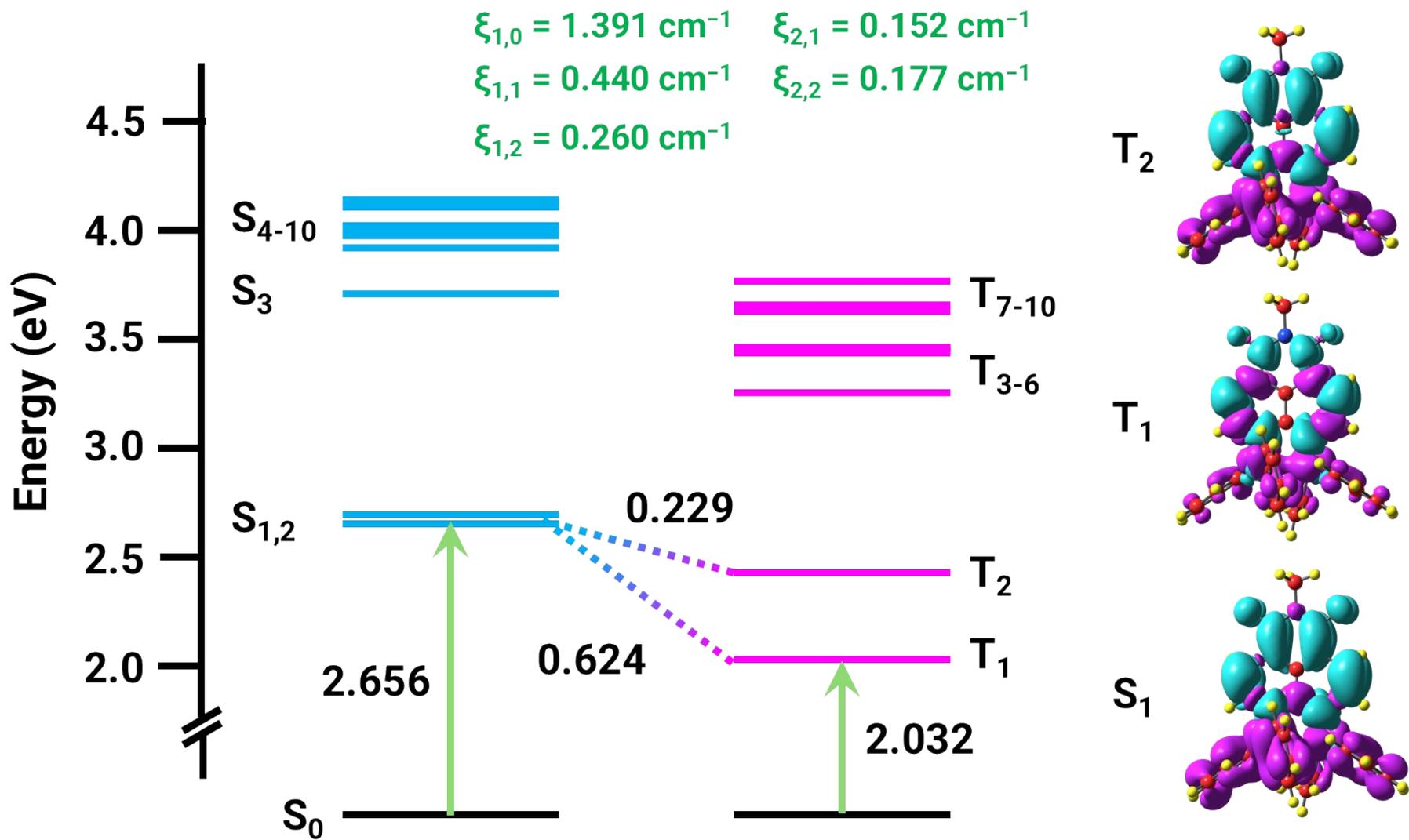


Figure S24. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2dpa**.

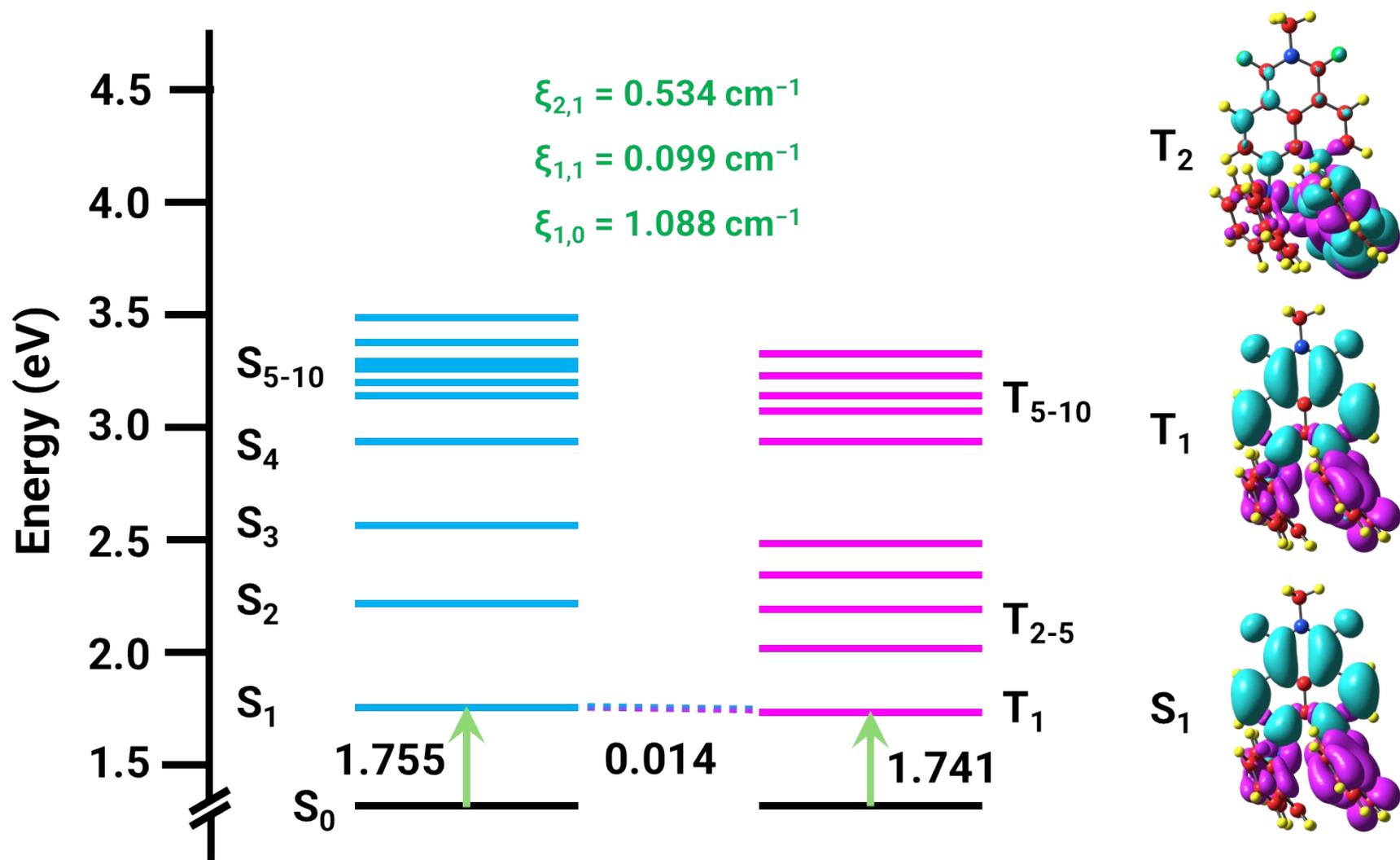


Figure S25. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2az1**.

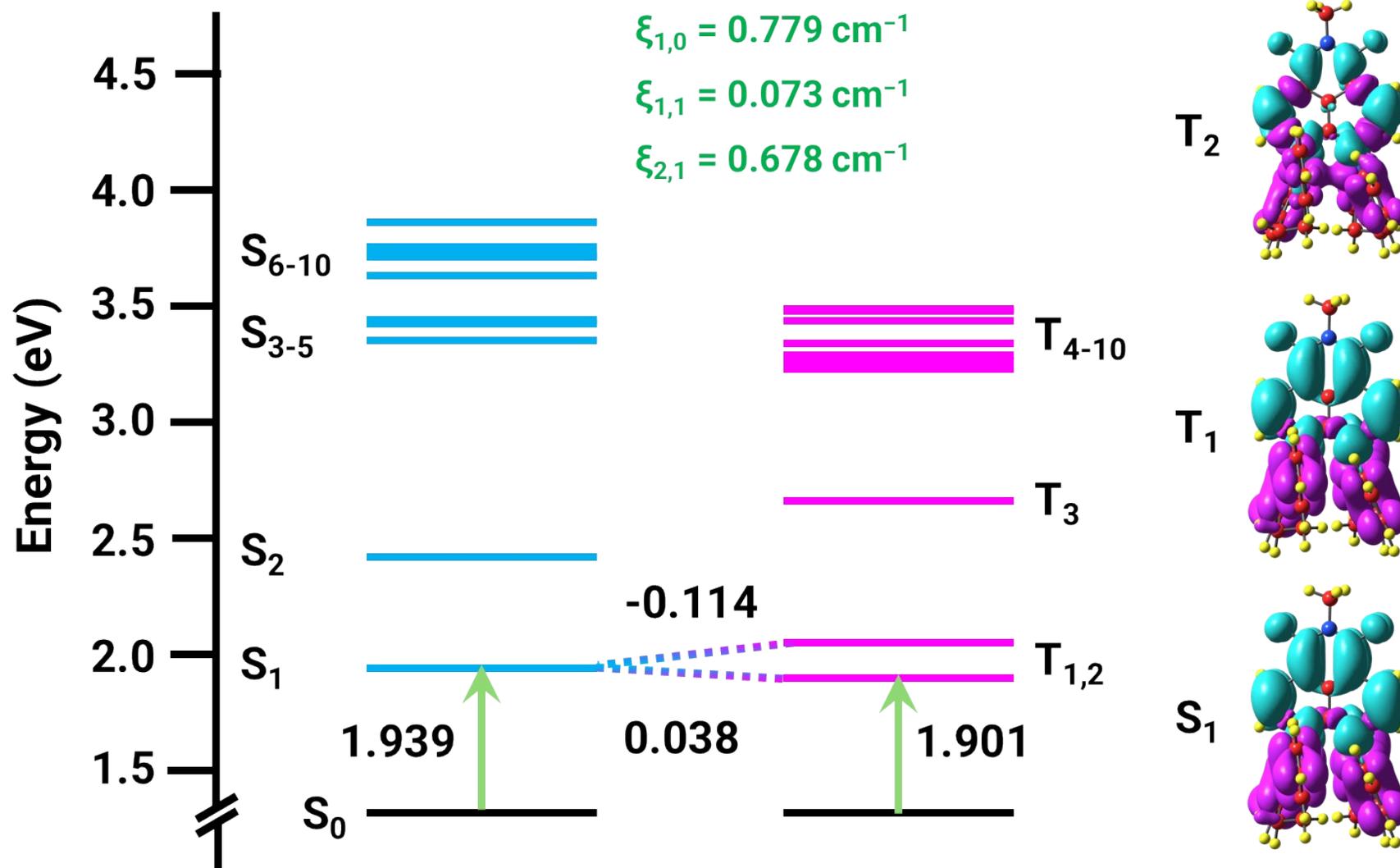


Figure S26. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2az2**.

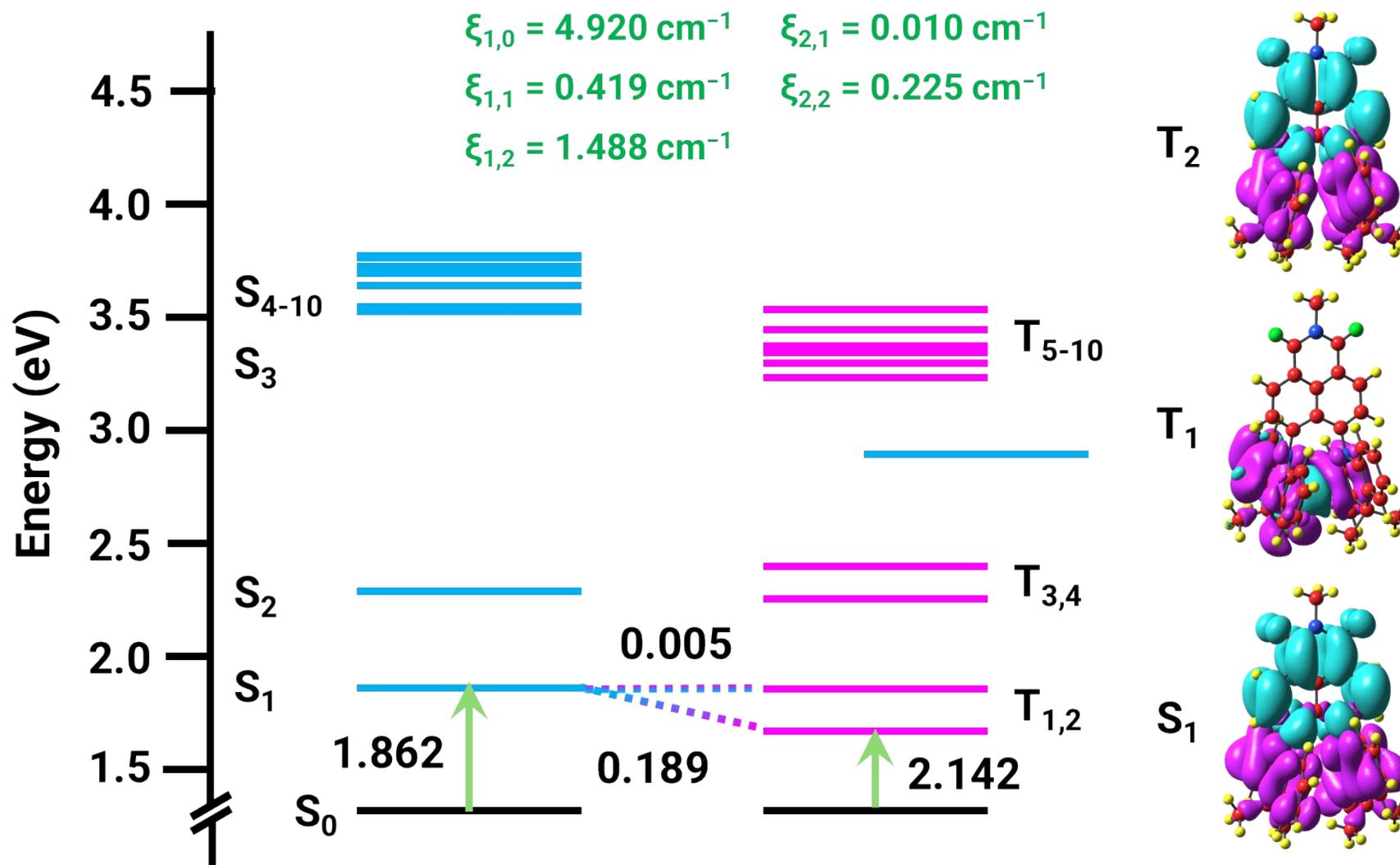


Figure S27. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of p2acr.

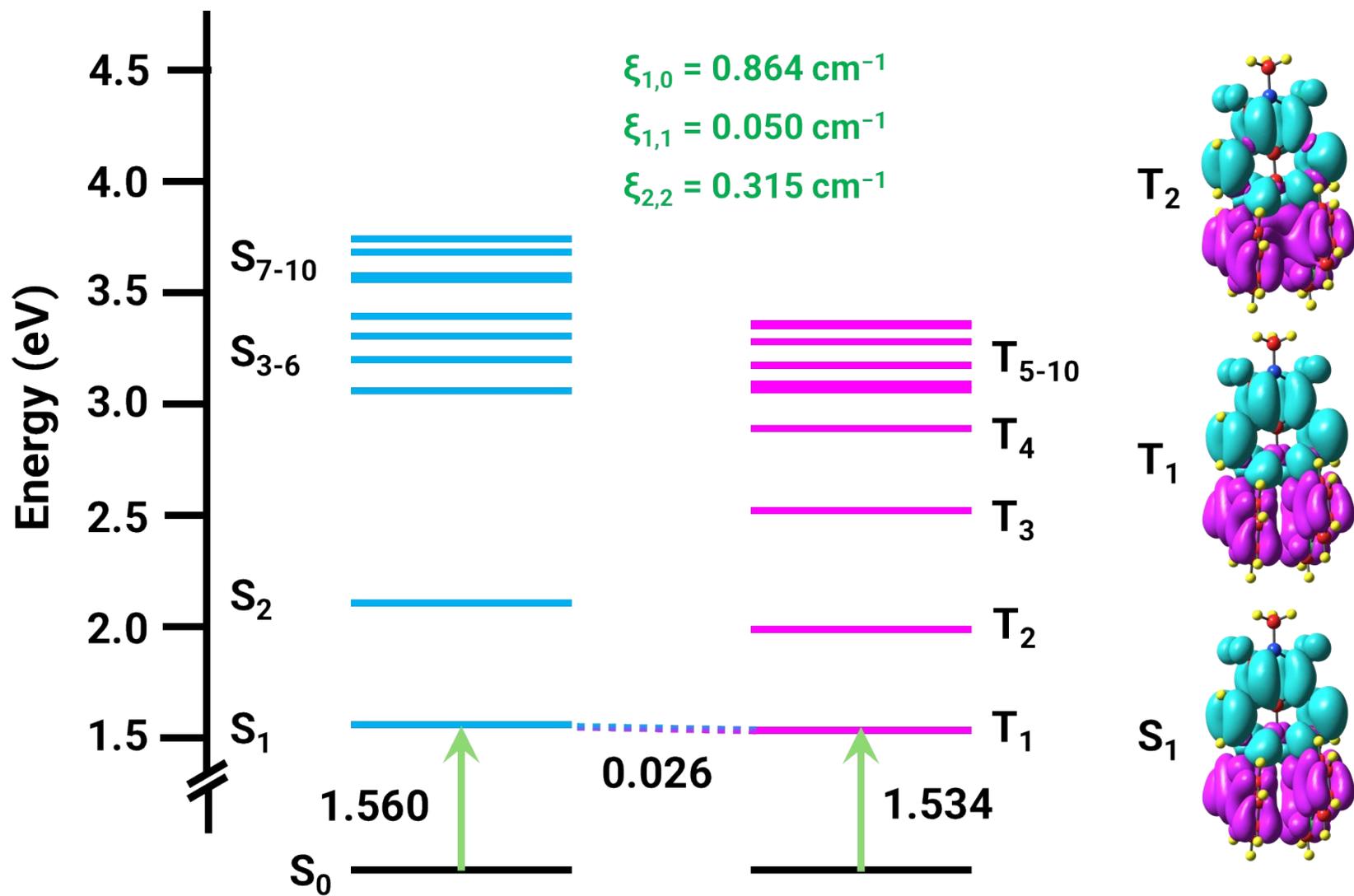


Figure S28. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2po**.

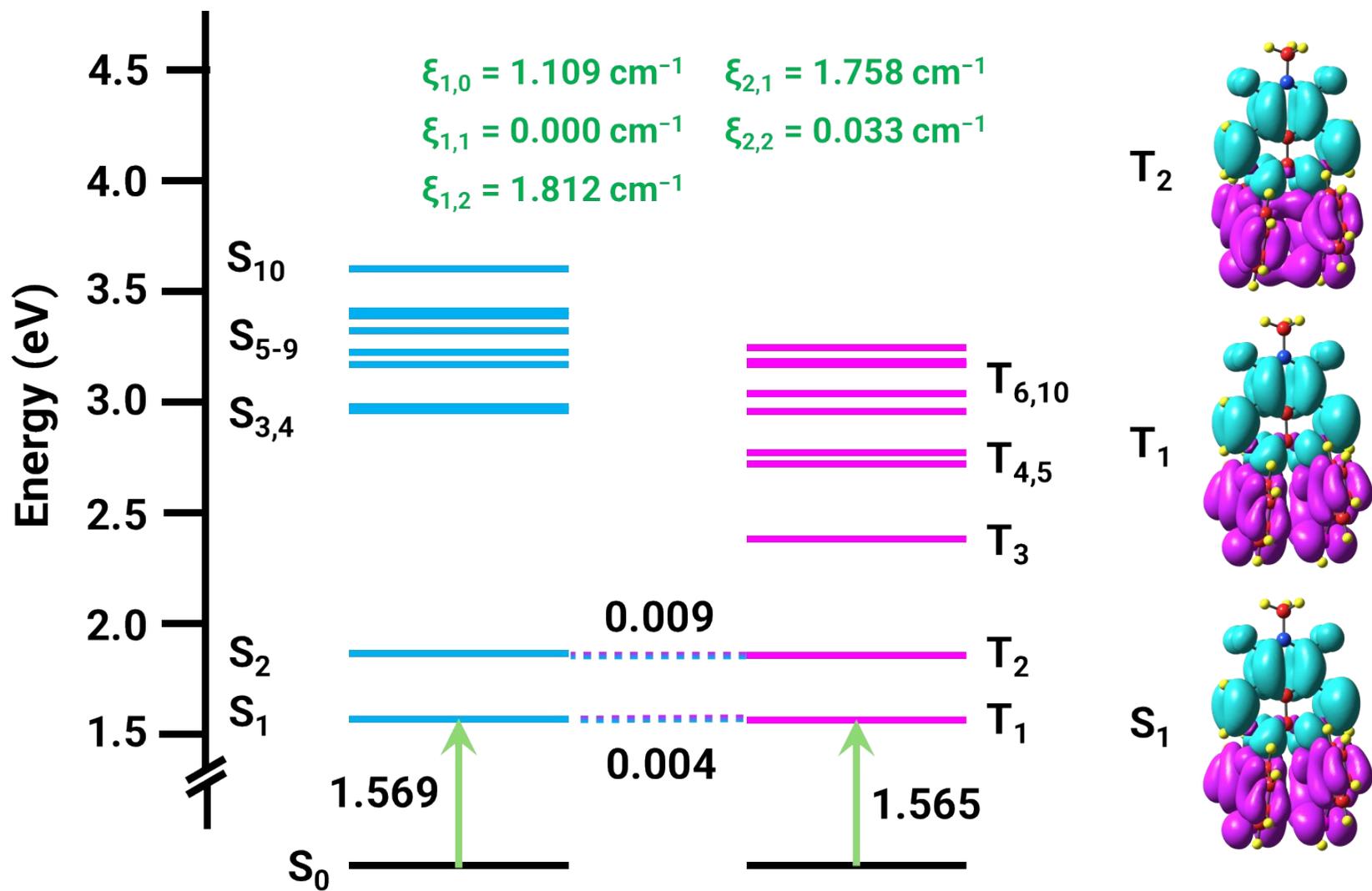


Figure S29. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2pt**.

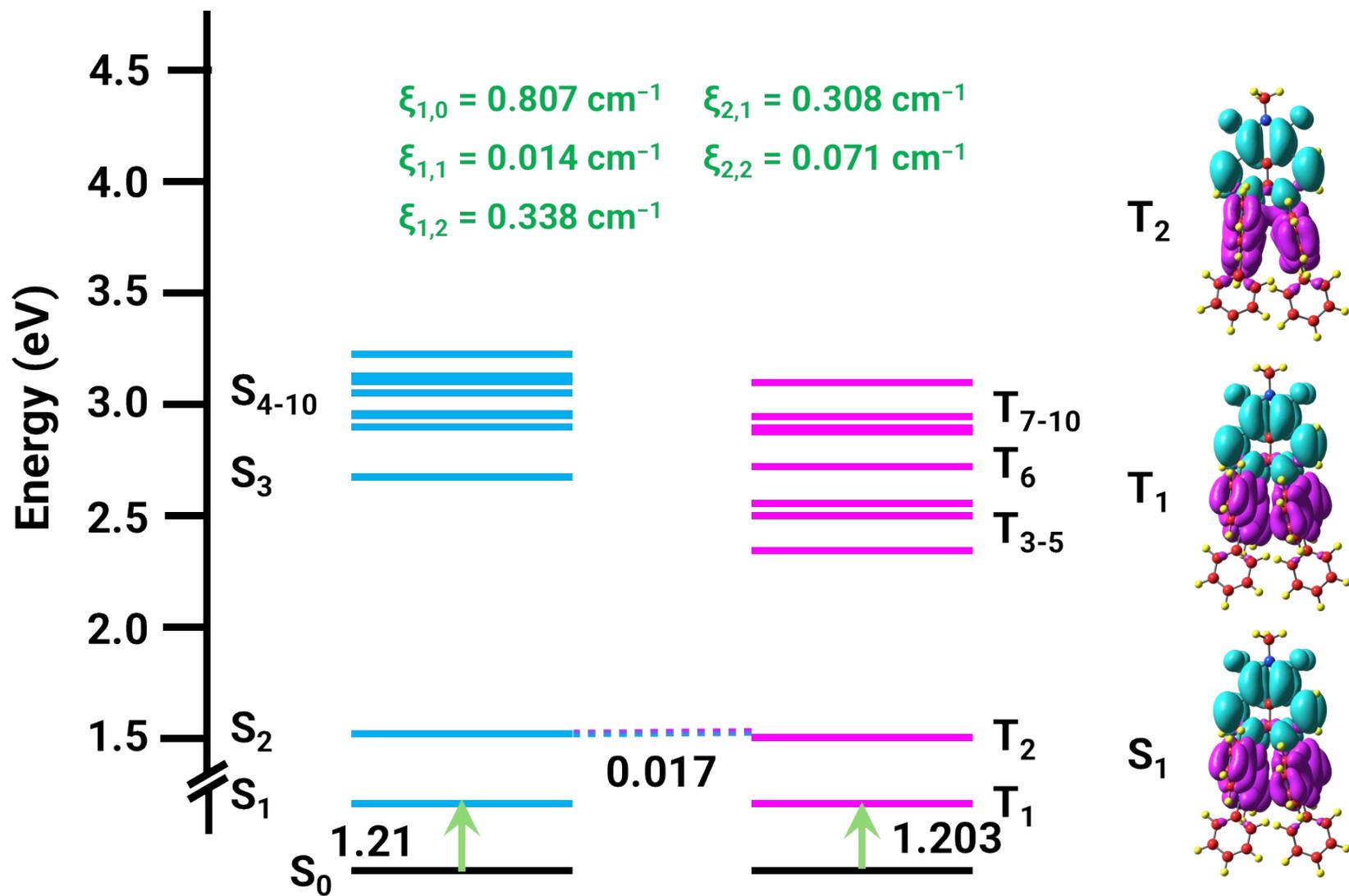


Figure S30. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2npp**.

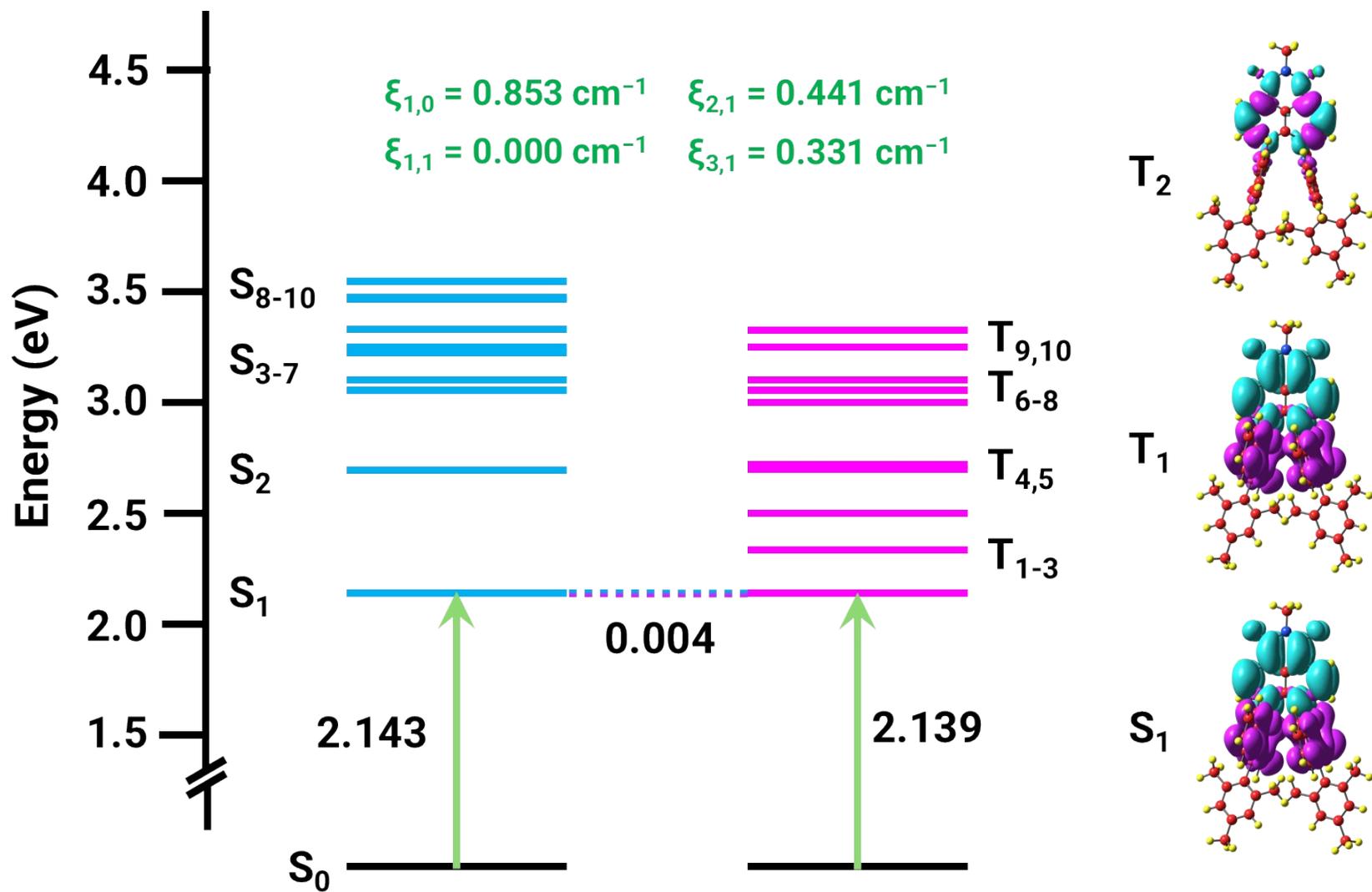
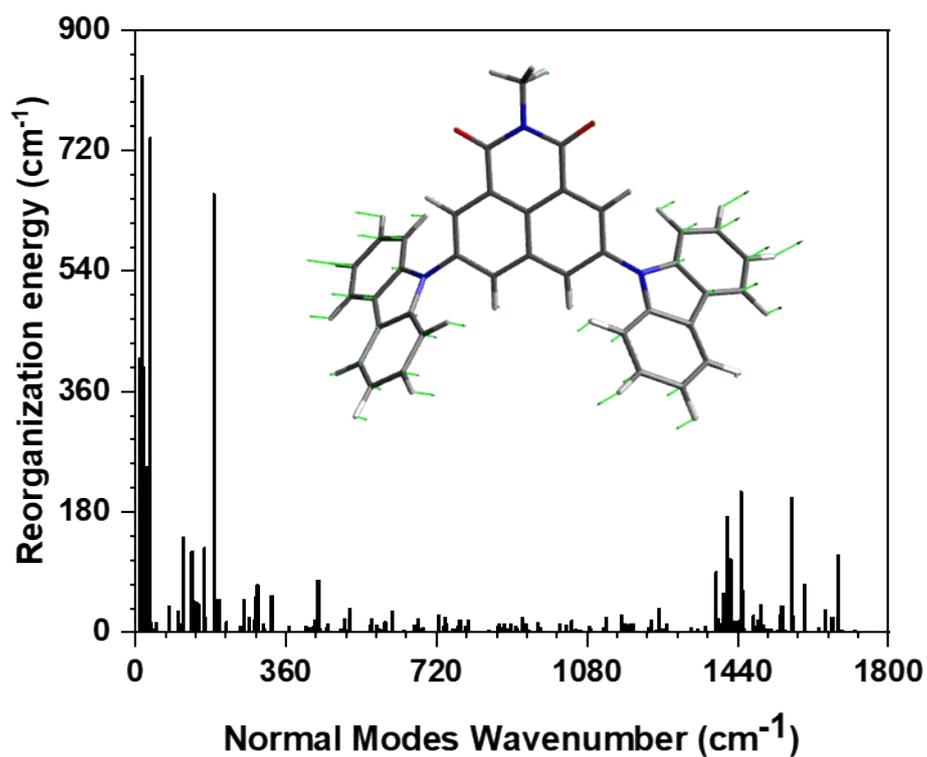
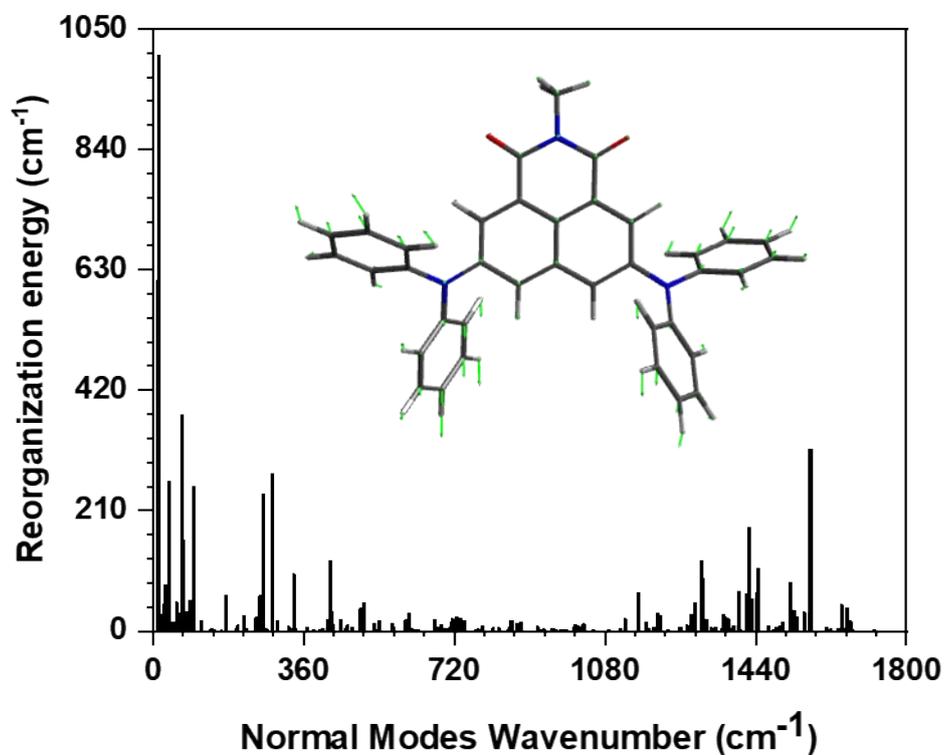


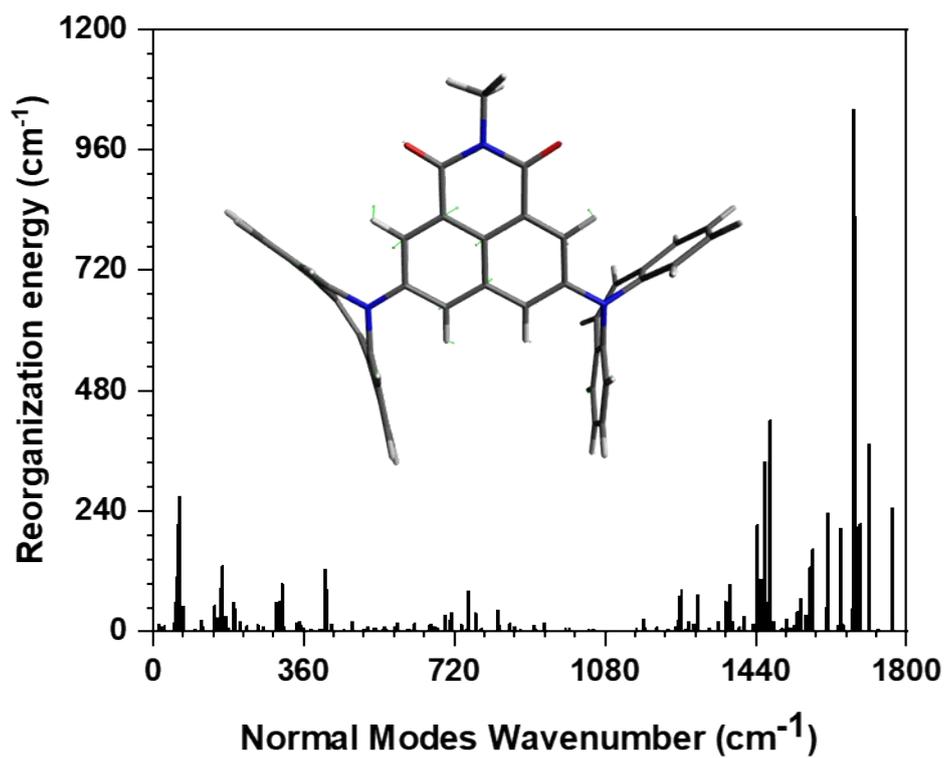
Figure S31. Energy profile diagram and difference density plots of  $S_1$ ,  $T_1$  and  $T_2$  states of **p2azb**.



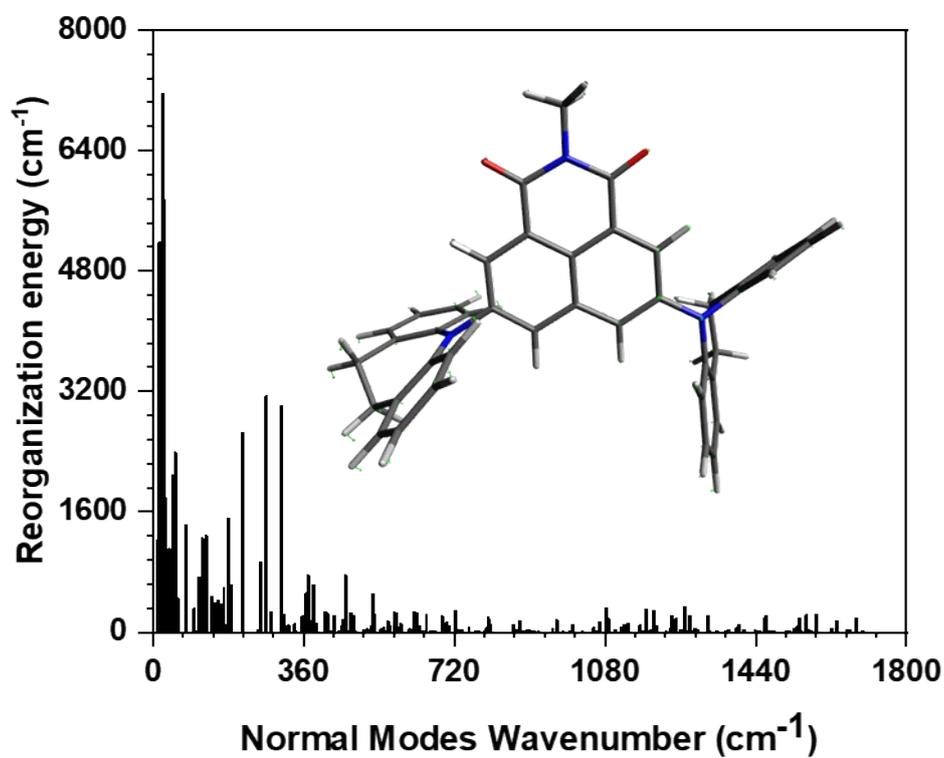
**Figure S32.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2cz**. Representative rotational modes are shown in the insets.



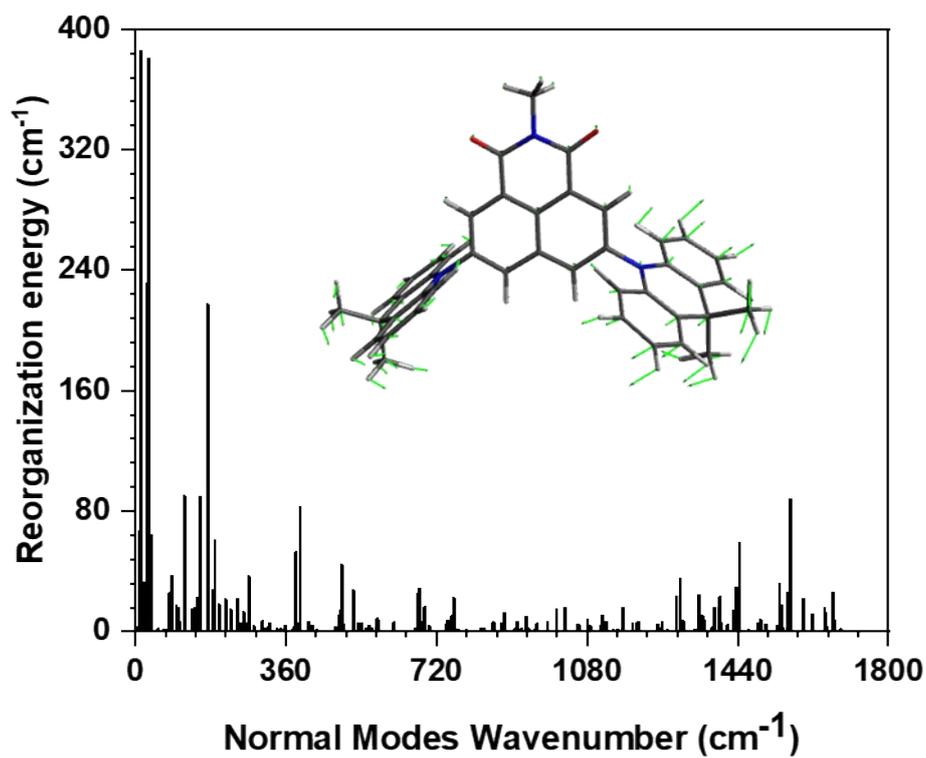
**Figure S33.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2dpa**. Representative rotational modes are shown in the insets.



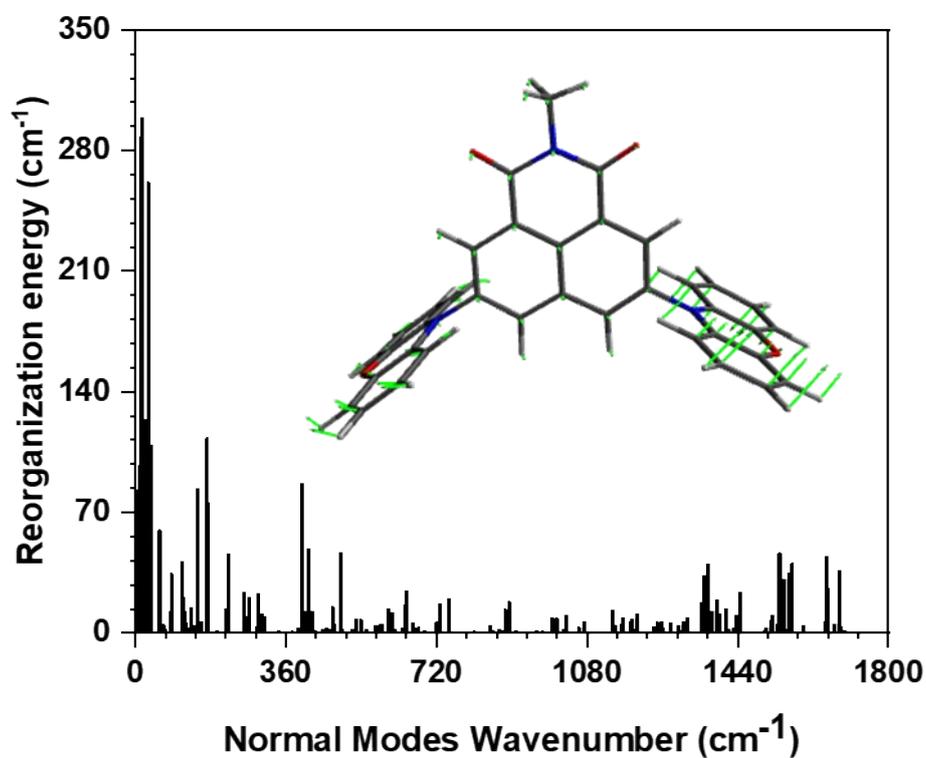
**Figure S34.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2az1**. Representative rotational modes are shown in the insets.



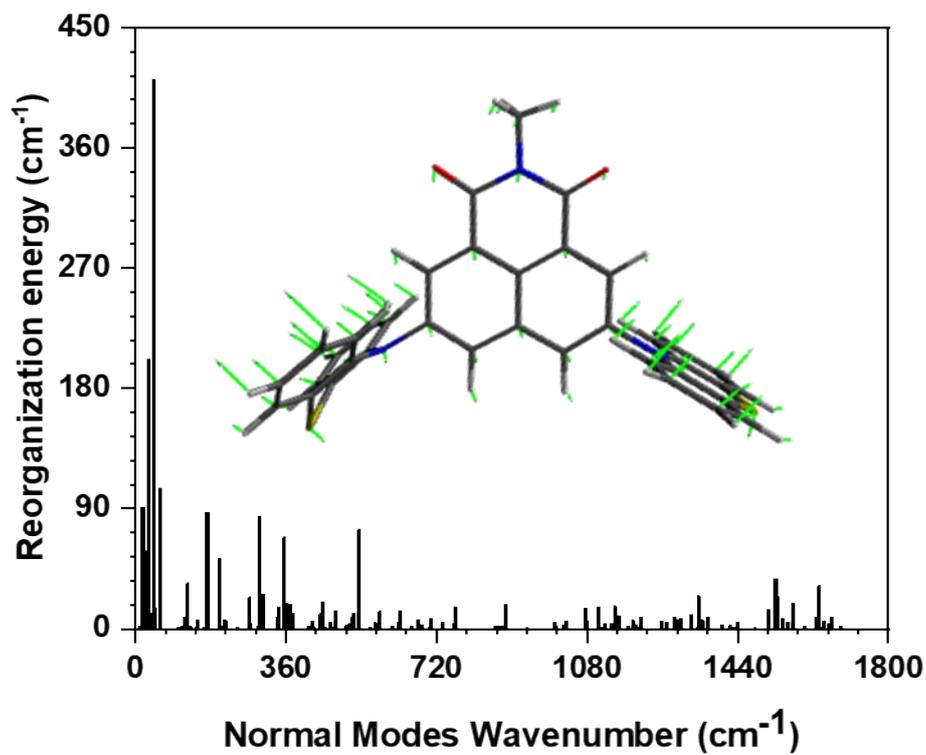
**Figure S35.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2az2**. Representative rotational modes are shown in the insets.



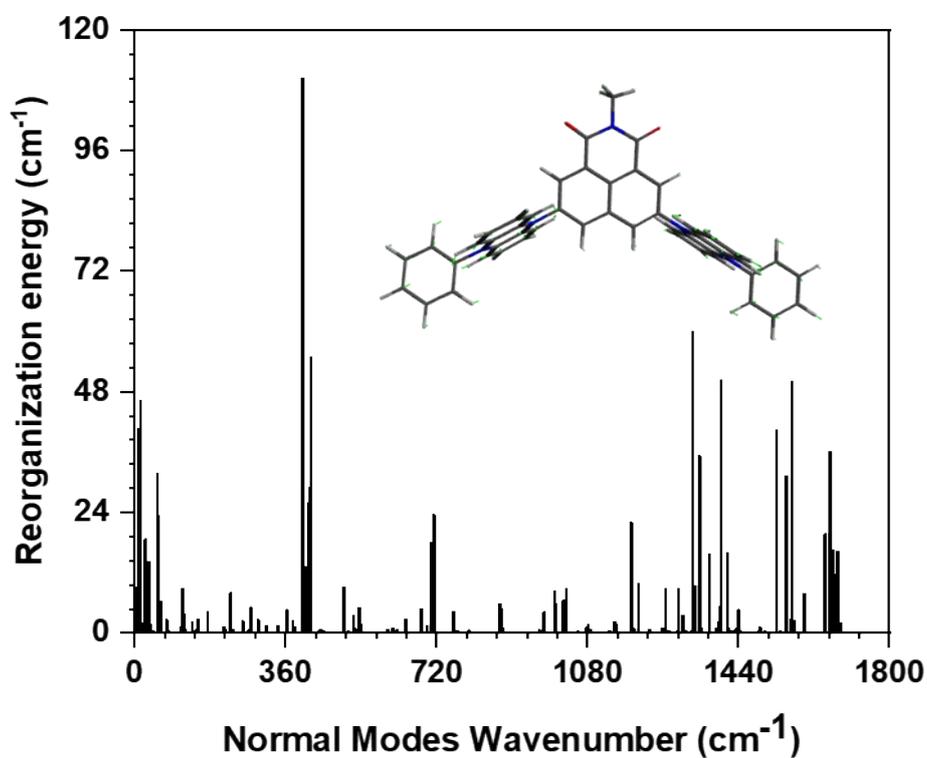
**Figure S36.** Reorganization energies for the  $S_1$  in the  $S_1-T_1$  transition versus the normal mode frequencies of **m2acr**. Representative rotational modes are shown in the insets.



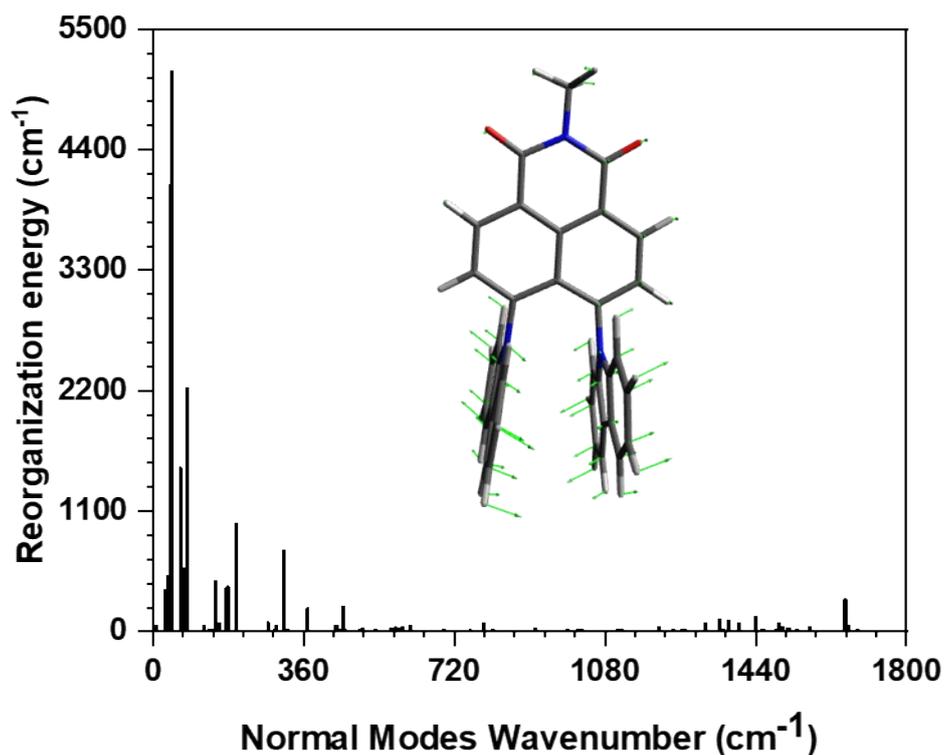
**Figure S37.** Reorganization energies for the  $S_1$  in the  $S_1-T_1$  transition versus the normal mode frequencies of **m2po**. Representative rotational modes are shown in the insets.



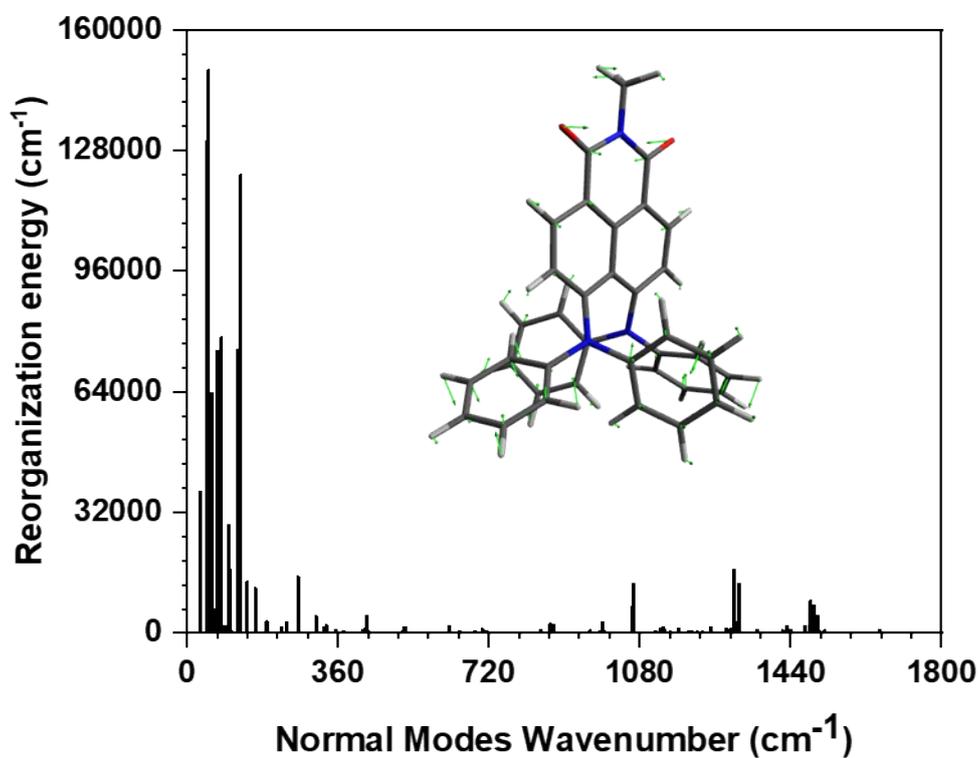
**Figure S38.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2pt**. Representative rotational modes are shown in the insets.



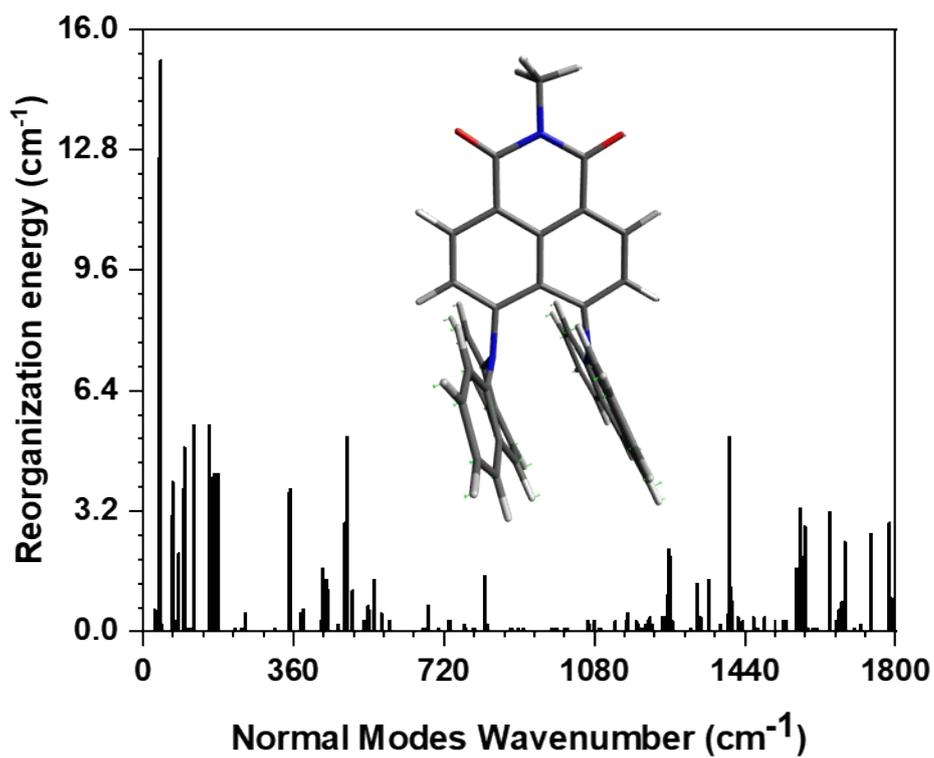
**Figure S39.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **m2npp**. Representative rotational modes are shown in the insets.



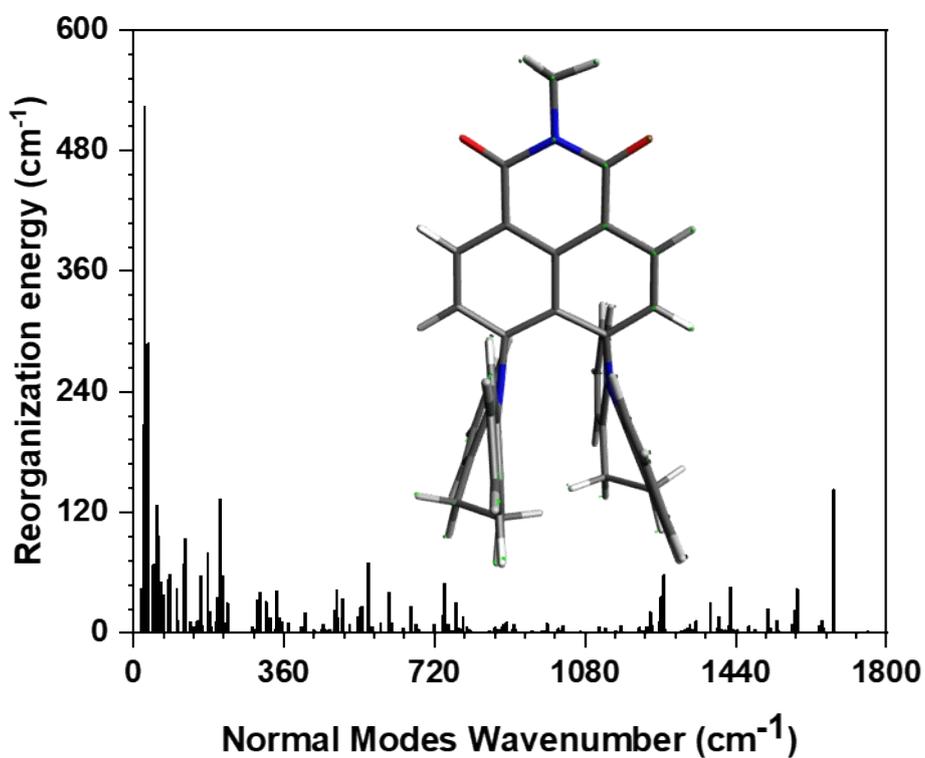
**Figure S40.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **p2cz**. Representative rotational modes are shown in the insets.



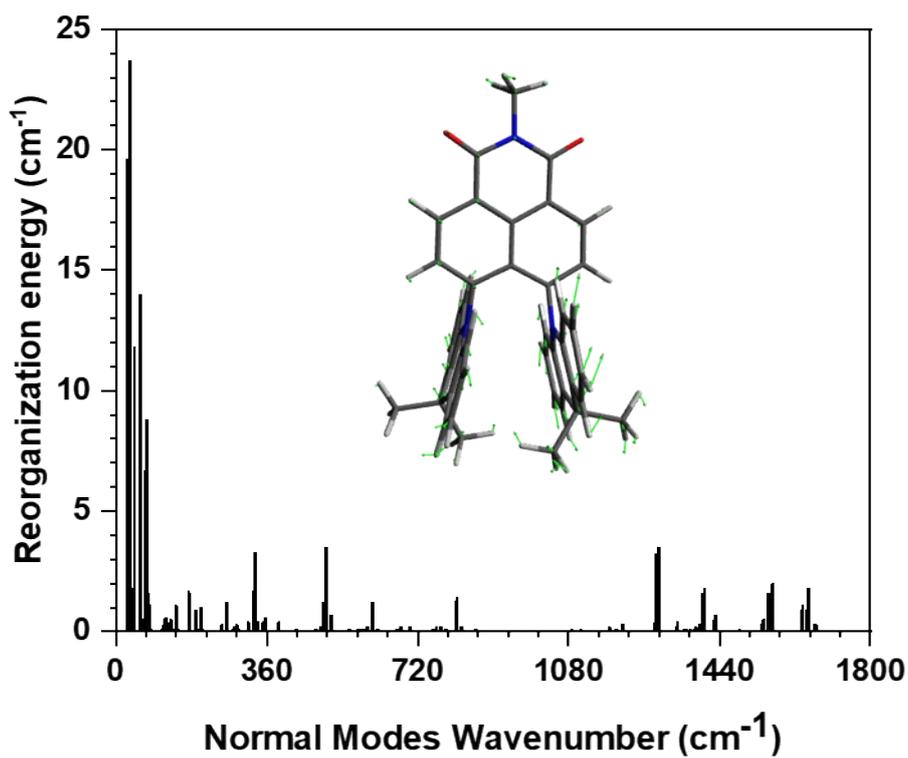
**Figure S41.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **p2dpa**. Representative rotational modes are shown in the insets.



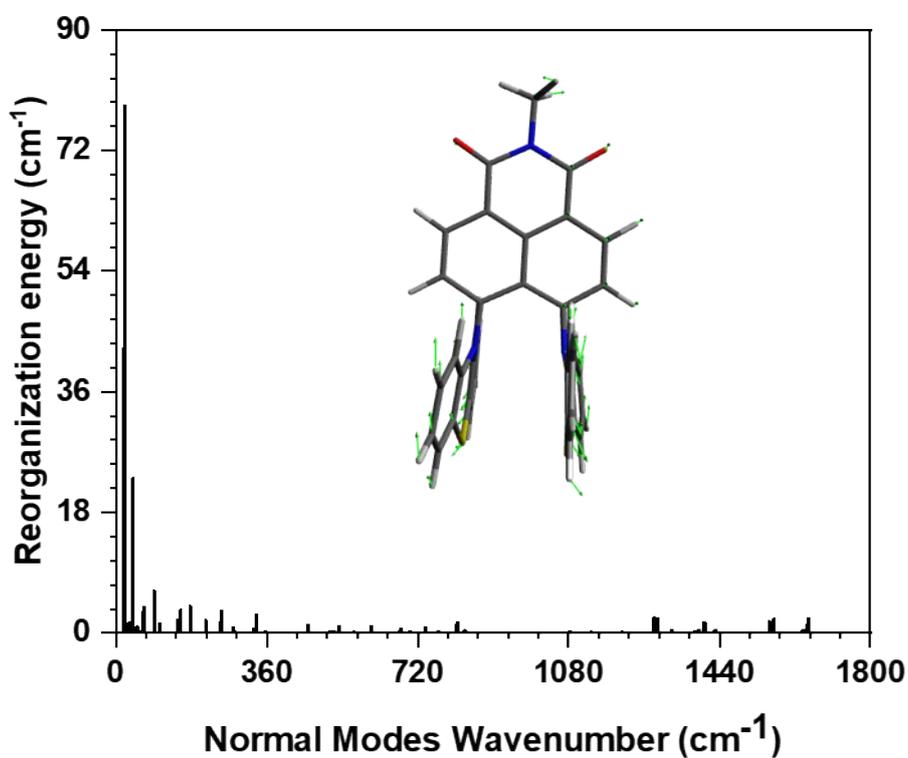
**Figure S42.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **p2az1**. Representative rotational modes are shown in the insets.



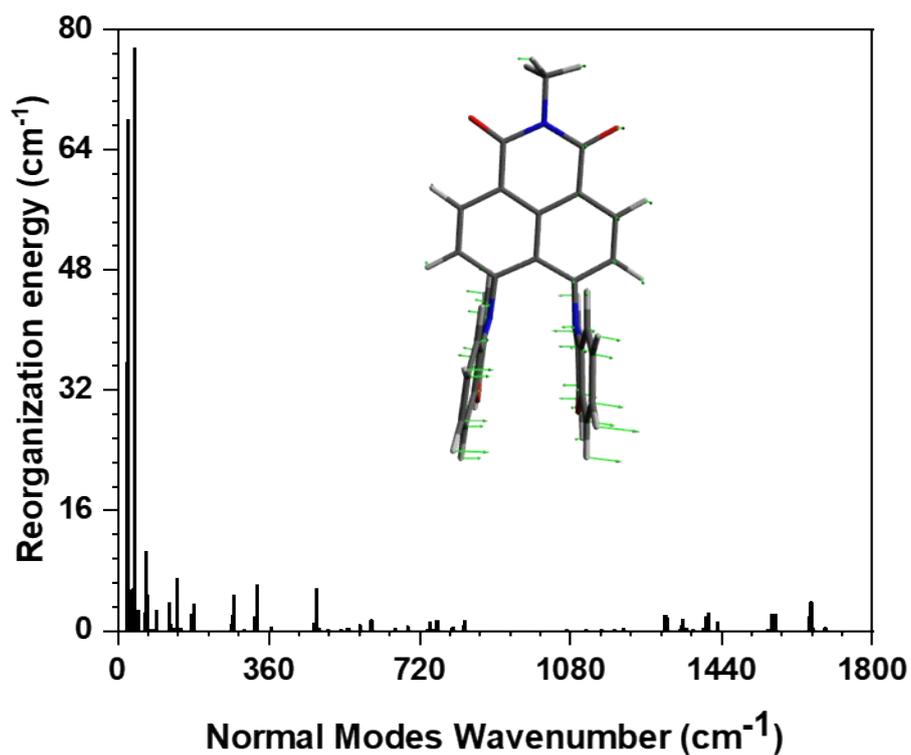
**Figure S43.** Reorganization energies for the  $S_1$  in the  $S_1$ - $T_1$  transition versus the normal mode frequencies of **p2az2**. Representative rotational modes are shown in the insets.



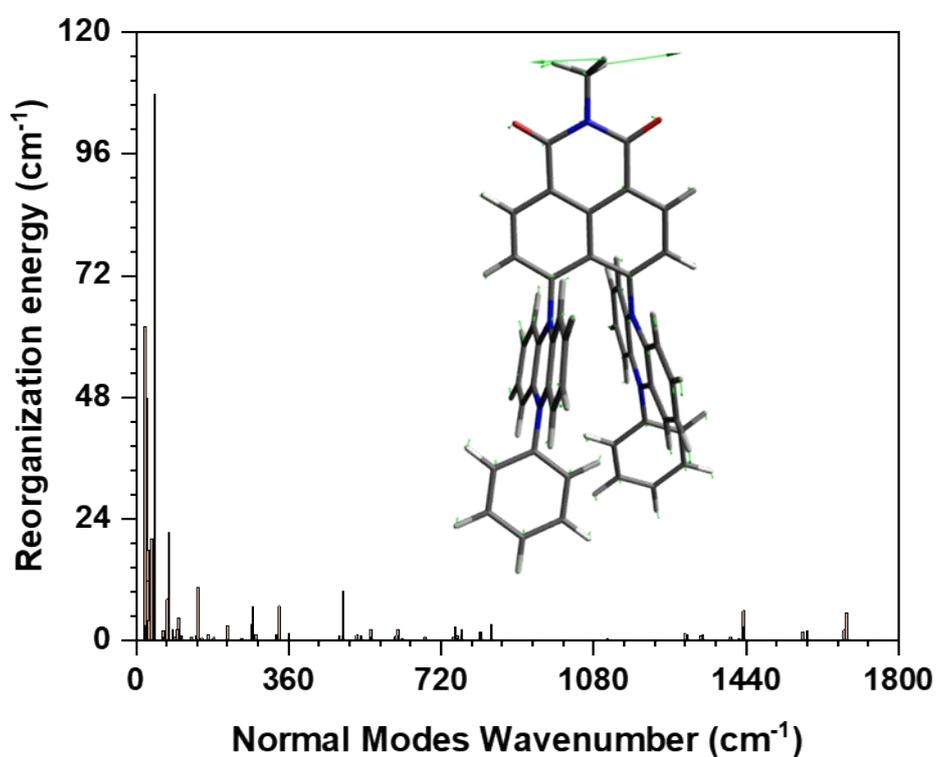
**Figure S44.** Reorganization energies for the S<sub>1</sub> in the S<sub>1</sub>-T<sub>1</sub> transition versus the normal mode frequencies of **p2acr**. Representative rotational modes are shown in the insets.



**Figure S45.** Reorganization energies for the S<sub>1</sub> in the S<sub>1</sub>-T<sub>1</sub> transition versus the normal mode frequencies of **p2pt**. Representative rotational modes are shown in the insets.



**Figure S46.** Reorganization energies for the S<sub>1</sub> in the S<sub>1</sub>-T<sub>1</sub> transition versus the normal mode frequencies of **p2po**. Representative rotational modes are shown in the insets.



**Figure S47.** Reorganization energies for the S<sub>1</sub> in the S<sub>1</sub>-T<sub>1</sub> transition versus the normal mode frequencies of **p2npp**. Representative rotational modes are shown in the insets.

**Table S1.** Computed  $S_1$ ,  $T_1$  energies and  $\Delta E_{ST}$  values of the compounds in  $S_0$ ,  $S_1$  and  $T_1$  geometries.

Compound	$S_0$ Geometry				$S_1$ Geometry				$T_1$ Geometry			
	$S_1$ , eV	$T_1$ , eV	$\Delta E_{ST}$ , eV	SOC, <sup>a</sup> $\text{cm}^{-1}$	$S_1$ , eV	$T_1$ , eV	$\Delta E_{ST}$ , eV	SOC, <sup>a</sup> $\text{cm}^{-1}$	$S_1$ , eV	$T_1$ , eV	$\Delta E_{ST}$ , eV	SOC, <sup>a</sup> $\text{cm}^{-1}$
<b>m2acr</b>	2.174	2.148	0.026	0.168	1.78	1.762	0.018	0.020	1.895	1.673	0.222	0.645
<b>p2acr</b>	1.884	1.879	0.005	0.000	1.41	1.404	0.006	0.000	1.412	1.403	0.009	0.010
<b>m2az1</b>	3.02	2.133	0.887	0.164	2.59	1.993	0.597	0.342	2.682	1.617	1.065	0.278
<b>p2az1</b>	1.748	1.735	0.013	0.095	1.164	1.155	0.009	0.063	1.159	1.146	0.013	0.077
<b>m2az2</b>	2.925	2.101	0.824	0.138	2.021	1.857	0.164	0.567	2.633	1.6	1.033	0.282
<b>p2az2</b>	1.949	1.909	0.04	0.073	1.544	1.526	0.018	0.028	1.706	1.508	0.198	0.540
<b>m2azb</b>	2.558	2.492	0.066	1.168	2.187	2.17	0.017	0.035	2.236	1.817	0.419	0.853
<b>p2azb</b>	2.159	2.155	0.004	0.000	1.749	1.745	0.004	0.000	1.83	1.716	0.114	0.364
<b>m2cz</b>	2.711	2.28	0.431	0.327	2.267	2.065	0.202	0.829	2.42	1.729	0.691	0.731
<b>p2cz</b>	2.358	2.245	0.113	0.753	1.735	1.732	0.003	0.014	2.267	1.719	0.548	0.624
<b>m2dpa</b>	2.567	2.081	0.486	0.575	2.031	1.794	0.237	0.587	2.316	1.537	0.779	0.433
<b>p2dpa</b>	2.675	2.04	0.635	0.457	1.564	1.54	0.024	0.046	2.406	1.618	0.788	0.283
<b>m2npp</b>	1.561	1.542	0.019	0.051	0.994	0.98	0.014	0.020	1.114	1.099	0.015	0.033
<b>p2npp</b>	1.201	1.192	0.009	0.014	0.735	0.731	0.004	0.000	0.754	0.741	0.013	0.028
<b>m2po</b>	1.998	1.975	0.023	0.095	1.392	1.377	0.015	0.022	1.598	1.483	0.115	0.382
<b>p2po</b>	1.594	1.555	0.039	0.062	1.045	1.04	0.005	0.010	1.066	1.054	0.012	0.030
<b>m2pt</b>	2.139	2.117	0.022	0.036	1.316	1.302	0.014	0.020	1.423	1.408	0.015	0.017
<b>p2pt</b>	1.585	1.581	0.004	0.000	0.89	0.886	0.004	0.000	0.925	0.918	0.007	0.000

<sup>a</sup> SOC means  $\langle \Psi_{S_1} | \hat{H}_{SOC} | \Psi_{T_1} \rangle$

**Table S2.** Charge transfer parameters of the compounds computed for the S<sub>1</sub> geometry at the M06/def2-TZVP level

Compound	State	CT (%)	LE (%)	S <sub>m</sub> (a.u.)	S <sub>r</sub> (a.u.)	D (Å)	H (Å)	t (Å)	HDI	EDI	Λ
<b>m2acr</b>	S <sub>1</sub>	92.91	7.10	0.04	0.18	4.80	2.89	3.09	8.93	6.89	0.16
	T <sub>1</sub>	92.72	7.28	0.04	0.18	4.79	2.86	3.09	9.09	6.90	0.16
<b>m2az1</b>	S <sub>1</sub>	60.24	39.76	0.13	0.36	3.01	2.90	1.40	9.50	6.71	0.55
	T <sub>1</sub>	28.61	71.39	0.51	0.79	1.41	2.93	-0.51	8.02	6.42	0.66
<b>m2az2</b>	S <sub>1</sub>	91.24	8.76	0.06	0.23	4.75	2.88	3.09	8.95	6.80	0.23
	T <sub>1</sub>	44.37	55.64	0.48	0.73	1.49	3.32	-0.68	6.38	6.63	0.52
<b>m2azb</b>	S <sub>1</sub>	93.59	6.41	0.04	0.17	4.87	2.91	3.14	8.25	6.95	0.15
	T <sub>1</sub>	93.46	6.54	0.04	0.18	4.84	2.91	3.11	8.26	6.95	0.15
<b>m2cz</b>	S <sub>1</sub>	94.09	5.91	0.04	0.16	5.22	2.80	3.55	8.86	6.98	0.14
	T <sub>1</sub>	37.66	62.34	0.53	0.76	1.78	3.24	-0.17	6.15	6.81	0.51
<b>m2dpa</b>	S <sub>1</sub>	89.38	10.62	0.08	0.28	4.63	2.91	2.90	9.21	6.78	0.27
	T <sub>1</sub>	52.01	47.99	0.44	0.71	1.72	3.47	-0.49	6.23	6.63	0.47
<b>m2npp</b>	S <sub>1</sub>	94.39	5.62	0.03	0.15	5.26	2.76	3.65	8.53	6.95	0.13
	T <sub>1</sub>	94.06	5.94	0.03	0.16	5.22	2.78	3.61	8.53	6.92	0.13
<b>m2po</b>	S <sub>1</sub>	93.91	6.09	0.03	0.16	5.07	2.73	3.45	9.23	6.90	0.14
	T <sub>1</sub>	93.35	6.65	0.04	0.17	5.02	2.74	3.39	9.23	6.85	0.14
<b>m2pt</b>	S <sub>1</sub>	94.05	5.95	0.03	0.15	5.39	2.73	3.77	7.89	6.91	0.13
	T <sub>1</sub>	93.23	6.77	0.04	0.17	5.32	2.75	3.68	7.91	6.84	0.13
<b>p2acr</b>	S <sub>1</sub>	92.18	7.82	0.05	0.19	3.98	3.00	2.37	7.01	7.04	0.17
	T <sub>1</sub>	90.08	9.92	0.05	0.19	3.96	3.00	2.35	7.03	7.03	0.17
<b>p2az1</b>	S <sub>1</sub>	91.96	8.04	0.06	0.21	4.12	3.01	2.43	6.73	6.90	0.19
	T <sub>1</sub>	91.34	8.66	0.08	0.24	4.04	3.05	2.33	6.67	6.77	0.20
<b>p2az2</b>	S <sub>1</sub>	91.39	8.62	0.07	0.24	3.72	3.06	2.17	6.89	7.02	0.22
	T <sub>1</sub>	91.06	8.94	0.07	0.25	3.70	3.06	2.14	6.90	7.02	0.22
<b>p2azb</b>	S <sub>1</sub>	93.11	6.90	0.05	0.18	4.13	3.07	2.52	6.14	7.03	0.16
	T <sub>1</sub>	93.09	6.91	0.05	0.18	4.13	3.07	2.51	6.14	7.03	0.16
<b>p2cz</b>	S <sub>1</sub>	92.89	7.11	0.04	0.16	4.40	2.95	2.75	6.64	6.98	0.15

<b>p2dpa</b>	T <sub>1</sub>	92.86	7.14	0.04	0.17	4.40	2.95	2.74	6.65	6.98	0.15
	S <sub>1</sub>	90.92	9.08	0.07	0.25	3.86	3.01	2.24	7.54	6.93	0.23
<b>p2npp</b>	T <sub>1</sub>	90.56	9.44	0.07	0.26	3.84	3.01	2.20	7.50	6.93	0.23
	S <sub>1</sub>	93.25	6.75	0.04	0.17	4.32	2.98	2.72	6.42	7.01	0.16
<b>p2po</b>	T <sub>1</sub>	93.24	6.76	0.04	0.17	4.32	2.98	2.72	6.42	7.01	0.16
	S <sub>1</sub>	92.56	7.44	0.05	0.18	4.21	2.91	2.63	7.15	7.00	0.16
<b>p2pt</b>	T <sub>1</sub>	92.53	7.47	0.05	0.18	4.21	2.91	2.63	7.16	7.00	0.16
	S <sub>1</sub>	93.64	6.36	0.04	0.16	4.64	2.94	2.98	6.11	7.03	0.14
	T <sub>1</sub>	93.62	6.38	0.04	0.16	4.64	2.94	2.98	6.12	7.03	0.14

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**Table S3.** Charge transfer parameters of the compounds computed for the T<sub>1</sub> geometry at the M06/def2-TZVP level.

Compound	State	CT (%)	LE (%)	S <sub>m</sub> (a.u.)	S <sub>r</sub> (a.u.)	D (Å)	H (Å)	t (Å)	HDI	EDI	Λ
<b>m2acr</b>	S <sub>1</sub>	89.76	10.24	0.09	0.30	2.55	3.95	0.25	6.65	6.85	0.31
	T <sub>1</sub>	61.54	38.46	0.36	0.63	1.99	3.56	-0.34	5.90	6.85	0.40
<b>m2az1</b>	S <sub>1</sub>	38.91	61.09	0.43	0.73	1.90	3.14	-0.15	8.02	6.48	0.72
	T <sub>1</sub>	23.49	76.51	0.57	0.83	1.00	2.92	-0.85	7.61	6.55	0.71
<b>m2az2</b>	S <sub>1</sub>	41.75	58.25	0.42	0.72	2.03	3.16	-0.16	8.17	6.53	0.71
	T <sub>1</sub>	26.23	73.78	0.57	0.82	1.05	2.98	-0.88	7.57	6.52	0.70
<b>m2azb</b>	S <sub>1</sub>	89.31	10.69	0.09	0.32	3.00	3.84	0.65	6.35	6.92	0.35
	T <sub>1</sub>	31.11	68.89	0.59	0.81	0.81	3.21	-1.38	6.06	6.90	0.58
<b>m2cz</b>	S <sub>1</sub>	79.91	20.09	0.19	0.45	2.47	3.97	0.03	5.94	6.84	0.50
	T <sub>1</sub>	32.06	67.94	0.60	0.81	0.86	3.23	-1.15	6.26	6.81	0.58
<b>m2dpa</b>	S <sub>1</sub>	71.06	28.94	0.26	0.55	1.86	3.84	-0.29	6.55	6.50	0.49
	T <sub>1</sub>	37.83	62.17	0.56	0.79	1.11	3.25	-0.75	6.72	6.57	0.63
<b>m2npp</b>	S <sub>1</sub>	94.36	5.64	0.04	0.19	3.11	4.02	0.84	6.55	6.85	0.18
	T <sub>1</sub>	94.14	5.86	0.05	0.21	2.63	4.17	0.28	6.18	6.81	0.18
<b>m2po</b>	S <sub>1</sub>	91.61	8.39	0.07	0.25	3.94	3.51	1.88	7.99	6.88	0.26
	T <sub>1</sub>	81.13	18.88	0.18	0.45	2.39	3.87	0.01	6.29	6.85	0.28
<b>m2pt</b>	S <sub>1</sub>	93.88	6.12	0.04	0.17	4.89	3.19	3.02	7.70	6.86	0.15
	T <sub>1</sub>	93.19	6.81	0.05	0.19	4.83	3.22	2.94	7.70	6.80	0.15
<b>p2acr</b>	S <sub>1</sub>	91.74	8.26	0.05	0.20	3.92	3.00	2.29	7.10	7.04	0.19
	T <sub>1</sub>	90.08	9.92	0.06	0.21	3.91	3.00	2.27	7.13	7.02	0.19
<b>p2az1</b>	S <sub>1</sub>	91.63	8.37	0.07	0.23	4.07	3.03	2.38	6.61	6.87	0.20
	T <sub>1</sub>	90.51	9.50	0.09	0.27	3.95	3.09	2.21	6.56	6.66	0.21
<b>p2az2</b>	S <sub>1</sub>	86.56	13.45	0.12	0.36	3.28	3.11	1.57	6.95	6.96	0.37
	T <sub>1</sub>	59.17	40.83	0.39	0.68	1.98	3.16	-0.16	6.64	7.07	0.44
<b>p2azb</b>	S <sub>1</sub>	90.93	9.07	0.07	0.25	3.90	3.11	2.21	6.12	7.05	0.25
	T <sub>1</sub>	59.64	40.36	0.38	0.66	2.26	3.26	0.06	5.28	7.00	0.36
<b>p2cz</b>	S <sub>1</sub>	83.26	16.74	0.15	0.42	3.59	3.19	1.60	6.23	6.60	0.39

<b>p2dpa</b>	T <sub>1</sub>	35.80	64.20	0.57	0.84	0.60	3.16	-1.70	6.10	6.64	0.62
	S <sub>1</sub>	64.54	35.46	0.34	0.64	2.34	3.24	0.10	7.61	6.32	0.67
<b>p2npp</b>	T <sub>1</sub>	40.36	59.64	0.54	0.82	0.39	3.19	-1.82	6.22	6.51	0.73
	S <sub>1</sub>	92.45	7.55	0.05	0.21	4.21	2.99	2.58	6.55	6.98	0.20
<b>p2po</b>	T <sub>1</sub>	92.38	7.62	0.06	0.22	4.21	3.00	2.57	6.50	6.98	0.20
	S <sub>1</sub>	91.87	8.13	0.06	0.21	4.12	2.92	2.52	7.14	6.95	0.20
<b>p2pt</b>	T <sub>1</sub>	91.78	8.22	0.06	0.22	4.12	2.92	2.51	7.15	6.95	0.20
	S <sub>1</sub>	93.06	6.94	0.05	0.19	4.53	2.95	2.85	6.50	7.01	0.17
	T <sub>1</sub>	93.04	6.96	0.05	0.19	4.52	2.95	2.85	6.50	7.01	0.17

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**Table S4.** Computed vertical excitation characteristics for **m2cz** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.697	459.8	0.147875	H-1 → L (97.42)
S <sub>2</sub>	2.738	452.9	0.002735	H → L (97.91)
S <sub>3</sub>	3.121	397.3	0.000187	H-2 → L (99.38)
S <sub>4</sub>	3.124	396.9	0.000151	H-3 → L (99.38)
S <sub>5</sub>	3.839	323.0	0.210264	H-4 → L (85.46); H-1 → L+1 (8.77)
S <sub>6</sub>	3.944	314.4	0.205137	H-7 → L (17.06); H → L+1 (73.48)
S <sub>7</sub>	3.954	313.6	0.001784	H-8 → L (92.46)
S <sub>8</sub>	4.054	305.9	0.157817	H-1 → L+3 (37.24); H → L+2 (30.67); H → L+3 (15.64)
S <sub>9</sub>	4.061	305.3	0.009168	H-1 → L+2 (40.48); H → L+2 (10.83); H → L+3 (31.58)
S <sub>10</sub>	4.119	301.0	0.250016	H-4 → L (6.90); H-1 → L+1 (82.64)
T <sub>1</sub>	2.272	545.8	0.000000	H-4 → L (29.65); H → L (64.30)
T <sub>2</sub>	2.483	499.4	0.000000	H-7 → L (5.76); H-1 → L (91.33)
T <sub>3</sub>	2.970	417.5	0.000000	H-4 → L (59.25); H → L (32.19)
T <sub>4</sub>	3.109	398.8	0.000000	H-2 → L (96.84)
T <sub>5</sub>	3.111	398.6	0.000000	H-3 → L (96.62)
T <sub>6</sub>	3.350	370.1	0.000000	H-2 → L+2 (9.48); H-2 → L+3 (69.39)
T <sub>7</sub>	3.352	369.9	0.000000	H-3 → L+2 (68.73); H-3 → L+3 (9.91)
T <sub>8</sub>	3.436	360.9	0.000000	H-1 → L+2 (41.16); H-1 → L+3 (6.95); H → L+2 (34.20)
T <sub>9</sub>	3.437	360.8	0.000000	H-1 → L+3 (33.89); H → L+2 (5.09); H → L+3 (42.92)
T <sub>10</sub>	3.584	346.0	0.000000	H-13 → L (11.75); H-7 → L (58.45); H-4 → L+4 (7.26); H → L+4 (7.50)

**Table S5.** Computed vertical excitation characteristics for **m2dpa** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.570	482.5	0.251942	H → L (95.98)
S <sub>2</sub>	2.692	460.6	0.015744	H-1 → L (97.33)
S <sub>3</sub>	3.780	328.0	0.008307	H-2 → L (30.37); H → L+1 (60.26)
S <sub>4</sub>	3.790	327.2	0.666558	H-1 → L+1 (75.24); H-1 → L+2 (8.32)
S <sub>5</sub>	4.006	309.5	0.273815	H-2 → L (58.03); H → L+1 (20.00); H → L+2 (6.85)
S <sub>6</sub>	4.019	308.5	0.006341	H-10 → L (88.00)
S <sub>7</sub>	4.036	307.2	0.064997	H-1 → L+1 (6.70); H-1 → L+2 (68.74); H → L+5 (13.17)
S <sub>8</sub>	4.073	304.4	0.257747	H → L+1 (5.62); H → L+2 (75.97)
S <sub>9</sub>	4.113	301.5	0.205309	H-3 → L (5.68); H-1 → L+3 (29.40); H-1 → L+4 (16.92); H → L+3 (36.72)
S <sub>10</sub>	4.123	300.8	0.309608	H-1 → L+3 (20.05); H-1 → L+4 (14.44); H → L+4 (55.76)
T <sub>1</sub>	2.077	597.0	0.000000	H-2 → L (11.35); H-1 → L (82.34)
T <sub>2</sub>	2.173	570.6	0.000000	H → L (93.11)
T <sub>3</sub>	3.104	399.5	0.000000	H-2 → L (56.77); H-1 → L (11.43); H → L+1 (16.39)
T <sub>4</sub>	3.378	367.1	0.000000	H-2 → L (12.94); H-1 → L+7 (6.79); H → L+1 (46.94); H → L+2 (16.64)
T <sub>5</sub>	3.400	364.7	0.000000	H-1 → L+3 (9.03); H-1 → L+4 (24.80); H → L+3 (26.87); H → L+4 (14.09)
T <sub>6</sub>	3.403	364.4	0.000000	H-1 → L+3 (33.75); H → L+4 (33.09)
T <sub>7</sub>	3.475	356.8	0.000000	H-1 → L+1 (38.33); H-1 → L+2 (24.65); H → L+7 (13.22)
T <sub>8</sub>	3.508	353.5	0.000000	H-13 → L (11.07); H-9 → L (5.78); H-1 → L+1 (36.03); H-1 → L+2 (17.80); H → L+5 (5.51)
T <sub>9</sub>	3.707	334.5	0.000000	H-1 → L+5 (20.43); H → L+1 (13.40); H → L+2 (43.19); H → L+6 (5.35)
T <sub>10</sub>	3.812	325.3	0.000000	H-13 → L (6.76); H-10 → L (6.20); H-1 → L+6 (30.50); H → L+5 (31.76)

**Table S6.** Computed vertical excitation characteristics for **m2az1** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	3.004	412.8	0.214986	H-1 → L (92.14)
S <sub>2</sub>	3.035	408.6	0.090484	H → L (95.29)
S <sub>3</sub>	3.357	369.4	0.039366	H-1 → L+2 (34.28); H → L+1 (57.47)
S <sub>4</sub>	3.364	368.6	0.017812	H-1 → L+1 (42.00); H → L+2 (49.89)
S <sub>5</sub>	3.585	345.9	0.045004	H-2 → L (98.39)
S <sub>6</sub>	3.591	345.3	0.016858	H-3 → L (98.45)
S <sub>7</sub>	3.776	328.4	0.005883	H-1 → L+2 (54.46); H → L+1 (34.03)
S <sub>8</sub>	3.779	328.1	0.000954	H-1 → L+1 (48.11); H-1 → L+2 (6.02); H → L+2 (40.75)
S <sub>9</sub>	4.015	308.8	0.000380	H-10 → L (74.76); H-9 → L (12.39)
S <sub>10</sub>	4.101	302.4	0.203043	H-3 → L+2 (41.74); H-2 → L+1 (49.92)
T <sub>1</sub>	2.117	585.7	0.000000	H → L (90.09)
T <sub>2</sub>	2.331	532.0	0.000000	H-1 → L (94.18)
T <sub>3</sub>	2.826	438.8	0.000000	H-3 → L+1 (17.05); H-3 → L+2 (14.73); H-2 → L+1 (22.07); H-2 → L+2 (22.31)
T <sub>4</sub>	2.833	437.7	0.000000	H-3 → L+1 (21.42); H-3 → L+2 (21.55); H-2 → L+1 (17.68); H-2 → L+2 (15.15)
T <sub>5</sub>	3.341	371.1	0.000000	H-1 → L+2 (25.47); H → L+1 (56.40)
T <sub>6</sub>	3.352	369.9	0.000000	H-1 → L+1 (37.37); H → L+2 (45.55)
T <sub>7</sub>	3.514	352.9	0.000000	H-12 → L (6.07); H-6 → L (11.39); H-2 → L (56.01); H-1 → L+5 (12.10)
T <sub>8</sub>	3.527	351.6	0.000000	H-13 → L (15.20); H-3 → L (11.63); H-1 → L+2 (9.82); H → L+5 (40.03)
T <sub>9</sub>	3.585	345.9	0.000000	H-3 → L (78.02); H → L+5 (5.50)
T <sub>10</sub>	3.630	341.6	0.000000	H-6 → L (7.85); H-2 → L (23.55); H-1 → L+1 (7.45); H-1 → L+5 (16.73); H → L+2 (12.39)

**Table S7.** Computed vertical excitation characteristics for **m2az2** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.913	425.7	0.269748	H-1 → L (93.76)
S <sub>2</sub>	2.963	418.5	0.093618	H → L (96.62)
S <sub>3</sub>	4.002	309.8	0.002913	H-10 → L (80.41); H-3 → L (8.25)
S <sub>4</sub>	4.048	306.3	0.046619	H-2 → L (82.78); H-1 → L+1 (8.95)
S <sub>5</sub>	4.082	303.8	0.161085	H-3 → L (14.95); H-1 → L+1 (6.52); H-1 → L+3 (14.05); H → L+2 (44.18)
S <sub>6</sub>	4.116	301.3	0.019052	H-10 → L (6.41); H-3 → L (69.08); H → L+2 (7.98)
S <sub>7</sub>	4.117	301.2	0.029699	H-1 → L+2 (36.07); H-1 → L+3 (6.87); H → L+1 (14.43); H → L+3 (30.54)
S <sub>8</sub>	4.199	295.3	0.190960	H → L+1 (49.12); H → L+3 (15.75)
S <sub>9</sub>	4.213	294.3	0.128847	H-6 → L (9.34); H-4 → L (10.48); H-2 → L (8.17); H-1 → L+1 (35.86); H → L+1 (10.27)
S <sub>10</sub>	4.304	288.1	0.018230	H-5 → L (45.79); H-4 → L (43.87)
T <sub>1</sub>	2.086	594.4	0.000000	H → L (89.71)
T <sub>2</sub>	2.265	547.5	0.000000	H-1 → L (94.38)
T <sub>3</sub>	3.469	357.5	0.000000	H-12 → L (11.66); H-8 → L (8.51); H-6 → L (14.46); H-2 → L (9.85); H-1 → L+1 (28.57)
T <sub>4</sub>	3.497	354.6	0.000000	H-14 → L (7.37); H-13 → L (10.00); H → L+1 (43.99); H → L+4 (5.22)
T <sub>5</sub>	3.658	339.0	0.000000	H-1 → L+2 (14.54); H → L+3 (7.87)
T <sub>6</sub>	3.685	336.5	0.000000	H → L+2 (13.98)
T <sub>7</sub>	3.802	326.1	0.000000	H-10 → L (85.23)
T <sub>8</sub>	3.841	322.8	0.000000	H-7 → L+3 (5.50); H-4 → L+6 (5.27)
T <sub>9</sub>	3.851	322.0	0.000000	H-8 → L+2 (6.03); H-8 → L+3 (8.06)
T <sub>10</sub>	3.893	318.5	0.000000	H-1 → L+4 (19.00); H-1 → L+6 (14.33); H-1 → L+10 (20.51)

**Table S8.** Computed vertical excitation characteristics for **m2acr** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.163	573.3	0.001127	H → L (98.57)
S <sub>2</sub>	2.195	564.9	0.000895	H-1 → L (98.55)
S <sub>3</sub>	3.534	350.9	0.000981	H → L+1 (94.35)
S <sub>4</sub>	3.564	347.9	0.000368	H-1 → L+1 (94.06)
S <sub>5</sub>	3.715	333.8	0.300340	H-2 → L (94.94)
S <sub>6</sub>	3.746	331.0	0.002417	H-3 → L (95.16)
S <sub>7</sub>	3.747	330.9	0.002547	H-4 → L (95.23)
S <sub>8</sub>	3.856	321.6	0.066098	H-5 → L (89.00)
S <sub>9</sub>	3.877	319.8	0.000001	H → L+2 (93.32)
S <sub>10</sub>	3.885	319.2	0.013304	H-6 → L (98.66)
T <sub>1</sub>	2.142	578.9	0.000000	H → L (97.87)
T <sub>2</sub>	2.174	570.4	0.000000	H-1 → L (98.08)
T <sub>3</sub>	2.507	494.6	0.000000	H-8 → L (8.29); H-6 → L (5.53); H-2 → L (78.27)
T <sub>4</sub>	3.334	371.9	0.000000	H-9 → L (75.21); H-7 → L (13.84)
T <sub>5</sub>	3.381	366.8	0.000000	H-1 → L+1 (5.33); H-1 → L+5 (17.41); H-1 → L+6 (18.32); H → L+1 (8.19); H → L+5 (12.27); H → L+6 (20.26)
T <sub>6</sub>	3.406	364.1	0.000000	H-1 → L+1 (6.25); H-1 → L+5 (15.77); H-1 → L+6 (15.81); H → L+1 (7.51); H → L+5 (24.21); H → L+6 (12.45)
T <sub>7</sub>	3.525	351.8	0.000000	H → L+1 (74.60); H → L+6 (6.33)
T <sub>8</sub>	3.548	349.5	0.000000	H-1 → L+1 (74.33)
T <sub>9</sub>	3.585	345.9	0.000000	H-1 → L+3 (9.68); H-1 → L+4 (34.94); H → L+3 (14.16); H → L+4 (27.29)
T <sub>10</sub>	3.599	344.5	0.000000	H-1 → L+3 (29.83); H-1 → L+4 (8.52); H → L+3 (31.06); H → L+4 (13.65)

**Table S9.** Computed vertical excitation characteristics for **m2po** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.987	624.1	0.001177	H → L (98.30)
S <sub>2</sub>	2.012	616.3	0.000037	H-1 → L (98.30)
S <sub>3</sub>	3.301	375.6	0.001023	H → L+1 (95.59)
S <sub>4</sub>	3.324	373.0	0.005295	H-1 → L+1 (95.54)
S <sub>5</sub>	3.446	359.8	0.004761	H-2 → L (97.13)
S <sub>6</sub>	3.453	359.1	0.001684	H-3 → L (97.10)
S <sub>7</sub>	3.671	337.8	0.000437	H → L+2 (84.13)
S <sub>8</sub>	3.693	335.8	0.001658	H-1 → L+2 (82.88); H-1 → L+4 (5.47); H → L+3 (5.61)
S <sub>9</sub>	3.802	326.1	0.318876	H-4 → L (94.05)
S <sub>10</sub>	3.860	321.2	0.045903	H-1 → L+3 (15.53); H → L+2 (9.47); H → L+3 (38.58); H → L+4 (26.90)
T <sub>1</sub>	1.968	630.1	0.000000	H → L (97.94)
T <sub>2</sub>	1.991	622.8	0.000000	H-1 → L (97.80)
T <sub>3</sub>	2.556	485.1	0.000000	H-4 → L (88.86)
T <sub>4</sub>	3.090	401.3	0.000000	H-1 → L+3 (13.16); H → L+1 (5.65); H → L+3 (39.44); H → L+4 (21.21)
T <sub>5</sub>	3.098	400.3	0.000000	H-1 → L+1 (5.78); H-1 → L+3 (19.56); H-1 → L+4 (39.89); H → L+3 (8.37); H → L+4 (9.09)
T <sub>6</sub>	3.278	378.3	0.000000	H → L+1 (84.10)
T <sub>7</sub>	3.300	375.8	0.000000	H-1 → L+1 (83.27)
T <sub>8</sub>	3.363	368.7	0.000000	H-9 → L (51.58); H-5 → L (23.92); H-2 → L (8.43)
T <sub>9</sub>	3.431	361.4	0.000000	H-3 → L (27.65); H-2 → L (63.43)
T <sub>10</sub>	3.436	360.9	0.000000	H-3 → L (66.70); H-2 → L (23.31)

**Table S10.** Computed vertical excitation characteristics for **m2pt** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.138	580.0	0.002188	H → L (97.89)
S <sub>2</sub>	2.190	566.2	0.000031	H-1 → L (97.94)
S <sub>3</sub>	3.280	378.0	0.006979	H-2 → L (97.53)
S <sub>4</sub>	3.299	375.9	0.000375	H-3 → L (97.68)
S <sub>5</sub>	3.469	357.5	0.000621	H-1 → L+1 (71.63); H-1 → L+4 (10.32); H → L+1 (13.95)
S <sub>6</sub>	3.522	352.1	0.001303	H-1 → L+1 (13.12); H → L+1 (78.01)
S <sub>7</sub>	3.594	345.0	0.000052	H → L+2 (26.45); H → L+3 (61.89)
S <sub>8</sub>	3.735	332.0	0.002416	H-1 → L+1 (9.47); H-1 → L+2 (17.55); H-1 → L+3 (7.60); H-1 → L+4 (55.95)
S <sub>9</sub>	3.754	330.3	0.305121	H-4 → L (93.65)
S <sub>10</sub>	3.885	319.2	0.013627	H → L+2 (63.92); H → L+3 (22.22)
T <sub>1</sub>	2.118	585.5	0.000000	H → L (97.15)
T <sub>2</sub>	2.178	569.3	0.000000	H-1 → L (97.53)
T <sub>3</sub>	2.518	492.5	0.000000	H-4 → L (87.75)
T <sub>4</sub>	3.101	399.9	0.000000	H → L+2 (10.72); H → L+3 (68.81)
T <sub>5</sub>	3.111	398.6	0.000000	H-1 → L+1 (21.51); H-1 → L+3 (5.39); H-1 → L+4 (56.60)
T <sub>6</sub>	3.256	380.8	0.000000	H-2 → L (88.93)
T <sub>7</sub>	3.289	377.0	0.000000	H-3 → L (96.02)
T <sub>8</sub>	3.378	367.1	0.000000	H-9 → L (56.86); H-7 → L (17.88); H-5 → L (8.99); H-2 → L (5.62)
T <sub>9</sub>	3.478	356.5	0.000000	H → L+1 (38.25); H → L+6 (48.84)
T <sub>10</sub>	3.521	352.2	0.000000	H-1 → L+1 (6.16); H-1 → L+5 (36.81); H → L+1 (20.68); H → L+6 (13.46)

**Table S11.** Computed vertical excitation characteristics for **m2npp** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.543	803.6	0.001300	H → L (98.34)
S <sub>2</sub>	1.569	790.3	0.000083	H-1 → L (98.36)
S <sub>3</sub>	2.900	427.6	0.001168	H → L+1 (93.33)
S <sub>4</sub>	2.921	424.5	0.007061	H-1 → L+1 (93.14)
S <sub>5</sub>	3.148	393.9	0.001020	H-2 → L (74.67); H → L+2 (15.15)
S <sub>6</sub>	3.155	393.0	0.000041	H-3 → L (54.88); H-2 → L (11.65); H → L+2 (14.27); H → L+3 (8.14)
S <sub>7</sub>	3.163	392.0	0.001195	H-3 → L (27.43); H-1 → L+3 (5.17); H → L+2 (8.11); H → L+3 (33.22); H → L+4 (8.25)
S <sub>8</sub>	3.194	388.2	0.002942	H-1 → L+2 (23.27); H-1 → L+3 (9.78); H-1 → L+4 (41.77); H-1 → L+8 (5.17); H → L+4 (5.18)
S <sub>9</sub>	3.280	378.0	0.013832	H-3 → L (5.96); H-2 → L (6.11); H-1 → L+3 (5.32); H → L+2 (52.80); H → L+3 (17.30); H → L+4 (8.32)
S <sub>10</sub>	3.299	375.9	0.041478	H-1 → L+2 (59.25); H-1 → L+4 (21.00)
T <sub>1</sub>	1.526	812.6	0.000000	H → L (98.13)
T <sub>2</sub>	1.553	798.5	0.000000	H-1 → L (98.18)
T <sub>3</sub>	2.531	489.9	0.000000	H-4 → L (84.93)
T <sub>4</sub>	2.667	464.9	0.000000	H → L+1 (6.40); H → L+3 (31.86); H → L+4 (6.98); H → L+7 (19.15); H → L+8 (12.04)
T <sub>5</sub>	2.700	459.3	0.000000	H-1 → L+1 (12.09); H-1 → L+3 (6.78); H-1 → L+4 (27.67); H-1 → L+7 (12.57); H-1 → L+8 (18.64)
T <sub>6</sub>	2.878	430.9	0.000000	H → L+1 (80.18); H → L+3 (5.19)
T <sub>7</sub>	2.903	427.1	0.000000	H-1 → L+1 (74.45); H-1 → L+4 (10.92)
T <sub>8</sub>	3.088	401.6	0.000000	H → L+2 (26.26); H → L+3 (12.36); H → L+7 (12.36); H → L+8 (5.69); H → L+9 (6.76); H → L+11 (9.34)
T <sub>9</sub>	3.130	396.2	0.000000	H-2 → L (59.25); H → L+2 (7.53)
T <sub>10</sub>	3.138	395.2	0.000000	H-3 → L (26.35); H-2 → L (24.96); H-1 → L+2 (15.44); H-1 → L+4 (6.17); H-1 → L+10 (5.78)

**Table S12.** Computed vertical excitation characteristics for **m2azb** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.546	487.0	0.003103	H → L (98.47)
S <sub>2</sub>	2.574	481.7	0.000496	H-1 → L (98.44)
S <sub>3</sub>	3.158	392.7	0.000153	H-2 → L (99.59)
S <sub>4</sub>	3.161	392.3	0.000152	H-3 → L (99.52)
S <sub>5</sub>	3.406	364.1	0.000001	H-4 → L (99.75)
S <sub>6</sub>	3.408	363.8	0.000005	H-5 → L (99.73)
S <sub>7</sub>	3.647	340.0	0.454175	H-1 → L+1 (10.10); H-1 → L+2 (32.06); H → L+1 (46.60)
S <sub>8</sub>	3.670	337.9	0.305559	H-6 → L (12.54); H-1 → L+1 (27.08); H-1 → L+2 (9.60); H → L+2 (39.36)
S <sub>9</sub>	3.713	334.0	0.027299	H-8 → L (5.99); H-6 → L (80.54)
S <sub>10</sub>	3.715	333.8	0.003214	H-7 → L (96.42)
T <sub>1</sub>	2.489	498.2	0.000000	H-10 → L (8.04); H-8 → L (32.44); H-6 → L (36.07); H → L (16.33)
T <sub>2</sub>	2.535	489.2	0.000000	H-8 → L (6.28); H-6 → L (7.01); H → L (81.41)
T <sub>3</sub>	2.555	485.3	0.000000	H-1 → L (96.35)
T <sub>4</sub>	2.918	424.9	0.000000	H-1 → L+1 (32.58); H-1 → L+2 (14.23); H → L+1 (34.14); H → L+2 (14.77)
T <sub>5</sub>	2.950	420.3	0.000000	H-1 → L+1 (14.45); H-1 → L+2 (32.78); H → L+1 (14.88); H → L+2 (34.09)
T <sub>6</sub>	3.157	392.8	0.000000	H-3 → L (11.10); H-2 → L (87.88)
T <sub>7</sub>	3.160	392.4	0.000000	H-3 → L (88.00); H-2 → L (11.33)
T <sub>8</sub>	3.360	369.0	0.000000	H-13 → L (80.43); H-9 → L (9.20)
T <sub>9</sub>	3.406	364.1	0.000000	H-4 → L (99.63)
T <sub>10</sub>	3.408	363.8	0.000000	H-5 → L (99.64)

**Table S13.** Computed vertical excitation characteristics for **p2cz** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.316	535.4	0.005208	H → L (98.53)
S <sub>2</sub>	2.679	462.9	0.096702	H-1 → L (96.61)
S <sub>3</sub>	2.863	433.1	0.124806	H-2 → L (96.40)
S <sub>4</sub>	3.067	404.3	0.000827	H-3 → L (99.21)
S <sub>5</sub>	3.683	336.7	0.243422	H-4 → L (94.68)
S <sub>6</sub>	3.847	322.3	0.020673	H → L+2 (90.27)
S <sub>7</sub>	3.848	322.2	0.016195	H → L+1 (95.24)
S <sub>8</sub>	3.885	319.2	0.069839	H-5 → L (90.48)
S <sub>9</sub>	3.895	318.4	0.003253	H-8 → L (68.52); H-7 → L (9.36); H-6 → L (6.45)
S <sub>10</sub>	3.919	316.4	0.007771	H-8 → L (20.72); H-7 → L (27.24); H-6 → L (15.06); H-2 → L+1 (11.87); H-1 → L+1 (11.70)
T <sub>1</sub>	2.247	551.8	0.000000	H-5 → L (5.49); H-4 → L (12.45); H-2 → L (21.30); H-1 → L (15.98); H → L (40.80)
T <sub>2</sub>	2.253	550.4	0.000000	H-4 → L (8.93); H-2 → L (15.37); H-1 → L (11.67); H → L (56.32)
T <sub>3</sub>	2.724	455.2	0.000000	H-4 → L (6.63); H-2 → L (21.29); H-1 → L (69.79)
T <sub>4</sub>	3.021	410.5	0.000000	H-5 → L (11.71); H-4 → L (42.48); H-2 → L (39.46)
T <sub>5</sub>	3.047	407.0	0.000000	H-3 → L (97.84)
T <sub>6</sub>	3.286	377.4	0.000000	H-3 → L+3 (15.17); H-3 → L+4 (11.77); H-2 → L+2 (16.53); H-1 → L+2 (32.95)
T <sub>7</sub>	3.295	376.3	0.000000	H-3 → L+2 (24.46); H-2 → L+3 (10.58); H-2 → L+4 (7.54); H-1 → L+3 (7.89); H → L+2 (25.59)
T <sub>8</sub>	3.359	369.2	0.000000	H-3 → L+2 (11.38); H-1 → L+3 (16.95); H-1 → L+4 (11.22); H → L+2 (48.64)
T <sub>9</sub>	3.400	364.7	0.000000	H-7 → L (67.91); H-6 → L (17.99)
T <sub>10</sub>	3.421	362.5	0.000000	H-2 → L+2 (14.31); H-1 → L+2 (15.23); H → L+3 (35.78); H → L+4 (24.42)

**Table S14.** Computed vertical excitation characteristics for **p2dpa** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.656	466.9	0.044787	H-1 → L (96.53)
S <sub>2</sub>	2.694	460.3	0.476830	H → L (95.68)
S <sub>3</sub>	3.704	334.8	0.021295	H-7 → L (6.76); H-4 → L (15.98); H → L+1 (69.60)
S <sub>4</sub>	3.919	316.4	0.047743	H-2 → L (69.26); H-1 → L+1 (20.31)
S <sub>5</sub>	3.973	312.1	0.022158	H-2 → L (22.81); H-1 → L+1 (65.36); H → L+3 (6.22)
S <sub>6</sub>	3.995	310.4	0.002220	H-10 → L (29.90); H-8 → L (57.37)
S <sub>7</sub>	4.025	308.1	0.057964	H → L+2 (90.23)
S <sub>8</sub>	4.104	302.1	0.014343	H-3 → L (15.85); H-1 → L+1 (6.29); H-1 → L+2 (9.05); H-1 → L+4 (5.85); H → L+3 (56.44)
S <sub>9</sub>	4.132	300.1	0.149071	H-4 → L (53.35); H-1 → L+3 (11.34); H → L+1 (16.18)
S <sub>10</sub>	4.138	299.7	0.003995	H-3 → L (75.06); H → L+3 (15.18)
T <sub>1</sub>	2.032	610.2	0.000000	H-2 → L (7.94); H → L (87.15)
T <sub>2</sub>	2.427	510.9	0.000000	H-1 → L (92.41)
T <sub>3</sub>	3.254	381.1	0.000000	H-2 → L (75.60); H → L (8.92)
T <sub>4</sub>	3.434	361.1	0.000000	H-7 → L (5.35); H-4 → L (10.27); H-1 → L+3 (20.00); H-1 → L+5 (11.75); H → L+2 (7.90); H → L+4 (21.47)
T <sub>5</sub>	3.442	360.3	0.000000	H-7 → L (12.52); H-4 → L (18.90); H-1 → L+3 (5.22); H → L+1 (40.21); H → L+2 (6.18)
T <sub>6</sub>	3.463	358.1	0.000000	H-1 → L+4 (28.45); H → L+3 (26.94); H → L+5 (12.75)
T <sub>7</sub>	3.538	350.5	0.000000	H-7 → L (15.26); H-4 → L (18.99); H-1 → L+5 (5.02); H → L+1 (44.23)
T <sub>8</sub>	3.624	342.2	0.000000	H → L+2 (57.14); H → L+4 (5.40)
T <sub>9</sub>	3.655	339.3	0.000000	H-1 → L+1 (51.96); H → L+3 (9.91); H → L+5 (13.56)
T <sub>10</sub>	3.764	329.4	0.000000	H-1 → L+1 (18.29); H-1 → L+2 (37.06); H-1 → L+10 (6.26)

**Table S15.** Computed vertical excitation characteristics for **p2az1** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.755	706.6	0.000028	H → L (97.23)
S <sub>2</sub>	2.217	559.3	0.001009	H-1 → L (95.77)
S <sub>3</sub>	2.563	483.8	0.005251	H → L+1 (96.10)
S <sub>4</sub>	2.937	422.2	0.000233	H-1 → L+2 (9.25); H → L+2 (87.94)
S <sub>5</sub>	3.141	394.8	0.000008	H-2 → L (97.40)
S <sub>6</sub>	3.200	387.5	0.001671	H-3 → L (16.09); H-1 → L+1 (46.97); H-1 → L+2 (26.22); H → L+2 (5.97)
S <sub>7</sub>	3.258	380.6	0.026017	H-3 → L (76.65); H-1 → L+1 (7.09); H-1 → L+2 (8.90)
S <sub>8</sub>	3.292	376.7	0.065016	H-1 → L+1 (40.37); H-1 → L+2 (49.86)
S <sub>9</sub>	3.374	367.5	0.000099	H → L+3 (95.00)
S <sub>10</sub>	3.488	355.5	0.276928	H-5 → L (9.24); H-4 → L (86.59)
T <sub>1</sub>	1.741	712.2	0.000000	H → L (94.84)
T <sub>2</sub>	2.021	613.6	0.000000	H → L+1 (78.27)
T <sub>3</sub>	2.190	566.2	0.000000	H-1 → L (83.57); H-1 → L+2 (6.47)
T <sub>4</sub>	2.344	529.0	0.000000	H-5 → L (8.90); H-4 → L (79.25)
T <sub>5</sub>	2.484	499.2	0.000000	H-1 → L (8.71); H-1 → L+2 (62.81); H → L+2 (9.90)
T <sub>6</sub>	2.934	422.6	0.000000	H-1 → L+2 (7.39); H → L+2 (80.97)
T <sub>7</sub>	3.072	403.6	0.000000	H-2 → L (24.00); H-2 → L+1 (10.43); H-1 → L+1 (41.95); H → L+1 (7.83)
T <sub>8</sub>	3.139	395.0	0.000000	H-2 → L (71.19); H-1 → L+1 (20.90)
T <sub>9</sub>	3.231	383.8	0.000000	H-3 → L (83.66); H-1 → L+1 (5.27)
T <sub>10</sub>	3.326	372.8	0.000000	H-9 → L (20.15); H-8 → L (44.27); H-7 → L (11.16); H-5 → L (13.85)

**Table S16.** Computed vertical excitation characteristics for **p2az2** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.939	639.5	0.004047	H → L (98.58)
S <sub>2</sub>	2.419	512.6	0.121716	H-1 → L (97.56)
S <sub>3</sub>	3.351	370.0	0.005950	H-2 → L (98.21)
S <sub>4</sub>	3.426	361.9	0.065576	H-3 → L (35.87); H → L+1 (62.04)
S <sub>5</sub>	3.439	360.6	0.032895	H-3 → L (59.97); H → L+1 (36.60)
S <sub>6</sub>	3.630	341.6	0.025012	H-4 → L (29.23); H → L+2 (66.85)
S <sub>7</sub>	3.709	334.3	0.147762	H-5 → L (10.68); H-4 → L (55.91); H → L+2 (24.23)
S <sub>8</sub>	3.720	333.3	0.003534	H-9 → L (6.55); H-8 → L (24.29); H-6 → L (13.72); H-1 → L+1 (43.67)
S <sub>9</sub>	3.754	330.3	0.083665	H-5 → L (83.39); H-4 → L (6.60); H → L+2 (5.51)
S <sub>10</sub>	3.859	321.3	0.011065	H-6 → L (80.18); H-1 → L+1 (10.92)
T <sub>1</sub>	1.901	652.3	0.000000	H → L (97.94)
T <sub>2</sub>	2.053	604.0	0.000000	H-4 → L (13.82); H-3 → L (15.35); H-1 → L (65.21)
T <sub>3</sub>	2.659	466.3	0.000000	H-4 → L (31.41); H-3 → L (30.44); H-1 → L (32.16)
T <sub>4</sub>	3.231	383.8	0.000000	H-9 → L (15.64); H-8 → L (20.50); H-6 → L (5.77); H-2 → L (51.32)
T <sub>5</sub>	3.263	380.0	0.000000	H-1 → L+4 (17.90); H → L+2 (9.67); H → L+3 (39.77); H → L+6 (7.47)
T <sub>6</sub>	3.290	376.9	0.000000	H-1 → L+3 (16.76); H → L+4 (49.82)
T <sub>7</sub>	3.340	371.3	0.000000	H → L+1 (93.60)
T <sub>8</sub>	3.435	361.0	0.000000	H-9 → L (17.15); H-8 → L (26.69); H-2 → L (44.88)
T <sub>9</sub>	3.478	356.5	0.000000	H-13 → L (29.19); H-6 → L (5.69); H-4 → L+2 (12.63); H-3 → L+2 (12.87); H-1 → L+2 (17.76)
T <sub>10</sub>	3.488	355.5	0.000000	H-4 → L (41.92); H-3 → L (46.41)

**Table S17.** Computed vertical excitation characteristics for **p2acr** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.862	666.0	0.000146	H → L (98.70)
S <sub>2</sub>	2.287	542.2	0.003268	H-1 → L (98.15)
S <sub>3</sub>	3.342	371.0	0.001617	H → L+1 (99.09)
S <sub>4</sub>	3.524	351.9	0.230316	H-2 → L (94.91)
S <sub>5</sub>	3.547	349.6	0.000366	H-3 → L (98.59)
S <sub>6</sub>	3.637	340.9	0.001270	H-4 → L (8.17); H → L+2 (89.42)
S <sub>7</sub>	3.695	335.6	0.013411	H-4 → L (88.36); H → L+2 (8.12)
S <sub>8</sub>	3.726	332.8	0.003862	H-5 → L (94.04)
S <sub>9</sub>	3.763	329.5	0.003050	H-1 → L+1 (93.43)
S <sub>10</sub>	3.773	328.7	0.165100	H-6 C L (93.90)
T <sub>1</sub>	1.673	741.2	0.000000	
T <sub>2</sub>	1.857	667.7	0.000000	H → L 98.6%
T <sub>3</sub>	2.254	550.1	0.000000	H-1 → L 83.3%; H-2 → L 10.0%
T <sub>4</sub>	2.400	516.7	0.000000	H-2 → L 55.5%; H-1 → L 14.8%; H-6 → L 10.1%; H-7 → L 8.6%; H-4 → L 5.0%
T <sub>5</sub>	3.235	383.3	0.000000	H → L+1 79.3%; H → L+6 5.7%
T <sub>6</sub>	3.298	376.0	0.000000	H-1 → L+3 28.1%
T <sub>7</sub>	3.343	370.9	0.000000	H-9 → L 48.7%; H-8 → L 34.7%; H-5 → L 5.6%
T <sub>8</sub>	3.372	367.7	0.000000	H → L+5 41.0%; H-1 → L+4 11.6%; H-1 → L+6 11.2%, H → L+3 10.2%; H-1 → L+1 9.3%
T <sub>9</sub>	3.443	360.2	0.000000	H → L+4 41.5%; H-1 → L+5 19.0%; H → L+1 11.6%; H → L+6 7.0%
T <sub>10</sub>	3.534	350.9	0.000000	H → L+3 56.3%; H-1 → L+4 10.3%; H → L+5 7.7%

**Table S18.** Computed vertical excitation characteristics for **p2po** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.560	794.9	0.001833	H → L (98.64)
S <sub>2</sub>	2.106	588.8	0.066732	H-1 → L (98.17)
S <sub>3</sub>	3.061	405.1	0.003739	H → L+1 (98.36)
S <sub>4</sub>	3.200	387.5	0.000006	H-2 → L (98.87)
S <sub>5</sub>	3.305	375.2	0.024279	H-3 → L (10.61); H → L+2 (84.66)
S <sub>6</sub>	3.396	365.1	0.003760	H-3 → L (86.32); H → L+2 (10.83)
S <sub>7</sub>	3.558	348.5	0.001775	H-1 → L+1 (89.61)
S <sub>8</sub>	3.576	346.8	0.002956	H → L+3 (91.81)
S <sub>9</sub>	3.680	337.0	0.243107	H-4 → L (89.79)
S <sub>10</sub>	3.739	331.6	0.027938	H-1 → L+2 (21.00); H-1 → L+3 (6.04); H → L+4 (48.67); H → L+5 (14.61)
T <sub>1</sub>	1.534	808.3	0.000000	H → L (98.39)
T <sub>2</sub>	1.991	622.8	0.000000	H-1 → L (89.03)
T <sub>3</sub>	2.519	492.3	0.000000	H-5 → L (15.84); H-4 → L (59.99); H-3 → L (8.51); H-1 → L (8.79)
T <sub>4</sub>	2.891	428.9	0.000000	H-1 → L+5 (7.25); H → L+1 (50.29); H → L+3 (28.75)
T <sub>5</sub>	3.064	404.7	0.000000	H-1 → L+1 (8.17); H-1 → L+3 (24.35); H → L+4 (15.39); H → L+5 (31.91)
T <sub>6</sub>	3.087	401.7	0.000000	H → L+1 (40.30); H → L+2 (5.57); H → L+3 (36.64)
T <sub>7</sub>	3.172	390.9	0.000000	H-2 → L (93.83)
T <sub>8</sub>	3.280	378.0	0.000000	H-3 → L (7.89); H → L+2 (71.24); H → L+3 (8.53)
T <sub>9</sub>	3.351	370.0	0.000000	H-1 → L+1 (5.35); H-1 → L+8 (10.16); H → L+4 (51.23); H → L+5 (18.48); H → L+7 (5.86)
T <sub>10</sub>	3.361	368.9	0.000000	H-9 → L (30.54); H-8 → L (25.06); H-7 → L (27.08)

**Table S19.** Computed vertical excitation characteristics for **p2pt** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.569	790.3	0.000060	H → L (98.30)
S <sub>2</sub>	1.867	664.2	0.002705	H-1 → L (98.30)
S <sub>3</sub>	2.962	418.6	0.000331	H-2 → L (98.21)
S <sub>4</sub>	2.977	416.5	0.000303	H → L+1 (95.05)
S <sub>5</sub>	3.169	391.3	0.002766	H-3 → L (88.39); H → L+2 (8.64)
S <sub>6</sub>	3.226	384.4	0.004175	H-1 → L+1 (67.93); H-1 → L+3 (7.79); H → L+4 (21.91)
S <sub>7</sub>	3.321	373.4	0.000304	H-1 → L+4 (8.52); H → L+2 (39.33); H → L+3 (42.92)
S <sub>8</sub>	3.387	366.1	0.000002	H-3 → L (5.04); H-1 → L+4 (5.77); H → L+2 (49.73); H → L+3 (35.89)
S <sub>9</sub>	3.412	363.4	0.020054	H-1 → L+1 (30.20); H-1 → L+3 (11.34); H → L+4 (52.11)
S <sub>10</sub>	3.603	344.2	0.004674	H → L+5 (91.93)
T <sub>1</sub>	1.565	792.3	0.000000	H → L (98.24)
T <sub>2</sub>	1.858	667.4	0.000000	H-1 → L (97.80)
T <sub>3</sub>	2.382	520.6	0.000000	H-5 → L (6.13); H-4 → L (83.54)
T <sub>4</sub>	2.722	455.5	0.000000	H-1 → L+4 (19.81); H → L+1 (40.41); H → L+3 (31.25)
T <sub>5</sub>	2.773	447.2	0.000000	H-1 → L+1 (18.18); H-1 → L+3 (26.73); H → L+4 (44.68)
T <sub>6</sub>	2.957	419.3	0.000000	H-2 → L (97.82)
T <sub>7</sub>	3.038	408.2	0.000000	H-1 → L+4 (5.60); H → L+1 (50.36); H → L+3 (30.34)
T <sub>8</sub>	3.167	391.5	0.000000	H-3 → L (84.82); H → L+2 (9.04)
T <sub>9</sub>	3.183	389.6	0.000000	H-1 → L+8 (10.22); H → L+5 (70.54)
T <sub>10</sub>	3.244	382.2	0.000000	H-1 → L+1 (59.11); H → L+4 (10.51); H → L+6 (13.42)

**Table S20.** Computed vertical excitation characteristics for **p2npp** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	1.210	1024.8	0.000231	H → L (98.61)
S <sub>2</sub>	1.522	814.7	0.009407	H-1 → L (98.52)
S <sub>3</sub>	2.675	463.6	0.000815	H → L+1 (97.72)
S <sub>4</sub>	2.899	427.7	0.000049	H-2 → L (97.94)
S <sub>5</sub>	2.949	420.5	0.004325	H-3 → L (8.23); H → L+2 (81.90)
S <sub>6</sub>	2.958	419.2	0.003037	H-1 → L+1 (65.74); H → L+2 (5.39); H → L+3 (18.38)
S <sub>7</sub>	3.051	406.4	0.038633	H-1 → L+1 (26.97); H → L+3 (64.21)
S <sub>8</sub>	3.102	399.7	0.001920	H-3 → L (11.12); H-1 → L+3 (23.26); H → L+4 (16.77); H → L+5 (33.49)
S <sub>9</sub>	3.124	396.9	0.003121	H-3 → L (77.78); H → L+2 (10.56)
S <sub>10</sub>	3.223	384.7	0.005020	H-1 → L+5 (6.32); H-1 → L+6 (7.09); H → L+4 (53.66); H → L+5 (23.26)
T <sub>1</sub>	1.203	1030.8	0.000000	H → L (98.55)
T <sub>2</sub>	1.507	822.8	0.000000	H-1 → L (98.11)
T <sub>3</sub>	2.345	528.8	0.000000	H-5 → L (22.82); H-4 → L (64.02); H-3 → L (5.81)
T <sub>4</sub>	2.500	496.0	0.000000	H-1 → L+3 (7.68); H-1 → L+7 (8.88); H → L+1 (48.24); H → L+5 (9.58); H → L+8 (9.03)
T <sub>5</sub>	2.558	484.8	0.000000	H-1 → L+1 (12.24); H-1 → L+5 (9.42); H-1 → L+8 (8.60); H → L+3 (30.73); H → L+7 (15.14); H → L+9 (5.64)
T <sub>6</sub>	2.723	455.4	0.000000	H-1 → L+3 (12.24); H → L+1 (42.66); H → L+4 (8.08); H → L+5 (17.00)
T <sub>7</sub>	2.878	430.9	0.000000	H-1 → L+1 (51.64); H → L+3 (19.78); H → L+10 (7.03)
T <sub>8</sub>	2.894	428.5	0.000000	H-2 → L (97.67)
T <sub>9</sub>	2.944	421.2	0.000000	H-3 → L (7.74); H → L+2 (84.82)
T <sub>10</sub>	3.098	400.3	0.000000	H-3 → L (5.88); H-1 → L+13 (6.18); H → L+4 (19.28); H → L+8 (14.80); H → L+9 (8.19); H → L+10 (5.89)

**Table S21.** Computed vertical excitation characteristics for **p2azb** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.143	578.6	0.000054	H → L (98.79)
S <sub>2</sub>	2.695	460.1	0.003454	H-3 → L (10.78); H-2 → L (52.85); H-1 → L (32.89)
S <sub>3</sub>	3.056	405.8	0.001034	H-2 → L (32.84); H-1 → L (65.27)
S <sub>4</sub>	3.101	399.9	0.000056	H-3 → L (86.45); H-2 → L (11.87)
S <sub>5</sub>	3.225	384.5	0.048477	H → L+1 (96.94)
S <sub>6</sub>	3.250	381.5	0.000121	H-4 → L (97.01)
S <sub>7</sub>	3.330	372.4	0.000021	H-5 → L (98.92)
S <sub>8</sub>	3.466	357.8	0.334980	H-7 → L (58.16); H-6 → L (24.10); H → L+2 (13.42)
S <sub>9</sub>	3.476	356.7	0.065092	H-7 → L (17.34); H-6 → L (74.00); H → L+2 (6.61)
S <sub>10</sub>	3.545	349.8	0.051688	H-9 → L (5.68); H-7 → L (16.32); H → L+2 (67.52); H → L+3 (5.96)
T <sub>1</sub>	2.139	579.7	0.000000	H → L (98.74)
T <sub>2</sub>	2.337	530.6	0.000000	H-9 → L (31.82); H-7 → L (56.33)
T <sub>3</sub>	2.502	495.6	0.000000	H-2 → L+1 (14.56); H-1 → L+1 (12.05); H → L+2 (6.25)
T <sub>4</sub>	2.699	459.4	0.000000	H-3 → L (10.47); H-2 → L (51.42); H-1 → L (30.79)
T <sub>5</sub>	2.719	456.1	0.000000	H-2 → L+2 (6.47); H → L+1 (77.97)
T <sub>6</sub>	3.001	413.2	0.000000	H → L+2 (68.16)
T <sub>7</sub>	3.056	405.8	0.000000	H-2 → L (32.73); H-1 → L (65.38)
T <sub>8</sub>	3.100	400.0	0.000000	H-3 → L (86.44); H-2 → L (11.75)
T <sub>9</sub>	3.250	381.5	0.000000	H-4 → L (96.97)
T <sub>10</sub>	3.328	372.6	0.000000	H-13 → L (10.99); H-11 → L (6.51); H-5 → L (75.22)

**Table S22.** Computed vertical excitation characteristics for **mcz** at M06/def2-TZVP level.

State	Energy (eV)	Wavelength (nm)	fosc	Assignment
S <sub>1</sub>	2.789	444.6	0.058241	H → L (97.80)
S <sub>2</sub>	3.206	386.8	0.000264	H-1 → L (99.38)
S <sub>3</sub>	3.829	323.8	0.289803	H-2 → L (88.09)
S <sub>4</sub>	3.991	310.7	0.000758	H-5 → L (93.18)
S <sub>5</sub>	4.039	307.0	0.044632	H-4 → L (41.14); H-2 → L (5.07); H-2 → L+2 (7.21); H → L+1 (29.69); H → L+2 (11.56)
S <sub>6</sub>	4.059	305.5	0.107390	H-4 → L (5.95); H-1 → L+4 (6.69); H → L+1 (48.43); H → L+2 (33.92)
S <sub>7</sub>	4.208	294.7	0.287378	H-4 → L (32.62); H → L+1 (10.14); H → L+2 (41.42)
S <sub>8</sub>	4.266	290.7	0.039514	H-3 → L (92.66)
S <sub>9</sub>	4.372	283.6	0.037762	H-8 → L (59.37); H-6 → L (22.85); H-5 → L+3 (5.25)
S <sub>10</sub>	4.458	278.2	0.065984	H-1 → L+1 (19.92); H → L+3 (70.08)
T <sub>1</sub>	2.378	521.4	0.000000	H-2 → L (35.65); H → L (58.55)
T <sub>2</sub>	2.831	438.0	0.000000	H-4 → L (5.54); H-2 → L (55.03); H → L (34.17)
T <sub>3</sub>	3.193	388.3	0.000000	H-1 → L (96.06)
T <sub>4</sub>	3.363	368.7	0.000000	H-1 → L+1 (60.75); H-1 → L+2 (18.10); H → L+4 (6.04)
T <sub>5</sub>	3.438	360.7	0.000000	H → L+1 (79.42); H → L+2 (10.98)
T <sub>6</sub>	3.548	349.5	0.000000	H-4 → L (74.20)
T <sub>7</sub>	3.800	326.3	0.000000	H-5 → L (15.28); H → L+1 (5.38); H → L+2 (47.78)
T <sub>8</sub>	3.805	325.9	0.000000	H-5 → L (74.49); H → L+2 (9.87)
T <sub>9</sub>	3.876	319.9	0.000000	H-11 → L (22.52); H-6 → L (5.32); H-4 → L (11.59); H-2 → L+3 (25.04); H → L+2 (13.83); H → L+3 (9.30)
T <sub>10</sub>	4.026	308.0	0.000000	H-6 → L (75.22)

### XYZ coordinates of m2az1 in S<sub>0</sub>

O	-1.69332957561568	0.96554122290430	2.38275541948234
O	1.83540622651479	0.22840220516971	5.14267274104186
N	0.07112950037838	0.59400381020115	3.74902236263123
C	1.64997042767653	-0.15039849268716	1.54400848562907
C	1.86200698236411	-0.52805453294970	-0.85836266035905
C	0.54039134255183	-0.13703196931762	-1.05397774335027
C	0.30849709392302	0.23310558839046	1.33595579231111
C	2.21364068989078	-0.16388165514733	2.83735409731332
C	2.44471666774243	-0.53995065024593	0.43113722975855
C	-0.23961523588092	0.24151370355868	0.07189071851574
C	3.52413052241818	-0.54262501142275	3.03441488093921
C	-0.53247727742891	0.62666944864097	2.48981128324379
C	1.39544240288952	0.22552634405712	4.01148514625183
C	4.33691315372810	-0.92868697066094	1.93459447325069
C	3.78591023468841	-0.93044928559176	0.65627692612091
C	-0.77325848691545	0.98093018403055	4.86488287596593
H	-1.28302828954226	0.54003054694751	-0.03477165257503
H	3.91286013430354	-0.54238976782476	4.05319863206425
H	4.39126948427737	-1.23696087192832	-0.19802393099952
H	-0.17430523432744	0.91926237294327	5.77870488409393
H	-1.14820797709230	2.00336654072805	4.71737384439968
H	-1.64355624771100	0.31275321870429	4.92976120405313
H	2.47117996810833	-0.83445106420999	-1.71005784856519
N	-0.02683895746322	-0.10512633600882	-2.32892644413776
C	-1.43019570041544	0.05443275788009	-2.48518198241896
C	0.64334685399272	-0.72805527554732	-3.41477206432438
C	-2.26596327802870	-1.08114881317243	-2.45690555572100
C	-1.97489818226077	1.33433484423094	-2.59852660914080
C	0.43288548629498	-2.10027365888260	-3.66421278125881
C	1.55036965095271	0.00282091301318	-4.18406640574601
C	-3.65714965935552	-0.87864252225356	-2.49046795898453
C	-1.73262922495175	-2.43819248557559	-2.41805707395559
C	-3.35415674734232	1.51040744097255	-2.65030578281939
H	-1.29448962644253	2.18821933123603	-2.61355298159847
C	1.19988104822307	-2.71394895737000	-4.67072183013652
C	-0.56455251611673	-2.87926083887294	-2.93886533288131
H	1.68550331280139	1.06270044610958	-3.95854915232304
C	2.28284836702473	-0.62017268898185	-5.18990718841176
C	-4.19621274171331	0.39796187940866	-2.58734493783564
H	-4.31852534173303	-1.74822258045796	-2.44897757791577
H	-2.40786656853401	-3.19416908393936	-2.00436633929730
H	-3.77431454020585	2.51613878960158	-2.72188327252087
C	2.11074042119797	-1.98612944658849	-5.42599805573658
H	1.05834939612927	-3.78043822136103	-4.86564057691052
H	-0.38325951331228	-3.95852462422406	-2.90768298626766
H	2.99749666282170	-0.04418020125440	-5.78232108938900
H	-5.28040441893091	0.52981969877213	-2.61229207800874
H	2.69020044821958	-2.48424611330563	-6.20693765526998

N	5.66685475788509	-1.29055733291832	2.15304314077808
C	6.40843592562820	-1.91722662582964	1.11722710210280
C	6.14583522063145	-1.51391147633667	3.47181686205349
C	6.36385596929765	-3.32056418040275	0.98275002371536
C	7.12188480684842	-1.13850827945135	0.20432636032824
C	6.02713406203767	-2.79603184045142	4.04711178671389
C	6.67259362713508	-0.45129040613511	4.20752269039119
C	7.01106846650911	-3.89877426630070	-0.12404342041240
C	5.70167515708674	-4.17594583484343	1.96142339457746
C	7.77258929268970	-1.73387879307744	-0.87195173837781
H	7.13215096485419	-0.05550703203584	0.34381014423659
C	6.40264699970997	-2.95336201143424	5.39314977638525
C	5.55752822730188	-3.94923026775664	3.28734694352340
H	6.74571242309206	0.52659185436126	3.72720345059082
C	7.05667634096311	-0.63426609778740	5.53216883382090
C	7.70790512202196	-3.11928598764202	-1.03867042036060
H	6.97210198911397	-4.98411340054073	-0.25029827752040
H	5.37924433297389	-5.15291226899118	1.58692112950397
H	8.32046025156123	-1.11757321277528	-1.58857443900649
C	6.91242569613850	-1.88968544688287	6.12688213617600
H	6.29899097388005	-3.93699105871572	5.85904109955258
H	5.12938285052768	-4.76021126749324	3.88537061344632
H	7.45321808835195	0.20569187926602	6.10692028088868
H	8.20740976349922	-3.59283740605523	-1.88722645412035
H	7.19914644246746	-2.03742527748819	7.17065040280581

#### XYZ coordinates of m2az1 in S<sub>1</sub>

O	-1.60389785955092	1.16238932855817	2.33119365928653
O	1.81969124492790	0.24713811736744	5.17154823514889
N	0.10241763976022	0.70333499382143	3.74625691573209
C	1.66931905618752	-0.15592286662645	1.56711093727863
C	1.87495608904479	-0.60277782865539	-0.83756096174232
C	0.57382880013608	-0.14354676983372	-1.05446303341887
C	0.36398843323360	0.29104517046001	1.34136878399662
C	2.21826992693728	-0.19317420768455	2.88064123417180
C	2.44109943231216	-0.61325783424477	0.46059577722331
C	-0.17720069196021	0.29971821393045	0.06449292992512
C	3.48629475471453	-0.64635500101156	3.10938202630604
C	-0.47209364120947	0.75546280292251	2.47813292051330
C	1.39541068150331	0.25849155480855	4.03955933740320
C	4.30449023838298	-1.07691016522735	2.00546824593977
C	3.74312240434289	-1.07624019228973	0.69501179850763
C	-0.73742301838983	1.15861713059319	4.84280470817793
H	-1.20284547737104	0.65344877899261	-0.05047979854885
H	3.86597597614714	-0.68132315297476	4.12956066238391
H	4.33915720647405	-1.45822667369110	-0.13241037043946
H	-0.16362045008436	1.06581980509050	5.76979333810304
H	-1.03607386928410	2.20290452578364	4.67794993139201
H	-1.65052873841909	0.54987625951671	4.89384421973807

H	2.47502378130357	-0.96557324565755	-1.67279582978870
N	0.01853087746541	-0.11375401915314	-2.32317556439320
C	-1.38357267111448	0.06829073947904	-2.48805195877773
C	0.68875151999323	-0.75493603556743	-3.40177581813537
C	-2.23025307777579	-1.05822832226190	-2.44556211206683
C	-1.90825767183309	1.35370713481886	-2.62380694524758
C	0.46214856952231	-2.12730983038248	-3.63192085940344
C	1.60924047262508	-0.04196617208294	-4.17053599882002
C	-3.61868908177192	-0.83823159166432	-2.48601511864762
C	-1.71331200301484	-2.42118382049962	-2.38932679606509
C	-3.28527405368197	1.54503686393839	-2.68363921430977
H	-1.21824923266004	2.19959877323574	-2.65345062330059
C	1.23230402121284	-2.76296466326805	-4.62236353390464
C	-0.54936266846385	-2.88365447081961	-2.90215687109221
H	1.75483416803569	1.01965294011081	-3.95979833899747
C	2.34346886030068	-0.68769049082964	-5.16071629310019
C	-4.14056470650735	0.44364934709763	-2.60487290999688
H	-4.29127382610574	-1.69847981381951	-2.43530832601372
H	-2.39966649513906	-3.16424560286365	-1.97091132678263
H	-3.69294099792626	2.55410705490481	-2.77542677037068
C	2.15828441112079	-2.05501929957110	-5.37810273415579
H	1.08298548979740	-3.83064070638196	-4.80314234447537
H	-0.38369704663486	-3.96484982470507	-2.85889408616515
H	3.07105191868959	-0.12901875547398	-5.75352878184625
H	-5.22280279618477	0.58837162694856	-2.63703868452012
H	2.74131005038983	-2.57083096522901	-6.14438636422186
N	5.56779191846094	-1.50199046347082	2.20103006799241
C	6.34689109984491	-1.98814035513782	1.09703932391561
C	6.09832104670710	-1.63709444825947	3.52608581239784
C	6.44208629981470	-3.40633302951454	0.94116311960174
C	6.84503242516334	-1.08236219973960	0.16889092819293
C	6.15327936053415	-2.95477901016817	4.07271822941668
C	6.42215317824876	-0.49519675960951	4.24945127642692
C	6.95888678017585	-3.81988980851458	-0.32619234049054
C	6.07624608157983	-4.34051916399496	1.94024858424025
C	7.42507827438369	-1.53440874658937	-1.01561563673437
H	6.74440875808069	-0.01206532461988	0.37031451311537
C	6.44520127368734	-2.99581725629259	5.46958067351772
C	5.94935110726922	-4.14223543480328	3.32250896520133
H	6.36478102822040	0.47811524013647	3.75453092328845
C	6.78209345802783	-0.59250369668563	5.59126039411493
C	7.44048020445136	-2.92290204288090	-1.25767700793972
H	7.00200848299539	-4.89313257644564	-0.53209032694862
H	6.02532297585736	-5.38015639606373	1.60319338241965
H	7.83798417915432	-0.82949329341175	-1.73838708324494
C	6.75725164020534	-1.86361119693219	6.19501581678125
H	6.45129159705180	-3.97356072730997	5.95911748358236
H	5.81668070699777	-5.04736434854012	3.92213611118118
H	7.05290465234032	0.29792068000539	6.16001109854745
H	7.85387288583066	-3.30144209466357	-2.19673995756093

H 6.99902352543833 -1.96086325640205 7.25687322650548

**XYZ coordinates of m2az1 in T<sub>1</sub>**

O -1.71370643657353 1.09505405659274 2.36223508720090  
O 1.77946129259435 0.26468759200345 5.17524647595671  
N 0.03664203755706 0.67567314789537 3.74935514913430  
C 1.57801568887110 -0.16945502827554 1.59444146506350  
C 1.79888778336096 -0.62082762853228 -0.80038017641297  
C 0.44715479628542 -0.17035417317555 -1.01994101701420  
C 0.26127325336271 0.25912858145243 1.36372850960310  
C 2.13756909879304 -0.18590577401065 2.88738132718361  
C 2.36685410693805 -0.62015646600661 0.48736640160233  
C -0.30339653115401 0.25727092708362 0.05871888572076  
C 3.46861867464348 -0.62656924606499 3.11289785862590  
C -0.55958168268188 0.70680889264441 2.48735645220366  
C 1.34179460526947 0.25599876016936 4.03176166462663  
C 4.25034294938794 -1.04553672638597 2.05263092752034  
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H 4.27587460467917 -1.42439460002372 -0.11680029838053  
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H -1.69233565671205 0.48989530977280 4.92659246097615  
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C -1.87602467658515 1.40323075579888 -2.64543123624716  
C 0.32252807151377 -2.19775341429809 -3.64308672911953  
C 1.61065801739352 -0.17633551882247 -4.09280249317883  
C -3.71860741966541 -0.68260292883475 -2.65557736369795  
C -1.91942026248060 -2.38026782450399 -2.50619908331881  
C -3.23451696577308 1.67949857505737 -2.76011952494435  
H -1.13696958121807 2.20610112221785 -2.61011651585701  
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C -0.76303754512244 -2.90491234646970 -2.97246232179425  
H 1.80737443363450 0.87138175526098 -3.85573797676098  
C 2.34758767555342 -0.84658452651326 -5.06451337034019  
C -4.15735338263304 0.63112577746249 -2.75777927364285  
H -4.44259355349240 -1.50174551342264 -2.65927502419657  
H -2.66752812701794 -3.08558259740373 -2.13027665332064  
H -3.57656159426838 2.71424431586118 -2.83295849928677  
C 2.09220291939733 -2.19637350779713 -5.31720379526876  
H 0.88827870459241 -3.91343705604992 -4.82224406815063  
H -0.66322158832456 -3.99463167633583 -2.94087846528700  
H 3.12937780876251 -0.32029866453771 -5.61688962728663

H	-5.22637720837488	0.84295718235703	-2.83266609265163
H	2.67439724953592	-2.73219217256807	-6.07059305070829
N	5.55336587397386	-1.48507760757021	2.21604110855455
C	6.34803641544367	-1.94318365811024	1.13369342270683
C	6.11462821369193	-1.64151044495671	3.51112357433507
C	6.56147069741639	-3.32727272809973	0.97045285417747
C	6.87169501801215	-1.02821453114793	0.21625069054343
C	6.24693722950441	-2.93596268636375	4.05040939269262
C	6.47890406165552	-0.51670592335264	4.25348969535345
C	7.26239475236555	-3.75369663378478	-0.17191839402677
C	6.09555515248805	-4.30953775246595	1.94331995914408
C	7.57580371069718	-1.47362036114703	-0.89756125849755
H	6.69034949731180	0.03613876290588	0.38068952086957
C	6.70486941914600	-3.05265241194911	5.37511688752332
C	5.95819289229649	-4.13876099429089	3.27753648269099
H	6.35669648539717	0.47054656263739	3.80357516785519
C	6.94676130311512	-0.65874982242661	5.55521092274584
C	7.76397379406225	-2.84364625524127	-1.09393861042210
H	7.41772028145228	-4.82516610779434	-0.32373261260108
H	5.93903770670063	-5.31959176920458	1.55121070330177
H	7.97022695624323	-0.75316113402170	-1.61771260760170
C	7.05155726468895	-1.93248565005876	6.11882438189680
H	6.79590828231895	-4.04931008558771	5.81489995351877
H	5.69875326611296	-5.02337126388463	3.86798279797587
H	7.21523190148985	0.22577968613661	6.13691379130927
H	8.30798041455090	-3.20202506957216	-1.97092114927036
H	7.40566576369046	-2.04956909024556	7.14553396568863

### XYZ coordinates of p2az1 in S<sub>0</sub>

O	-0.02272270329463	5.95085522161274	-2.04839424568725
C	-0.74039319422442	5.08761406451278	-1.59006757638457
C	-0.22328365237295	3.73844249127373	-1.24348925692800
C	-1.06284411463120	2.73098404477644	-0.70047669340136
C	-0.54553568171696	1.42942286562692	-0.36753350191617
C	-1.47028266690167	0.47373010862639	0.18193975271550
N	-1.08203620435900	-0.85253142285553	0.55186874505987
C	-0.91547542853327	-1.09670630989113	1.95547849490560
C	-1.56614707095518	-0.29504860791272	2.90402545223396
C	-1.33780441728709	-0.43288031513506	4.27189438373750
C	-0.44720232493932	-1.39135428891613	4.73795405864955
C	0.20386941699325	-2.19438938347984	3.81054085967102
C	-0.00973543619296	-2.07752532944495	2.42927742083458
C	0.77238986451240	-2.95693995675997	1.57150738222958
C	0.46968340200679	-3.39244592759424	0.33861572294069
C	-0.71468237328253	-3.09379479293374	-0.45487543730991
C	-1.47282653962867	-1.90220575326093	-0.34381313976662
C	-2.55777405379133	-1.73476322803654	-1.21631510890804
C	-2.89508119718560	-2.69108473228374	-2.17204383052549
C	-2.15324333748435	-3.86014392825796	-2.28193417274441

C	-1.07405425336340	-4.03979164902783	-1.42639792855431
C	-2.79740560023652	0.84055286053194	0.36507970105309
C	-3.28594954616742	2.10760291617768	0.03305016467726
C	-2.42782251803305	3.04643576509512	-0.49572336037094
C	-2.97894349922844	4.38092491715493	-0.83961666118785
N	-2.09637619981757	5.31680605189343	-1.36363509676912
C	-2.65308614874255	6.61884739114931	-1.68765687410271
O	-4.14768147768603	4.66294318048313	-0.67661692595153
C	0.85496145650337	1.21496996846425	-0.62172498560153
N	1.55224392514144	-0.00691594460730	-0.36336724822551
C	1.55368723843163	-0.92165408278135	-1.44654599906863
C	0.54527792538950	-0.77966449742165	-2.41513334784167
C	0.44847585704726	-1.60201166760449	-3.53337544443482
C	1.37568531586533	-2.61416545517213	-3.73494290692281
C	2.39952811976134	-2.74949413460872	-2.80598659644063
C	2.52599792952306	-1.92978291110033	-1.67258818282942
C	3.69382306911358	-2.19395612416699	-0.84173442367250
C	3.99420641826289	-1.75910940054026	0.39024269577129
C	3.24533637335821	-0.88739048118859	1.28642763275308
C	2.12895233301927	-0.08833709707599	0.92956208249974
C	1.59108851438947	0.73992951205430	1.92964820358331
C	2.08110041718190	0.77042275085960	3.23149667996719
C	3.15042819483553	-0.03709592478209	3.59131914704390
C	3.71479282250293	-0.84111387038330	2.60923426721629
C	1.63393552596324	2.22443784427876	-1.15242214047249
C	1.11188888711688	3.48531165272185	-1.46530090654668
H	-2.24233554499562	0.49258804238801	2.58104071366599
H	-1.85933459910764	0.22904948888674	4.96746588618080
H	-0.24690499382649	-1.50273524847448	5.80557503297863
H	0.92998116799742	-2.93637926100508	4.15173158002977
H	1.68458971013141	-3.35029147952768	2.02854013195966
H	1.15730967796098	-4.10915431895123	-0.11877900466814
H	-3.14154488159861	-0.81800979270068	-1.19131462485310
H	-3.74110633284914	-2.50216959132142	-2.83723036198055
H	-2.39667452850700	-4.61316819929780	-3.03428908989566
H	-0.45645493613504	-4.93707585228649	-1.51467102652040
H	-3.47865492968781	0.09843489488842	0.78467873785399
H	-4.33366117852678	2.37601117711111	0.18156562735575
H	-3.08204094905627	7.07879802932687	-0.78665330756038
H	-1.84661571080525	7.24040980693105	-2.08866688175969
H	-3.45922385240861	6.50959384454902	-2.42628911193977
H	-0.21012150601999	-0.00690960254004	-2.29937938105498
H	-0.37244900337795	-1.44266041988672	-4.23555353942649
H	1.31665822596829	-3.27474619397589	-4.60193297712562
H	3.16159753419459	-3.51903939221006	-2.95657197780525
H	4.41688104000078	-2.87498227343488	-1.30076154900574
H	4.93246954384274	-2.12803039075562	0.81556416861321
H	0.74532080096551	1.38279760151057	1.69977051872566
H	1.60264935811309	1.42795077702803	3.96029084568727
H	3.54871303622829	-0.03435244430479	4.60767198416122

H	4.57664806483656	-1.46637302076271	2.85774978231726
H	2.68929884559840	2.00510656464054	-1.32391629309657
H	1.73604257418608	4.27740086412480	-1.88308673782016

**XYZ coordinates of p2az1 in S<sub>1</sub>**

O	-0.12372332132216	5.90681054026678	-2.01604300807475
C	-0.83140035635783	5.02549527466166	-1.54605902194468
C	-0.31878108367228	3.69460283747866	-1.21504396151283
C	-1.16596922346728	2.69795586500280	-0.66905284795476
C	-0.64227085486623	1.38805696451791	-0.34078446723227
C	-1.55233282224347	0.44232632975741	0.20645176730250
N	-1.11211878309841	-0.88457412420582	0.56969291455898
C	-0.82424069623657	-1.07635645868748	1.94424104360436
C	-1.33196505833093	-0.13964185814903	2.86778924784640
C	-1.02205806115740	-0.18192595106663	4.21921761256914
C	-0.16481635996629	-1.16182195885389	4.71447569617851
C	0.34401751684785	-2.09470605343487	3.82611015035875
C	0.03151786085538	-2.09469573013935	2.45486422003360
C	0.66197113937200	-3.14065107038338	1.67431618421877
C	0.36779723824668	-3.57718136634278	0.43809804009537
C	-0.66533427709270	-3.12900488997624	-0.47431290158346
C	-1.37813439599484	-1.89847556870811	-0.38419452266690
C	-2.34329731917456	-1.63923634013251	-1.37896506963052
C	-2.60249947670596	-2.52466723528890	-2.41483800622592
C	-1.88766643733516	-3.71581144757861	-2.51801211439612
C	-0.93591396180246	-3.99308452251190	-1.55051090696041
C	-2.90513980649680	0.77752089032046	0.41161023447349
C	-3.39635994754896	2.02654084224645	0.09521850702740
C	-2.53289435404016	2.99484090528623	-0.44436343362692
C	-3.07695934298353	4.31199577609676	-0.76500116745007
N	-2.18790778939732	5.24629508958605	-1.29499090581753
C	-2.74502160658732	6.54807521908208	-1.60302220340477
O	-4.24983995845123	4.61657237647841	-0.58882569252539
C	0.74000439197001	1.18195714054200	-0.60046112329240
N	1.41994407048651	-0.07398306466720	-0.32065420642486
C	1.49003694535813	-0.94517167599022	-1.42103079910064
C	0.58103961618979	-0.69414084679585	-2.47558859376547
C	0.53255659770717	-1.46169797340981	-3.62577462096944
C	1.41286419532228	-2.52879925116856	-3.79943277333771
C	2.32078869998453	-2.79298837608331	-2.79105464391112
C	2.39058527767435	-2.04300113954671	-1.59956602843596
C	3.40307643999819	-2.48308024907099	-0.67748156743226
C	3.69965772350824	-2.04497826975192	0.56462668258536
C	3.09463457688321	-1.00240233450075	1.34953313470543
C	2.05254825002585	-0.11419276458691	0.93388379460647
C	1.62202396396644	0.84363270716805	1.88178866150857
C	2.15301821975683	0.93216005329365	3.15629318538093
C	3.17051645580867	0.06813238921789	3.55836296253083
C	3.62045855522620	-0.87243366874739	2.65091766047646

C	1.55220537592704	2.18500151942237	-1.14422481501605
C	1.04035695139743	3.43018203671457	-1.45160403941772
H	-1.97324096828020	0.66124387247486	2.51023189058251
H	-1.44960815582132	0.57256179107738	4.88352738192282
H	0.10405533734314	-1.19624647043834	5.77204247444196
H	1.02744590816883	-2.86700305862403	4.18736980912582
H	1.46327280984208	-3.67000512605570	2.19764791677008
H	0.95699095717138	-4.42162790556079	0.06952557889496
H	-2.89269195096947	-0.70227033031554	-1.35089228421917
H	-3.36492352792100	-2.26604682923828	-3.15323424214026
H	-2.06687131697080	-4.41366939616629	-3.33826769439362
H	-0.35378347294658	-4.91559225926424	-1.61506778609038
H	-3.56640851483986	0.01687139114422	0.83410869342693
H	-4.44149887080099	2.29724335888166	0.25069326233957
H	-3.17123580883988	7.00087727259486	-0.69638866691365
H	-1.93916907365643	7.17052241872239	-2.00491851180011
H	-3.56013409971548	6.44739241195121	-2.33392653456465
H	-0.11256657123000	0.13528639023219	-2.38181863937980
H	-0.20636380983139	-1.21651545755773	-4.39069313136307
H	1.39133697731027	-3.13836533168676	-4.70450000219047
H	3.02739230082507	-3.61832572068796	-2.90548974247036
H	4.01417550469652	-3.31030812609314	-1.04857303467790
H	4.51957021511423	-2.56336462492183	1.06911685347746
H	0.83918688575010	1.54135082205219	1.60232223839505
H	1.76007826048657	1.68851229606930	3.83803855802794
H	3.60415289364176	0.13100671126786	4.55793720328353
H	4.42282916896384	-1.55623560629606	2.93757698499340
H	2.60640537599256	1.95892272546717	-1.31907783035762
H	1.65662877831919	4.22433421362963	-1.87388900307655

### XYZ coordinates of p2az1 in T<sub>1</sub>

O	-0.13791052377084	5.89076551463315	-2.01780877016142
C	-0.84330163139621	5.01114930283279	-1.54788443848151
C	-0.32514562263543	3.68085691922020	-1.20771180495101
C	-1.16996442092675	2.68573684208088	-0.66099924588917
C	-0.64427222619796	1.38043754658594	-0.32843370355494
C	-1.55090591219216	0.43036316369619	0.22046270573524
N	-1.11950916274134	-0.89620514263208	0.58196117867452
C	-0.81962631667929	-1.08259311409473	1.95449460136059
C	-1.31511495837040	-0.13627787975620	2.87616636314978
C	-0.98818003853884	-0.16747866539107	4.22302406545896
C	-0.12182627989913	-1.14453162339361	4.71387719551381
C	0.37348016101594	-2.08547038594424	3.82975475497866
C	0.04052679815939	-2.10160856672669	2.46048224066803
C	0.64292107536151	-3.16200432076391	1.68684021034284
C	0.34459276905734	-3.59767105504900	0.44681581348999
C	-0.66269865267211	-3.13127059521204	-0.47719609056128
C	-1.37664245102299	-1.89993657356575	-0.38416530762103
C	-2.32715143971627	-1.62407484915978	-1.38971543781155

C	-2.57173626839805	-2.49303181278163	-2.44149985009633
C	-1.85346941331942	-3.68404478467289	-2.55061151280372
C	-0.91887786991386	-3.97797970601019	-1.57450897023747
C	-2.90412085568991	0.76323233157176	0.42536338502436
C	-3.39543862925533	2.01306190746794	0.10168393956463
C	-2.53949055094654	2.97949630645575	-0.44051533603170
C	-3.08952056098559	4.29454942213792	-0.77314230707666
N	-2.20234071654677	5.22898250908100	-1.30553092861553
C	-2.76298994325505	6.52774887403069	-1.62306570124607
O	-4.26278242475076	4.59306772788772	-0.60463537837867
C	0.74054355134970	1.17099225443693	-0.58448631368120
N	1.39802426350336	-0.08799315412672	-0.30317371922866
C	1.47135969104836	-0.94790520692677	-1.41659999958172
C	0.58538369560588	-0.66817720569238	-2.48161768217470
C	0.55299856248028	-1.40995286584670	-3.65049488257297
C	1.42759016701712	-2.48191711746029	-3.82494913491804
C	2.30447176274030	-2.78124454681719	-2.79924698739329
C	2.35670928288718	-2.05793756382525	-1.58875521332668
C	3.32885015486810	-2.53750820747480	-0.64345689065071
C	3.63178202205797	-2.09909740094692	0.59859024348810
C	3.07248176719946	-1.01900249326400	1.36592412160925
C	2.03898192682819	-0.12191497036576	0.95140703880437
C	1.62463580280109	0.85085090161463	1.88906642543613
C	2.17935232308298	0.96464625780834	3.15264026112356
C	3.20269427986859	0.10412989176368	3.54878946662646
C	3.62495815473615	-0.86197663597549	2.65489296765973
C	1.55083676898527	2.17493997418412	-1.12716721947807
C	1.03348098819091	3.41854481180419	-1.43766128623221
H	-1.96131849660112	0.66207749166163	2.52013005636968
H	-1.40737429697115	0.59133615487527	4.88756741104070
H	0.16376562688559	-1.16792752974282	5.76739330071186
H	1.06176160307513	-2.85442394978832	4.18837973425399
H	1.42556518910993	-3.71368489250968	2.21488533343961
H	0.91375782849705	-4.46071163877181	0.09069563957951
H	-2.87681824783335	-0.68695810583465	-1.35583960339134
H	-3.32319071099730	-2.22348775143980	-3.18701315808632
H	-2.01886198966680	-4.36803615824018	-3.38533014293084
H	-0.33671627816550	-4.89992985192133	-1.64403924943390
H	-3.56376224392473	0.00194321754209	0.84902219971640
H	-4.44234175604273	2.28015568827944	0.25560709536659
H	-3.18416308509963	6.98908702483211	-0.71836604991274
H	-1.96041853404476	7.14799546367670	-2.03464228937640
H	-3.58130078075709	6.41881293030262	-2.34901013726089
H	-0.10130375876930	0.16855858766941	-2.38839460984989
H	-0.16694734801830	-1.14094194781354	-4.42554743106531
H	1.42369502538469	-3.07086076803106	-4.74402912962602
H	3.00068761519354	-3.61561578132402	-2.91347658331197
H	3.90805956225392	-3.39448341432040	-0.99835332559832
H	4.42354483637963	-2.64809864496004	1.11595775771289
H	0.83790071544710	1.54617921948100	1.61035147816135

H	1.80070947042588	1.73419456580152	3.82773854648355
H	3.66030554058393	0.18637282787197	4.53644458819229
H	4.42508570599731	-1.54822471642364	2.94256063957573
H	2.60569071518594	1.94918883181431	-1.29977623675267
H	1.65034899343314	4.21273713191490	-1.86011869996547

### XYZ coordinates of m2az2 in S<sub>0</sub>

O	-1.71870200504185	1.11767662230306	2.21701187554592
O	1.62987495177952	0.20907699479819	5.14577366196322
N	-0.04439419810496	0.65942207454424	3.66807638383349
C	1.59047223547322	-0.19382810440059	1.54605426824330
C	1.89017720253694	-0.61661559743202	-0.83945443447847
C	0.60723910559709	-0.14085650993387	-1.10582749020732
C	0.28439976568428	0.26136986809061	1.27129293239004
C	2.09265420857071	-0.22608930537070	2.86399307201510
C	2.41085165692645	-0.64414868349285	0.47597975672098
C	-0.20162347166132	0.29036123728957	-0.01758960171018
C	3.36801922416226	-0.67715275154590	3.12672477215492
C	-0.58578863843511	0.71437677876391	2.38153540164951
C	1.24298900903744	0.21962786997762	3.99569025870535
C	4.21449624329746	-1.11280662091620	2.06905635454396
C	3.71674198943611	-1.10449683265543	0.76702974079884
C	-0.91724098766186	1.10350631460804	4.74022567861222
H	-1.21902018020136	0.64943592075062	-0.17577559482565
H	3.70168799397320	-0.69600798285389	4.16446521588490
H	4.34118610964391	-1.45332457487754	-0.05641830991586
H	-0.36749305416661	1.01429575423604	5.68224398628562
H	-1.22416223416617	2.14487100255761	4.56992034480594
H	-1.82709320667257	0.48749527209169	4.76606577567048
H	2.51814281889269	-0.97720499249702	-1.65524477732520
N	0.09291532092816	-0.09724578746451	-2.39891634364589
C	-1.30049502606157	0.10128491564517	-2.62159343815818
C	0.86387379024959	-0.51408299284805	-3.51892422436449
C	-2.10984215749785	-1.03557978565752	-2.75501864446144
C	-1.84092097871921	1.38299170676398	-2.71352528712933
C	1.93862886220476	0.29743920980558	-3.91072257948882
C	0.56284822838068	-1.68540041913393	-4.23838797623555
C	-3.47576194466121	-0.86009380843943	-2.98544977089567
C	-1.44064897514258	-2.37713461947676	-2.69833078104596
C	-3.20832090994823	1.54250422022509	-2.93050596942945
H	-1.18015795326242	2.24594700565392	-2.60653269908508
C	2.73397504652536	-0.03850182343367	-4.99709826366916
H	2.13434861475561	1.20288077360354	-3.33177879011620
C	-0.57069210617696	-2.64170744873371	-3.92824928872140
C	1.36836941774659	-1.98939598692008	-5.34741126724888
H	-4.11840623570898	-1.73815631675186	-3.09549034228787
C	-4.02394908185564	0.41973701683163	-3.06570289984589
H	-2.19861505312811	-3.17190464781507	-2.63154211803702
H	-0.82737609581606	-2.44604773569310	-1.78455222756966

H	-3.63714698946959	2.54507795455657	-2.99519619032033
C	2.44201645135931	-1.19326054292021	-5.72467850173030
H	3.56881633667899	0.60466103287224	-5.28496216617816
H	-0.13928464981156	-3.65350017111298	-3.84288290613773
H	-1.22693400709040	-2.67460819080147	-4.81592405184030
H	1.14144823882903	-2.89189417229457	-5.92315278394210
H	-5.09650681763812	0.54149579095070	-3.23524336033784
H	3.05009857023506	-1.47039150252323	-6.58906214936392
N	5.50131884984804	-1.56709037901847	2.34517213980258
C	6.24194639578164	-2.26075714696765	1.34700703087649
C	6.03787633672432	-1.57300755623153	3.66261494508353
C	6.18884476449535	-3.66169718519512	1.35062255914668
C	6.99601299635998	-1.57270238000652	0.39718173774331
C	6.31385188596662	-0.33739308806225	4.26591526186811
C	6.31177866613766	-2.77090218127348	4.34798201282966
C	6.91043032996514	-4.36030709721304	0.38030703685352
C	5.40290348017126	-4.32402064463106	2.44328758267462
C	7.70116883782175	-2.28329655853302	-0.57277040194452
H	7.01740530808935	-0.48113188166244	0.42688970733872
C	6.83990690833033	-0.26502552945134	5.54794830546984
H	6.09600822186815	0.57092763594441	3.69968537951458
C	6.06977611060521	-4.16693126227782	3.81138136997960
C	6.86720367122511	-2.66971780190161	5.63295192726058
H	6.88295531467009	-5.45365504280006	0.37536170079037
C	7.65593893824364	-3.67713503424573	-0.58031715465215
H	5.29546942310164	-5.39814633434635	2.23033019759785
H	4.38490594248941	-3.90130950881317	2.47198421469219
H	8.29084178934077	-1.74782949684177	-1.32055146703690
C	7.12292770650212	-1.44512350904924	6.23640416448301
H	7.03786276669738	0.70735198483958	6.00444313996092
H	5.46931500515570	-4.71200963917055	4.55911437726319
H	7.04522754910339	-4.68410839681222	3.78208692578531
H	7.09078515930490	-3.59270334120864	6.17651723099485
H	8.20919631478574	-4.23741438456296	-1.33802186208261
H	7.54399713241088	-1.41011378943123	7.24389323763211

### XYZ coordinates of m2az2 in S<sub>1</sub>

O	-2.27865223014485	-0.31917827335591	2.10609032392625
O	0.76541325992419	-1.94789423825139	5.09061042257884
N	-0.74350344941331	-1.12537262105605	3.57129733660820
C	1.24652172263236	-0.98751791128374	1.62070163642564
C	1.91617529548209	-0.43995795129045	-0.67650189033028
C	0.60798910347370	-0.01603406520533	-0.97275037050937
C	-0.06407441965755	-0.57974356196202	1.29820234643095
C	1.55905267418194	-1.46738034018710	2.91921674227402
C	2.25914827989209	-0.91572752387654	0.60427349931276
C	-0.38006016868673	-0.09992344405845	0.01882376547081
C	2.86975069323846	-1.88585461198566	3.22528322255073
C	-1.11742149357105	-0.65076326299606	2.31045727010094

C	0.53785107735086	-1.54385332766639	3.95162639944199
C	3.82630413041327	-1.81459179272567	2.23241815637395
C	3.57191478573462	-1.33754993241417	0.94320228824584
C	-1.80236527722832	-1.18265668393028	4.55794515620391
H	-1.41148218007409	0.19817609522226	-0.16565072394838
H	3.08056131683702	-2.26032033823301	4.22749963021185
H	4.36831671889907	-1.30063697634253	0.19756371048316
H	-1.37126242210578	-1.56543531057748	5.48865544716520
H	-2.23323329338945	-0.18248539681929	4.71005464640756
H	-2.61354251507792	-1.83673549825188	4.20660008034686
H	2.68807225549117	-0.41009995092048	-1.44574840899010
N	0.28212218824829	0.45603102704568	-2.25133778632234
C	-1.08053156988697	0.56144942103291	-2.64708865135912
C	1.25768334781514	0.57611940891151	-3.27311518906632
C	-1.65601963251837	-0.52375292523447	-3.32226197280366
C	-1.82456972009834	1.70777131807079	-2.37215217221936
C	2.23402965794285	1.57492408100869	-3.13274902128942
C	1.26186399823998	-0.25247330135899	-4.41187391915533
C	-2.99008237187245	-0.43422075177971	-3.72420154171743
C	-0.77255424401158	-1.69774086676180	-3.62286034552125
C	-3.15945261175986	1.77863903283791	-2.76647477238448
H	-1.34698645126990	2.53183361044552	-1.83814118388918
C	3.21975063089733	1.76168532075765	-4.09148618820147
H	2.19417276790075	2.20083368687048	-2.23861332259560
C	0.27468080968393	-1.36831015744217	-4.68781676959361
C	2.25458311214703	-0.02692829176709	-5.37861667164718
H	-3.44821434020596	-1.27337074642507	-4.25565700224087
C	-3.74072888650624	0.70689595419548	-3.44262830548754
H	-1.37940995875106	-2.54336665348438	-3.98028987510639
H	-0.27476594269822	-2.02831418850062	-2.69615553860388
H	-3.74724021939040	2.67217506315431	-2.54365640689176
C	3.22669391430583	0.95410316744908	-5.23001872606762
H	3.97024286036001	2.54511609256982	-3.96072350183669
H	0.85631045127931	-2.28019661312158	-4.90648435771149
H	-0.25238858277537	-1.12213118928044	-5.62695016379316
H	2.26169251342763	-0.65865763974352	-6.27236895040927
H	-4.78750780147019	0.75916726042344	-3.75201843005470
H	3.98674886389486	1.09227246175828	-6.00288643898362
N	5.18281142363262	-2.27570972211998	2.53626423954569
C	5.34329755595300	-3.66663823868462	2.50267049692784
C	6.09800271442262	-1.26837361848968	2.80358862657371
C	6.38231474110022	-4.38567869947774	3.16186917361263
C	4.33790401582730	-4.40886094908499	1.82609928232399
C	5.56737296132424	0.04569561832395	2.98138948453255
C	7.52288128730417	-1.42453800461185	2.84436955383018
C	6.34246073083155	-5.77959176564080	3.14857177334084
C	7.54376893387317	-3.70810679262210	3.80859538920505
C	4.34254235991057	-5.78814717217756	1.81414581693232
H	3.55184156669216	-3.86860096094941	1.30317115458096
C	6.38444370263218	1.14389786472839	3.14151321308612

H	4.48848617510086	0.17380630955919	2.99435411960331
C	8.20012007872124	-2.75512812150015	2.81314923739536
C	8.31222470350519	-0.28748724552430	2.98694895268311
H	7.13539286539324	-6.32157542530954	3.66931541477753
C	5.34080755519947	-6.48977524333387	2.49466276824987
H	8.25796510853413	-4.47127476164788	4.14709648600241
H	7.23172525183339	-3.14916580785935	4.70885237696061
H	3.55617211411878	-6.32022365093595	1.27613022494544
C	7.77266812961797	0.99039053589417	3.12379493130478
H	5.93426597685916	2.12837336189493	3.27857009577234
H	9.26377724312442	-2.61223621071011	3.04986985083446
H	8.16363988672086	-3.19696347578679	1.80111800526910
H	9.39697771233009	-0.41558552169839	3.00695645954825
H	5.34466973465581	-7.58156343459200	2.50771465440271
H	8.43141906365100	1.85389234889274	3.23539028593011

### XYZ coordinates of m2az2 in T<sub>1</sub>

O	-1.73678385908077	1.12313391720870	2.25124959648170
O	1.65676462975579	0.26388218233698	5.17503729336494
N	-0.03590025379034	0.68802898363077	3.69464385552647
C	1.56587556894161	-0.18668397245882	1.59611517920682
C	1.85838837161689	-0.65626829641926	-0.78685891317901
C	0.52169238588852	-0.16702194379955	-1.05689001731417
C	0.25825196600827	0.25790097620594	1.31977746476756
C	2.08210875363149	-0.20056998919172	2.90163152725413
C	2.38348129579816	-0.65940489840936	0.51929370366354
C	-0.25998306967915	0.26488340030505	-0.00092647386963
C	3.39815277174209	-0.66272776674057	3.17411456802202
C	-0.59179978932123	0.72155939968064	2.41363896540206
C	1.25445163189571	0.25574949092193	4.01943158802276
C	4.20749338572998	-1.10820600701069	2.14409031022012
C	3.68396780645687	-1.11846659712074	0.79985634282874
C	-0.89816968807830	1.14648675211640	4.76693540289252
H	-1.28202666229332	0.61538279109543	-0.13749034379661
H	3.72853653725964	-0.65477425084861	4.21186440276424
H	4.30371149236500	-1.48600368295694	-0.01852640410038
H	-0.33671372251548	1.07486252550551	5.70383383110680
H	-1.21316906294148	2.18309561958576	4.58127440768973
H	-1.80636884513181	0.52859730362500	4.81217561999223
H	2.46290570332734	-1.05573897177298	-1.60147394429369
N	0.04811843756684	-0.20515941301646	-2.35736706308260
C	-1.33357683748851	0.02829914117256	-2.62374175487698
C	0.86162790305798	-0.54501802439105	-3.47153525504606
C	-2.14271538307503	-1.09007548359987	-2.85957141376825
C	-1.85483213456362	1.32046836889668	-2.65462468149999
C	1.95582369841345	0.28196743156194	-3.76978843376677
C	0.57232608079991	-1.65921057632581	-4.28204548967946
C	-3.49592879255939	-0.88463060840845	-3.13582610328585
C	-1.48583197127987	-2.43816086380163	-2.86106892365860

C	-3.21023270168864	1.50680064538852	-2.91787962891814
H	-1.19436444771903	2.16827055210151	-2.46162415750628
C	2.78591581280690	0.01044997471204	-4.84865696258832
H	2.13577160801970	1.14849877445226	-3.12946892122944
C	-0.57308060317162	-2.62887291584398	-4.07361029208342
C	1.41523066314357	-1.89570657096528	-5.37816108036958
H	-4.14036093161229	-1.74703571600130	-3.32753857460752
C	-4.02873231472800	0.40356722922428	-3.15791099458994
H	-2.24966611253859	-3.22970354003443	-2.87210449164405
H	-0.90877136675069	-2.56583561313214	-1.93027810881820
H	-3.62738550764250	2.51607002244874	-2.93541321894064
C	2.50994297659878	-1.08851259451804	-5.66254155596608
H	3.63536503303178	0.66299700726000	-5.06293279014695
H	-0.14631712794658	-3.64565372186350	-4.03849645608230
H	-1.19756392665503	-2.60196192827670	-4.98397196747638
H	1.20240654257325	-2.75670794546332	-6.01882696110346
H	-5.09202099387114	0.54790392259749	-3.36369777438640
H	3.14592880681888	-1.31372614497607	-6.52176743434373
N	5.50077769134539	-1.56466614520234	2.35358364656527
C	6.20575630793341	-2.28347406980508	1.34502414531881
C	6.08159815235538	-1.55540830991241	3.65409049282355
C	6.14362331882517	-3.68370450696876	1.37896600844420
C	6.94201846604704	-1.61834083040520	0.36543169732319
C	6.38199447124050	-0.30995635661182	4.22329091577039
C	6.36562375660033	-2.74360488669154	4.34984949712992
C	6.83403378307156	-4.40463549461554	0.40218860775218
C	5.38378963518819	-4.32124021102809	2.50453410737956
C	7.61535171897936	-2.35211726455310	-0.60982194896129
H	6.97409873352401	-0.52668194426863	0.37630067615136
C	6.95488378698761	-0.21978012397188	5.48328258740789
H	6.14334327254108	0.58907575884284	3.65125741909905
C	6.09187626609828	-4.14672533421528	3.84918586846001
C	6.96366086912579	-2.62347614384821	5.61419348834982
H	6.79744410149836	-5.49757244676634	0.41753661793606
C	7.55868816656861	-3.74533462207350	-0.59058790933418
H	5.26111050743516	-5.39749337696241	2.31228555860731
H	4.37069289108346	-3.88946120870356	2.55939396516995
H	8.18894701011569	-1.83486364929068	-1.38243124437462
C	7.25094396119021	-1.39014607837418	6.18367705795737
H	7.17560445144814	0.75877133665418	5.91523195944818
H	5.50502657397927	-4.66813463917030	4.62388747881299
H	7.05951164885795	-4.67713427766727	3.80362599922850
H	7.19618048000170	-3.53811411484839	6.16780823841693
H	8.08693089186053	-4.32397410727486	-1.35227536017239
H	7.70609556897141	-1.33997744695428	7.17555850610238

**XYZ coordinates of p2az2 in S<sub>0</sub>**

O	2.13526689353421	5.96468785168353	0.09677028052428
C	1.12960916027353	5.30850195975191	-0.07552523885798

C	1.14002628884160	3.82572682309362	-0.02279327030772
C	-0.04802837020063	3.07251155523324	-0.18782880075137
C	-0.02260080170036	1.64059096640221	-0.10691064016825
C	-1.28680154837465	0.96706586860859	-0.10952319508116
N	-1.42482940868568	-0.38647093671305	0.33259736709430
C	-1.41251243238503	-0.50242379668864	1.75280026467730
C	-1.52837828880880	0.67636766466821	2.52257996550087
C	-1.43045980005616	0.66943854841929	3.90880886621155
C	-1.23884799962871	-0.52526710504637	4.59225490058426
C	-1.16288947278022	-1.69691797697895	3.84903006770760
C	-1.23277971572109	-1.71634136502162	2.45372367887865
C	-1.18022582622135	-3.03790573100335	1.76251251015777
C	-2.44205173021557	-3.25997181267393	0.93086084127595
C	-2.36254809626462	-2.61091525826101	-0.42080510467070
C	-1.85086666949221	-1.31101148871090	-0.65587166397790
C	-1.74522546730911	-0.88989366389801	-1.99955917144160
C	-2.16010069264464	-1.67304272185370	-3.06485707880316
C	-2.68670680522756	-2.93931461273019	-2.83381140003534
C	-2.76092399642666	-3.38357597442116	-1.52066885116581
C	-2.44867081881348	1.66918819305737	-0.38300057987634
C	-2.44162185340245	3.05533343821202	-0.57623224462907
C	-1.26241584561372	3.75876289940573	-0.43184875825896
C	-1.29813602019820	5.23633320701060	-0.53442528823838
N	-0.09869684565046	5.91478488614732	-0.33743607992238
C	-0.16107478268159	7.36388482333012	-0.41799533464045
O	-2.31658016175176	5.85153748850562	-0.77180161516873
C	1.26348323325994	1.01620983417780	-0.02670058327364
N	1.44763396149397	-0.37559349361673	-0.29933790698993
C	1.45245056264712	-0.66441551191856	-1.69484145705044
C	1.54993549304476	0.41244122006231	-2.60362215134843
C	1.46886931451265	0.23088303195755	-3.97924289925401
C	1.31108926715469	-1.04379052457556	-4.51034679017853
C	1.24842470788035	-2.11542532542107	-3.62787835351908
C	1.30271655652320	-1.95912400700920	-2.24071048867539
C	1.25778739464877	-3.18212248143134	-1.38738604729774
C	2.51663913902325	-3.28687261889534	-0.52901963863587
C	2.42978131429483	-2.46808915801302	0.72712179259589
C	1.89404131363571	-1.15848141878310	0.79683181546723
C	1.78117824644007	-0.57278511147418	2.07696552753798
C	2.21546230576292	-1.20456209577754	3.23120606228339
C	2.76953775598664	-2.47818435132501	3.16051996217222
C	2.84844811206506	-3.08492988941389	1.91451684807449
C	2.39931221886749	1.78574281427410	0.16208922287637
C	2.34283103246411	3.18358837217480	0.19647572286464
H	-1.69421880152355	1.63523741827936	2.03678127034463
H	-1.51854461598020	1.61489753640971	4.44935040646065
H	-1.16127406517828	-0.54881309963094	5.68117623050305
H	-1.02115432336339	-2.65242341456795	4.36108709105652
H	-1.07858462219089	-3.82824353423491	2.51980449079390
H	-0.28382939501483	-3.10534367307708	1.12476085678034

H	-3.31173896226175	-2.89088148604270	1.50166771718733
H	-2.61116685953577	-4.33659946293478	0.77943009549916
H	-1.29826930095956	0.07644448098412	-2.22611443027689
H	-2.03990068031845	-1.28874887459496	-4.07992753881895
H	-3.01604463530857	-3.57614256888382	-3.65728132894050
H	-3.14633301642238	-4.38653535631241	-1.31624700350146
H	-3.39110499913532	1.11772125412558	-0.38252763506840
H	-3.36124172916426	3.60970949903566	-0.77394267802594
H	-0.51329835225624	7.67080028834452	-1.41265085519326
H	0.84269336921607	7.75621816254036	-0.22794307150838
H	-0.87292394718533	7.75065327623739	0.32424220454038
H	1.68711734461417	1.42791145253215	-2.23933790452810
H	1.54256590706020	1.10361833648620	-4.63250360620555
H	1.24698298908252	-1.20419820136220	-5.58853805020898
H	1.12797490270079	-3.12965389330966	-4.01798432213402
H	1.16493466768908	-4.06401290985280	-2.03700671466044
H	0.35910091921241	-3.17138282187659	-0.74958604549343
H	2.68911904607944	-4.33363391420159	-0.23716336510005
H	3.38758201899702	-2.99292616086529	-1.14022789184359
H	1.31185083982997	0.40358317998364	2.18074718143190
H	2.08890349272906	-0.69718558771456	4.18981260907703
H	3.11498242277566	-2.99784297527295	4.05649263119172
H	3.25305616456920	-4.09824007129008	1.83776813164845
H	3.36039090488652	1.27156623071746	0.22714324664446
H	3.24182249425560	3.78829387582885	0.33103321408302

### XYZ coordinates of p2az2 in S<sub>1</sub>

O	2.18962530762972	5.99546591452491	-0.26061341248904
C	1.16162740916236	5.33115132272011	-0.27081359123526
C	1.16427396434662	3.86970798215564	-0.19527546680893
C	-0.04799825283834	3.13507656505289	-0.18763410540685
C	-0.02492300553102	1.69138788083619	-0.09803359640935
C	-1.28307033542633	1.03896598965275	-0.00244086307853
N	-1.38889002037658	-0.36672082668556	0.33706682853352
C	-1.33398878841186	-0.62153438180928	1.72569119757438
C	-1.34457385672688	0.50590528535463	2.59168761399655
C	-1.23302109707490	0.39078427631380	3.96628888731016
C	-1.09177021489958	-0.86266607591081	4.55481775958124
C	-1.09043266081546	-1.97952415121438	3.72858820545820
C	-1.20915616463649	-1.90042436377175	2.33943960201273
C	-1.26026906700631	-3.19073225612871	1.59124226659834
C	-2.47566991381356	-3.25618925983131	0.67910307232432
C	-2.26782312475460	-2.53745878573720	-0.61779835358028
C	-1.76883675441181	-1.20871053075539	-0.72652039174804
C	-1.68979579596560	-0.65129582306130	-2.02925409933441
C	-2.03975721002515	-1.35846892967732	-3.16596789519027
C	-2.48909850889339	-2.66992764409935	-3.05754459752146
C	-2.59485568593310	-3.22866046782569	-1.78746833926225
C	-2.48987369131121	1.74848228834052	-0.09770573240881

C	-2.50015728498016	3.12091544916576	-0.24959817120915
C	-1.28352311019316	3.82363585082578	-0.26996912383201
C	-1.31941717630832	5.28101160969137	-0.38000866174386
N	-0.09199052015726	5.94261510598295	-0.36294081303028
C	-0.15063986235465	7.38781077634977	-0.45347851847165
O	-2.35718311135214	5.92242371600824	-0.47778316720719
C	1.25327308598323	1.07228453247581	-0.11543658207544
N	1.40483260944880	-0.35942118744421	-0.28754053051969
C	1.36345088622270	-0.77561365384073	-1.63743610300051
C	1.34503022898295	0.24284008536644	-2.62916979965363
C	1.24332277474511	-0.03512799360381	-3.98104525296655
C	1.14210841298133	-1.35235402393665	-4.41945518696648
C	1.16857686972900	-2.36454472509360	-3.46835115310443
C	1.27744876468346	-2.12013416500045	-2.09770652249809
C	1.35712563978562	-3.31110402014187	-1.20239114038895
C	2.57149689276695	-3.23896713618374	-0.28966356887175
C	2.34407969355568	-2.37747494001565	0.91359479764278
C	1.80813393857627	-1.05926615439954	0.86639802889251
C	1.71355192700475	-0.35444279580033	2.09472559047211
C	2.08470071640621	-0.91191253933453	3.30558119288716
C	2.57124484091050	-2.21379335154601	3.35100108927493
C	2.69185754417539	-2.91572125539371	2.15546824213526
C	2.43630302913245	1.82711666366646	-0.10879005883927
C	2.40238116047290	3.20721890307439	-0.12852979614523
H	-1.45211285300592	1.50021842350087	2.16826465079195
H	-1.25684623459326	1.29672829339769	4.57553702548748
H	-0.99392926233280	-0.97231614440848	5.63684803609516
H	-0.99107744555284	-2.97348633707614	4.17176911326573
H	-1.28811831482851	-4.01327552440305	2.31964943375537
H	-0.33833015293229	-3.33624435848717	1.00798058553537
H	-3.34746533832342	-2.84019262903208	1.21481050535604
H	-2.72584064482402	-4.30339661966753	0.45536018784101
H	-1.36171193877689	0.37775395176991	-2.13813364107654
H	-1.95283069548287	-0.87228003102586	-4.13913623388275
H	-2.76717657079224	-3.24800809402997	-3.94114188530700
H	-2.96509931225395	-4.25206982241319	-1.68339387689517
H	-3.42536850743114	1.18842461611195	-0.02836266061052
H	-3.42682755661738	3.69016453933974	-0.33231659195385
H	-0.64092710390128	7.68922084228506	-1.39025154727430
H	0.87518590065503	7.76784212180520	-0.41441476751801
H	-0.74836060497880	7.79381479438506	0.37498565975516
H	1.42118090174833	1.28263684899431	-2.32499153437800
H	1.24339354964984	0.79395231274716	-4.69178086071354
H	1.05294215455825	-1.59031927514847	-5.48142102762635
H	1.09923332445531	-3.40593540521098	-3.79226940646800
H	1.40586546895105	-4.21333592290726	-1.82805132913837
H	0.43737397805603	-3.40725496151481	-0.60570410441023
H	2.84645104645845	-4.24605681019334	0.05602617390039
H	3.43420382690682	-2.86833301839344	-0.87147241921793
H	1.35651457969162	0.67067256120181	2.08252182559771

H	1.98476784986064	-0.31677179267650	4.21487627244542
H	2.86626223320104	-2.67533510214904	4.29558632964083
H	3.09061142848900	-3.93355988742359	2.17178305207676
H	3.38960150086977	1.29337202810228	-0.10928414798352
H	3.31070431057136	3.81076164320454	-0.11820259678589

### XYZ coordinates of p2az2 in T<sub>1</sub>

O	2.02842501382183	5.99337280391801	0.23853664928419
C	1.04178927772130	5.30648937678877	0.02977670605486
C	1.09146057804070	3.83793074500063	0.04979074344039
C	-0.06610745515066	3.06610180012379	-0.15697812240518
C	-0.00060153725242	1.62714993545272	-0.10636023822560
C	-1.24333920893421	0.92019070693060	-0.24125873602436
N	-1.42519124019149	-0.39698778846698	0.25490640952259
C	-1.31594453464893	-0.51845259451642	1.66465933538025
C	-1.37917256051638	0.67891538756586	2.41356729733479
C	-1.17740963468051	0.69651299390728	3.78476896052925
C	-0.94197090482545	-0.49372458848383	4.46703020265746
C	-0.95398453227839	-1.68606446080492	3.75163398935434
C	-1.14007461458885	-1.73404854482687	2.36911027336122
C	-1.26846700822184	-3.07134373422487	1.71626446012861
C	-2.60490938904425	-3.16405244679294	0.97836951901573
C	-2.51791001152294	-2.57455632115700	-0.39775646243757
C	-1.88763828805379	-1.33371933676460	-0.68911040270400
C	-1.71479899720289	-0.97656772306681	-2.04783662697856
C	-2.22046968205341	-1.74839185186928	-3.08212221043347
C	-2.88564473591693	-2.93493593792191	-2.79507909501224
C	-2.99966153551412	-3.33446329142003	-1.46472555966048
C	-2.44064955132153	1.60413445972626	-0.64419654292546
C	-2.47147907115702	2.96598770900014	-0.73277148707859
C	-1.29558446191525	3.71718829136969	-0.45313013978797
C	-1.37211240449780	5.17476705244216	-0.50814237205717
N	-0.19852342906543	5.88116205978086	-0.24828767182900
C	-0.30222391021407	7.32740656282695	-0.29253352300298
O	-2.40660427108333	5.77610078074523	-0.76123732825866
C	1.27490877496559	1.03813330350501	-0.00350117655147
N	1.47420839030777	-0.35862667472425	-0.26871101222274
C	1.52054887240463	-0.64726071527974	-1.66209728050128
C	1.66757849700012	0.43026571418450	-2.56456954589973
C	1.62613483275550	0.25287260180281	-3.94173260061205
C	1.44566671669911	-1.01621251303599	-4.48227595435187
C	1.31839816218481	-2.08746505744154	-3.60668033842984
C	1.33838817916306	-1.93477450464815	-2.21708615007121
C	1.20965418177711	-3.15485799939344	-1.36801529651808
C	2.42746218656294	-3.32579996210394	-0.46621864704881
C	2.37347153990598	-2.48242162291454	0.77635362507608
C	1.91578420077429	-1.14084112585906	0.82797372483607
C	1.89351056508167	-0.51759960134624	2.09659623433130
C	2.31607319696300	-1.15181840074233	3.25320805453382

C	2.77225983249986	-2.46480490919903	3.20200123742587
C	2.77846824848471	-3.10058084523060	1.96822359529923
C	2.42487625841849	1.84199880070201	0.20214358630736
C	2.33996140390717	3.21108816825058	0.26163527945472
H	-1.61109275788130	1.61498882617092	1.90812962579322
H	-1.22792640057948	1.64776304989572	4.31876232694412
H	-0.78100919492590	-0.49920528831669	5.54713758938857
H	-0.80648099557886	-2.63207500621372	4.27831819097069
H	-1.20276482930368	-3.84814983015515	2.49076549408232
H	-0.43414603940949	-3.25756992762649	1.02145586409575
H	-3.38390664940175	-2.66543735158484	1.58111889014094
H	-2.91681634295834	-4.21414095239204	0.88062047670932
H	-1.14134010418394	-0.08233243437415	-2.28814604178827
H	-2.05678640162284	-1.42813183382780	-4.11271860666401
H	-3.28324317286024	-3.56418013916163	-3.59416958243349
H	-3.47812734834256	-4.28991013019625	-1.23333493456461
H	-3.34614250575910	1.01055675146461	-0.78662532009073
H	-3.38039556191674	3.51360977320027	-0.98535492073224
H	-0.63512540124198	7.65222677001262	-1.28858780423412
H	0.68411839705991	7.74228340930124	-0.06203366461863
H	-1.04877879706882	7.67373577695248	0.43591979560470
H	1.81411712026487	1.43928271721608	-2.18573348578283
H	1.74370507381041	1.12439805459837	-4.59006540357883
H	1.40957162155948	-1.17110498317038	-5.56266332246764
H	1.17424596283450	-3.09599809906153	-4.00409863374153
H	1.09554651430300	-4.03189272071428	-2.02119708497043
H	0.29289141732847	-3.10226944657856	-0.75860454419435
H	2.51968037867089	-4.37744354687791	-0.15518939108626
H	3.33459929660783	-3.10258719268515	-1.05462706905606
H	1.51807944431756	0.50096953068825	2.17963622068892
H	2.26953405259649	-0.60895257930091	4.19984155022323
H	3.11003361411996	-2.98587847678687	4.10009556940922
H	3.11926249113965	-4.13812659084704	1.90441049970732
H	3.38682273627167	1.33487686242605	0.30521566570050
H	3.21331844256169	3.84329830615650	0.42758668824640

### XYZ coordinates of m2azb in S<sub>0</sub>

O	-2.200313	1.847396	2.258499
O	0.939713	0.244021	5.103422
N	-0.630050	1.055568	3.674443
C	0.435380	-0.537510	1.611472
C	0.379922	-1.276006	-0.704887
C	-0.685623	-0.446465	-0.937748
C	-0.666478	0.297845	1.349380
C	1.009028	-0.580546	2.896116
C	0.969835	-1.341335	0.573827
C	-1.216924	0.345058	0.092866
C	2.082580	-1.399741	3.146182
C	-1.241065	1.128514	2.428327

C	0.464155	0.254525	3.990507
C	2.607325	-2.203715	2.122368
C	2.066088	-2.177688	0.863501
C	-1.204524	1.892703	4.715997
H	-2.064008	0.993796	-0.095807
H	2.516658	-1.424104	4.138632
H	2.487697	-2.806961	0.087584
H	-0.654864	1.711770	5.634211
H	-1.131403	2.941660	4.428472
H	-2.258718	1.648675	4.843771
H	0.772305	-1.881670	-1.514133
N	3.711628	-3.062583	2.395651
C	4.990876	-2.588297	2.133964
C	3.440799	-4.335592	2.882019
C	6.116628	-3.418929	2.318522
C	5.165719	-1.269304	1.679890
C	4.488956	-5.248604	3.124519
C	2.111185	-4.719872	3.128759
C	7.384264	-2.890304	2.021344
B	5.933209	-4.846294	2.830786
C	6.429362	-0.794323	1.407642
H	4.315191	-0.615375	1.543227
C	4.156008	-6.520923	3.619176
C	1.834876	-5.978479	3.614702
H	1.294444	-4.036007	2.942445
C	7.555498	-1.601756	1.571518
H	8.242825	-3.539930	2.160401
C	7.133306	-5.838763	3.028577
H	6.541604	0.227206	1.061302
C	2.855991	-6.895085	3.867698
H	4.969651	-7.215987	3.801716
H	0.802423	-6.252669	3.801554
H	8.543248	-1.216014	1.349782
C	7.467023	-6.749901	2.015843
C	7.880086	-5.839757	4.213634
H	2.624091	-7.881686	4.250431
C	8.523859	-7.632821	2.198894
C	6.682966	-6.765134	0.734574
C	8.931498	-6.737530	4.368898
C	7.540770	-4.876836	5.315226
C	9.267498	-7.645608	3.373549
H	8.774866	-8.330318	1.403974
H	5.632054	-7.007998	0.919180
H	6.700029	-5.784331	0.249362
H	7.080038	-7.497541	0.029967
H	9.502674	-6.727757	5.293427
H	7.626179	-3.840272	4.975475
H	6.509066	-5.013986	5.653689
H	8.197841	-5.005084	6.176727
C	10.381070	-8.630982	3.565690

H	9.989698	-9.611796	3.853836
H	10.954122	-8.768998	2.646006
H	11.068287	-8.308640	4.350049
N	-1.264881	-0.382258	-2.238426
C	-0.715715	0.506449	-3.155184
C	-2.362249	-1.191962	-2.504935
C	-1.246720	0.612294	-4.458390
C	0.375582	1.310444	-2.781595
C	-2.990932	-1.155476	-3.767707
C	-2.849461	-2.057175	-1.509635
C	-0.643634	1.517831	-5.347576
B	-2.455525	-0.231208	-4.859448
C	0.929418	2.187826	-3.687378
H	0.788554	1.252580	-1.783809
C	-4.102042	-1.989462	-3.977617
C	-3.941993	-2.856567	-1.763333
H	-2.375863	-2.103787	-0.538470
C	0.428304	2.299448	-4.984820
H	-1.057904	1.587239	-6.348559
C	-3.105580	-0.150804	-6.286305
H	1.769448	2.799550	-3.377150
C	-4.583485	-2.831147	-3.002170
H	-4.579616	-1.950812	-4.951716
H	-4.302723	-3.514168	-0.980061
H	0.876020	2.991850	-5.687510
C	-4.047287	0.845082	-6.583746
C	-2.753819	-1.069631	-7.283366
H	-5.442912	-3.464188	-3.187146
C	-4.614032	0.905346	-7.850960
C	-4.443978	1.840817	-5.531767
C	-3.336978	-0.982757	-8.543152
C	-1.741689	-2.140793	-6.993654
C	-4.273393	-0.003088	-8.846351
H	-5.341314	1.683137	-8.068507
H	-4.870582	1.340414	-4.656844
H	-3.578820	2.409703	-5.178407
H	-5.183591	2.549204	-5.908054
H	-3.049569	-1.698209	-9.309046
H	-0.796530	-1.707987	-6.651411
H	-2.089455	-2.808453	-6.199298
H	-1.535425	-2.746772	-7.877218
C	-4.918571	0.061278	-10.198339
H	-5.907203	-0.408236	-10.182650
H	-5.056482	1.094375	-10.525255
H	-4.320873	-0.457104	-10.950326

**XYZ coordinates of m2azb in S<sub>1</sub>**

O	-2.04229280531137	2.12254683363179	2.39049954403150
O	1.08730142556877	0.34968953483737	5.17714975334711

N	-0.47712587346383	1.22575301081431	3.75926463131322
C	0.46057466620403	-0.38399743598754	1.68925434619624
C	0.31971490254928	-1.12486958080889	-0.62845115127944
C	-0.74124155139727	-0.24992606777251	-0.82803620028456
C	-0.61472233841896	0.49093605535283	1.45203462254823
C	1.06487800924125	-0.44929358591969	2.96442254120178
C	0.94104915197449	-1.21428871963214	0.62638954587058
C	-1.21418303807768	0.55378811048466	0.18818712946314
C	2.13639324266510	-1.32541207242180	3.19722117522266
C	-1.11330811670779	1.33830583442893	2.52465084751474
C	0.59013368328937	0.38006636420217	4.05487476588265
C	2.57377302170744	-2.11379158829575	2.16061375096455
C	2.01716575351933	-2.08943217041413	0.88928742814487
C	-0.99284916531037	2.07920132749370	4.81242626269727
H	-2.04121921345403	1.23391813877697	0.03002802380135
H	2.58151581422297	-1.35789338109724	4.18317247730861
H	2.39855710393653	-2.73173178823761	0.10518682296638
H	-0.41451194743356	1.88666906033000	5.71097051789646
H	-0.90984907047737	3.12555092360677	4.51647998167923
H	-2.04915098786586	1.86564423039308	4.97890677914482
H	0.66217912339652	-1.74146222583429	-1.45105650691520
N	3.67969104051815	-3.03332199641201	2.39360948693353
C	4.95654092374816	-2.58580203752421	2.15368260725026
C	3.38271391351852	-4.30815292806740	2.81147498424230
C	6.07624821157289	-3.44354175262785	2.30736543745703
C	5.14066899604362	-1.24677598054770	1.74267103418952
C	4.40417480700956	-5.27328417364393	3.00633972462323
C	2.03181192900158	-4.64872607398011	3.04634424656863
C	7.33602047079662	-2.92605519136827	2.03692707552075
B	5.87414405554908	-4.90215758982031	2.74993155356253
C	6.40955779354437	-0.77514920698638	1.49070640921523
H	4.28509398083824	-0.59851962883083	1.63029320689066
C	4.03096483113908	-6.54072137662289	3.43297165564665
C	1.70817442358305	-5.91877979320665	3.46846016743652
H	1.25949186212265	-3.90950963719762	2.89848795262965
C	7.51644049114896	-1.60601510263148	1.63364602531321
H	8.19271633790988	-3.58242288685655	2.14877924951715
C	7.04895933694425	-5.91570540083693	2.91662568741686
H	6.53778854192340	0.25389938599706	1.17882709713511
C	2.69975481329723	-6.87470875856758	3.66578719054700
H	4.81131675839679	-7.27941373614623	3.58322387363673
H	0.66939534283829	-6.16654688132742	3.64781174615168
H	8.51150123406362	-1.22799389519755	1.43279958122741
C	7.39903225876943	-6.76888156811355	1.86027268757908
C	7.76577939355628	-5.98275057638331	4.11923918052065
H	2.43744762831332	-7.87178210295656	3.99809652417009
C	8.44806977666460	-7.66517406613761	2.02041600088796
C	6.65169438076815	-6.70115391274833	0.55903996803174
C	8.80785138847626	-6.89323092070002	4.24732023333588
C	7.40204934049537	-5.08045517416533	5.26359141081242

C	9.16385577254109	-7.74576261312828	3.20933012399368
H	8.71635607330877	-8.31690406312421	1.19368393029770
H	5.58374467276802	-6.89303080622323	0.70212997439447
H	6.73876788786358	-5.71036874998744	0.10174024555364
H	7.02754328983560	-7.43145947114700	-0.15822026968305
H	9.35755103772345	-6.93761903928507	5.18324725433495
H	7.47283150002557	-4.02603211790729	4.97918105863931
H	6.37239269104628	-5.25215869821503	5.59301440915443
H	8.05518877734687	-5.23784769493539	6.12245692839641
C	10.26976680589218	-8.74324759114672	3.37483381717083
H	9.87613189462490	-9.70517006142117	3.71755707378479
H	10.78972812431794	-8.92208726123091	2.43184945514030
H	11.00195064191810	-8.40865102585397	4.11169602270959
N	-1.34407979749682	-0.20103880011713	-2.12811107927350
C	-0.82403918849476	0.68303532083173	-3.05787192482161
C	-2.37249053818210	-1.08576404759087	-2.40456525258477
C	-1.32075216220863	0.72168015372369	-4.38012810064068
C	0.21437823199007	1.55557689979087	-2.68094156768875
C	-2.95089343949957	-1.14733888619907	-3.69222922842209
C	-2.84895801840505	-1.93603046984082	-1.38874824098998
C	-0.75211757986564	1.64474628200084	-5.27581418273573
B	-2.44135904430164	-0.22557237814483	-4.79497063914668
C	0.73696564058058	2.44209609243885	-3.59343127036194
H	0.59735941528388	1.53826229363131	-1.67007655559660
C	-3.99103409841710	-2.06853772199681	-3.90931364532378
C	-3.87117183662561	-2.81857940264065	-1.64961019639555
H	-2.41941072583205	-1.89067877164927	-0.39767793945147
C	0.25989326529774	2.49783454563118	-4.90558400429785
H	-1.14265450098038	1.66658447220159	-6.28866369062829
C	-3.02734320556712	-0.25576635185773	-6.25355612705897
H	1.53149242279780	3.11009522691545	-3.27845959381510
C	-4.45551238148520	-2.89770573698986	-2.91643705877256
H	-4.42753661610632	-2.10678661536324	-4.90269465800824
H	-4.22700010727957	-3.45874636419402	-0.84943108759743
H	0.68026612278134	3.20337510907745	-5.61251042476399
C	-4.13631208296355	0.53064696980786	-6.59421758566012
C	-2.44893033695160	-1.06958599729008	-7.23660243281006
H	-5.26089154069380	-3.59740799824138	-3.10625928591048
C	-4.64308690952996	0.49199112241605	-7.88825859275987
C	-4.76800166734690	1.41771911220387	-5.56037152944067
C	-2.97771837634909	-1.08862767034153	-8.52243304508946
C	-1.25683500210511	-1.91778940877366	-6.89748568808482
C	-4.07887247195838	-0.31551645574823	-8.86815832841386
H	-5.50085067170270	1.11083287932711	-8.13895045888810
H	-5.11423484895846	0.83558562255594	-4.70107856610185
H	-4.04870207524564	2.14716526997762	-5.17578692951489
H	-5.62092111437847	1.96401220430974	-5.96639623399933
H	-2.51648002238158	-1.72284755399099	-9.27521364538647
H	-0.42207974854806	-1.30131359449172	-6.55024150463679
H	-1.49004095997420	-2.61667262445017	-6.08826065552482

H	-0.91771646329238	-2.49618388190209	-7.75865566418322
C	-4.65948657217002	-0.37188339245438	-10.24962370842433
H	-5.45223909962193	-1.12451891079389	-10.31130441328083
H	-5.09815855498161	0.58604915467489	-10.53708828296710
H	-3.90151096095169	-0.63544312717077	-10.99016990159997

**XYZ coordinates of m2azb T<sub>1</sub>**

O	-2.54951330176057	1.58331888064448	2.56180702208906
O	0.60347168633341	-0.12246855335508	5.36062181057820
N	-0.97368996417067	0.73666220688168	3.95391146204095
C	0.21238745778552	-0.61258048350829	1.81724567033167
C	0.27124362966997	-1.14018677144185	-0.55727194555026
C	-0.88762863020624	-0.32916527243665	-0.74993335928529
C	-0.92659278947530	0.18188910761319	1.59447254846242
C	0.75258472576064	-0.73390668751785	3.10008702404344
C	0.82618152577448	-1.29660737288804	0.71820944406512
C	-1.47632016340529	0.31630423794314	0.29425632712858
C	1.90647581988724	-1.53506676116205	3.32885411583842
C	-1.55472092488588	0.88785586538229	2.70164435194084
C	0.15030091518294	-0.03565539586011	4.23034964929858
C	2.48573753701472	-2.18624993820688	2.28297778783354
C	1.96461358695073	-2.07454615495949	0.96938906573124
C	-1.61185066158658	1.45231844574981	5.04504783477310
H	-2.35920906119325	0.92792569040803	0.16197469366060
H	2.29431397320000	-1.61768202774063	4.33562471051799
H	2.45152109704150	-2.60957252844194	0.16288985750873
H	-1.08298229460741	1.20752850410174	5.96095071929363
H	-1.57316934743351	2.52574397565540	4.85710281450980
H	-2.65956930099574	1.16024431114161	5.11336552949776
H	0.69999764960360	-1.65318563797101	-1.40937800940606
N	3.61764409496858	-3.02745364997578	2.47888402095956
C	4.84259335705886	-2.56034220198932	2.02758329753985
C	3.43005219762183	-4.28923464914890	3.03855694675595
C	5.99163491243454	-3.37941529629052	2.06957721572647
C	4.94435735500745	-1.24217899530982	1.54436096577184
C	4.52126143264882	-5.16908065866477	3.20010357684243
C	2.14282094045821	-4.70338185076606	3.42055510845985
C	7.19508971229251	-2.85573163580840	1.57440172936538
B	5.90622744981716	-4.77215783678914	2.69285297814657
C	6.14819007835052	-0.77302194316404	1.06599987950967
H	4.08766488719487	-0.58255487350004	1.56470828049745
C	4.28062272541299	-6.42342082409728	3.78605668689939
C	1.95476184063427	-5.94459707752200	3.98522815923197
H	1.29111560783260	-4.05372892819955	3.27660427183512
C	7.28658444713411	-1.57866457108777	1.06562565980729
H	8.07249663133295	-3.49393810905314	1.61089849308021
C	7.14460502012863	-5.72950580807536	2.79936784865321
H	6.20547670742206	0.24592415082925	0.69953715092909
C	3.02512491769432	-6.81776852612269	4.18460617523868

H	5.12907574314702	-7.08887999454433	3.91028254538314
H	0.95273110163519	-6.24037457792962	4.27558380835243
H	8.22794529979080	-1.19640053959281	0.68950879340603
C	7.35417861130704	-6.72803265222457	1.83777396538083
C	8.05442887092402	-5.60581119530175	3.85808576202139
H	2.86325281368090	-7.78974452487380	4.63488417236030
C	8.45002531902363	-7.57564336518212	1.94725598995346
C	6.39784295451436	-6.87671036227061	0.68906778063367
C	9.13921311401531	-6.47166634345781	3.94295202821284
C	7.85524242494650	-4.54108980256337	4.89904851829753
C	9.35328636435417	-7.46701055267360	2.99781238110697
H	8.60421248822132	-8.34110882022083	1.19124124801213
H	5.39191965985971	-7.12238944480334	1.04279717070335
H	6.31364773449431	-5.94518268215954	0.12073034173767
H	6.71549071390012	-7.66299313113748	0.00251243868365
H	9.83695738759078	-6.36512331929920	4.76938655879556
H	7.87028802167038	-3.54294270620971	4.45127489904664
H	6.88589850898288	-4.64893646658044	5.39549336987855
H	8.63151903277476	-4.58006465704377	5.66460791622741
C	10.50907900523420	-8.41379071588331	3.12120877256811
H	10.21293749332149	-9.32549593110050	3.64983460753838
H	10.88436250687731	-8.71474374256016	2.14082948803253
H	11.33353564104656	-7.96613197149494	3.67958723460457
N	-1.42177153132268	-0.25737763221671	-2.06265405860104
C	-0.63764127090734	0.36024508330569	-3.02763554156675
C	-2.65049519289491	-0.86195801618466	-2.34037487386516
C	-1.01365791220555	0.35190265873936	-4.38782810726001
C	0.53203123939078	1.03714948029837	-2.63371600786343
C	-3.17680366457019	-0.83863037476917	-3.64974546727035
C	-3.35022816513157	-1.53430599764704	-1.32545470531712
C	-0.15538430265916	0.95792972843750	-5.31431288095743
B	-2.36700622079358	-0.23216202911066	-4.79576891030560
C	1.35334636556618	1.60790419865098	-3.58276413811258
H	0.78184108750750	1.13793854668937	-1.58646511776276
C	-4.41885224920247	-1.45195067599676	-3.87733330945587
C	-4.56499554251207	-2.12406964965947	-1.59564275698000
H	-2.94561725977980	-1.59770805692950	-0.32578537525865
C	1.02653203554316	1.56099466026736	-4.93614377359259
H	-0.45441943762465	0.94921078680745	-6.35773945852684
C	-2.88560255958866	-0.20005339901147	-6.27483426584862
H	2.25327775486009	2.11856850451240	-3.25908184682789
C	-5.12058098523864	-2.08003473964562	-2.87388322425699
H	-4.81326800443701	-1.42643399139850	-4.88815641811245
H	-5.08831125228767	-2.63266711226776	-0.79378190547331
H	1.67577540092117	2.01890092366642	-5.67266841861663
C	-3.64960258711617	0.88180334963118	-6.73270555196589
C	-2.58954900358455	-1.24615053333736	-7.15908644642336
H	-6.07863734574873	-2.54537530392004	-3.07185691459844
C	-4.10243660973092	0.90121693542121	-8.04683152960928
C	-3.96879644982272	2.01838316822042	-5.80468935155046

C	-3.05559682855971	-1.19793822199373	-8.46741569515364
C	-1.77223023230815	-2.41420258326930	-6.68772704906555
C	-3.81815841370834	-0.13233861038039	-8.93069654921616
H	-4.69215186366776	1.74682399408613	-8.39041358804556
H	-4.48589951752183	1.66216857987899	-4.90852698059142
H	-3.05606074634440	2.51850045009222	-5.46580441435424
H	-4.60215239172758	2.76500822403825	-6.28580904473043
H	-2.81724482803956	-2.01403065151538	-9.14435476838367
H	-0.79247883338453	-2.08961705662284	-6.32348489926717
H	-2.26401583114591	-2.92898202020212	-5.85628093824628
H	-1.61143486692886	-3.14110066266795	-7.48523009223577
C	-4.34335181743700	-0.11444272652348	-10.33476921053705
H	-5.30003403620303	-0.64233495138634	-10.40003306996281
H	-4.50885470691334	0.90585027918984	-10.68594329313150
H	-3.65384211398291	-0.60528019146456	-11.02470122218818

### XYZ coordinates of m2cz in S<sub>0</sub>

O	-1.509533	1.500717	2.390298
O	1.551235	-0.256862	5.229022
N	0.019902	0.629097	3.802565
C	1.448819	-0.421914	1.620589
C	1.675252	-0.737212	-0.778875
C	0.519839	-0.019200	-0.983493
C	0.265651	0.301989	1.390687
C	1.920811	-0.630646	2.929135
C	2.176045	-0.941534	0.521802
C	-0.186580	0.511593	0.112660
C	3.084220	-1.323949	3.145952
C	-0.489072	0.863531	2.530262
C	1.178589	-0.088348	4.089158
C	3.806106	-1.854972	2.059914
C	3.352655	-1.673326	0.773763
C	-0.745194	1.186090	4.906702
H	-1.084253	1.097552	-0.042249
H	3.446312	-1.445623	4.159301
H	3.903385	-2.103975	-0.054455
H	-0.247206	0.913434	5.831735
H	-0.801311	2.270068	4.807442
H	-1.760783	0.791239	4.886720
H	2.202094	-1.157530	-1.627845
N	0.042054	0.199321	-2.284205
C	0.780700	0.700633	-3.349058
C	-1.241339	-0.089283	-2.732085
C	-0.040080	0.740824	-4.492981
C	2.092184	1.156863	-3.378173
C	-1.329353	0.233247	-4.099952
C	-2.310912	-0.647870	-2.044331
C	0.472438	1.229785	-5.689861
C	2.578404	1.638754	-4.581912

H	2.713353	1.147615	-2.491218
C	-2.519443	0.008910	-4.783564
C	-3.484542	-0.860176	-2.747601
H	-2.234730	-0.916809	-0.998224
H	-0.149193	1.266753	-6.577328
C	1.782212	1.672205	-5.729227
H	3.599198	1.999555	-4.631367
C	-3.593372	-0.533418	-4.101293
H	-2.600898	0.250691	-5.837281
H	-4.335256	-1.292546	-2.233946
H	2.195724	2.054186	-6.654874
H	-4.527319	-0.713180	-4.620113
N	4.997403	-2.554608	2.299985
C	6.217917	-2.316456	1.679067
C	5.153072	-3.607406	3.193639
C	7.168818	-3.225707	2.181844
C	6.562703	-1.343210	0.749876
C	6.488969	-4.050045	3.147946
C	4.208503	-4.222223	4.005370
C	8.481104	-3.170517	1.724637
C	7.875843	-1.308167	0.312227
H	5.837244	-0.626085	0.386886
C	6.888565	-5.112255	3.952081
C	4.632108	-5.276159	4.796986
H	3.175578	-3.897846	4.020841
H	9.222630	-3.865098	2.102833
C	8.826765	-2.214503	0.786831
H	8.169805	-0.557782	-0.412485
C	5.957440	-5.716497	4.777222
H	7.914332	-5.462525	3.928826
H	3.915971	-5.769879	5.443403
H	9.844853	-2.160565	0.420318
H	6.254394	-6.543234	5.411273

### XYZ coordinates of m2cz in S<sub>1</sub>

O	-1.16780566490347	2.05366806214075	2.28866872886845
O	1.87330994921764	0.27381214612780	5.16889044611644
N	0.36130506855964	1.15623310925966	3.70661462414753
C	1.58905197236641	-0.18649468279611	1.59822590630898
C	1.69130061918410	-0.72510412670971	-0.78231265725005
C	0.58401286796947	0.09505910618462	-0.96472846143361
C	0.46564911479850	0.63287342187327	1.35299456793265
C	2.09544601108616	-0.33113387697301	2.90197492992531
C	2.22061949420983	-0.88160353696243	0.51738093655391
C	-0.04095173247701	0.77468220948148	0.05384437133983
C	3.21549116225333	-1.13517559937821	3.14294503314093
C	-0.18403562981936	1.33327283202235	2.44046616449903
C	1.46948716716063	0.36450697569903	4.01724371337555
C	3.81128083792761	-1.81414567662358	2.09632818948258

C	3.32460629168611	-1.70102205903074	0.79630853782632
C	-0.30033144574845	1.86532907175842	4.78442436142584
H	-0.90447481011261	1.40661632393347	-0.10716237527996
H	3.59982122719431	-1.20777360510374	4.15180171119205
H	3.79982034501021	-2.25925718872710	-0.00132307774760
H	0.22300668330954	1.63179922670809	5.70671727251262
H	-0.28048078874808	2.93848259710605	4.59104057780275
H	-1.34511565584263	1.55855083726852	4.84448097164440
H	2.14344469823557	-1.24172019660102	-1.61966729166021
N	0.05818913505937	0.22997584436532	-2.30185408366366
C	0.45450222284040	1.16280196581961	-3.21452047188036
C	-0.90783566367169	-0.56368000148133	-2.85038458656865
C	-0.27274450858375	0.98180141727445	-4.41669731680294
C	1.41241093766839	2.16262454261829	-3.05366927430444
C	-1.16180127791120	-0.14393635088871	-4.17841788188556
C	-1.57920309099849	-1.62803647476278	-2.25252157543364
C	-0.03054518355024	1.81985295364751	-5.47756790588768
C	1.63940515128332	2.99477383764421	-4.13659251592262
H	1.94164155691400	2.26917985813472	-2.11648285517272
C	-2.10890569118880	-0.80719991872283	-4.92027623044958
C	-2.52875956023108	-2.28213093132663	-3.01971051979851
H	-1.35777646257849	-1.91327585309025	-1.23301975638728
H	-0.56578159371230	1.71526306683367	-6.41351089153298
C	0.93397484185275	2.82854320172660	-5.32599838818912
H	2.37325229857139	3.78624036716032	-4.05740617831594
C	-2.79024692144472	-1.88191490088822	-4.32743630561843
H	-2.33428881565825	-0.51585429531598	-5.93898906914234
H	-3.07639266619850	-3.11394618024090	-2.59614349741840
H	1.13189612953629	3.49508273760340	-6.15634395029979
H	-3.53948843568852	-2.41085831708867	-4.90341592956750
N	4.92728905136079	-2.64804771628303	2.33877736046517
C	6.15143122594667	-2.56103605551677	1.70353140031372
C	4.95781371493321	-3.72419937075564	3.20820384519744
C	6.98913542125646	-3.59657986866456	2.16904367963023
C	6.59716799986763	-1.62746740452114	0.77470232420892
C	6.22317979706699	-4.34286046779953	3.13201824946987
C	3.95701680259946	-4.21309516594074	4.03964059248637
C	8.28746303172392	-3.70162127970695	1.68032551429709
C	7.89286217966564	-1.75520075934599	0.30525228091636
H	5.95213762701619	-0.82457904005787	0.44032377534171
C	6.48847239488633	-5.46373998376581	3.91264450499751
C	4.24718359906784	-5.32952948229297	4.80380943047060
H	2.98846377197790	-3.73194227198701	4.09031453731963
H	8.94265051312389	-4.49153895646676	2.03078095271732
C	8.73206079578700	-2.78242744833248	0.74701985213350
H	8.26562594590175	-1.03810409418124	-0.41749369304795
C	5.49876874438061	-5.95053774299136	4.74684490079974
H	7.45758731007133	-5.94815757188986	3.86537792884383
H	3.48556444276124	-5.72759673566710	5.46461636000333
H	9.74125950144414	-2.85241248874459	0.35849666893002

H 5.69173994433348 -6.82057803476822 5.36337553802397

**XYZ coordinates of m2cz T<sub>1</sub>**

O -1.59254743061485 1.46466239474977 2.42977774469769  
O 1.47016058253223 -0.30095462973872 5.29086625662540  
N -0.05928669315473 0.58857495350057 3.84969095312825  
C 1.42397767116763 -0.35383408573739 1.68924770035535  
C 1.71416028378205 -0.59692440137384 -0.71632469466547  
C 0.49664336566260 0.11984744482751 -0.92704142421760  
C 0.23113791432816 0.33993454488134 1.45463780083979  
C 1.87632537728048 -0.58936491079649 2.99491215660690  
C 2.18907156672579 -0.83398596743635 0.57985508699741  
C -0.22991159140414 0.57770461211982 0.13577908067414  
C 3.08816490760058 -1.28322213855844 3.23240207580241  
C -0.54965638559867 0.84478120317026 2.57529686823701  
C 1.11140091255202 -0.10725685265069 4.13883946294210  
C 3.82814868386022 -1.73492498939109 2.17601495023366  
C 3.37974961523747 -1.52422649216661 0.83465621717939  
C -0.85867075792528 1.09295212387904 4.95231485789985  
H -1.14576932278327 1.13766193232634 0.00326516878183  
H 3.41290907559811 -1.41510786914242 4.25541456954007  
H 3.94585025393734 -1.94885197576559 0.01508173471674  
H -0.37098190696803 0.80514633021887 5.87853111459721  
H -0.94228231610312 2.17777394959208 4.88335105964697  
H -1.86413077589674 0.67494975627139 4.90024535483808  
H 2.24446172588396 -1.00062479910858 -1.56995220058508  
N 0.04734558384634 0.27191865058805 -2.24108494115283  
C 0.82554179771545 0.69281518619486 -3.31219454151254  
C -1.22709021938580 -0.03463663894169 -2.71444696459838  
C 0.05374842843199 0.64033075048502 -4.48867293555459  
C 2.12894663884246 1.17413580708668 -3.31637904220551  
C -1.25548359104853 0.17147474328037 -4.10696311854198  
C -2.33038559624054 -0.52518423046622 -2.02894624284213  
C 0.61226318110739 1.03904464913921 -5.69545829644769  
C 2.66656116785399 1.55979988478290 -4.53371029404963  
H 2.69957818425351 1.26677443885800 -2.40098489464024  
C -2.41406664422395 -0.10436715811429 -4.82142775464236  
C -3.47345044107946 -0.79404092871972 -2.76337648677180  
H -2.30372515492683 -0.69509795640906 -0.96075628289621  
H 0.02835779439423 1.00774623648916 -6.60823157840658  
C 1.92252367660902 1.48884330443707 -5.71238892341699  
H 3.68205565235178 1.93661487486394 -4.56635557551675  
C -3.52165381185127 -0.58252711984128 -4.14225262312347  
H -2.44735500053041 0.04711925236908 -5.89431602704969  
H -4.34943094038009 -1.17451070514384 -2.25141949553057  
H 2.37157181660599 1.80447980766174 -6.64644784872305  
H -4.43449113806204 -0.79890549580243 -4.68416569447977  
N 5.00191268575907 -2.46742959475639 2.36152307075603  
C 6.18514566450067 -2.27492812005658 1.65817714364249

C	5.17362537230901	-3.54662325343204	3.22676426499332
C	7.11913049016974	-3.25083783968449	2.05455603549809
C	6.51705078642119	-1.27237570056595	0.75515735109328
C	6.47212085797395	-4.06372720515476	3.05544095209284
C	4.26799211926847	-4.12853978530762	4.10379548285699
C	8.39139796610321	-3.24910550056086	1.49913242352334
C	7.79046270148663	-1.29491942882539	0.21011688506177
H	5.81660622372538	-0.48693120713225	0.50174335255459
C	6.87501381355222	-5.17129167386726	3.79031620259177
C	4.69254468007380	-5.23273889050894	4.82407728568011
H	3.26583330298827	-3.73928365547456	4.22422510069665
H	9.12185428354312	-3.99321051265889	1.79534594739985
C	8.71690173505464	-2.27459333459727	0.56937506986163
H	8.07472232820215	-0.52613357927837	-0.49875233591100
C	5.98151869935283	-5.74765868910274	4.67735201010194
H	7.87185063080542	-5.57928081033389	3.66779153531701
H	4.00636343324893	-5.70211084912247	5.51903609453093
H	9.70626066491966	-2.26031689791114	0.12810362019866
H	6.28223942055854	-6.60899095813647	5.26164417469042

#### XYZ coordinates of m2dpa in S<sub>0</sub>

O	-0.200892	0.192466	5.377068
O	3.111639	-1.269991	8.095230
N	1.457166	-0.535087	6.723021
C	2.480284	-2.112230	4.638958
C	2.325181	-2.910292	2.347963
C	1.204119	-2.131682	2.138417
C	1.330032	-1.336108	4.416378
C	3.128519	-2.107300	5.886531
C	2.993972	-2.909026	3.587186
C	0.710558	-1.333169	3.193882
C	4.250746	-2.867483	6.093216
C	0.785990	-0.499762	5.505079
C	2.595435	-1.291220	6.999094
C	4.781275	-3.657857	5.050599
C	4.157419	-3.667721	3.820101
C	0.899505	0.292155	7.779842
H	-0.161475	-0.707424	3.051761
H	4.721856	-2.854388	7.068116
H	4.563630	-4.272974	3.017857
H	1.502145	0.149294	8.671234
H	0.910175	1.338945	7.475303
H	-0.135519	0.005725	7.965550
H	2.707450	-3.528592	1.544196
N	0.558354	-2.106972	0.896991
C	-0.846604	-2.010904	0.825597
C	1.297131	-2.302028	-0.290492
C	-1.443189	-1.252778	-0.181126
C	-1.655727	-2.671176	1.748692

C	0.847488	-3.193857	-1.261225
C	2.479685	-1.597135	-0.508244
C	-2.821895	-1.159944	-0.258778
H	-0.816601	-0.739696	-0.900886
C	-3.034345	-2.556244	1.675403
H	-1.199097	-3.271609	2.526481
C	1.567414	-3.370787	-2.431650
H	-0.072335	-3.741483	-1.093661
C	3.201076	-1.790303	-1.673781
H	2.827491	-0.899959	0.244945
C	-3.626299	-1.804897	0.670969
H	-3.270977	-0.564291	-1.045315
H	-3.649638	-3.070345	2.404825
C	2.748262	-2.674489	-2.643892
H	1.206140	-4.068621	-3.178455
H	4.117599	-1.233199	-1.831068
H	-4.704845	-1.720872	0.613499
H	3.311634	-2.817878	-3.558170
N	5.927139	-4.429735	5.288409
C	6.064571	-5.693421	4.676846
C	6.999463	-3.888511	6.024280
C	7.262691	-6.060868	4.067680
C	5.000737	-6.594557	4.682995
C	7.742689	-4.700266	6.881021
C	7.334778	-2.540624	5.905733
C	7.393168	-7.310654	3.483886
H	8.091631	-5.363254	4.061530
C	5.134272	-7.835096	4.083466
H	4.069642	-6.312803	5.160488
C	8.802194	-4.171191	7.596884
H	7.483765	-5.747870	6.977514
C	8.385005	-2.015586	6.641103
H	6.768171	-1.906280	5.234496
C	6.331545	-8.203526	3.484397
H	8.331890	-7.582803	3.014882
H	4.299021	-8.526012	4.099038
C	9.128007	-2.825874	7.486471
H	9.369122	-4.814902	8.259781
H	8.630359	-0.964532	6.540644
H	6.435696	-9.178579	3.023798
H	9.952228	-2.413525	8.055905

### XYZ coordinates of m2dpa in S<sub>1</sub>

O	-0.34185549257731	-0.10763445508440	5.47530345122304
O	2.91372039251848	-1.73136887204836	8.21055510418768
N	1.28803762047183	-0.92940189768273	6.81625170082814
C	2.43437762040961	-2.27268381279593	4.66553225339068
C	2.40428213340400	-2.85643363445336	2.29587971067320
C	1.26209685979919	-2.07677088504255	2.11685191341993

C	1.27283252196045	-1.50471185398625	4.46120208428370
C	3.01830748135028	-2.36602827789729	5.94670803461024
C	3.01417519448488	-2.96108434398224	3.55257951892099
C	0.70354575200903	-1.39970612815917	3.19140244541150
C	4.17623197848722	-3.13554182142658	6.14258972352023
C	0.66536106080892	-0.79602423216548	5.57752222246759
C	2.43691318069075	-1.67417942191802	7.07907694028590
C	4.70992758981503	-3.79103976434849	5.05910373748584
C	4.17021822961660	-3.74305989391466	3.78201445537667
C	0.66375211969255	-0.21663181607857	7.91362646538171
H	-0.18147856671137	-0.78845067120363	3.06989470960171
H	4.61384680083659	-3.18748603729420	7.13070817492514
H	4.63551956822604	-4.28046793450445	2.96457181306419
H	1.24024070554868	-0.41689399453177	8.81178349156883
H	0.64257191151205	0.85255304491062	7.69896201568755
H	-0.36786559803635	-0.54959070526724	8.03277176995362
H	2.82830595916643	-3.38330549808022	1.44922619861252
N	0.67454998157996	-1.98286007835687	0.83446308312762
C	-0.71872202712661	-2.09976646844437	0.69971753121024
C	1.49041262134877	-1.77459903529713	-0.28703060178755
C	-1.41421742190208	-1.32403833031668	-0.22904343333992
C	-1.43415654302280	-2.98587507369448	1.50619734642149
C	1.21061528074132	-2.39939577942458	-1.50415113879440
C	2.60935761727323	-0.94339998405647	-0.20138821955428
C	-2.78773005070400	-1.44489263958624	-0.35333658828364
H	-0.86951026207170	-0.62296012822502	-0.84975723676875
C	-2.80927084711836	-3.08802810576404	1.38555078875498
H	-0.90271400809154	-3.58378545706178	2.23641467786760
C	2.02306509638092	-2.18686406209604	-2.60481721638092
H	0.34776794234819	-3.05010686508038	-1.57949488560538
C	3.42351023028053	-0.74812328948381	-1.30392951339224
H	2.83087847346885	-0.45319446346157	0.73887112305088
C	-3.49680813661588	-2.32403439394534	0.45295959904978
H	-3.31035761124646	-0.82937233751168	-1.07704650254176
H	-3.34742166871425	-3.77829407277060	2.02543327385828
C	3.13716250892176	-1.36364287121162	-2.51469105477506
H	1.78746783952419	-2.68168908311770	-3.54054813492337
H	4.28409801016635	-0.09386259431635	-1.21773268922973
H	-4.57303604908883	-2.40760248448652	0.36052981553708
H	3.77230300179485	-1.20210645600061	-3.37751347438443
N	5.92516179652895	-4.56442200919481	5.24266263783133
C	5.84210379884073	-5.92900984014115	5.23163537952283
C	7.11755465386894	-3.87769976628452	5.43257912162049
C	6.95408527778110	-6.73245546726309	4.88894092348764
C	4.60455202984476	-6.54888953433131	5.51326965355984
C	8.11333075826785	-4.38639155874433	6.28096083570741
C	7.29660565379149	-2.62893681237814	4.82037926045569
C	6.83515555261881	-8.10186416743812	4.88052599804097
H	7.87697231430607	-6.26111421754582	4.57895511084994
C	4.51278002390586	-7.91996310504863	5.51322153955204

H	3.75309475880469	-5.92874955464660	5.75461732915305
C	9.28065646659559	-3.67589523824132	6.47374362047579
H	7.93384622113733	-5.30369080897289	6.82698294241070
C	8.47315194454689	-1.94030440460986	5.01205221498599
H	6.50964551169398	-2.23326999703873	4.19234368225492
C	5.62187199806496	-8.70583895174953	5.20438508185854
H	7.68411423774416	-8.70999448698772	4.59364950010611
H	3.56740181697875	-8.38918489432460	5.75483616074639
C	9.47194257726383	-2.45853337075260	5.83352498768994
H	10.03446971932961	-4.06074014612642	7.14955453453845
H	8.61630342494584	-0.98551723482695	4.52160162448975
H	5.53515630037275	-9.78527799602261	5.19373577734260
H	10.38744649115648	-1.90147665666488	5.99055364932194

### XYZ coordinates of m2dpa T<sub>1</sub>

O	-0.20390294077280	0.17780786542899	5.35983148035881
O	3.23703296758087	-1.15349555250339	8.01703156799596
N	1.51971142507205	-0.48967193515070	6.66960626844264
C	2.51406508943335	-2.06198024042797	4.60790382268701
C	2.33753966892940	-2.90118798116562	2.32748623005771
C	1.14412176117890	-2.13095429132000	2.13740159128882
C	1.34225690426901	-1.32308415793469	4.39963050823714
C	3.19440700671203	-2.02572145231601	5.83172765353086
C	3.02467428715853	-2.87441480056569	3.54684415815698
C	0.66234963069864	-1.35797809515156	3.16384127194544
C	4.36674034084382	-2.78538742991197	6.03901224738240
C	0.81291614827082	-0.49233743442932	5.47185024859723
C	2.68385174008731	-1.21171089170780	6.92817735249663
C	4.86145362080964	-3.57436692677082	5.03157787844037
C	4.19091797771836	-3.61710325673202	3.76699438976799
C	0.97074403343864	0.33993122709368	7.72649435785663
H	-0.23746977122144	-0.76691937329484	3.05847252856803
H	4.85026331637608	-2.72567707519823	7.00483916222544
H	4.61253327115749	-4.20543121319880	2.96165423875253
H	1.61079091721933	0.23872643428993	8.59759812475529
H	0.92895518851714	1.37905862639863	7.39846421281202
H	-0.04653103498720	0.02189318440436	7.95632673145948
H	2.68700972828332	-3.54491917413759	1.53011924585382
N	0.48482260610044	-2.24050056404410	0.91448695553268
C	-0.91860270962099	-2.10270300150960	0.83748960229158
C	1.22545581246276	-2.37574532097157	-0.27400686863008
C	-1.49282424579128	-1.32854344920743	-0.16788760629898
C	-1.73932123128955	-2.75255087781480	1.75789869106248
C	0.78207366058934	-3.23177064151029	-1.28302141299305
C	2.40932225552304	-1.66017184106194	-0.45335268029929
C	-2.87070752831734	-1.21266748932191	-0.25247171150527
H	-0.85360653486165	-0.81874294058266	-0.87852862510031
C	-3.11341631443161	-2.62213956666529	1.67216738135835
H	-1.29069121156333	-3.35102472323004	2.54124507171596

C	1.51659338840210	-3.36948953472907	-2.44620594777464
H	-0.13790004246713	-3.78631885205979	-1.14214232224247
C	3.14434933572373	-1.81463579259439	-1.61768263041325
H	2.73817055687121	-0.97720441436961	0.32081629900691
C	-3.68723318903227	-1.85463623590953	0.66635340261486
H	-3.30662889881033	-0.60325710823385	-1.03559753276964
H	-3.74205143546731	-3.13101359711659	2.39353080009392
C	2.70290754326167	-2.66609391320196	-2.61931792731663
H	1.16620726895927	-4.04188657417382	-3.22081963694740
H	4.06122986361349	-1.25125826675176	-1.74678716164128
H	-4.76423021413553	-1.75567220342326	0.60286159742405
H	3.27636925815006	-2.77961647278178	-3.53148759693910
N	6.03385525662714	-4.31689952949087	5.17298208909238
C	6.13305363956137	-5.59195476088206	4.58927607205514
C	7.06150985009750	-3.87058247706441	6.03338987912668
C	7.34718447547488	-6.02692085707266	4.05467018041640
C	5.02258114507429	-6.43547708213660	4.54022340853934
C	7.65575008022267	-4.75026001604340	6.93444057645099
C	7.49106503321878	-2.54598998005394	5.97964958771802
C	7.44139103068428	-7.28037719746157	3.47892347621150
H	8.20950967943716	-5.37235962504891	4.09528654930591
C	5.12434123217337	-7.68385273162890	3.94759536586747
H	4.08846803192348	-6.10971678688943	4.98196298657345
C	8.67056596252541	-4.30821323309167	7.76752416498940
H	7.31558673737057	-5.77776289389660	6.97921382030655
C	8.49789741182638	-2.11080414522247	6.82229915329126
H	7.02273177043042	-1.86423049281618	5.28015656882929
C	6.33108325357984	-8.11449451576291	3.41708064415105
H	8.38840164802920	-7.60560335911360	3.06389648213387
H	4.25509754074484	-8.33070859912827	3.91800197241605
C	9.09441625739397	-2.98873412924769	7.71852390454572
H	9.12223998477933	-4.99939273811353	8.46967307320859
H	8.82392389344080	-1.07837839988921	6.77436431385471
H	6.40950097669873	-9.09466635034835	2.96229801481156
H	9.88283816804295	-2.64370995402978	8.37662835420553

### XYZ coordinates of m2acr in S<sub>0</sub>

O	-1.248050	-0.767639	-3.711759
O	1.927214	-2.476727	-0.970405
N	0.338445	-1.615656	-2.348161
C	1.361168	-3.147203	-4.476881
C	1.265205	-3.810538	-6.813399
C	0.197820	-2.971102	-7.006943
C	0.258908	-2.299706	-4.694738
C	1.955754	-3.233514	-3.203741
C	1.874920	-3.921004	-5.547112
C	-0.312486	-2.212379	-5.940055
C	3.027558	-4.066253	-2.998380
C	-0.291821	-1.499463	-3.581636

C	1.434317	-2.430792	-2.075310
C	3.532303	-4.847520	-4.052039
C	2.967923	-4.776843	-5.300063
C	-0.213865	-0.808761	-1.271808
H	-1.160260	-1.555351	-6.093780
H	3.476708	-4.124491	-2.014137
H	3.368927	-5.387089	-6.101728
H	0.344523	-1.027741	-0.367202
H	-0.131888	0.248917	-1.523141
H	-1.269374	-1.044872	-1.140075
H	1.642328	-4.391075	-7.648048
N	4.624300	-5.720253	-3.808225
C	5.922369	-5.278008	-4.061170
C	4.369975	-6.961805	-3.226587
C	7.022443	-6.087143	-3.753769
C	6.130137	-4.013379	-4.624963
C	5.422226	-7.815854	-2.877142
C	3.048203	-7.363501	-2.997643
C	8.292306	-5.597097	-4.042112
C	6.881257	-7.457963	-3.110839
C	7.405137	-3.557272	-4.896835
H	5.282051	-3.381106	-4.850493
C	5.102963	-9.038970	-2.296244
C	2.766756	-8.584943	-2.417879
H	2.232277	-6.711236	-3.277928
C	8.502256	-4.352508	-4.609028
H	9.152974	-6.214121	-3.810015
C	7.513797	-8.514063	-4.032460
C	7.617572	-7.450430	-1.760455
H	7.535805	-2.574052	-5.333799
C	3.798724	-9.435839	-2.058221
H	5.908409	-9.708851	-2.017245
H	1.734105	-8.867567	-2.249238
H	9.508049	-4.009081	-4.817535
H	7.004245	-8.535868	-4.997661
H	7.447675	-9.509548	-3.589445
H	8.568976	-8.296947	-4.208970
H	8.674496	-7.211238	-1.892923
H	7.554507	-8.425927	-1.274445
H	7.181925	-6.707255	-1.090016
H	3.594110	-10.396039	-1.600824
N	-0.393589	-2.864222	-8.292368
C	0.104054	-1.918111	-9.187908
C	-1.500321	-3.655497	-8.596868
C	-0.448842	-1.789435	-10.467315
C	1.166097	-1.089094	-8.806527
C	-2.109151	-3.574209	-9.854610
C	-2.005430	-4.543258	-7.639214
C	0.100809	-0.839171	-11.321930
C	-1.599726	-2.655561	-10.954447

C	1.684417	-0.152152	-9.679072
H	1.588794	-1.179871	-7.815024
C	-3.207660	-4.391787	-10.100054
C	-3.100368	-5.338695	-7.915592
H	-1.534457	-4.608999	-6.667618
C	1.154412	-0.021860	-10.952131
H	-0.310562	-0.736593	-12.319636
C	-2.748268	-1.750607	-11.428403
C	-1.109086	-3.516604	-12.130770
H	2.506001	0.476908	-9.356603
C	-3.713170	-5.268163	-9.155725
H	-3.685599	-4.343624	-11.071772
H	-3.471538	-6.014799	-7.154131
H	1.552889	0.705638	-11.648579
H	-3.114940	-1.133714	-10.606041
H	-3.581895	-2.342884	-11.809146
H	-2.421690	-1.088554	-12.231935
H	-0.740646	-2.889358	-12.945296
H	-1.917986	-4.138115	-12.520310
H	-0.297240	-4.173959	-11.813262
H	-4.571728	-5.886417	-9.387372

### XYZ coordinates of m2acr in S<sub>1</sub>

O	-1.15675100435419	-0.52455228156305	-3.69510316620257
O	1.96809315226427	-2.29130831396277	-0.89942522302800
N	0.40539056932932	-1.42008003666752	-2.32251226054434
C	1.35687019292887	-3.02248861022790	-4.39140688874358
C	1.22992444042687	-3.75529400610805	-6.71241432748139
C	0.16849533168394	-2.88067741805630	-6.91994252868698
C	0.28041884821004	-2.14993863563712	-4.63189211246811
C	1.95632780907998	-3.08779713629793	-3.11366874645370
C	1.84419871856513	-3.84861772978327	-5.45448160339138
C	-0.31018726453580	-2.08374535766186	-5.89934711865322
C	3.03109891062692	-3.95936890521287	-2.87919239158897
C	-0.22572839428058	-1.30677021645589	-3.55963500987006
C	1.47515547709078	-2.26221259244614	-2.02426417676638
C	3.47470095274137	-4.74487773743432	-3.91541969348634
C	2.92262465448382	-4.72127405862284	-5.18856076038499
C	-0.11736785143205	-0.57068558246974	-1.26995504500308
H	-1.13659775427379	-1.40353160644281	-6.06032587794519
H	3.47371502698941	-3.99088181496434	-1.89218920637831
H	3.30992903146882	-5.35966192965493	-5.97292088224941
H	0.45523729702202	-0.76649080511963	-0.36839333693116
H	-0.03262993720098	0.47699744603355	-1.56107311550488
H	-1.17482409114243	-0.78476970826040	-1.11148317354203
H	1.58016350811709	-4.36777817983271	-7.53502568011924
N	4.58449658307279	-5.65339204436919	-3.67732698748694
C	5.86360335494897	-5.20991754860311	-3.90438476739332
C	4.31395604608468	-6.93057230045843	-3.25307055757314

C	6.96830764748132	-6.06943292133578	-3.72022674214351
C	6.05984398977743	-3.87849970295240	-4.32668376884735
C	5.35833218026468	-7.85661516339909	-3.04177084033021
C	2.97286251273428	-7.30655068825092	-3.03023331224936
C	8.23247444399260	-5.55829543298263	-3.97035716347249
C	6.80655775824457	-7.50132350783286	-3.27254981563166
C	7.32587513399003	-3.41018391502307	-4.56289073893806
H	5.20002615354340	-3.23938501520598	-4.45690412763017
C	5.01522033377729	-9.12992787686615	-2.61423929908300
C	2.67429991927820	-8.57518599266391	-2.60674343589849
H	2.19209660398669	-6.58002842499169	-3.19538047771761
C	8.42332408120610	-4.25143654607316	-4.38570934205695
H	9.09765674115376	-6.19601476646510	-3.83830898273011
C	7.37795256663561	-8.43097125705809	-4.36302151358010
C	7.58819692037537	-7.70625100575771	-1.95908938690313
H	7.46672444978995	-2.38647031025146	-4.88519866772355
C	3.69837471409219	-9.49738170787727	-2.39581292525755
H	5.79642816004734	-9.86057259259558	-2.44538753738801
H	1.64233638437243	-8.85394372923449	-2.43634458759219
H	9.42615573042608	-3.88664830859249	-4.57083460029086
H	6.83966610964175	-8.30282348315720	-5.30345488836218
H	7.29452610488857	-9.47484782730363	-4.05864618020560
H	8.43225093356665	-8.21374917851041	-4.53793516821375
H	8.64517620280161	-7.47966556275799	-2.10212505481818
H	7.50998600746070	-8.74057348503860	-1.62291237739777
H	7.20052687836238	-7.05797745820935	-1.17178713939125
H	3.46831332654599	-10.50123753574810	-2.06059896180529
N	-0.42273708594201	-2.81803430677875	-8.21758503043628
C	0.09746127705503	-1.93477434365170	-9.15562522316774
C	-1.44960553103826	-3.69792275621955	-8.53664444192870
C	-0.40551717002248	-1.89325395783812	-10.46269145465739
C	1.13812774907699	-1.06962852425826	-8.79131963309759
C	-2.00517122511536	-3.72103179993646	-9.82271497126256
C	-1.94139853423811	-4.57353619145160	-7.55911974952563
C	0.15618295806696	-0.98274998399565	-11.35227265256348
C	-1.53439419418623	-2.79615615422616	-10.93386772239521
C	1.67232591030567	-0.17816631815698	-9.69958776449883
H	1.51883696592271	-1.09928973822216	-7.77960627453322
C	-3.03204951412288	-4.62493872453885	-10.07661614897538
C	-2.96207323337988	-5.45759934570258	-7.84521693080968
H	-1.51650543668953	-4.54596603464276	-6.56505151719429
C	1.18356664138910	-0.12715682145635	-10.99584383610327
H	-0.22763609280664	-0.94030384200352	-12.36556304221989
C	-2.71576765148280	-1.92439602659977	-11.39223212987640
C	-1.03802250943853	-3.64340996792639	-12.11768362316461
H	2.47282160251345	0.48258511534379	-9.38646829028805
C	-3.51847010694968	-5.49231316328462	-9.11452445733826
H	-3.47066170550531	-4.64953531412854	-11.06803192126666
H	-3.32507322218867	-6.11890466469660	-7.06653165817178
H	1.59131077729264	0.56966145169047	-11.71818616924118

H	-3.08465769204017	-1.31491629566032	-10.56523795069952
H	-3.53970960978185	-2.54271330475383	-11.75431140699638
H	-2.41688506995147	-1.25565254609236	-12.20204650251130
H	-0.70890927572975	-3.00795872823735	-12.94227992624825
H	-1.83021861347069	-4.29427501035869	-12.49315919768876
H	-0.19743415126820	-4.27013641681198	-11.81337611575203
H	-4.32166385262641	-6.17927877898943	-9.35235258385219

### XYZ coordinates of m2acr T<sub>1</sub>

O	-1.65634304425396	-1.04705443454311	-3.47680084244948
O	1.47695306982988	-2.81754103875020	-0.69634575310425
N	-0.08570499938532	-1.93131212396735	-2.10290693260780
C	1.13297149156494	-3.19824930875142	-4.26336666665428
C	1.22384103713813	-3.65123193710270	-6.65591336254642
C	0.06547622112562	-2.85207994660777	-6.83494368609811
C	-0.01143164347151	-2.40726892450469	-4.47663499361902
C	1.66367330548909	-3.35739445539585	-2.97706865040179
C	1.76783596749323	-3.83800485873973	-5.37708080974597
C	-0.54040456787620	-2.23773053809793	-5.77221973023233
C	2.82067363296191	-4.14184033997876	-2.76756133805835
C	-0.65647531559991	-1.74214039807132	-3.35698917462176
C	1.04300911965605	-2.70301566029277	-1.83365642069600
C	3.42940235282593	-4.74553731991668	-3.83379459688414
C	2.92236527880363	-4.60037588845748	-5.14232018031176
C	-0.74200844462118	-1.25653226561762	-0.99826597125054
H	-1.42194842697971	-1.62225628068199	-5.89715334430277
H	3.20153612611450	-4.25216780822818	-1.76050426725587
H	3.42522499656352	-5.09708482627114	-5.96361110654352
H	-0.21590107211987	-1.52009850350235	-0.08582774400352
H	-0.71918835179651	-0.17750115848751	-1.15538943947232
H	-1.78645381275645	-1.56433113134078	-0.94571890475446
H	1.67069994227406	-4.13604475231324	-7.51536482657116
N	4.57422543989712	-5.56762901866938	-3.65246655959675
C	5.79800434754472	-5.09403115687275	-4.10451548603121
C	4.44147831330068	-6.84177545484547	-3.09931277707899
C	6.94505474749154	-5.90037276741894	-4.06235368206790
C	5.89329918304413	-3.77632885421580	-4.58073243396581
C	5.55234407332240	-7.68770728804650	-2.98641955206217
C	3.18235104905296	-7.29385912317209	-2.68196035278367
C	8.13211811881910	-5.37018738216941	-4.55264075411912
C	6.93706599848598	-7.29640408471515	-3.46937382060658
C	7.08813697022048	-3.28372411525005	-5.06218826573234
H	5.02162314723421	-3.13764362498895	-4.55262312364898
C	5.36037076572932	-8.94638010721418	-2.42391404799248
C	3.02707044582340	-8.54772153171450	-2.13136010748069
H	2.32279733978269	-6.64784295763975	-2.79111494965652
C	8.21949467219629	-4.08556181448912	-5.06217603224193
H	9.02623138108832	-5.98241121963716	-4.53008975312078
C	7.39827588530010	-8.30232902629339	-4.53797404924359

C	7.90935543559519	-7.33179088688899	-2.27698984995366
H	7.13581857686627	-2.26340605468958	-5.42395800760780
C	4.12382448931378	-9.38610893259873	-1.99028661897863
H	6.21277366275121	-9.60844571133415	-2.32532978190995
H	2.04260915281113	-8.86914900670960	-1.81244289391018
H	9.16488004112400	-3.71013429626845	-5.43449337848644
H	6.71255567626504	-8.30237646567787	-5.38739776346397
H	7.43701664190284	-9.31408936573795	-4.13086045050662
H	8.39569839186605	-8.05205714279148	-4.90385639226491
H	8.92289149751406	-7.07610291833742	-2.59144473948491
H	7.93730881607399	-8.32667563376756	-1.82900267431535
H	7.59996913438755	-6.62030732014196	-1.50925402562627
H	4.01612983582304	-10.37219008837813	-1.55524152917551
N	-0.45700597733850	-2.75285871521864	-8.14843414290124
C	0.33886813612909	-2.15390968595314	-9.11711959684323
C	-1.69794370729248	-3.31178271875765	-8.47128423432310
C	-0.01358403577475	-2.19449224089329	-10.47390899539470
C	1.49936164698528	-1.46748828837443	-8.72080467336078
C	-2.14510215705250	-3.32620301679955	-9.80022652611378
C	-2.48298561966565	-3.90351890541304	-7.47208894362364
C	0.86063781326746	-1.62261162990414	-11.38997591200668
C	-1.31186117156091	-2.80791313619815	-10.95733965524946
C	2.34521263519112	-0.91220945354021	-9.65708307646552
H	1.71930378340720	-1.36172501803671	-7.66783922574838
C	-3.38821721106463	-3.89363590926125	-10.06507717046486
C	-3.70833066492505	-4.45781598427292	-7.76970767265602
H	-2.12429302361445	-3.92534885168133	-6.45366407531547
C	2.03811302052811	-1.00269975340777	-11.00652739093345
H	0.61096993333894	-1.65859264522007	-12.44384626807139
C	-2.10994550890528	-1.73536176725630	-11.71995253639822
C	-0.99251211559545	-3.97794739178539	-11.90469163349349
H	3.23707207797109	-0.39255224698588	-9.32794391003347
C	-4.17790663010553	-4.44701617893702	-9.07533769116643
H	-3.74649807337918	-3.91253639056437	-11.08753124600489
H	-4.29653552016801	-4.90122877183884	-6.97519873419482
H	2.69372812330527	-0.57154144654130	-11.75327149451842
H	-2.34196597113620	-0.89140006435133	-11.06808203156282
H	-3.04819826058675	-2.14240697406039	-12.09986170176323
H	-1.54182146759747	-1.36242449420067	-12.57343295781717
H	-0.40317794581604	-3.63290606603551	-12.75635029036826
H	-1.90889481050281	-4.42883699331042	-12.28931758521564
H	-0.42349104721538	-4.75138213556556	-11.38543940984655
H	-5.14169434443418	-4.87554887533936	-9.32175862284519

### XYZ coordinates of m2pt in S<sub>0</sub>

O	1.936100	-0.306562	6.194327
O	4.944564	-1.801909	9.232774
N	3.436796	-1.050977	7.707587
C	4.496453	-2.825428	5.796845

C	4.475881	-3.723580	3.536448
C	3.437375	-2.889893	3.213650
C	3.426298	-1.980760	5.446410
C	5.040620	-2.789176	7.093454
C	5.033434	-3.713303	4.832190
C	2.906566	-2.011152	4.176958
C	6.087906	-3.613847	7.425742
C	2.860066	-1.049007	6.443904
C	4.496696	-1.861228	8.110055
C	6.625458	-4.495627	6.475218
C	6.111583	-4.540795	5.201900
C	2.868310	-0.119380	8.668911
H	2.086887	-1.348964	3.923342
H	6.502016	-3.578308	8.426090
H	6.544477	-5.218098	4.473643
H	3.393639	-0.245671	9.610233
H	2.979435	0.901676	8.303731
H	1.804601	-0.321393	8.792062
H	4.872302	-4.391284	2.779731
N	2.921497	-2.918554	1.888458
C	1.713729	-3.604664	1.662592
C	3.378953	-1.934258	0.991748
C	1.294729	-3.873331	0.354302
C	0.918392	-4.054293	2.714792
C	3.114063	-2.053232	-0.377300
C	4.118374	-0.835889	1.426863
S	2.343035	-3.499747	-1.002460
C	0.093462	-4.525536	0.119963
C	-0.260831	-4.743164	2.471723
H	1.224610	-3.877849	3.737195
C	3.541176	-1.076236	-1.264332
C	4.576861	0.115558	0.527547
H	4.351216	-0.723478	2.477288
C	-0.685708	-4.974400	1.175256
H	-0.216039	-4.698432	-0.904653
H	-0.852155	-5.087854	3.311718
C	4.284544	0.006683	-0.820601
H	3.302126	-1.184638	-2.316298
H	5.157772	0.952618	0.896340
H	-1.612596	-5.499939	0.981347
H	4.629676	0.753813	-1.524577
N	7.724896	-5.312981	6.856885
C	7.502306	-6.685902	7.073447
C	9.015287	-4.807547	6.606435
C	8.495204	-7.471330	7.672959
C	6.298912	-7.300805	6.730976
C	10.138647	-5.419482	7.174394
C	9.212991	-3.684418	5.804299
S	9.944235	-6.728064	8.325392
C	8.301991	-8.832719	7.855585

C	6.097786	-8.654410	6.958512
H	5.498406	-6.717332	6.297854
C	11.412307	-4.941890	6.904036
C	10.487614	-3.187304	5.574571
H	8.363193	-3.181855	5.362873
C	7.100835	-9.431818	7.509010
H	9.099893	-9.417658	8.299149
H	5.145605	-9.096969	6.690762
C	11.594787	-3.816499	6.115080
H	12.264339	-5.451397	7.339926
H	10.605615	-2.304488	4.957450
H	6.953643	-10.491750	7.675435
H	12.592870	-3.439422	5.929319

### XYZ coordinates of m2pt in S<sub>1</sub>

O	1.91522839108325	-0.43011224933868	6.25909942203944
O	4.98273086924403	-2.01727887450889	9.22223059720126
N	3.45159137556805	-1.23391022854408	7.71595248600084
C	4.52890921408364	-2.86656815089107	5.73347091770559
C	4.50828750231489	-3.67133401583739	3.43246021254622
C	3.43419953975878	-2.83421247534554	3.15791820528069
C	3.43872934993727	-2.03247380542234	5.42682439222982
C	5.07898446918893	-2.87752753518020	7.03452529062543
C	5.07892863582656	-3.70841132398566	4.71478838719428
C	2.89771186965208	-2.01772579294103	4.13670743768575
C	6.16751008228325	-3.71125014502809	7.33475219106069
C	2.86545935047948	-1.17647815236618	6.45380949197845
C	4.53295623983227	-2.03525552228509	8.07925562650916
C	6.67455715174385	-4.51166214326647	6.34009207207255
C	6.17123395591578	-4.53976226668701	5.04678802014958
C	2.86423048719717	-0.37101636469209	8.72251187778694
H	2.06142815662762	-1.36261947383951	3.92742123123558
H	6.57181183588738	-3.70237709978198	8.33858791889178
H	6.60632488310105	-5.18844753421208	4.29654439607244
H	3.40801113589323	-0.52280657660347	9.65003097536362
H	2.92866008261526	0.66989257391648	8.40330898302278
H	1.80843674669372	-0.61300345438141	8.84831623533764
H	4.90301336391831	-4.29719269084845	2.64097084415206
N	2.90869064314097	-2.84308923555218	1.82789813153139
C	1.74650996253005	-3.58607814548868	1.57651683013339
C	3.35171340992939	-1.85392992633159	0.93846387782913
C	1.34633771836246	-3.86101752412083	0.26216891413906
C	0.96281713387135	-4.08736758978965	2.61606616703467
C	3.10508398656410	-1.96630698162276	-0.43598092722006
C	4.06126088358292	-0.73937246456058	1.38634232606872
S	2.38957657306890	-3.43254971987311	-1.08291938422820
C	0.17626950732820	-4.56156900551558	0.00980616812532
C	-0.18252692677734	-4.82371599385952	2.35501110866293
H	1.25642375842767	-3.89884857053798	3.63957419280695

C	3.51116208919034	-0.97064566245948	-1.31202477521611
C	4.50118688737891	0.23008582999717	0.49821787249640
H	4.27133027174403	-0.63474750666440	2.44206682772281
C	-0.59061937045852	-5.05779398643996	1.05291923746804
H	-0.11656759702365	-4.73505455446095	-1.01983989810957
H	-0.76462175790402	-5.20222010808007	3.18728759492844
C	4.22235099787975	0.12802794982399	-0.85411583351361
H	3.28272795746097	-1.07800246616491	-2.36669224234538
H	5.05521174924885	1.07992390589524	0.87987400627700
H	-1.49356193256734	-5.61909797207935	0.84567853713451
H	4.55154234815036	0.89130054344376	-1.54867284922273
N	7.80019551123437	-5.38003302666206	6.65286228889006
C	7.52014876523968	-6.64681779811709	7.10783632578383
C	9.06605908624291	-4.87634938580057	6.46881587750383
C	8.52674040835903	-7.58085574005959	7.44341619809847
C	6.18178383523296	-7.05571048084587	7.25531141225096
C	10.23512586702356	-5.62516801890953	6.73478268890623
C	9.23236922182721	-3.56143028078192	5.99620331578704
S	10.20416871963669	-7.23913821155821	7.31804622975415
C	8.19640551405908	-8.85898147626388	7.90494762294973
C	5.87622123504098	-8.31342964205127	7.70747271120435
H	5.39755060095530	-6.35752536278347	7.00713388148465
C	11.50395847052975	-5.07285255191160	6.53273287536927
C	10.48407574408093	-3.03648578950053	5.80296610527217
H	8.35310779791396	-2.97103518504395	5.79012881333521
C	6.88184757815562	-9.22840817036451	8.03793014226615
H	8.99321408255408	-9.55027736123630	8.15539634467325
H	4.83586819867198	-8.59526780933323	7.80994175801547
C	11.63365725082771	-3.78804958428536	6.06951763855287
H	12.38006933358201	-5.67423862417941	6.74792674240428
H	10.57625113244770	-2.02100763016722	5.43881586472305
H	6.62884680790764	-10.21801077920994	8.39586635861032
H	12.61681588650198	-3.36285405442228	5.91439958951820

### XYZ coordinates of m2pt T<sub>1</sub>

O	1.76686127779550	-0.47661557252453	6.34516472884936
O	4.89668523821246	-2.02190053519281	9.26145937219401
N	3.33925414806158	-1.25514686206777	7.77943847828251
C	4.45341754248703	-2.82245375692022	5.76464375181478
C	4.45768335056281	-3.57270558252074	3.44198121863847
C	3.36064951222314	-2.75048135829457	3.20109588431628
C	3.34099167188741	-2.00746571889182	5.47866960507554
C	5.00665660363503	-2.85123996723742	7.06049628013412
C	5.02645377178005	-3.62880387989529	4.72804609354601
C	2.79611727830952	-1.97292337513959	4.18781146388089
C	6.10974108604406	-3.67097179323026	7.34197342375712
C	2.74400993094619	-1.19344848762828	6.52270996897734
C	4.44428503540195	-2.03617304148525	8.12340868198794
C	6.64279557659410	-4.44588365895117	6.33749175576304

C	6.13201327956131	-4.44200208201066	5.04180893034472
C	2.73714700194059	-0.42530892766184	8.80517945606426
H	1.94126277518363	-1.33670842369645	3.99466875551049
H	6.51438135138426	-3.68208034670214	8.34633463784747
H	6.58140647910457	-5.06953446739579	4.28082951705506
H	3.27637895398976	-0.59720077353230	9.73189250890598
H	2.79588619868894	0.62513666686940	8.51662861941562
H	1.68281182722196	-0.68007009425186	8.91621760099633
H	4.87072978671096	-4.16983486954735	2.63730763020661
N	2.81928703816834	-2.72910749749127	1.87056726631769
C	1.73679156025053	-3.55322216409028	1.59258830861522
C	3.39200501392450	-1.84847937491349	0.96332117856056
C	1.20482007305516	-3.69245337978859	0.29770777930466
C	1.13732160027829	-4.28784222091054	2.62494184103727
C	3.04211741360125	-1.82692383925997	-0.39896215002560
C	4.35898089842321	-0.93270865609039	1.40276613205929
S	1.90111626867932	-2.93252365536313	-1.10143300095501
C	0.09904241024010	-4.50797854798556	0.07211129737514
C	0.04898611685112	-5.10008430731439	2.38509814735312
H	1.53712140004956	-4.20062490837700	3.62514251027254
C	3.64014473541567	-0.91815005976314	-1.26760235537302
C	4.94798946141282	-0.04266499980558	0.52953549962219
H	4.63311784826025	-0.92805923425552	2.44809667126114
C	-0.48433635202107	-5.21147864153193	1.10602704217210
H	-0.29721886432578	-4.58481695543310	-0.93458952069409
H	-0.39092781364346	-5.64751172733312	3.20983227037296
C	4.59303009390150	-0.02850162411103	-0.81455728266808
H	3.34481706357943	-0.92013960611696	-2.31120618083493
H	5.68819399542254	0.65277505985120	0.90613690531648
H	-1.34494302356074	-5.84088371488224	0.91712496400462
H	5.05033981208604	0.67312185679360	-1.50100013201868
N	7.75390391348260	-5.31227780323973	6.62349271154594
C	7.47076212696332	-6.58615895001820	7.09543474598297
C	9.02803619103148	-4.82525792762841	6.37616808980651
C	8.47272473788941	-7.53050164593635	7.38491895167656
C	6.13674581088632	-6.96961877143515	7.29655081890115
C	10.19052450499107	-5.59275333879438	6.57862215723076
C	9.18701333825086	-3.51162024942028	5.90965986345755
S	10.16710076547911	-7.22523314649942	7.16642117274421
C	8.13513560651482	-8.79338270832205	7.86695361355862
C	5.81775117754025	-8.22302946536851	7.77255632808436
H	5.35303726946672	-6.25907861050143	7.07657443495217
C	11.44706903718594	-5.05362736320800	6.31209117824026
C	10.43699781564123	-2.99283623108532	5.64856271056489
H	8.30573742404120	-2.90439669105311	5.76001098716727
C	6.81673564115033	-9.14592710836301	8.06471051403242
H	8.92913775233584	-9.49928967895212	8.08552963533040
H	4.77604447213794	-8.48119251394143	7.91898553296157
C	11.57885235077601	-3.76201939220144	5.84617212558125
H	12.32569341794034	-5.66723787267499	6.47950228938797

H	10.52037016641768	-1.97374229676104	5.29112584762562
H	6.56885912523927	-10.13015934448739	8.44194806887221
H	12.56206495686205	-3.35611323402644	5.64356654765495

**XYZ coordinates of m2po in S<sub>0</sub>**

O	-3.068177	0.089773	-6.249799
O	0.046797	-1.598505	-3.427520
N	-1.506924	-0.740686	-4.846604
C	-0.477127	-2.336549	-6.927134
C	-0.541137	-3.039126	-9.254275
C	-1.597131	-2.193637	-9.477354
C	-1.563751	-1.477697	-7.178095
C	0.092208	-2.408006	-5.641469
C	0.042369	-3.138150	-7.973432
C	-2.117177	-1.410258	-8.431540
C	1.140022	-3.259895	-5.398197
C	-2.121238	-0.647664	-6.089745
C	-0.430691	-1.569023	-4.539395
C	1.646524	-4.073722	-6.427477
C	1.112692	-4.011850	-7.689007
C	-2.059248	0.102414	-3.798061
H	-2.956685	-0.748131	-8.608581
H	1.567853	-3.306725	-4.403606
H	1.517350	-4.646785	-8.469214
H	-1.503525	-0.088507	-2.885510
H	-1.973639	1.150649	-4.084720
H	-3.115709	-0.126100	-3.660120
H	-0.158909	-3.637990	-10.073316
N	2.710362	-4.970764	-6.153516
C	2.447452	-6.122326	-5.401646
C	4.031885	-4.514787	-6.233949
C	1.160588	-6.524031	-5.064863
C	3.519585	-6.919683	-4.991037
C	5.062390	-5.357887	-5.808071
C	4.367207	-3.261344	-6.730600
C	0.947198	-7.684500	-4.331284
H	0.316135	-5.926745	-5.384212
O	4.810272	-6.614745	-5.328295
C	3.308869	-8.066674	-4.255765
C	6.380034	-4.959150	-5.882704
C	5.695899	-2.863360	-6.815681
H	3.581470	-2.593120	-7.059755
C	2.017694	-8.457615	-3.922498
H	-0.066488	-7.975272	-4.083980
H	4.173171	-8.648109	-3.958118
C	6.705124	-3.708605	-6.394007
H	7.142312	-5.647982	-5.538982
H	5.930739	-1.883260	-7.212705
H	1.859501	-9.361895	-3.348159

H	7.742655	-3.404829	-6.455877
N	-2.176146	-2.113812	-10.770287
C	-1.909119	-0.991491	-11.564482
C	-3.334347	-2.854326	-11.040634
C	-0.958893	-0.036410	-11.224876
C	-2.610989	-0.832292	-12.762456
C	-3.998287	-2.646578	-12.252755
C	-3.845664	-3.799475	-10.160013
C	-0.714206	1.049283	-12.056658
H	-0.400368	-0.146946	-10.304047
O	-3.529120	-1.756955	-13.181741
C	-2.376346	0.250460	-13.583035
C	-5.135918	-3.359125	-12.567836
C	-4.985310	-4.525923	-10.482381
H	-3.344025	-3.972691	-9.216366
C	-1.421327	1.198044	-13.235097
H	0.035171	1.777211	-11.770490
H	-2.949298	0.330708	-14.498972
C	-5.633948	-4.308695	-11.683576
H	-5.616821	-3.161124	-13.518211
H	-5.360630	-5.260899	-9.780707
H	-1.237938	2.042960	-13.887079
H	-6.524043	-4.869570	-11.940019

### XYZ coordinates of m2po in S<sub>1</sub>

O	-3.12690165089979	0.36961776843864	-5.91560902878047
O	0.00446050871779	-1.44454922661480	-3.15840877495669
N	-1.56225186719586	-0.54876189984510	-4.56137880744510
C	-0.62780675187246	-2.13010140964493	-6.65583441669057
C	-0.77254713918859	-2.83675664918519	-8.98405928607434
C	-1.83216999929784	-1.95380016039825	-9.17387115154773
C	-1.70218075963720	-1.25064643228392	-6.87884608877685
C	-0.02242530473642	-2.21252234200699	-5.38197734410758
C	-0.14849752448186	-2.94440552236970	-7.73243109626516
C	-2.29953896684376	-1.16545161917714	-8.14223085189451
C	1.05220044519221	-3.08779378607475	-5.16372682128405
C	-2.19902105121709	-0.41807352334533	-5.79394678848514
C	-0.49503061895763	-1.39881063591426	-4.27951920140175
C	1.49082299913050	-3.85768367500604	-6.21383546614283
C	0.93317233052556	-3.81882100388259	-7.48459495522788
C	-2.07602432875859	0.29020877053464	-3.49594980325363
H	-3.12319416702508	-0.47932024424951	-8.29110305718647
H	1.49998982977264	-3.13115453505206	-4.17949959060883
H	1.31762515520890	-4.44529045095020	-8.27985044364494
H	-1.49603724620405	0.08543201634394	-2.60116548081666
H	-1.99368872434488	1.34050356182824	-3.77785060912946
H	-3.13206506839221	0.07445768137203	-3.33040013552108
H	-0.42960844819943	-3.44119270018661	-9.81573988709798
N	2.60522698316909	-4.76032950898409	-5.99170580551465

C	2.37460071342351	-6.04645206572491	-5.58578034040801
C	3.88735431014822	-4.32843790178831	-6.19682228176997
C	1.08259395037061	-6.53741865741932	-5.35279182318274
C	3.46852550049132	-6.91448899028983	-5.39116774451023
C	4.95726151684313	-5.22380093969219	-5.99290116787260
C	4.18020712038249	-3.01949323604415	-6.60356866838120
C	0.91099267909508	-7.83720874193494	-4.94558639690723
H	0.24257048685334	-5.87390917728931	-5.49739980480791
O	4.73403304805915	-6.49547147032542	-5.60041950566998
C	3.28859314390917	-8.22442099879023	-4.97995599869459
C	6.27241889861222	-4.83596361050518	-6.18631853821664
C	5.48617488871161	-2.64126163158458	-6.79369630789105
H	3.36323287573523	-2.32976125527091	-6.75707529604917
C	2.00936732960819	-8.68537521934446	-4.75738802506406
H	-0.09002519743679	-8.20784796624340	-4.76637173448206
H	4.16034013025276	-8.85122663364950	-4.84323617303933
C	6.53641407584215	-3.54432168812094	-6.58685129729682
H	7.05878173539733	-5.55987810125707	-6.01570364912122
H	5.70346288119418	-1.62809559194861	-7.10643896765482
H	1.85554366211367	-9.70708998721196	-4.43468949792080
H	7.56033331258376	-3.22853805140183	-6.74032672224747
N	-2.43576924776287	-1.86990799597861	-10.46190568803648
C	-1.85057452755214	-1.08334132336577	-11.45099485735392
C	-3.43146238858800	-2.77471855000673	-10.82172600823677
C	-0.75682133839136	-0.26077767113381	-11.20512241074774
C	-2.38226446814095	-1.10418250834045	-12.74528217779060
C	-3.93009255541275	-2.75880498446471	-12.12908902776037
C	-3.96496426885355	-3.69650158819975	-9.92800010734338
C	-0.20926953768518	0.51768010168096	-12.21753050473888
H	-0.34310459210904	-0.22831750801483	-10.20545654506754
O	-3.47676171124445	-1.86396384590066	-13.06127052514373
C	-1.83408205360023	-0.33803051726703	-13.75168417541789
C	-4.91829722797699	-3.63494189685906	-12.52401997728458
C	-4.96670811990238	-4.57432900899180	-10.32377250848742
H	-3.59343836473361	-3.71222922429274	-8.91146430362291
C	-0.74156587539167	0.48225213391166	-13.49293269771901
H	0.63760056545463	1.15581944590285	-11.99455853113542
H	-2.28400453820984	-0.39119091573269	-14.73596211307115
C	-5.44659227891657	-4.54982981090531	-11.62006069799303
H	-5.26912315278528	-3.58048735163217	-13.54774902109102
H	-5.36983943287074	-5.27601823818509	-9.60321060859045
H	-0.32074338805922	1.08718709485927	-14.28664336193160
H	-6.22818105392211	-5.23015666459183	-11.93513304839205

### XYZ coordinates of m2po T<sub>1</sub>

O	-3.56746965364566	-0.19795999632827	-5.87506958661491
O	-0.46678198591667	-1.94954321942738	-3.04619883857874
N	-2.00865476540949	-1.07137863919316	-4.48140080584820
C	-0.74516320272220	-2.32085536998394	-6.62551733406576

C	-0.62442783704846	-2.78420363215483	-9.01786962267386
C	-1.77825692338633	-2.00020192843335	-9.20634507152507
C	-1.89387646246543	-1.54148702332852	-6.85397394019583
C	-0.23321961663853	-2.47901878681771	-5.32689829387193
C	-0.08922359532766	-2.95538500959973	-7.73042845040512
C	-2.40438292770349	-1.38037742822872	-8.15248101633063
C	0.92004677931131	-3.25253992792140	-5.10259171194299
C	-2.56266984903291	-0.88474640716892	-5.74409311854634
C	-0.87818633938437	-1.83554179884657	-4.19303513915952
C	1.54763014593186	-3.85149688422571	-6.16622566734251
C	1.06823675305836	-3.71216204719482	-7.47912356456093
C	-2.68830449188098	-0.40401018115644	-3.38702651941807
H	-3.28875542427419	-0.77167741667743	-8.29254821271510
H	1.28916112913017	-3.35943933885587	-4.09043792367536
H	1.58317369222162	-4.20861113820468	-8.29323889991239
H	-2.16957901440830	-0.65800467683080	-2.46762245192625
H	-2.68000503576789	0.67486659965245	-3.54708211234604
H	-3.72909834913601	-0.72621167583445	-3.34623965815627
H	-0.16374530336543	-3.27278794351095	-9.86830534278794
N	2.69328737970487	-4.66915064773893	-5.95922884571230
C	2.58733227801298	-5.91824307919545	-5.35786508527209
C	3.93393140268638	-4.22813752372634	-6.39020412279441
C	1.37918017869039	-6.42515138437768	-4.88148734477391
C	3.73051488459006	-6.72207306756859	-5.25181858816741
C	5.04582645851891	-5.07516570250626	-6.27291770882502
C	4.12918807536852	-2.94867528127126	-6.91352691926368
C	1.32231320085441	-7.67997890067455	-4.30280132624538
H	0.48703245983810	-5.81981211161097	-4.96753580306279
O	4.94043607317342	-6.31861702907755	-5.73170173180293
C	3.67245693769028	-7.97419832051321	-4.67091101717525
C	6.29687552687773	-4.67123053220201	-6.69465758516447
C	5.38324328135486	-2.54789171839520	-7.33828044954924
H	3.28516933045331	-2.27487065002266	-6.97359830317168
C	2.46706065416794	-8.45780233893856	-4.19008701051672
H	0.37279880147826	-8.05009194427157	-3.93630033169887
H	4.58534714581304	-8.55393457613012	-4.61064785703179
C	6.46878784528378	-3.40702988905903	-7.23691017217682
H	7.12367531065421	-5.36195757693508	-6.58367753339743
H	5.51286876266962	-1.55050756092162	-7.73992118091958
H	2.42329568188232	-9.43849342538560	-3.73310647175476
H	7.45153066381426	-3.09196119065850	-7.56491902737324
N	-2.30718831801648	-1.90575612014522	-10.52121100062395
C	-1.56131099467726	-1.29365832609805	-11.51801846556646
C	-3.54833981382736	-2.44886443819420	-10.84369853955736
C	-0.36684423278373	-0.62108681015076	-11.24963392673464
C	-2.02746548457234	-1.31334011278193	-12.84081739538501
C	-3.98112134939225	-2.41540095990241	-12.17672447465454
C	-4.37349798720056	-3.06616193450693	-9.90342270609649
C	0.35803978745716	-0.04129155228399	-12.27459960011307
H	-0.02186359181571	-0.55650284900711	-10.22670368884240

O	-3.21386693753309	-1.88825491273023	-13.17039938460000
C	-1.30145603036710	-0.73358306755675	-13.86277268626048
C	-5.20235626259754	-2.94473027686338	-12.54855822769376
C	-5.59327185446597	-3.59814902144523	-10.27744157250811
H	-4.04860254547138	-3.12036379756774	-8.87378908497859
C	-0.09939220374871	-0.10370667556698	-13.58413370413268
H	1.28228146717670	0.47392608763445	-12.04396620569425
H	-1.70113440792157	-0.78312237819582	-14.86810335003743
C	-6.01781894646762	-3.53390720550024	-11.59817586487128
H	-5.48763655097942	-2.88810833887181	-13.59182545984294
H	-6.21678894761609	-4.06590906001245	-9.52566805983683
H	0.46817163717480	0.35100426312000	-14.38650459497431
H	-6.97591034807148	-3.94578246192068	-11.88956803854426

### XYZ coordinates of m2npp in S<sub>0</sub>

O	-2.050870	1.645222	2.052255
O	1.108347	0.011659	4.856824
N	-0.469591	0.838232	3.446210
C	0.586443	-0.725636	1.356446
C	0.518226	-1.433137	-0.968847
C	-0.553965	-0.606252	-1.187273
C	-0.519741	0.109756	1.112450
C	1.165894	-0.786321	2.638247
C	1.117059	-1.514392	0.305760
C	-1.079474	0.169077	-0.138914
C	2.236631	-1.612161	2.872202
C	-1.088916	0.925213	2.204863
C	0.627538	0.034277	3.745825
C	2.757000	-2.411102	1.838196
C	2.210937	-2.361280	0.581542
C	-1.038895	1.660983	4.501292
H	-1.931538	0.815678	-0.312053
H	2.672168	-1.651340	3.863607
H	2.625788	-2.984279	-0.202910
H	-0.479838	1.473045	5.412451
H	-0.974290	2.713362	4.224262
H	-2.090727	1.410277	4.636388
H	0.905338	-2.027593	-1.788925
N	3.846399	-3.279322	2.103745
C	5.151435	-2.778532	1.989022
C	3.596547	-4.458038	2.821190
C	6.231819	-3.599669	2.358801
C	5.403383	-1.506043	1.499568
C	4.680350	-5.270366	3.200237
C	2.306981	-4.861394	3.132960
C	7.524795	-3.119371	2.208868
C	6.705747	-1.038622	1.347704
H	4.571655	-0.871758	1.221710
C	4.430537	-6.448323	3.889427

C	2.069493	-6.048318	3.819620
H	1.470473	-4.246055	2.828906
C	7.765077	-1.846882	1.699436
H	8.356484	-3.752374	2.489177
H	6.872775	-0.043218	0.954855
C	3.131619	-6.840124	4.198824
H	5.263869	-7.073809	4.181352
H	1.050945	-6.338039	4.046729
H	8.785937	-1.502764	1.586735
H	2.968608	-7.767581	4.734117
N	-1.141707	-0.527871	-2.474556
C	-0.690753	0.457302	-3.363647
C	-2.337302	-1.219111	-2.709421
C	-1.368924	0.644395	-4.581477
C	0.415078	1.243445	-3.077434
C	-3.016152	-1.023380	-3.925463
C	-2.853796	-2.110231	-1.780676
C	-0.904535	1.602985	-5.470757
C	0.872827	2.199523	-3.979721
H	0.932678	1.106270	-2.137030
C	-4.190375	-1.724065	-4.160449
C	-4.030834	-2.809735	-2.030624
H	-2.327540	-2.266125	-0.847931
C	0.213575	2.377317	-5.176417
H	-1.425314	1.744717	-6.408683
H	1.741666	2.796007	-3.730006
C	-4.698915	-2.614907	-3.219749
H	-4.714550	-1.573100	-5.095054
H	-4.409003	-3.499955	-1.286585
H	0.552905	3.115759	-5.892527
H	-5.616916	-3.148519	-3.433710
C	7.070429	-5.713896	3.218448
C	7.630774	-5.612662	4.485709
C	7.574999	-6.628332	2.305076
C	8.694335	-6.429389	4.837698
H	7.224558	-4.892805	5.187030
C	8.640143	-7.443476	2.659038
H	7.124366	-6.690951	1.321487
C	9.199894	-7.344857	3.924596
H	9.130116	-6.351188	5.826995
H	9.032866	-8.157323	1.944302
H	10.031691	-7.982556	4.200560
N	5.976889	-4.883772	2.848877
N	-2.484680	-0.144741	-4.873337
C	-3.200080	0.087766	-6.079141
C	-4.201554	1.049459	-6.118600
C	-2.895481	-0.647832	-7.215638
C	-4.897925	1.274337	-7.295870
H	-4.426087	1.614025	-5.220910
C	-3.593594	-0.420837	-8.392732

H	-2.110775	-1.393713	-7.165438
C	-4.594139	0.539556	-8.433863
H	-5.679204	2.024941	-7.324964
H	-3.355119	-0.995959	-9.279868
H	-5.138799	0.715896	-9.354173

**XYZ coordinates of m2npp in S<sub>1</sub>**

O	-2.05686284579570	2.07451546909414	2.24758713520805
O	1.01858668292498	0.38774473988036	5.14620316715849
N	-0.51366704715874	1.21720362659177	3.67432586733597
C	0.49075992085100	-0.42942310369583	1.66713667156628
C	0.40914952513247	-1.22254814254469	-0.64281043021489
C	-0.64743162550091	-0.34973968299010	-0.86127741053440
C	-0.58831574403172	0.43859730227674	1.39080051034086
C	1.06731287064293	-0.46832524535905	2.95018179390365
C	1.00622666663772	-1.27926971913888	0.63598696494314
C	-1.15885966826517	0.47776571360554	0.10992016267096
C	2.14060430295400	-1.32849642938432	3.21789848378977
C	-1.11973289832150	1.29956985894823	2.42576983354508
C	0.55579107996153	0.38407049330609	4.01323871512247
C	2.63175884724858	-2.14334205007986	2.21833071672107
C	2.07971141241055	-2.12889454529876	0.94103101770691
C	-1.05852145958749	2.08599979576355	4.69895698275328
H	-1.98392588876079	1.15309099820757	-0.07526981066839
H	2.56973285471703	-1.34160906015320	4.21129284590105
H	2.48872051340173	-2.78254294995940	0.17943056450585
H	-0.49654971363604	1.91570444035978	5.61236831930116
H	-0.97828551255372	3.12744783973837	4.38504349763205
H	-2.11607396241250	1.86600675433089	4.84932093080041
H	0.77840684291266	-1.85502834096204	-1.44065275024612
N	3.72188682301629	-3.02384883977768	2.48147193000873
C	5.01826065403067	-2.60950423554789	2.17559013051581
C	3.45364101500744	-4.34404108830080	2.84376289313151
C	6.08671616468937	-3.51685651362952	2.30882158541293
C	5.28497152851816	-1.31584808831556	1.75062971561662
C	4.51723727750336	-5.25651215001393	2.97999953369145
C	2.15890885271955	-4.78104664751030	3.08452273361737
C	7.37433923545213	-3.09754778691664	2.00863364904621
C	6.58240626146094	-0.90589740832590	1.45649978225355
H	4.46217928135138	-0.61935543823474	1.65832577319261
C	4.24494870407741	-6.56574119276822	3.34837242466881
C	1.89898779296584	-6.09685822639010	3.45725329552056
H	1.34538903365127	-4.07453994119845	2.98664827397409
C	7.62717268815879	-1.79552695202081	1.58401771561596
H	8.19317598367758	-3.79767833719253	2.11218325508488
H	6.75798350618578	0.11335957738368	1.13377568678775
C	2.94042570975449	-6.98978777186458	3.58884249431080
H	5.06507760526751	-7.26413325784721	3.45336384112882

H	0.87733639746593	-6.40451396801575	3.64543106414226
H	8.64408433351562	-1.49518833570945	1.36177212277807
H	2.75907415022760	-8.01726364313338	3.88056031458640
N	-1.23639836749365	-0.31328883014988	-2.18630084371764
C	-0.73186036003893	0.54988856809140	-3.12294229831566
C	-2.28377411716180	-1.14599747409235	-2.48132595635510
C	-1.29355298618634	0.58432074668434	-4.42304204551819
C	0.33556145474022	1.40375729500995	-2.82133390761433
C	-2.85790811546459	-1.12255963445003	-3.77609969394757
C	-2.80250212924406	-2.02566543562826	-1.52415124832314
C	-0.77625740265468	1.46348563853169	-5.37804871908527
C	0.82863508897831	2.26049030012269	-3.77522009934305
H	0.75568654641788	1.37293953916634	-1.82717213225734
C	-3.92711579482826	-1.97109567737238	-4.07525047107808
C	-3.85334723714204	-2.85228104103515	-1.83977267870039
H	-2.36066459439631	-2.03472536612434	-0.53897652987236
C	0.27394544671261	2.29223624783472	-5.05682141687674
H	-1.20964546064208	1.48520332700662	-6.36818685980252
H	1.65377128737135	2.91493515849304	-3.52509117667111
C	-4.41879125988782	-2.82689949015992	-3.11682267242278
H	-4.36213529669651	-1.94702781385413	-5.06460296563540
H	-4.24325451675519	-3.52574585198653	-1.08735582390148
H	0.66673899894071	2.97026567004285	-5.80379739064778
H	-5.24793518110871	-3.47961525146879	-3.35860903704698
C	6.89843330901423	-5.73604908653173	2.87937543366246
C	7.56144040851730	-5.85824270211617	4.09296938377143
C	7.28685031794751	-6.51237313424344	1.79496225116238
C	8.61149657362385	-6.75540671923064	4.22137759197350
H	7.24443963223822	-5.24421058059507	4.92784004290264
C	8.33650089405651	-7.40890623743602	1.92505279750073
H	6.75778604383577	-6.40373065528227	0.85524201820529
C	8.99974810613256	-7.53125461516142	3.13827763378470
H	9.12744513071473	-6.84855309826309	5.17007922669556
H	8.63761997093819	-8.01360729535350	1.07726012396913
H	9.82041202396397	-8.23214726052321	3.23951648071206
N	5.82447687646487	-4.81781397015687	2.74865368730948
N	-2.34539190461630	-0.25630428056680	-4.71797450415939
C	-2.91390680534602	-0.23395814850915	-6.03310602703915
C	-3.96201629821424	0.62994762002038	-6.30736917475343
C	-2.40461124951001	-1.07878536453346	-7.00626702152033
C	-4.50849100442514	0.64604470660487	-7.58169932829765
H	-4.34085883351568	1.27992739914570	-5.52739728866335
C	-2.95706875213985	-1.05631793085424	-8.27771684706269
H	-1.58442614091720	-1.74426883391992	-6.76378367887247
C	-4.00720036727409	-0.19562045595915	-8.56456848230064
H	-5.32812967011769	1.31802104611834	-7.80525376895998
H	-2.56539845359888	-1.71345543293716	-9.04460373073691
H	-4.43689886370119	-0.18062917158440	-9.55898828647839

XYZ coordinates of m2npp T<sub>1</sub>

O	-2.07379375177207	1.92668969958145	2.26930822882654
O	1.05088280044724	0.20602872360024	5.09111947057194
N	-0.50480367857866	1.05797375181002	3.65471667291086
C	0.47572501827846	-0.54729928274646	1.60181274565372
C	0.37085400580627	-1.29167624969769	-0.72127481221186
C	-0.68911354704748	-0.41168563861353	-0.92785656205692
C	-0.60569577755909	0.32046415992944	1.35242075755284
C	1.06510261044143	-0.60861282596072	2.88055671396081
C	0.98134513973926	-1.37291084145881	0.54470221449788
C	-1.18272204064649	0.38995627534387	0.07710515049075
C	2.14666688414447	-1.46833462515435	3.12122695751216
C	-1.13049488789120	1.15777072465991	2.41481343533898
C	0.56946413906039	0.22174069637024	3.96420328272824
C	2.62523449140368	-2.25115143574439	2.09482025500790
C	2.06898503357629	-2.22406980779072	0.81821180803181
C	-1.03588713391558	1.91140064267000	4.69966008072304
H	-2.00898461165238	1.06926504115498	-0.09097483337490
H	2.58695334008116	-1.49582685620150	4.11003797813441
H	2.47499478163797	-2.85746220667286	0.03780117169995
H	-0.48264475775114	1.70551766169959	5.61112734761702
H	-0.92954040510339	2.95934768419011	4.41513384330607
H	-2.09910174632404	1.71191700548589	4.83650048948397
H	0.72896488990926	-1.90662516081707	-1.53896219296107
N	3.73847278889459	-3.12110979220788	2.33305531642509
C	5.02125577304307	-2.64776789875633	2.12670303095875
C	3.51312907239089	-4.42439348438021	2.73724784251505
C	6.12444443728108	-3.50159177532219	2.34186865919096
C	5.24789885946610	-1.33579820152824	1.71305637053558
C	4.60882986908546	-5.28771802304088	2.95193487931613
C	2.22006648213945	-4.90357670281752	2.94032701478892
C	7.41374558875765	-3.01584341020491	2.13998791752475
C	6.53494792756782	-0.87081660848152	1.51483066517043
H	4.39554691275210	-0.68898177819240	1.55638877556776
C	4.37557096102099	-6.59904710906343	3.35791223598192
C	2.00667416540747	-6.20835213545126	3.34577242779215
H	1.38886241119394	-4.23079383270026	2.77820081538097
C	7.61899556545681	-1.70991005989363	1.72865613280476
H	8.25762572564783	-3.67083705228786	2.31024182463427
H	6.68786918118398	0.15282870983541	1.19611741009425
C	3.08414330869772	-7.05748719388887	3.55393540356631
H	5.21720039153466	-7.25859625663968	3.52158403431002
H	0.99371933200882	-6.55856836127028	3.50103695642824
H	8.62994684526595	-1.35156106974642	1.57826623208472
H	2.92435358359061	-8.08045509848218	3.87181616313608
N	-1.27750548364457	-0.34766998935961	-2.23240491847943
C	-0.67596933784686	0.42345611575033	-3.21047569497728
C	-2.42195749844447	-1.07765859905224	-2.50079982280628
C	-1.23949660253509	0.47644675419605	-4.50350931174175
C	0.47576970590327	1.16185145940277	-2.94177702036660

C	-3.00483041458458	-1.01515525979364	-3.78473491004956
C	-3.01507581086541	-1.87590545276194	-1.52399413643981
C	-0.62097251676629	1.24296548211754	-5.48783354681706
C	1.07377252932973	1.92253495163229	-3.92977118234374
H	0.89033858652071	1.12807222038573	-1.94363943345095
C	-4.16871975287360	-1.73487059349415	-4.04200496090577
C	-4.16752892346402	-2.58884263255778	-1.79843474963985
H	-2.55930904641679	-1.91791607990466	-0.54419737849382
C	0.52879525391131	1.96023800697812	-5.20508998818480
H	-1.05223555078000	1.27601337240050	-6.47932479767270
H	1.96725544101949	2.48884733920786	-3.69778607200029
C	-4.74816167395844	-2.51528763987049	-3.05644972805822
H	-4.61964332018066	-1.67698238201763	-5.02355091721203
H	-4.61309636225331	-3.19890401870778	-1.02249634055137
H	0.99316056612066	2.55157375348945	-5.98467862035420
H	-5.65477970482242	-3.06536177534299	-3.27663485143442
C	7.00851543154894	-5.66900480409628	2.98862755530770
C	7.56620751837429	-5.73902791486775	4.25685123789578
C	7.52528269724383	-6.42538612183509	1.94693690656150
C	8.65110468599104	-6.57251753968645	4.48276025810235
H	7.14598293360253	-5.13870651384120	5.05531738451165
C	8.61103357968481	-7.25668533045028	2.17770766047632
H	7.07341987197600	-6.35430809005206	0.96443500706999
C	9.17387458401089	-7.33016741930387	3.44412982095674
H	9.08915989295783	-6.62893370503409	5.47226211760710
H	9.01759530202711	-7.84850452433612	1.36610854675723
H	10.02234759808582	-7.98033832769570	3.62231615456990
N	5.89683156575760	-4.80804037095997	2.75380922034190
N	-2.40326099347663	-0.23461627654026	-4.76334509260092
C	-3.01172310816789	-0.13144026276365	-6.04836619419179
C	-3.90356677008146	0.90068719608136	-6.30171593057972
C	-2.70852154918766	-1.05991213196076	-7.03322879044323
C	-4.49497783797190	1.00382310180533	-7.55147716532703
H	-4.12553175340970	1.61521132268157	-5.51767459956224
C	-3.30516989123202	-0.95421033384565	-8.28080900719400
H	-2.00924828750593	-1.85825759628341	-6.81348500447192
C	-4.19692276950268	0.07697251925634	-8.54046762922241
H	-5.19158064969726	1.80929111293539	-7.75183883728558
H	-3.07130866728735	-1.67890739673746	-9.05175468278983
H	-4.66085834578057	0.15858831371581	-9.51641430616076

### XYZ coordinates of p2azb in S<sub>0</sub>

O	1.845277	8.082357	-0.323306
C	0.865390	7.385130	-0.475604
C	0.914766	5.906985	-0.348603
C	-0.249847	5.116911	-0.510719
C	-0.192460	3.687988	-0.371409
C	-1.435747	2.981872	-0.449313
C	-2.604163	3.650513	-0.761657

C	-2.630215	5.036490	-0.964689
C	-1.471720	5.768270	-0.812188
C	1.102615	3.112884	-0.167456
C	2.212669	3.918912	0.001222
C	2.127375	5.315147	-0.066997
N	-0.364793	7.956064	-0.783622
C	-0.386061	9.403281	-0.916146
C	-1.548021	7.244983	-0.971700
O	-2.587069	7.804313	-1.248304
C	-0.451754	-3.105857	1.872904
C	-1.824192	-3.542260	1.446351
C	-2.231862	-4.863490	1.661383
C	-3.515609	-5.298786	1.330631
C	-3.930112	-6.728372	1.534086
C	-4.400978	-4.366733	0.780364
C	-4.020659	-3.044989	0.538149
C	-5.005612	-2.076641	-0.060392
C	-2.713425	-2.619966	0.862002
B	-2.269395	-1.139404	0.540722
C	-1.927908	-0.690938	-0.887924
C	-1.950496	-1.585614	-1.980145
C	-1.659258	-1.184199	-3.270216
C	-1.346214	0.162110	-3.502149
C	-1.328876	1.077770	-2.465602
C	-1.604851	0.663921	-1.146133
N	-1.572073	1.599772	-0.113105
C	-1.921108	1.304961	1.206675
C	-2.222725	-0.025133	1.594827
C	-2.538969	-0.268744	2.948328
C	-2.576028	0.741010	3.892692
C	-2.312268	2.054219	3.480791
C	-1.994055	2.341049	2.164870
C	5.134027	-1.505750	0.504108
C	4.286852	-2.677022	0.082935
C	4.819190	-3.965611	0.109752
C	4.067316	-5.082390	-0.274967
C	4.668634	-6.458755	-0.243277
C	2.761337	-4.869558	-0.710780
C	2.200743	-3.586476	-0.765529
C	0.802450	-3.425033	-1.294368
C	2.954335	-2.474426	-0.348918
B	2.346602	-1.017201	-0.326068
C	1.941688	-0.330835	0.987351
C	2.048528	-0.979805	2.237103
C	1.701086	-0.361634	3.423172
C	1.238723	0.961112	3.382714
C	1.134515	1.641991	2.183538
C	1.471317	1.004668	0.971427
N	1.354585	1.707391	-0.227340
C	1.750449	1.193702	-1.464541

C	2.197012	-0.146757	-1.581694
C	2.557380	-0.619803	-2.861718
C	2.501356	0.180134	-3.988435
C	2.092403	1.512904	-3.845129
C	1.726208	2.019860	-2.610677
H	-3.526444	3.068012	-0.810374
H	-3.556057	5.562003	-1.206240
H	3.177112	3.430971	0.155808
H	3.005600	5.950681	0.062086
H	-0.050233	9.869831	0.020085
H	-1.410618	9.706741	-1.151974
H	0.301087	9.717096	-1.714067
H	0.264675	-3.940351	1.887052
H	-0.045580	-2.329577	1.211278
H	-0.473152	-2.664308	2.883164
H	-1.523422	-5.571375	2.104160
H	-4.983528	-6.803388	1.843769
H	-3.313203	-7.224541	2.297561
H	-3.825060	-7.306610	0.600356
H	-5.419626	-4.681021	0.529568
H	-4.698945	-1.769393	-1.073523
H	-5.075883	-1.155585	0.540613
H	-6.012070	-2.513191	-0.130603
H	-2.200564	-2.629825	-1.771948
H	-1.671024	-1.898804	-4.095785
H	-1.107164	0.503573	-4.512263
H	-1.086640	2.118114	-2.678440
H	-2.771584	-1.298854	3.234048
H	-2.823267	0.526392	4.934530
H	-2.358327	2.873656	4.203118
H	-1.792615	3.374776	1.884489
H	5.132699	-0.715594	-0.264227
H	4.751319	-1.045322	1.429105
H	6.177276	-1.803608	0.680931
H	5.852492	-4.107570	0.443781
H	5.229415	-6.631584	0.688377
H	3.898792	-7.239379	-0.327052
H	5.377111	-6.601150	-1.076566
H	2.154565	-5.726319	-1.022353
H	0.101290	-4.133306	-0.826745
H	0.411059	-2.413114	-1.129009
H	0.770144	-3.603221	-2.382204
H	2.413630	-2.010857	2.239786
H	1.782481	-0.889550	4.375586
H	0.951175	1.470434	4.305685
H	0.779507	2.671599	2.185622
H	2.900647	-1.655612	-2.938179
H	2.785954	-0.209903	-4.968029
H	2.059369	2.171641	-4.717055
H	1.411304	3.060899	-2.541199

### XYZ coordinates of p2azb in S<sub>1</sub>

O	1.83998128274715	8.11909579075711	-0.40105822957028
C	0.85856083433465	7.39601547720097	-0.51056217099078
C	0.91851442020596	5.94016096144746	-0.39277483341982
C	-0.25494428545911	5.15581024805206	-0.51681600804545
C	-0.18465972662432	3.71638253964369	-0.38400937193456
C	-1.41499516898614	3.01051733800023	-0.45686121126312
C	-2.62930965915762	3.66565422556193	-0.71640886885137
C	-2.67758340826813	5.03424616383794	-0.88665806879834
C	-1.49727785965204	5.79008085876971	-0.76884107999249
C	1.10749628935121	3.15991179481564	-0.19249572781250
C	2.25226623704657	3.96353095028030	-0.07348812155405
C	2.16656997894415	5.33833193435200	-0.15634160218639
N	-0.39327101681988	7.95483082677703	-0.76363179651042
C	-0.42953868540577	9.39866699093570	-0.88423472789784
C	-1.58822984878316	7.24406595506439	-0.90680837148314
O	-2.64405346587372	7.82153901404369	-1.12985833012508
C	-0.38081408294554	-3.22859124126477	1.83768499793779
C	-1.76539299200303	-3.60570231162049	1.39319424492582
C	-2.22989987256193	-4.90775494486714	1.60884161385710
C	-3.52414811073717	-5.29297114767891	1.25826856697132
C	-4.00131475405123	-6.70215586497565	1.46333131137226
C	-4.36134192623267	-4.32837263531452	0.68867993373424
C	-3.92563116867595	-3.02436375920764	0.44584260076629
C	-4.87132765344474	-2.02133907556124	-0.15991800880746
C	-2.60560205597033	-2.65095659400601	0.78800774713163
B	-2.12243714455402	-1.18203370486514	0.48351349997248
C	-1.83431165487525	-0.68882550294595	-0.94652026288397
C	-1.88146987959100	-1.55197385636112	-2.05320954616914
C	-1.65713059609967	-1.10632435470492	-3.35066747831007
C	-1.40738203488641	0.25243589149151	-3.56665397132180
C	-1.37017642607640	1.14522536988529	-2.50879753031945
C	-1.56395795665766	0.68731429596080	-1.18361967260161
N	-1.51029831753746	1.60229448761226	-0.14458432445095
C	-1.76354592531102	1.26120151042343	1.17616435357979
C	-2.02077545301524	-0.08543525955131	1.55857450851272
C	-2.27022363395657	-0.35377402092348	2.91317676751612
C	-2.28058253470646	0.64870403519503	3.87795152522165
C	-2.05631742760997	1.97060959123671	3.48336256117703
C	-1.79744972809441	2.28275034945281	2.15859499786467
C	4.98559099202906	-1.47249799946723	0.66155545849864
C	4.17475083435645	-2.65929325561673	0.21014551298284
C	4.74427482572164	-3.93064051436792	0.24550450535177
C	4.04631343718777	-5.06689030785556	-0.18282523085738
C	4.67972890705667	-6.42603387344212	-0.10393640100459
C	2.75922118985479	-4.88824579163466	-0.68267350935248
C	2.15989661294091	-3.62310828696708	-0.74738075561625
C	0.78084159101624	-3.51306069746152	-1.33622008263965
C	2.85321052906364	-2.49239620851291	-0.27650962077712

B	2.22337264547107	-1.04755104112757	-0.27608081799430
C	1.86653380496973	-0.30676701373011	1.02753880049174
C	1.96888204496715	-0.92156614653593	2.28600169554149
C	1.68656275454916	-0.24609812139397	3.46734399085557
C	1.31529478746438	1.10071779642391	3.40616924772870
C	1.21201193299444	1.75351849399108	2.18978266580909
C	1.46562136592107	1.05687266617697	0.98365235761704
N	1.33794234031279	1.73352397644720	-0.21832263215830
C	1.63456796703702	1.15904116610758	-1.44531831169784
C	2.02628786734812	-0.20516991513221	-1.55052941634195
C	2.31328127538490	-0.71476054110706	-2.82631836867192
C	2.23310113618455	0.06857833761751	-3.97313167161013
C	1.87543868072253	1.41429143621333	-3.85120620017538
C	1.57559033568402	1.95990721201522	-2.61374831017939
H	-3.54106738582353	3.06566731712200	-0.76278268165588
H	-3.60997335160927	5.56155366890818	-1.09088751752074
H	3.21682881486970	3.47206702537725	0.07275822073553
H	3.04108865318882	5.98303140887705	-0.06221074648280
H	-0.05555861282780	9.86411194633336	0.03873455158142
H	-1.46649889993684	9.69302596666490	-1.07477431276602
H	0.22426337125452	9.72598112550418	-1.70527584576408
H	0.30473744795205	-4.08860985845660	1.83605382404743
H	0.05562003923951	-2.45495505253712	1.19316865769113
H	-0.39074084641123	-2.81253648957708	2.85907062218070
H	-1.55889977792172	-5.64077758523972	2.06844794712964
H	-5.05885911455874	-6.73012890038730	1.76602526870300
H	-3.41134938431750	-7.22269714576203	2.23162249184475
H	-3.91592883399677	-7.28604799122962	0.53134459266476
H	-5.38851154215038	-4.60171955410862	0.42618050437746
H	-4.55860948254419	-1.73281464197155	-1.17617199401195
H	-4.90810604059189	-1.09337621446405	0.43355698529575
H	-5.89383217435480	-2.41891513119909	-0.22415012821923
H	-2.10192994607709	-2.60677431695147	-1.86688711212867
H	-1.69157807342989	-1.80250766146843	-4.19125692476132
H	-1.24319046692472	0.62573366358673	-4.57996018058159
H	-1.21529299659544	2.20627775125253	-2.69246775889934
H	-2.48307643896778	-1.38825462940624	3.19701969644206
H	-2.48273988068254	0.41020728359874	4.92438417761863
H	-2.08473426250487	2.77672757730362	4.22028992241357
H	-1.63879743510496	3.31937243422426	1.86773333803740
H	4.93283464101521	-0.64648875552347	-0.06580244771781
H	4.62194699290446	-1.07019530698076	1.62015318784686
H	6.04429874607400	-1.73749208955632	0.79087792606320
H	5.76956632916519	-4.04254645621418	0.61316040234002
H	4.84154163338238	-6.72704028681966	0.94408489767329
H	4.05401872514463	-7.19433758518585	-0.57980364227674
H	5.66510701554468	-6.43689229957102	-0.59588949687154
H	2.19855406665761	-5.75763955946815	-1.04158396342352
H	0.06071367752094	-4.16386718059680	-0.81604973881310
H	0.39238558640375	-2.48804731908269	-1.29032455816020

H	0.78002217716387	-3.81452924082830	-2.39675915488657
H	2.28281188928537	-1.96855496723773	2.31754296446742
H	1.76956051933950	-0.75340888896931	4.43080477362359
H	1.10416230260044	1.65440172667820	4.32365475354018
H	0.95759214249613	2.81060668304702	2.15547188340284
H	2.62682534024242	-1.75968928794041	-2.89947002106648
H	2.46686556278573	-0.35541917009549	-4.95209535558645
H	1.82979067245986	2.05347188823122	-4.73610927203911
H	1.31182815439746	3.01285040253030	-2.53528955712861

### XYZ coordinates of p2azb in T<sub>1</sub>

O	1.90579389580518	8.01791702445425	-0.17102861576276
C	0.93156616372901	7.32086604977122	-0.41520621708504
C	0.92872714770575	5.87192774971562	-0.22495840169962
C	-0.22217679109445	5.10296897740495	-0.53090098512898
C	-0.20682588025204	3.66864725294111	-0.35478874759953
C	-1.43558172554854	2.98866697557225	-0.51557453350639
C	-2.60965196467723	3.67998976275353	-0.91358757561057
C	-2.58855003776754	5.02483814110370	-1.17821846722047
C	-1.39162288766933	5.75507494160463	-0.96994544759738
C	1.02849094477275	3.08783683272960	0.05927165558472
C	2.13298836070834	3.90107579164411	0.46079597795584
C	2.09782925037497	5.25764024580134	0.30644299022138
N	-0.23854265191889	7.89717579667063	-0.90555907697387
C	-0.20722310272624	9.33438253179502	-1.10359175622678
C	-1.41506573453697	7.20607530062041	-1.19303061378538
O	-2.40943625640694	7.78309322608394	-1.60405700763135
C	-0.54323973363599	-3.00815652250172	2.14866187570517
C	-1.86338407864764	-3.47608653478879	1.60052118300754
C	-2.25970038342332	-4.79870218909428	1.83995190133604
C	-3.48477180182242	-5.28963052065562	1.39526740745365
C	-3.89658378867463	-6.71352582764809	1.63785060278970
C	-4.32863146597419	-4.41193979644403	0.70340493530415
C	-3.95953727875815	-3.09460892877864	0.43506505535044
C	-4.90942942558133	-2.18973104471754	-0.30394269185457
C	-2.70217313541019	-2.61201673622794	0.87321684174503
B	-2.27475651183638	-1.13286565945010	0.52595968490759
C	-1.89348046504935	-0.70743461687955	-0.90040320032190
C	-1.87906312019923	-1.62019451476027	-1.97639936308996
C	-1.58827661041107	-1.23174417356016	-3.27144178816703
C	-1.32036986044626	0.12063520000571	-3.52636315085572
C	-1.33892713651167	1.05405485524079	-2.50651165791287
C	-1.60068455436850	0.65142101120675	-1.17921215682998
N	-1.59624719065119	1.60818817181631	-0.16796885456181
C	-1.96591754152555	1.33332438218014	1.14460468897646
C	-2.28140361606291	0.01013109916128	1.55394562182674
C	-2.62930410995515	-0.20263319304949	2.90215969789420
C	-2.67810092507994	0.82924478979618	3.82601786614343
C	-2.38262219622341	2.13007397855911	3.40008500549761

C	-2.02911104487727	2.38830200878239	2.08604552149084
C	5.16047175723514	-1.42926323681448	0.20089807341241
C	4.30806103007440	-2.62773697141045	-0.12161147169777
C	4.88166933172224	-3.89852072505306	-0.17507303059082
C	4.12467056610492	-5.03741671027229	-0.47241220009518
C	4.76313704051683	-6.39691445731443	-0.48898256277403
C	2.76632061332971	-4.86776710050406	-0.73834148109566
C	2.16171696537714	-3.60543687080069	-0.70813218133380
C	0.70762643163063	-3.46532077293328	-1.05848464782913
C	2.92755654832825	-2.47072355956202	-0.38298304288573
B	2.28406286094208	-1.03604116894196	-0.28904395426218
C	1.98837210873437	-0.36423316488972	1.06542012129622
C	2.17196766329242	-1.03534926680461	2.28612864563704
C	1.84882470338108	-0.45337462018391	3.50526951029740
C	1.31401130372891	0.83904310405148	3.52011953622937
C	1.12338638660809	1.54123035896185	2.34087991124765
C	1.47600252188573	0.95796951081845	1.10352417008799
N	1.30128230829343	1.69680665163529	-0.06219635837857
C	1.61980947060606	1.20433082777803	-1.33307579303299
C	2.00805824099074	-0.14808915420145	-1.51508560929802
C	2.29201495370060	-0.58629691428932	-2.82125015294280
C	2.23015886673808	0.26474278511037	-3.91521407456036
C	1.91760773183812	1.61210536202095	-3.70506818949066
C	1.62465616745377	2.08534087358171	-2.43650947730048
H	-3.52717732974312	3.09769582483294	-1.02374618563028
H	-3.47089602026905	5.56798982055143	-1.51887354183221
H	3.03320000794052	3.39597670028614	0.81780824187666
H	2.94567584467027	5.89746998029621	0.55425276185052
H	0.01199438096360	9.84117913804712	-0.15321401067823
H	-1.18446764780786	9.64295746083714	-1.48794044808970
H	0.58965864082826	9.59889663117870	-1.81270959792949
H	0.27899608937021	-3.68182935058147	1.86097909767819
H	-0.28440442471280	-1.99952511432342	1.80191616529541
H	-0.56271097993392	-2.97297269039188	3.25062364880617
H	-1.58784151072764	-5.46006545082117	2.39745398706315
H	-4.91375251993236	-6.77095063010806	2.05598475631417
H	-3.21337398036266	-7.22066327872177	2.33410446676954
H	-3.90285432625114	-7.28945313545356	0.69756113311382
H	-5.30751550889639	-4.76854189061388	0.36588997556924
H	-4.54356270136467	-1.96110390661955	-1.31771377376262
H	-5.02748577244503	-1.22338150957099	0.21202632106882
H	-5.90531611080957	-2.64472439399082	-0.40092179391635
H	-2.10546383387238	-2.66693416235528	-1.75470226266616
H	-1.57817070318769	-1.95972694599291	-4.08549498702842
H	-1.10024301357812	0.45306546873433	-4.54366017259524
H	-1.15819352958886	2.10521960266901	-2.72979929931657
H	-2.87341471945130	-1.22439174465270	3.20698343321642
H	-2.95254951372053	0.63639100332423	4.86539746601878
H	-2.42900052959144	2.96207270352683	4.10756525351197
H	-1.79883562012631	3.40948864674407	1.78440711155481

H	5.06407812273787	-0.64883223882844	-0.57162504444504
H	4.85999202247937	-0.96795952486208	1.15549481958375
H	6.22372527317350	-1.69693744008033	0.27693927351117
H	5.95323819553521	-4.00635882431710	0.02305913700158
H	5.05285015044013	-6.71082536721716	0.52749375562070
H	4.08197581697705	-7.16028684345972	-0.89119258048921
H	5.67963445748413	-6.40255646699737	-1.09956478079733
H	2.15436383871799	-5.74296969293751	-0.97956190171954
H	0.13143964869475	-4.37199510320584	-0.82242886090741
H	0.23652445714289	-2.62681641293488	-0.52860520478722
H	0.58000168239222	-3.25935314003201	-2.13412186344557
H	2.56627052643595	-2.05494475756407	2.25173183592157
H	1.99260888567167	-1.00209449218763	4.43845559029771
H	1.02613050089404	1.30468294681037	4.46547004520896
H	0.68777378874275	2.53817583263557	2.36918108613870
H	2.59538968252791	-1.62894241849590	-2.95249176298899
H	2.45786927598831	-0.10049743873994	-4.91898362198514
H	1.91133133805366	2.31150170134619	-4.54474209338973
H	1.41490934062572	3.14526428539601	-2.29581951899989

#### XYZ coordinates of p2cz in S<sub>0</sub>

O	1.530039	5.787757	-1.769254
C	0.734700	5.159940	-1.104336
C	0.829504	3.694231	-0.943541
C	-0.150738	2.981483	-0.224966
C	-0.068703	1.567135	-0.115524
C	-1.202647	0.883619	0.415419
N	-1.365543	-0.492205	0.201734
C	-1.587438	-1.482572	1.150258
C	-1.616133	-1.385141	2.533227
C	-1.818418	-2.549747	3.252724
C	-1.984653	-3.781133	2.614572
C	-1.953455	-3.870422	1.234476
C	-1.757346	-2.713851	0.488232
C	-1.675075	-2.445081	-0.925381
C	-1.452846	-1.062747	-1.063792
C	-1.402884	-0.449323	-2.307556
C	-1.539369	-1.255747	-3.425183
C	-1.719604	-2.635033	-3.308547
C	-1.794077	-3.234439	-2.063537
C	-2.212385	1.591269	1.026753
C	-2.198753	2.987529	1.050286
C	-1.214189	3.676222	0.383864
C	1.139776	0.943634	-0.546086
N	1.452567	-0.359426	-0.133134
C	1.577127	-0.729950	1.201652
C	1.457850	0.050166	2.342974
C	1.652358	-0.570558	3.565522

C	1.955626	-1.930475	3.650694
C	2.096657	-2.695177	2.506203
C	1.920398	-2.092831	1.265848
C	2.037636	-2.556693	-0.093334
C	1.766569	-1.454909	-0.927932
C	1.796777	-1.560925	-2.310420
C	2.102737	-2.797834	-2.850510
C	2.369933	-3.903096	-2.039197
C	2.337576	-3.789899	-0.661049
C	2.068051	1.662392	-1.264274
C	1.894127	3.027906	-1.501508
N	-0.315453	5.792141	-0.445557
C	-0.428522	7.238430	-0.536816
C	-1.288878	5.147310	0.306252
O	-2.157705	5.788215	0.857943
H	-1.462176	-0.437741	3.033022
H	-1.836240	-2.503441	4.335274
H	-2.136321	-4.673945	3.209379
H	-2.078117	-4.827070	0.739941
H	-1.262189	0.619873	-2.406310
H	-1.501641	-0.803591	-4.409565
H	-1.810694	-3.238874	-4.203405
H	-1.950479	-4.303443	-1.975245
H	-3.059603	1.045809	1.424539
H	-2.998988	3.546721	1.519423
H	1.220882	1.105172	2.284783
H	1.563761	0.013892	4.474090
H	2.090563	-2.387252	4.623774
H	2.347001	-3.747642	2.573801
H	1.566097	-0.715564	-2.945467
H	2.124043	-2.910682	-3.928098
H	2.601600	-4.857308	-2.497122
H	2.540380	-4.648360	-0.030790
H	2.976380	1.164526	-1.581707
H	2.629916	3.595501	-2.057854
H	0.376448	7.598479	-1.169723
H	-1.397063	7.506809	-0.958237
H	-0.358757	7.677967	0.458300

### XYZ coordinates of p2cz in S<sub>1</sub>

O	1.93691281682429	5.92907602080175	-0.83985758820047
C	0.94872363465988	5.24530064048587	-0.60503885351506
C	1.00641809061257	3.79492458787171	-0.49123719777291
C	-0.15947489224523	3.04395794564125	-0.23177413501911
C	-0.08480753578875	1.61120704307797	-0.12933820107361
C	-1.30504393659833	0.92332666878290	0.06606556508571
N	-1.36462872974091	-0.50242191558619	-0.01331715300183
C	-1.38853831231464	-1.39012519522856	1.03220021501636
C	-1.30747581928149	-1.12318627349961	2.39546381624459

C	-1.32107978832630	-2.20608603231624	3.25488959345545
C	-1.41518473152304	-3.51241841317898	2.77126880697539
C	-1.52211483178246	-3.77150584052184	1.40764549555389
C	-1.51368154146388	-2.70602103321707	0.52709375867774
C	-1.62443689236553	-2.57819719802485	-0.91073799923169
C	-1.55285688294617	-1.19629834977121	-1.18831498663022
C	-1.66481767945683	-0.69067036169888	-2.47677177566795
C	-1.84815016981915	-1.60474150946259	-3.50518825290284
C	-1.89989238631212	-2.97218891495402	-3.25119377548464
C	-1.78603145734126	-3.47002968394623	-1.95291806929136
C	-2.51693944906657	1.59756660556141	0.21949170129928
C	-2.56867603990285	2.97025814852609	0.17281806339785
C	-1.39846811514380	3.69786283624039	-0.06994192334768
C	1.20158576107408	1.03240159124323	-0.23136731668760
N	1.40970204237150	-0.35074488314749	0.06230632417241
C	1.66132198535417	-0.83141463518560	1.32852603474600
C	1.71022478876673	-0.12349977660780	2.52223740719014
C	1.98147225936939	-0.84299583352837	3.67778915904876
C	2.17867398273472	-2.22013366663742	3.63750576938308
C	2.12770869553713	-2.92194295158190	2.43274173354100
C	1.88124026767788	-2.22397459257646	1.26676385232585
C	1.79691287801170	-2.58267670738780	-0.13336620591875
C	1.53625368248700	-1.38119823539269	-0.83426401406241
C	1.43873896864939	-1.33799643281791	-2.22166316594292
C	1.57637704083068	-2.53262742652444	-2.90387192888730
C	1.80656630846415	-3.73092903006822	-2.22549377437813
C	1.92816039330910	-3.76385139007796	-0.83904926149991
C	2.33812571509163	1.80027301349114	-0.48768296563217
C	2.24703907767644	3.16326331377675	-0.63737850671681
N	-0.30238376027524	5.83053127282427	-0.42567015146076
C	-0.41217144428435	7.27345690597603	-0.51914623202130
C	-1.48186514011038	5.14738166801572	-0.15668272492562
O	-2.52586445565166	5.77028258080536	-0.00932325430670
H	-1.24592002790288	-0.10449718069084	2.75424425339815
H	-1.25161055553159	-2.03779993003576	4.32234960215371
H	-1.42024306061058	-4.33807813701290	3.47269623550818
H	-1.61020424549369	-4.78995285026303	1.04757831397553
H	-1.62071652081294	0.37593404997050	-2.65637010800517
H	-1.94854291519180	-1.24575758475928	-4.52221703708924
H	-2.03589822661132	-3.66215267634549	-4.07526602557173
H	-1.83409821140860	-4.53712140051286	-1.77009444336243
H	-3.41912188894471	1.01412902590574	0.36315419770396
H	-3.49680293683007	3.51165647355011	0.29774514966928
H	1.55276135389288	0.94742724967720	2.53508764107619
H	2.03612354890874	-0.32248241230054	4.62614220998997
H	2.38023089143013	-2.75631525916063	4.55703583231213
H	2.28934778400183	-3.99340759462395	2.41680135426912
H	1.27156584525482	-0.39938158780196	-2.73282036244006
H	1.49869154428808	-2.53935514516352	-3.98394389361280
H	1.90695849245191	-4.64937703037695	-2.79130057956882

H	2.12227493743523	-4.69905399690907	-0.32684702715503
H	3.29732803884973	1.29949680380764	-0.55168501325456
H	3.11573088932530	3.77393526089315	-0.84314483382646
H	0.57529003249925	7.66928224033103	-0.73632696564255
H	-1.11786229327833	7.54127325824658	-1.30619135255695
H	-0.79285687347217	7.67840386343055	0.41915496955223

### XYZ coordinates of p2cz T<sub>1</sub>

O	1.63039536914901	5.80937306934127	-1.63612343521055
C	0.77507047928500	5.17945154701469	-1.03346811828756
C	0.83968762913249	3.72604593563656	-0.90401442226587
C	-0.15875761225961	3.00269380108395	-0.22988201362533
C	-0.08398095930645	1.56581384318245	-0.12364750596609
C	-1.21415164896253	0.91486260276837	0.44017737155066
N	-1.41903933059821	-0.46266994820106	0.35957068289502
C	-1.80667478242032	-1.29997511305492	1.40752977021122
C	-1.98243471091629	-1.00555899341057	2.75165325460410
C	-2.35028899488255	-2.04110015689441	3.59528275226617
C	-2.51649472944481	-3.34162268720422	3.11906819856267
C	-2.31566527089267	-3.63338160161798	1.77985461275004
C	-1.96238257434929	-2.60772232735116	0.91360305089289
C	-1.68868289307034	-2.55523958210405	-0.50211243336767
C	-1.38347043811889	-1.21640111185308	-0.80833459670292
C	-1.18669712654163	-0.79222255545796	-2.11491671701314
C	-1.23834861968195	-1.74918129764794	-3.11219941009156
C	-1.48794556898108	-3.09162673489237	-2.82044106182664
C	-1.72767954071505	-3.49974897164346	-1.51900486524827
C	-2.26579351202622	1.66897325320803	1.04264768296982
C	-2.27851445273086	3.02258836820873	1.01034481340710
C	-1.23221626876628	3.70776155565751	0.33972035791100
C	1.11216540966847	0.95986455666156	-0.59221657999861
N	1.46130730569821	-0.36050464409503	-0.30617430363989
C	1.50051176991950	-0.92679006396493	0.96344455112331
C	1.24574465387420	-0.33359140970850	2.19171616394651
C	1.39508891149954	-1.11527510157421	3.32303255894568
C	1.79430384623735	-2.45046660634827	3.23673010657710
C	2.08760266364515	-3.02322786224044	2.01055809282460
C	1.95312279227816	-2.25504453155901	0.86176885432014
C	2.23908043561901	-2.49291328454714	-0.53198890765950
C	1.94443453523411	-1.30096771254746	-1.21821008998091
C	2.09607006039736	-1.19916123573400	-2.59342117370155
C	2.57867388185057	-2.30647054547851	-3.27192627759995
C	2.88239881318060	-3.49286566466373	-2.60422202801035
C	2.70696556839581	-3.59533694496290	-1.23415970379337
C	2.08357466712614	1.72247148493312	-1.30723629327975
C	1.95564697561846	3.06007100565205	-1.47497302846038
N	-0.30373560193558	5.81453440073207	-0.43494936931840
C	-0.40763058774837	7.26015898466640	-0.52137119374326
C	-1.31158350318904	5.16164912777120	0.25422211131945

O	-2.22497089066910	5.79617771497381	0.75984490117184
H	-1.81796448673359	-0.00755140386096	3.13649093474292
H	-2.49906877464842	-1.83509672393868	4.64873425907223
H	-2.79826380374894	-4.13046889586135	3.80613528043470
H	-2.43056868785809	-4.64677633832459	1.41251564597005
H	-0.99140943258486	0.24712685879110	-2.34519021195866
H	-1.07508472058881	-1.44925572674488	-4.14052619994188
H	-1.50854546364544	-3.81694051622549	-3.62480816979351
H	-1.95470370178991	-4.53641987135857	-1.29844247710920
H	-3.09294000210446	1.12093220511837	1.47608048855073
H	-3.08446360614289	3.60421806264143	1.43678798562186
H	0.93412590564274	0.70043059987447	2.26266869358516
H	1.19086247008075	-0.68200868000065	4.29497928857392
H	1.88849046194260	-3.03810426254332	4.14191094067679
H	2.42748292444145	-4.05067335910438	1.94895769311495
H	1.82715737871238	-0.29609131670983	-3.12571711111179
H	2.71063760568098	-2.24971737224730	-4.34605726408815
H	3.25213101044526	-4.34254738726519	-3.16556587700843
H	2.92963918164177	-4.52152399359310	-0.71676856020117
H	2.96717159543000	1.20602507294296	-1.66086035914774
H	2.70138254212716	3.65188409140297	-1.98797318377683
H	0.42767429010711	7.62072894020147	-1.11373913686908
H	-1.35567670112449	7.53414914315827	-0.98396532075483
H	-0.38277213487363	7.69425631094997	0.47857630201655

### XYZ coordinates of p2dpa in S<sub>0</sub>

O	0.263522	6.027997	0.526916
C	-0.381289	5.117993	0.046519
C	0.022188	3.708012	0.186540
C	-0.766908	2.659204	-0.328747
C	-1.954132	2.984069	-1.015750
C	-2.767134	1.983524	-1.490352
C	-2.474972	0.655649	-1.206403
C	-1.335046	0.293435	-0.509948
C	-0.374018	1.296599	-0.156724
C	0.943947	1.059080	0.355762
C	1.669298	2.113654	0.882356
C	1.201409	3.420565	0.831075
N	-1.543031	5.365408	-0.676787
C	-1.965360	6.740037	-0.878418
C	-2.351799	4.383935	-1.231418
O	-3.344959	4.697377	-1.856911
C	-1.758809	-2.056490	-0.915655
N	-1.205208	-1.041148	-0.092710
C	-1.052269	-1.310992	1.284163
C	-0.484841	-2.517953	1.693447
C	-0.373044	-2.819260	3.038079
C	-0.813008	-1.921300	4.002290

C	-1.371897	-0.718064	3.599831
C	-1.499673	-0.413292	2.252295
C	-1.372225	-2.137842	-2.249963
C	-1.914598	-3.107150	-3.074460
C	-2.839665	-4.016572	-2.579311
C	-3.224976	-3.936741	-1.249430
C	-2.697838	-2.958223	-0.420795
C	1.662090	-0.812995	-1.006012
N	1.562748	-0.196754	0.260460
C	2.520293	-0.552570	1.247095
C	2.153878	-0.548628	2.589267
C	3.077648	-0.885762	3.562864
C	4.373582	-1.240033	3.213149
C	4.740532	-1.240050	1.875669
C	3.824675	-0.890581	0.895578
C	1.638277	-0.063556	-2.181137
C	1.778772	-0.689412	-3.411285
C	1.957467	-2.061924	-3.489543
C	1.988610	-2.808493	-2.318417
C	1.837992	-2.194223	-1.089267
H	-3.671854	2.254015	-2.021071
H	-3.182581	-0.116014	-1.480254
H	2.654205	1.915747	1.284803
H	1.790539	4.237785	1.228946
H	-2.000080	6.963928	-1.944858
H	-1.252418	7.386208	-0.375785
H	-2.966359	6.883209	-0.471313
H	-0.146852	-3.221902	0.943616
H	0.075389	-3.759915	3.335977
H	-0.720425	-2.158272	5.055309
H	-1.727863	-0.008719	4.338261
H	-1.958817	0.519992	1.951337
H	-0.639823	-1.438761	-2.632065
H	-1.596956	-3.159475	-4.109594
H	-3.256889	-4.780439	-3.224696
H	-3.954480	-4.632808	-0.851346
H	-3.013232	-2.893128	0.613249
H	1.139276	-0.288233	2.861243
H	2.773723	-0.887374	4.603440
H	5.091762	-1.512956	3.977274
H	5.752422	-1.502174	1.588452
H	4.118902	-0.882428	-0.146694
H	1.521311	1.011805	-2.132212
H	1.760386	-0.090173	-4.314463
H	2.072026	-2.546303	-4.451738
H	2.118402	-3.883585	-2.362498
H	1.870058	-2.776562	-0.177229

**XYZ coordinates of p2dpa in S<sub>1</sub>**

O	0.63621246425200	6.04215126962152	-0.75389135330264
C	-0.18760550728118	5.14312893411246	-0.64368807448256
C	0.19172778482080	3.74639403144980	-0.47855026075602
C	-0.78664352997186	2.73889795435479	-0.34332273027488
C	-2.15357083433133	3.08412123735364	-0.37452071609851
C	-3.14253515689997	2.10457121279294	-0.24673449859114
C	-2.77544332407613	0.79320503883398	-0.06033774809999
C	-1.43252489285882	0.42083027596079	-0.00235549100804
C	-0.39159283052844	1.36250305064501	-0.17295370945631
C	0.99619877020391	1.09437490715028	-0.19376693041363
C	1.93867816248365	2.11575846772981	-0.31111653781607
C	1.55283933291743	3.42750988711296	-0.44841738521964
N	-1.55280832208638	5.41420354999449	-0.67153705737002
C	-1.98453475487616	6.78825960077237	-0.83985740751967
C	-2.56326136951000	4.46950997536552	-0.54819401242001
O	-3.73487832915685	4.82349712551271	-0.58646664717473
C	-1.36289158835331	-1.85253774938207	-0.82540598492533
N	-1.16372927605965	-0.97429037968322	0.23483224772294
C	-1.02816680389171	-1.39840453291170	1.56213160101330
C	-0.30249208540150	-2.55292809041877	1.89051704244562
C	-0.14387207335206	-2.93572788226849	3.20779508109356
C	-0.69857089154140	-2.18209001602793	4.23211885157620
C	-1.40318619906202	-1.02769461299401	3.91804632600521
C	-1.55917099949096	-0.62785733786131	2.60450492703651
C	-1.26616011861390	-1.36464336039207	-2.13895111858286
C	-1.43828135110687	-2.20923160826593	-3.21490412108795
C	-1.73393240622444	-3.55231054585109	-3.02222550325832
C	-1.89011742684585	-4.03165208693674	-1.72723474056891
C	-1.71643650638299	-3.19965837109221	-0.63948195365698
C	1.70917979413317	-0.96885642722203	-1.26910362574614
N	1.51397921846042	-0.24541340385290	-0.08699037223569
C	2.07644119480289	-0.61489375198505	1.13108027862546
C	1.65003170277024	0.03462037399732	2.30116727187464
C	2.17068228942443	-0.31786603786606	3.52809335722631
C	3.14365060489443	-1.30348569560369	3.62898885872714
C	3.61521270880739	-1.90963531115372	2.47088198064425
C	3.10024596304295	-1.57117177035021	1.23546170324163
C	1.81725657259992	-0.29831561928624	-2.49438356149249
C	1.98276663528486	-1.00929598680336	-3.66761423243473
C	2.01882917534771	-2.39726577613946	-3.66018694735192
C	1.88215630076402	-3.07081496847478	-2.45490532096760
C	1.72853752313589	-2.37152709063907	-1.27422736770003
H	-4.18010010478521	2.40705019784119	-0.29513700867846
H	-3.52847938111265	0.02055283753290	0.04804404432123
H	2.98976377691299	1.85002266757135	-0.29239459774041
H	2.27386360015809	4.22898629044626	-0.53709969129849
H	-2.59818478413938	6.87692162084723	-1.73703345889030
H	-1.09713429150574	7.40905575455794	-0.91774843996734
H	-2.59541321902060	7.09195486909892	0.01086972629688
H	0.16017942489472	-3.13576479350737	1.10829038910505

H	0.43861854972568	-3.82047794126228	3.43497684133646
H	-0.57182401915816	-2.48382564575648	5.26470039295474
H	-1.83695751608145	-0.42402999005591	4.70659169712851
H	-2.09876415315915	0.27982103064827	2.37267246390527
H	-1.05705823739384	-0.31729840193107	-2.29900474318354
H	-1.34059009423118	-1.81117623081189	-4.21745474420662
H	-1.87157695784606	-4.21172638883172	-3.87046306387423
H	-2.17391021547753	-5.06438567721100	-1.56089620610537
H	-1.89548985145275	-3.58079286757360	0.35594299564377
H	0.90904594534811	0.81715089871387	2.23094599342206
H	1.81119205151927	0.18612192537078	4.41685902738643
H	3.55247080280246	-1.57495996245146	4.59462242675818
H	4.41260759395522	-2.64157333716028	2.52698484608921
H	3.51928553612396	-2.01629779859667	0.34414114275056
H	1.77733412151824	0.78187586007107	-2.51394049414418
H	2.08074983357834	-0.46793994985474	-4.60126256521442
H	2.13852509221260	-2.94827018729755	-4.58506174485484
H	1.87290400887116	-4.15394528998274	-2.43292923370188
H	1.59672286750018	-2.91301796971355	-0.34951011245786

### XYZ coordinates of p2dpa T<sub>1</sub>

O	0.31549187174631	6.01770216688966	0.45933172687732
C	-0.36128734074156	5.10429231727408	0.01096748077436
C	0.02766821785244	3.70585283921420	0.16916136488562
C	-0.76687635681904	2.65764264983436	-0.32834766618714
C	-1.95790370162849	2.98215400873706	-1.00147443060339
C	-2.80837668902417	1.96358660812516	-1.49351753064631
C	-2.50379245911347	0.66832261570391	-1.23792844294698
C	-1.32759823653281	0.29626077356243	-0.51623943480123
C	-0.37067990655217	1.28205608648880	-0.15191155188182
C	0.93498222673474	1.06033875361956	0.36723644910663
C	1.68314073400996	2.14884944782061	0.91288896549668
C	1.24553446136138	3.42873180111537	0.83681462811816
N	-1.53780912973086	5.35293003097091	-0.68209199379392
C	-1.96004968124754	6.72650591821394	-0.88472261382286
C	-2.36030072805395	4.36911441206598	-1.20444158932504
O	-3.38134946778870	4.67567122447213	-1.80259118272654
C	-1.75603281134820	-2.05250385124794	-0.92075843361125
N	-1.25729609476531	-1.03349284620679	-0.08012434925339
C	-1.05420914416076	-1.31010489087912	1.28599928025491
C	-0.45731425201534	-2.50808505981844	1.67994481762203
C	-0.29956572643911	-2.80232692493846	3.02180678722013
C	-0.72657819821165	-1.90800179707689	3.99442323840141
C	-1.31447700081794	-0.71227550942436	3.60601533983412
C	-1.47930466448044	-0.41033222528365	2.26411152423302
C	-1.42182822225656	-2.04828039056825	-2.27332284763797
C	-1.93061328703641	-3.01620824859274	-3.12052366115972
C	-2.77003321252668	-4.00794515377536	-2.63330905908155
C	-3.10492615429821	-4.01292847797683	-1.28585994736050

C	-2.61204209863287	-3.04039198120389	-0.43280642800048
C	1.66827791469570	-0.80204672080002	-1.00981538811957
N	1.60763459676063	-0.16195057866616	0.24368754197718
C	2.51528940543881	-0.54933862715769	1.25414068429198
C	2.14135938874146	-0.43872885064209	2.59163124406676
C	3.02781253602436	-0.78994588814974	3.59406663430056
C	4.29451742601547	-1.26241057999907	3.28150682504552
C	4.67056113090515	-1.36786681143446	1.94903259644129
C	3.79482054550009	-1.00798092139652	0.93926218008937
C	1.61472715329536	-0.06043793173560	-2.19076055304657
C	1.71879226576958	-0.69621015128487	-3.41697109401342
C	1.87586584409615	-2.07324723205111	-3.48817371552709
C	1.92659053350018	-2.81255438564947	-2.31374804213112
C	1.82092907200711	-2.18680153331403	-1.08543236243235
H	-3.70966723341469	2.25093593980379	-2.01782934465439
H	-3.18436370846726	-0.11739945479438	-1.53989764171684
H	2.64929875495497	1.93250267583600	1.35047598004214
H	1.82247851886520	4.25743180064647	1.22408352135929
H	-2.02966208947209	6.93884163191117	-1.95191553696387
H	-1.22760357222439	7.37429751831500	-0.41285667147505
H	-2.94684456365873	6.87890954105021	-0.44702559283838
H	-0.13054258109299	-3.20887633917135	0.92249241549249
H	0.17219940017900	-3.73441116440512	3.31005553798465
H	-0.60094388683907	-2.14059582458756	5.04501044042112
H	-1.66014352748459	-0.00743805200519	4.35351005866822
H	-1.95357727850907	0.51650851326156	1.96693596709977
H	-0.75049060987746	-1.28649071501591	-2.64753603186647
H	-1.65328290546433	-3.00070104696996	-4.16828492150334
H	-3.16257718185197	-4.76913018665296	-3.29691808663240
H	-3.77219997615535	-4.77243071707309	-0.89475580924229
H	-2.89605070284184	-3.03831636654765	0.61202141964665
H	1.14597381843573	-0.08967881341566	2.83320929074211
H	2.71597836675161	-0.70753299771097	4.62892296762719
H	4.98442991039467	-1.54337709552072	4.06825667984406
H	5.66297237459283	-1.71887437796841	1.69033798975195
H	4.10253476946755	-1.07406871056530	-0.09674308524433
H	1.50838091291445	1.01587578478840	-2.14054987540117
H	1.68599642490085	-0.10434628456411	-4.32451849997840
H	1.95766037466939	-2.56628005450695	-4.44933177973099
H	2.03806419919825	-3.88974823233382	-2.35378579784994
H	1.86823123179633	-2.76322105663833	-0.17052058450822

### XYZ coordinates of p2acr in S<sub>0</sub>

C	1.087905	0.486829	0.793103
C	-0.102862	0.993374	0.330788
H	-0.870710	1.227836	1.058584
C	-0.360042	1.139574	-1.032662
H	-1.304984	1.530090	-1.389297
C	0.572148	0.718234	-1.946734

C	1.818453	0.220954	-1.512838
C	2.747621	-0.222512	-2.475663
C	3.976850	-0.692798	-2.089650
H	4.668321	-1.038555	-2.848009
C	4.333401	-0.657722	-0.741607
H	5.334662	-0.935909	-0.434491
C	3.463171	-0.215903	0.225924
C	2.133659	0.163077	-0.120002
C	0.233028	0.795772	-3.385415
O	-0.824334	1.244260	-3.771291
N	1.186292	0.322465	-4.278616
C	2.421764	-0.192613	-3.916397
O	3.187811	-0.594048	-4.765539
C	0.895859	0.359171	-5.702331
H	-0.096220	0.780174	-5.831613
H	0.941755	-0.648861	-6.114120
H	1.639939	0.968808	-6.214951
N	1.154169	0.166572	2.177526
C	1.417091	1.172267	3.107522
C	0.586615	-1.050882	2.569433
C	1.231502	0.952839	4.476237
C	1.883012	2.411614	2.661208
C	0.396997	-1.347503	3.923092
C	0.218019	-1.994296	1.601567
C	1.531958	1.997060	5.346972
C	0.705993	-0.358869	5.035018
C	2.183288	3.423196	3.549913
H	2.030426	2.574514	1.602417
C	-0.108231	-2.601464	4.252420
C	-0.288569	-3.226870	1.961943
H	0.342340	-1.767177	0.551348
C	2.007233	3.220511	4.909489
H	1.394183	1.843403	6.411319
C	1.753395	-0.968807	5.979295
C	-0.587111	-0.078710	5.819764
H	2.566539	4.363945	3.173230
C	-0.446169	-3.546431	3.300675
H	-0.245561	-2.845800	5.299398
H	-0.557456	-3.937084	1.188486
H	2.237702	4.003015	5.622059
H	2.665071	-1.216703	5.435345
H	1.374666	-1.883269	6.440243
H	2.007245	-0.271457	6.780209
H	-0.399568	0.602775	6.651681
H	-1.001075	-1.000808	6.231913
H	-1.340736	0.373370	5.171925
H	-0.835657	-4.511463	3.600938
N	3.999003	-0.028922	1.530464
C	4.132799	-1.128026	2.378791
C	4.716006	1.150758	1.756268

C	4.885721	-1.042010	3.554445
C	3.492263	-2.326256	2.052209
C	5.478044	1.312360	2.917647
C	4.660913	2.191115	0.819693
C	4.947832	-2.169761	4.368616
C	5.635319	0.217143	3.959366
C	3.563631	-3.423401	2.885432
H	2.911751	-2.390001	1.142205
C	6.119633	2.531343	3.113458
C	5.315105	3.386233	1.041531
H	4.087826	2.068330	-0.089458
C	4.296006	-3.350467	4.059614
H	5.523714	-2.118870	5.285875
C	5.096568	0.723551	5.306147
C	7.129569	-0.119595	4.101421
H	3.032825	-4.328942	2.617179
C	6.046747	3.570189	2.203383
H	6.703625	2.671142	4.015783
H	5.247793	4.174141	0.300183
H	4.359569	-4.200457	4.727953
H	4.049133	1.013430	5.217802
H	5.661233	1.593732	5.646602
H	5.178093	-0.049309	6.073438
H	7.285937	-0.894461	4.854226
H	7.699991	0.759680	4.406424
H	7.535969	-0.477520	3.153441
H	6.561119	4.503774	2.395674

### XYZ coordinates of p2acr in S<sub>1</sub>

C	1.10410220457945	0.53971274924396	0.74619284948733
C	-0.11815499501657	1.03964087056782	0.29573208583291
H	-0.86459415996826	1.31594863216034	1.03196365684996
C	-0.38510103196552	1.15696301066343	-1.04688047978814
H	-1.32527914953972	1.54955125710591	-1.41018943008244
C	0.56335365265307	0.72362560427838	-1.98042313093856
C	1.81081000622851	0.21842886692193	-1.55650362031081
C	2.74908823720186	-0.22716468106517	-2.51038465372916
C	3.99825035426633	-0.71573132102501	-2.11287810947804
H	4.68615537909319	-1.05662972323400	-2.87499499952942
C	4.33115265739436	-0.71733005303785	-0.77980052165756
H	5.31498230694153	-1.03935962542121	-0.45749812861990
C	3.42524791645574	-0.28394928298680	0.18871050573256
C	2.12585349798590	0.15611188866239	-0.15225167985575
C	0.22914852762261	0.79816368267920	-3.39550162425738
O	-0.84033264286015	1.23635414735927	-3.80000164158769
N	1.19563535360654	0.33393724389826	-4.28451878160460
C	2.43704841298112	-0.17934333801843	-3.93002060599834
O	3.20951640039839	-0.56033249681364	-4.80059538068211
C	0.90916586918538	0.37902489590575	-5.70523660504598

H	-0.08477158783267	0.79755049207752	-5.83125408578683
H	0.96210027377326	-0.62543322623299	-6.12650913071073
H	1.65370976864852	0.99172447562286	-6.21472839626437
N	1.19416851056050	0.25590930157509	2.15418728775563
C	1.48935685246201	1.26173596022975	3.05754568539961
C	0.75468259475271	-0.98642671803146	2.58281682213345
C	1.40643834568596	1.04270072578500	4.44508800579943
C	1.86686486834452	2.52325089796165	2.57220850154815
C	0.65634305559097	-1.29139738245744	3.95221825588964
C	0.39805352411139	-1.95756425672397	1.62863779563377
C	1.73860884530233	2.09621416471686	5.28707090650939
C	0.85668417379159	-0.24439143028248	5.02712093477802
C	2.19932438516736	3.54180219755232	3.43690131923716
H	1.87608248666084	2.68580108427125	1.50488634806161
C	0.26940857279590	-2.57597836184262	4.30673794554395
C	-0.00267542704795	-3.21508246948778	2.01717532805414
H	0.43919036010414	-1.70509274772760	0.57969105524901
C	2.14562434982818	3.33018895267276	4.80676847193968
H	1.66644998716355	1.95400533492438	6.35883341314422
C	1.77493690726178	-0.78651069097634	6.13006388056495
C	-0.52626187975710	0.07346860028197	5.63595603049571
H	2.49822369271862	4.50300976622359	3.03790555115817
C	-0.05027812011800	-3.54050337458034	3.36546708330487
H	0.19312826214655	-2.83061512093703	5.35658195955117
H	-0.27256775679360	-3.94428602688601	1.26295958985063
H	2.40087842398313	4.12370126372471	5.49850295899020
H	2.72915426260047	-1.10694651489724	5.71407107679967
H	1.31747945174000	-1.64017128096876	6.63129458018573
H	1.96144539116307	-0.03061524795305	6.89354475208945
H	-0.43158365293636	0.81530875392821	6.43168187843840
H	-0.97392385904780	-0.82989823989668	6.05529566973060
H	-1.20266079986517	0.47034570521503	4.87665891616016
H	-0.35323209551485	-4.53030911522372	3.68488701680021
N	3.94630959637593	-0.13214069092706	1.52155990430891
C	4.04451122302637	-1.22411174579314	2.36606134412788
C	4.55207416173392	1.07396874778799	1.83567856308803
C	4.71732883545392	-1.13384784685629	3.59858871187139
C	3.46972721472723	-2.44257413945410	1.97289612784827
C	5.23375935528617	1.25141914202708	3.05287990574392
C	4.48529058226037	2.13780444063197	0.91682844101834
C	4.75590784521878	-2.26834048052656	4.39899170457945
C	5.49203603126282	0.10390072600956	4.00577520971734
C	3.51870383732703	-3.54451937584537	2.79701751888177
H	3.00124859678822	-2.50495071413470	1.00216987154434
C	5.76199901511469	2.50512480264632	3.32634332749398
C	5.04028145209022	3.36164958818288	1.21223017501666
H	3.99307990859990	1.98396147569643	-0.03175997904541
C	4.15762746040078	-3.46066929125742	4.02545561781497
H	5.28293515758577	-2.22532371297332	5.34475484687728
C	5.15091408584569	0.52115669905269	5.44223983160946

C	6.99456878286410	-0.24294284992417	3.92598409178650
H	3.05874076889449	-4.47070792429337	2.47591105675003
C	5.66794634790015	3.56013170782747	2.43384821065264
H	6.28608614550790	2.66187785123128	4.26099363947283
H	4.97615520430722	4.16401060328765	0.48729301305023
H	4.20709985088484	-4.32088351072016	4.68188492711689
H	4.11937831363784	0.86439960762797	5.50906838182084
H	5.80202604827621	1.32939309597703	5.77687445831184
H	5.29001364866383	-0.30804423025089	6.13660597884278
H	7.23438530234689	-1.05938906503846	4.61035219820565
H	7.60039072783515	0.62492408383201	4.19457868484959
H	7.26804955023668	-0.55205897496540	2.91538130011849
H	6.09952494485862	4.52177518164006	2.68389538375293

### XYZ coordinates of p2acr T<sub>1</sub>

C	1.14108447458532	0.59822579026383	0.75910881932748
C	-0.06238126430096	1.15551259097438	0.31259445072349
H	-0.79012385910782	1.47254337423863	1.05157055131883
C	-0.33096637811808	1.26486830871583	-1.02928796101578
H	-1.25589660356059	1.69417614495187	-1.39158284638858
C	0.58714814082907	0.77324304042455	-1.96650747576154
C	1.81512258639447	0.22057897028297	-1.54722251464830
C	2.72736988209016	-0.28176237606206	-2.49730117935504
C	3.95854475090030	-0.81477729481834	-2.09710000499671
H	4.62623200236712	-1.19686458718051	-2.85831825337983
C	4.30434896195461	-0.80831190271587	-0.76829180443057
H	5.27658298981157	-1.16443473871642	-0.44565807517258
C	3.41979410569220	-0.31719976205283	0.19767691559445
C	2.13690974338173	0.16503165271016	-0.14612602474442
C	0.24385095418517	0.83684651111278	-3.37958198019435
O	-0.80689254307415	1.31537672810484	-3.78528884345341
N	1.18084817703987	0.31004894161408	-4.26750881643871
C	2.40352503292373	-0.24970649839543	-3.91465929468601
O	3.14780982177389	-0.68156179576593	-4.78502291373614
C	0.88207807392958	0.33786706531941	-5.68629738830894
H	-0.09458786248412	0.79541425746868	-5.81209274193503
H	0.88816686524901	-0.67645055150650	-6.08693138810237
H	1.64629883283516	0.90811765805484	-6.21574873978606
N	1.22416938406776	0.29048124152116	2.15834194020159
C	1.48897967429387	1.28792904520304	3.08356046584433
C	0.77852289743937	-0.96152704452381	2.56254916946998
C	1.37880397268725	1.04926042552528	4.46474002815426
C	1.86924078252468	2.55616633812854	2.62030940802386
C	0.66080131901842	-1.28568398723507	3.92459279042652
C	0.42790717734440	-1.91268734923579	1.58786134559606
C	1.68322437472393	2.09571567232497	5.32688380129057
C	0.84467742022038	-0.25623173993855	5.01971840006373
C	2.17410638211604	3.56718304123920	3.50390201629562

H	1.90619158891755	2.72716274308688	1.55443902198019
C	0.26536193063398	-2.57518001197533	4.25412514646784
C	0.01864418603819	-3.17572144087182	1.95125193023740
H	0.47631509029453	-1.63964524346059	0.54352946942197
C	2.08885254478359	3.33875979235378	4.86975945916926
H	1.59129955840451	1.93940543362181	6.39520913440627
C	1.77009940525802	-0.80887118745670	6.11189802619870
C	-0.54307270816247	0.03100102291405	5.63209950274441
H	2.47606092706814	4.53479789288661	3.12289347873286
C	-0.04516287044021	-3.52288817828047	3.29334302206989
H	0.17475645901745	-2.84567480409331	5.29903998702193
H	-0.24768070330916	-3.89065739747781	1.18210261006070
H	2.32074147947092	4.12635062315486	5.57648984858879
H	2.72435383152100	-1.11898023107298	5.68802379726086
H	1.31929197619178	-1.67299481792945	6.60157561323647
H	1.95679739145871	-0.06255615847652	6.88476685821844
H	-0.46077089382590	0.76207311304411	6.43887735267679
H	-0.97853339655796	-0.88460849893679	6.03716879677270
H	-1.22392293066199	0.42944010047615	4.87760520633301
H	-0.35599638512795	-4.51661578519357	3.59275026267208
N	3.94582897899615	-0.15089398936355	1.52240895795244
C	4.06971741817504	-1.24152331802553	2.36839534512533
C	4.54565149818445	1.06411243068834	1.82532102818976
C	4.75067999549780	-1.13817629503873	3.59415448088102
C	3.50494573307951	-2.46604576317217	1.98156940309412
C	5.23416835283629	1.25250628815656	3.03525832212022
C	4.46845220510343	2.11707725599672	0.89648523034262
C	4.80669341592082	-2.27041948878199	4.39772552826059
C	5.50033223303215	0.11577792270465	3.99970829087926
C	3.57148126155009	-3.56537099702950	2.80804503393435
H	3.02655203907598	-2.53344942865548	1.01547512748054
C	5.75898399268841	2.51147781012854	3.29513933160863
C	5.01732065731959	3.34747279030415	1.17948151221023
H	3.97408304341661	1.94909294317780	-0.04954398714653
C	4.21978444108261	-3.47043233704139	4.03092988238704
H	5.33732598012863	-2.22006628120612	5.34129125480802
C	5.12828168342032	0.54085768153201	5.42624527001656
C	7.00896822286940	-0.20673488497107	3.94582844753004
H	3.11825111570124	-4.49708144270010	2.49308674257738
C	5.65176012573149	3.55852124881219	2.39541728528128
H	6.28909456729578	2.67786709593208	4.22486129447168
H	4.94538567556170	4.14351458122996	0.44819844579715
H	4.28318945919025	-4.32781671052183	4.69003649911739
H	4.09129342093351	0.87151411925407	5.47110300073454
H	5.76192204834349	1.36145858846996	5.76479041493635
H	5.26458144734466	-0.28141661739759	6.12944542670103
H	7.25233635734398	-1.00976850174464	4.64461400167561
H	7.59751013113046	0.67363891267458	4.21166309996860
H	7.30208535610667	-0.52437185972763	2.94342693183103
H	6.07894335223279	4.52480510997080	2.63517757716629

### XYZ coordinates of p2pt in S<sub>0</sub>

C	1.104263	0.540344	0.779811
C	-0.079637	1.068803	0.323765
H	-0.826862	1.350681	1.056215
C	-0.350679	1.191071	-1.039775
H	-1.289961	1.598415	-1.392652
C	0.563515	0.738740	-1.957670
C	1.800551	0.215309	-1.529334
C	2.716244	-0.250625	-2.493846
C	3.933916	-0.752512	-2.110004
H	4.616710	-1.110820	-2.870442
C	4.287623	-0.746795	-0.760305
H	5.274651	-1.071767	-0.453034
C	3.428125	-0.286890	0.208724
C	2.120846	0.155170	-0.138713
C	0.215899	0.811704	-3.394941
O	-0.838498	1.270447	-3.776134
N	1.158496	0.322987	-4.291365
C	2.388186	-0.209344	-3.934202
O	3.147202	-0.617548	-4.786107
C	0.862637	0.362499	-5.714148
H	-0.125665	0.793383	-5.839584
H	0.896834	-0.646023	-6.125745
H	1.610674	0.964664	-6.229823
N	1.219487	0.289522	2.175344
C	1.522134	1.373555	3.014772
C	0.644925	-0.912807	2.627327
C	1.791601	2.628612	2.469859
C	1.599182	1.232833	4.404987
C	0.656240	-1.272739	3.980920
C	0.063181	-1.805633	1.725064
C	2.123627	3.709490	3.270551
H	1.768235	2.759999	1.396748
S	1.452321	-0.314923	5.209896
C	1.897820	2.329608	5.201376
C	0.091389	-2.472043	4.391388
C	-0.470207	-3.015498	2.141915
H	0.037751	-1.565941	0.671372
C	2.170717	3.568750	4.645341
H	2.349544	4.660930	2.804780
H	1.939872	2.193843	6.276623
C	-0.462403	-3.357390	3.481021
H	0.106353	-2.715942	5.448197
H	-0.898296	-3.683548	1.404043
H	2.423074	4.407089	5.282683
H	-0.882783	-4.295799	3.820573
N	3.933156	-0.169744	1.533723
C	4.001839	-1.337611	2.312653

C	4.689539	0.987191	1.799841
C	3.510673	-2.544689	1.816351
C	4.523927	-1.327501	3.610869
C	5.266502	1.215236	3.055586
C	4.866775	1.964736	0.818751
C	3.534158	-3.702723	2.577010
H	3.074307	-2.577033	0.827491
S	5.013749	0.146641	4.417555
C	4.577857	-2.500103	4.351326
C	6.002930	2.367665	3.290135
C	5.576679	3.128141	1.073926
H	4.430023	1.830203	-0.160834
C	4.077121	-3.689793	3.848756
H	3.117406	-4.613023	2.163667
H	4.998688	-2.463799	5.350213
C	6.155145	3.336722	2.311805
H	6.447008	2.507664	4.269763
H	5.676795	3.866215	0.286956
H	4.107240	-4.589662	4.450401
H	6.719408	4.237253	2.520183

### XYZ coordinates of p2pt in S<sub>1</sub>

C	1.10639005480523	0.55806284874552	0.72094882899912
C	-0.13174599344267	1.02060867245655	0.27510298369863
H	-0.86858713997066	1.31249493243393	1.01519112505848
C	-0.42136183766605	1.09844073072325	-1.06541200715519
H	-1.37551670623916	1.45946056555286	-1.42475570197288
C	0.53348431816629	0.68621539239912	-2.00214826048236
C	1.79538709314416	0.21337020130429	-1.58372409781670
C	2.73947837974206	-0.20218707123650	-2.54554899588761
C	4.00120247055163	-0.66672545245805	-2.15877550674068
H	4.69606229455619	-0.97716355610905	-2.92745181817580
C	4.32625828024328	-0.70495770426601	-0.82463344475337
H	5.30637106625800	-1.04189934407049	-0.50583095263965
C	3.41311107556302	-0.30820398932646	0.15219318516556
C	2.11842447666999	0.15264127283088	-0.17876530183998
C	0.18906354457952	0.75339725386671	-3.41528439335419
O	-0.89573807185548	1.16038994401997	-3.81184524978643
N	1.16418727164146	0.32340753862842	-4.31122358016885
C	2.42134707333422	-0.15364514005969	-3.96391525568817
O	3.20161316315189	-0.50780719063124	-4.83910421601955
C	0.87017828617064	0.36686168138204	-5.73040691334631
H	-0.13644159475681	0.75589097758527	-5.85005961825286
H	0.95145980183225	-0.63343630915402	-6.15699672433406
H	1.59376320237808	1.00418582863842	-6.23985724054102
N	1.27259606810024	0.42738793894719	2.14585517265298
C	1.58251676165228	1.56686354928757	2.88024100810255
C	0.83367602547911	-0.75799543003147	2.72365628213913
C	1.76332838338607	2.79214879377055	2.22580630395671

C	1.73754013847499	1.55294214920994	4.27797372374732
C	0.96011514787431	-1.02595763450194	4.09939010051921
C	0.25586456378490	-1.75533287543696	1.92397137833943
C	2.07964616737880	3.93879326400738	2.92282686689024
H	1.65249558180821	2.82541889696859	1.15206670923325
S	1.64810524342557	0.10104378562520	5.22169336004732
C	2.04232045193546	2.71995533441728	4.97304272067772
C	0.54866408805798	-2.24842610954222	4.62680297973932
C	-0.15138827712172	-2.95699906167710	2.45939918446210
H	0.13660788790949	-1.57005729875575	0.86708147706980
C	2.21827460681269	3.91379107701248	4.30508663566340
H	2.21642686370492	4.86428345407508	2.37708842678266
H	2.14750478548526	2.67366109120066	6.05155571579469
C	0.00157204895827	-3.21929893697312	3.81658627622649
H	0.66494497749907	-2.42352969026362	5.69079154152821
H	-0.59054697226599	-3.70102969055641	1.80601314204948
H	2.45945133007089	4.81465930287920	4.85512039998081
H	-0.31284661088112	-4.16575580467172	4.23800596004846
N	3.88275998462672	-0.31443235373514	1.51387410434499
C	3.89738647777982	-1.52535592647906	2.19763501179132
C	4.55320342723736	0.82028921856734	1.95384351443400
C	3.41543081321214	-2.68433170969789	1.57563263170948
C	4.37139889557773	-1.65030054529247	3.51567755905389
C	5.05006885808594	0.95044808919955	3.26408201785288
C	4.74022892946686	1.90469751032175	1.08366455632544
C	3.40713205093946	-3.89904449056653	2.22750506625985
H	3.04260607848469	-2.61105435876510	0.56478181757848
S	4.90170132836132	-0.29563960340706	4.45888973425178
C	4.37206498392488	-2.88495132589605	4.15895599112051
C	5.67744119211081	2.12551319913027	3.67361432716136
C	5.36604033762941	3.05848044217850	1.50041597960826
H	4.37811072039577	1.82547562543668	0.06964198411414
C	3.89016730903113	-4.01131383649818	3.52543555809533
H	3.02009724940443	-4.76917794041795	1.71162450734431
H	4.75170802331866	-2.94568575561029	5.17315083017050
C	5.83247894911556	3.18349422397851	2.80471676034446
H	6.04509408348118	2.19341001060490	4.69169435866630
H	5.48759023734890	3.87333846267053	0.79714458059819
H	3.89142751873122	-4.96574708806876	4.03661992853686
H	6.32036269134851	4.09176742409994	3.13524516101992

### XYZ coordinates of p2pt T<sub>1</sub>

C	1.14783607676109	0.63830680931679	0.72761443865605
C	-0.05837265001907	1.18944648544766	0.28183779387722
H	-0.77188947416260	1.53535507015387	1.02189851961623
C	-0.34227949255236	1.27100468937885	-1.05851048044116
H	-1.26988896292535	1.69468020169748	-1.42044221891148
C	0.57229977156641	0.77169391515204	-1.99468414406395
C	1.79899558611264	0.21517246395420	-1.57640851186845

C	2.70597543516640	-0.28768802465814	-2.53127492290392
C	3.93376911192891	-0.83335146018210	-2.13800723756017
H	4.60042890265478	-1.20738519460143	-2.90404458066498
C	4.26953426846032	-0.86314824824297	-0.80733798974741
H	5.22960898228616	-1.25209596325131	-0.48583088893172
C	3.38798596053516	-0.37897915202836	0.16465708723999
C	2.12442461240312	0.15671164574035	-0.17389790055502
C	0.22319507119398	0.83341467121175	-3.40694021628727
O	-0.83080563180720	1.30864404491255	-3.80789894398537
N	1.15874966194078	0.31230813321795	-4.29870935385728
C	2.38246844130669	-0.24589152507935	-3.94876558691268
O	3.12784376288797	-0.67161089948451	-4.82114586657309
C	0.85762139797688	0.34479301773116	-5.71690917441925
H	-0.12096515640744	0.79915355748563	-5.83927301925022
H	0.86686667637127	-0.66783899382987	-6.12163512076098
H	1.61881248071475	0.92017565175204	-6.24514544637524
N	1.29234095113772	0.45029434153511	2.14441884765613
C	1.59940570021409	1.55275014780838	2.93619053475865
C	0.84485581190992	-0.76223101082433	2.65968532911361
C	1.81878289774463	2.79885253775419	2.33526166412299
C	1.72385367148200	1.47343676631610	4.33413418758238
C	0.96109088195124	-1.09881679499491	4.02041098229406
C	0.26855355709290	-1.71204082506470	1.80214298778652
C	2.14183890514796	3.90975737083078	3.08539195508905
H	1.73457886984050	2.87395098781031	1.26055781053221
S	1.60189944803903	-0.01625897398806	5.21334310176915
C	2.03621886134538	2.60519370730794	5.08239980418217
C	0.55768479387162	-2.35265917693249	4.47481078297826
C	-0.13733073901443	-2.94283305504388	2.26805497035353
H	0.14640453903321	-1.46315254619311	0.75776075013378
C	2.24851171140788	3.82213499700000	4.46787484584360
H	2.31069244109784	4.85389569265797	2.58245035065507
H	2.12117788553561	2.51266533330806	6.15971550152650
C	0.01965742599755	-3.27964593251027	3.60828742802721
H	0.66895443206362	-2.58725728287836	5.52779422982496
H	-0.57698010627697	-3.64912197069699	1.57438860824115
H	2.49659859193652	4.69379000664178	5.06060274205614
H	-0.28969780880432	-4.25015515393778	3.97567289126928
N	3.87334922683473	-0.33195716390581	1.51583712516848
C	3.91480942754931	-1.51457009180807	2.24939757072597
C	4.51990153931282	0.83597359437516	1.90692526616147
C	3.43175480681808	-2.70075245078710	1.68186884156311
C	4.40733760259429	-1.57625350384629	3.56451962444242
C	5.00776953862250	1.03390575124485	3.21139615834039
C	4.68542741840867	1.88139411794183	0.98541378569196
C	3.44113386888593	-3.88752952765510	2.38397778701847
H	3.04277988048111	-2.66954617666823	0.67417351461218
S	4.92422319763946	-0.17678311947640	4.44926176708753
C	4.42652727105294	-2.78350332778997	4.25767403095000
C	5.58737107245518	2.24861644990111	3.57152020541418

C	5.27322046058713	3.07168716176827	1.35217915949120
H	4.33869108588313	1.73937898308681	-0.02815173457053
C	3.94510794116611	-3.93921143445501	3.67766711317265
H	3.05120711864446	-4.78115739076464	1.91250547585721
H	4.81745750531214	-2.79928701095662	5.26923651456968
C	5.71512108894711	3.27075451157859	2.65592782725325
H	5.94427575575730	2.37598512002841	4.58767460975272
H	5.38215712179120	3.85509300753841	0.61204450866131
H	3.96048436338412	-4.87082595667153	4.22946125150253
H	6.16834506272475	4.20901585562134	2.95059124601724

### XYZ coordinates of p2po in S<sub>0</sub>

C	1.195207	0.748596	0.706517
C	0.125261	1.479481	0.244949
H	-0.556879	1.906037	0.970579
C	-0.125816	1.621431	-1.120620
H	-0.975059	2.190386	-1.478280
C	0.666177	0.969655	-2.032738
C	1.779946	0.222274	-1.598231
C	2.562708	-0.459960	-2.551441
C	3.670272	-1.168673	-2.158987
H	4.255346	-1.683150	-2.911338
C	4.063626	-1.155996	-0.819696
H	4.990516	-1.630238	-0.520046
C	3.328556	-0.497873	0.138952
C	2.110330	0.156664	-0.214615
C	0.317911	1.063084	-3.466908
O	-0.619505	1.724313	-3.857600
N	1.116489	0.346821	-4.350972
C	2.213514	-0.419606	-3.985408
O	2.845619	-1.019380	-4.828196
C	0.803192	0.385152	-5.769979
H	-0.059954	1.029175	-5.905590
H	0.589764	-0.621900	-6.128342
H	1.658749	0.768099	-6.326002
N	1.288169	0.487046	2.089693
C	0.920856	-0.788215	2.541785
C	1.512466	1.492125	3.037339
C	0.377159	-1.757639	1.707306
C	1.102141	-1.102128	3.890383
C	1.649925	1.120809	4.378307
C	1.664776	2.833944	2.709470
C	0.078141	-3.024345	2.191423
H	0.198099	-1.527608	0.665233
O	1.604568	-0.189229	4.772341
C	0.803101	-2.358619	4.372929
C	1.895813	2.062574	5.354998
C	1.925983	3.779635	3.690386
H	1.615133	3.136675	1.672143

C	0.299347	-3.332161	3.520800
H	-0.329441	-3.766535	1.515865
H	0.984875	-2.558863	5.421581
C	2.035379	3.401356	5.016322
H	1.997975	1.719979	6.377526
H	2.057239	4.815321	3.402059
H	0.079069	-4.321003	3.903260
H	2.240443	4.134936	5.785986
N	3.865721	-0.377283	1.438102
C	4.048421	-1.473404	2.288966
C	4.413469	0.857553	1.811899
C	3.754985	-2.782870	1.928376
C	4.494764	-1.232482	3.592283
C	4.823188	1.038943	3.134497
C	4.571476	1.913629	0.922441
C	3.919964	-3.822626	2.832152
H	3.360526	-2.988298	0.942350
O	4.716236	0.036979	4.055256
C	4.673730	-2.267581	4.485588
C	5.322732	2.250377	3.563047
C	5.072482	3.135239	1.353117
H	4.286958	1.786489	-0.113995
C	4.386967	-3.572620	4.109934
H	3.666356	-4.830566	2.527475
H	5.017528	-2.024297	5.483552
C	5.439611	3.310758	2.674468
H	5.601503	2.347491	4.604985
H	5.171410	3.946977	0.642675
H	4.517904	-4.380489	4.819028
H	5.820268	4.263544	3.020706

### XYZ coordinates of p2po in S<sub>1</sub>

C	1.08768239567468	0.54484931047333	0.67905991277825
C	-0.15567558889207	1.00655263987770	0.24685415352739
H	-0.89373389483190	1.28220319575696	0.99172897274188
C	-0.44640327743538	1.09965158905369	-1.09345555919522
H	-1.40229646880487	1.46280815785541	-1.44616111011159
C	0.50425986983699	0.69566875124627	-2.03834381986341
C	1.76908956210353	0.22232550052003	-1.63057320653616
C	2.71214790674409	-0.19031363135174	-2.59420503394087
C	3.97620018769360	-0.65160567749499	-2.21036693049546
H	4.66859815213614	-0.96197956954723	-2.98137082480837
C	4.31153015937020	-0.68177792108035	-0.87754443065182
H	5.29741940552903	-1.00565651118401	-0.56351004608684
C	3.39671640674901	-0.28779891775837	0.09898908239225
C	2.09715168181785	0.15811277657224	-0.23083366899587
C	0.15529011161472	0.76856515462122	-3.45031050465334
O	-0.93024150864524	1.17701611564166	-3.84199690464806

N	1.12819582802511	0.34093627970782	-4.35077298466571
C	2.38713574740843	-0.13884782731947	-4.01115928450854
O	3.16245120564944	-0.49139580024709	-4.89079116844740
C	0.82876857760292	0.38936736522437	-5.76888395556641
H	-0.17530219999802	0.78624353315556	-5.88390750756460
H	0.90018332748036	-0.61068093605701	-6.19790844042913
H	1.55548467827338	1.02191964089879	-6.27967169497308
N	1.26365879111976	0.35401694459388	2.09015966010742
C	0.87697109263105	-0.84699417358247	2.65688161244963
C	1.57791151564659	1.41061678973510	2.92738137833359
C	0.33015180865484	-1.88810871118330	1.90193868982689
C	1.05447533018266	-1.04565906181783	4.03522347285784
C	1.71614127400528	1.17827855777227	4.30494113230824
C	1.77764981935774	2.70681310172903	2.45252671564995
C	-0.00127135940104	-3.08528206434236	2.50233415319239
H	0.17748702833193	-1.73688159086338	0.84251620140478
O	1.55275384358949	-0.06447312237593	4.83379505306128
C	0.73436012030032	-2.24976129359191	4.62999599193287
C	2.04361661667293	2.20021616613887	5.17319296314134
C	2.10823018432954	3.72798455327430	3.32232158640513
H	1.66769370565264	2.89083999991605	1.39273064118318
C	0.21068804242056	-3.27631236901767	3.86350458344789
H	-0.42273869215104	-3.88073188413716	1.90044990813421
H	0.90329642750626	-2.35933378022998	5.69386701680281
C	2.24283774849581	3.48005639479835	4.68264025793306
H	2.14238796446031	1.96893147198362	6.22644428459588
H	2.26314423924578	4.72610600532860	2.93265962642944
H	-0.04127433739011	-4.22034750533302	4.33020133022291
H	2.50190123860138	4.28183273264479	5.36273580364697
N	3.86502580493600	-0.23763680381469	1.45418274777159
C	3.92906424634213	-1.37858551608010	2.23560094908566
C	4.48928495081746	0.91064551088470	1.90653222783152
C	3.50677123259916	-2.62528190303597	1.77410183228596
C	4.42242971980461	-1.28703804955024	3.54659633327743
C	4.94767251828028	0.96742447247000	3.23227614341497
C	4.66661757128551	2.03455580589861	1.09521120140176
C	3.57103280281288	-3.73446593395599	2.59510205306722
H	3.13030216149487	-2.70114012374914	0.76337648665189
O	4.83445852068059	-0.09963475981447	4.06706583155707
C	4.48928924105931	-2.39688010388367	4.36469811607061
C	5.52622930567508	2.11382795003525	3.73929912797602
C	5.25729337902117	3.17397337886404	1.60164210557305
H	4.32867608339525	1.99276825596009	0.06921182695227
C	4.06086854904707	-3.62566720243028	3.89061820222184
H	3.23398317976432	-4.69194629354135	2.21867802063303
H	4.87419815635088	-2.27332747740436	5.36926409413376
C	5.67756358117536	3.22372532511182	2.92649703687209
H	5.85045878693860	2.11305773339882	4.77238395115648
H	5.38469413036563	4.03537544274212	0.95791852308842
H	4.11060319792107	-4.49632815071725	4.53245857477942

H 6.13214207286777 4.12251567260730 3.32402405583214

**XYZ coordinates of p2po T<sub>1</sub>**

C 1.14011745968972 0.63835790046937 0.68661886110190  
C -0.06632942924304 1.19962967587221 0.25395915406843  
H -0.77842751013030 1.53853781920037 0.99844294063760  
C -0.35221626914739 1.29308634179823 -1.08641000461370  
H -1.27885605316000 1.72474739303572 -1.44146813618795  
C 0.55235308656587 0.79040754768533 -2.03110590999678  
C 1.77817740794002 0.22508031650525 -1.62340353003929  
C 2.67836339093742 -0.28818678301651 -2.57890070973367  
C 3.90391904094532 -0.84080761510677 -2.18693532948780  
H 4.56365538463368 -1.22506803371339 -2.95397830940193  
C 4.25174587627646 -0.85999555301647 -0.85800219650861  
H 5.21457910800857 -1.24538542466646 -0.54091153935471  
C 3.37559755015887 -0.36215042175243 0.11206934234907  
C 2.10981512260142 0.16633991029002 -0.22681785023128  
C 0.19667367957363 0.85306236218026 -3.44180878315963  
O -0.85515531290904 1.33580928243616 -3.83841336247106  
N 1.12410068257310 0.32151986504036 -4.33703072062134  
C 2.34506510830075 -0.24878495115510 -3.99435369898221  
O 3.07920237853776 -0.68495037308200 -4.87062976156474  
C 0.81480716914002 0.35253581796172 -5.75373777046115  
H -0.15395039042652 0.82820617618473 -5.87291304723618  
H 0.79772597304011 -0.66233465842903 -6.15281246842325  
H 1.58620138409722 0.90679700615340 -6.28944101869422  
N 1.29852502764255 0.39923591085746 2.08764857391547  
C 0.91059649945447 -0.82784268769676 2.60284032643558  
C 1.58485680765973 1.42549058182310 2.97378273459851  
C 0.37055374467563 -1.83406165972018 1.79822123378548  
C 1.07517198984823 -1.08104373337691 3.97212715444374  
C 1.71154520273374 1.13531605681693 4.34070514774530  
C 1.77629361319418 2.74139128114197 2.55282603547379  
C 0.03049970067544 -3.05509388431141 2.34507484841269  
H 0.22467315957386 -1.63423845874370 0.74495308423094  
O 1.56147328198304 -0.13064103824263 4.81566371305735  
C 0.74657713027845 -2.30814940476084 4.51315179976042  
C 2.02011603657163 2.12472960813747 5.25327349740597  
C 2.08514226228734 3.72961364674482 3.46726829377873  
H 1.67857313225890 2.96536969931636 1.49910226985605  
C 0.22850192134221 -3.30093502615706 3.69909397524134  
H -0.38831558261834 -3.82353669294895 1.70725773778591  
H 0.90230539588146 -2.46190295141328 5.57357553777467  
C 2.20852180531191 3.42587857457863 4.81759859950805  
H 2.11302056607102 1.85168228461091 6.29704104182530  
H 2.23380610096338 4.74450656853484 3.12075749145942  
H -0.03100727034664 -4.26236012922045 4.12463138087326  
H 2.45174596574385 4.20158236197252 5.53308416312357  
N 3.85481685937802 -0.27041918816014 1.45617756254198

C	3.95636622296310	-1.39053157296848	2.26601654413811
C	4.45003881884034	0.90727297684857	1.87800679877605
C	3.55270540082453	-2.65564381004378	1.83881568679717
C	4.45413194385321	-1.25112658084073	3.57012781127691
C	4.90936754118829	1.01008303894891	3.19885946969929
C	4.59422182005757	2.01061023798206	1.03341865628705
C	3.64557122176357	-3.74199595061342	2.68678235279258
H	3.16539913318049	-2.76119222493682	0.83443217822834
O	4.83573222464345	-0.04055214220742	4.05971358096050
C	4.54805111273643	-2.33885668642628	4.41574212732109
C	5.45721347837415	2.18599863384728	3.67163473269229
C	5.15636239481191	3.17966389883071	1.50523450992238
H	4.25668840235108	1.92662878808027	0.00890781468958
C	4.14343094220022	-3.58809643345073	3.97495817261099
H	3.32307819489057	-4.71520777641771	2.33895372187525
H	4.93324425546271	-2.18228496435511	5.41559245723622
C	5.57689923644045	3.27632856385770	2.82705026777081
H	5.78499177663380	2.22342114841304	4.70293537566756
H	5.26067738578590	4.02533945083846	0.83689441995949
H	4.21574885530775	-4.44037439959714	4.63923774593941
H	6.00830530912240	4.19739809355284	3.19885977133773

### XYZ coordinates of p2npp at $S_0$

O	-2.341036	7.064278	-1.305206
C	-1.318259	6.455323	-1.073515
C	-1.291747	4.987328	-0.864360
C	-0.071168	4.310126	-0.625766
C	-0.055148	2.891786	-0.434812
C	1.222011	2.254487	-0.337244
C	2.376192	3.015019	-0.284895
C	2.337750	4.414264	-0.373542
C	1.132576	5.055175	-0.576989
C	-1.318257	2.223499	-0.353592
C	-2.488140	2.914701	-0.611851
C	-2.481133	4.288469	-0.897032
N	-0.103830	7.130721	-0.984086
C	-0.158503	8.571514	-1.164576
C	1.131914	6.531240	-0.740799
O	2.150224	7.185693	-0.669238
C	1.935280	-1.290928	0.567425
C	2.255343	-2.036386	1.704293
C	2.269688	-1.452436	2.974790
C	1.978147	-0.105008	3.115406
C	1.692669	0.659879	1.981952
C	1.666719	0.089453	0.711020
N	1.357640	0.846926	-0.428446
C	1.441663	0.287477	-1.715777
C	1.665498	-1.102132	-1.848729
C	1.686376	-1.666421	-3.123951
C	1.507525	-0.881821	-4.266646
C	1.327320	0.485880	-4.138920

C	1.304770	1.064419	-2.866222
N	1.866375	-1.877428	-0.701121
C	2.145212	-3.265707	-0.837911
C	1.098500	-4.188322	-0.816977
C	1.370677	-5.550922	-0.926633
C	2.686646	-5.992226	-1.063795
C	3.732067	-5.068257	-1.095181
C	3.463566	-3.705591	-0.983141
C	-1.886051	-1.462619	-0.189412
C	-2.146606	-2.523549	-1.059434
C	-2.190037	-2.333269	-2.443736
C	-1.990068	-1.067148	-2.970565
C	-1.757081	0.007955	-2.109832
C	-1.696759	-0.169863	-0.729439
N	-1.421679	0.897848	0.137851
C	-1.505956	0.736364	1.532385
C	-1.667266	-0.562932	2.066129
C	-1.695758	-0.728763	3.450642
C	-1.576190	0.363717	4.313958
C	-1.450702	1.640779	3.791554
C	-1.426637	1.821680	2.405380
N	-1.798481	-1.650624	1.195101
C	-2.002610	-2.951393	1.734669
C	-0.901964	-3.745551	2.058721
C	-1.095653	-5.026915	2.572020
C	-2.387981	-5.514660	2.764476
C	-3.488566	-4.716496	2.448778
C	-3.298391	-3.434270	1.937236
H	3.332267	2.492289	-0.214459
H	3.249036	5.014370	-0.334589
H	-3.432311	2.371338	-0.536325
H	-3.405318	4.836584	-1.091224
H	0.855546	8.965721	-1.047434
H	-0.833856	9.016620	-0.421012
H	-0.552247	8.811070	-2.162117
H	2.494358	-3.094508	1.590132
H	2.504918	-2.067226	3.845989
H	1.960642	0.367090	4.099122
H	1.456927	1.718170	2.093505
H	1.842023	-2.741105	-3.221833
H	1.521131	-1.355161	-5.250594
H	1.202067	1.119520	-5.019329
H	1.156075	2.140253	-2.771408
H	0.077294	-3.817759	-0.718950
H	0.548073	-6.269854	-0.903042
H	2.899883	-7.060573	-1.148952
H	4.763542	-5.411413	-1.205977
H	4.269974	-2.968997	-1.001860
H	-2.317164	-3.517155	-0.643209
H	-2.377245	-3.187682	-3.097379
H	-2.001170	-0.898325	-4.048646
H	-1.587133	1.002225	-2.522809
H	-1.808072	-1.733505	3.858487
H	-1.592516	0.199684	5.393417
H	-1.372064	2.510033	4.447737

H	-1.323361	2.828818	2.001285
H	0.098490	-3.336984	1.909283
H	-0.230047	-5.645978	2.820096
H	-2.539803	-6.519804	3.165435
H	-4.502014	-5.094768	2.603174
H	-4.148615	-2.797348	1.683061

**XYZ coordinates of p2npp at S<sub>1</sub>**

O	-2.40520249036942	7.11620171955594	-1.05918940315173
C	-1.36351133316687	6.48038448174165	-0.95990240032524
C	-1.32064357252629	5.04024357890867	-0.71583381591215
C	-0.07992810787311	4.36170912883407	-0.62787290742487
C	-0.05047969869415	2.93493097169967	-0.40447133714049
C	1.22629990090244	2.31258423088752	-0.38967254895847
C	2.40877747100372	3.05631312384148	-0.52612135476684
C	2.37226287569694	4.42691347184292	-0.69275351546625
C	1.13114406454228	5.08539018232613	-0.76579201244809
C	-1.30116632695527	2.28652086184314	-0.22570953839297
C	-2.51368061192826	2.98820016755743	-0.30926001003607
C	-2.53375796653003	4.34467939237098	-0.56961028897156
N	-0.13685572982333	7.13374797196349	-1.07851643981192
C	-0.20208614642722	8.56248559539639	-1.31100228709813
C	1.12170560183149	6.52946794803738	-0.99730026233894
O	2.14713469574737	7.18729264487186	-1.12052241344559
C	1.89510900438052	-1.22313257190353	0.67915532490169
C	2.19095628621416	-1.92141282217427	1.85563751039850
C	2.26430077986357	-1.26117201825997	3.07978149751309
C	2.05759988050416	0.11419864575410	3.14288926376052
C	1.76705476081113	0.82346422649466	1.98315305878722
C	1.66467937173038	0.17629632619846	0.74547831524324
N	1.34894754607296	0.88053834750209	-0.40917761529160
C	1.37200493199285	0.24996507518534	-1.64615569699773
C	1.58035424773489	-1.15216862225867	-1.72318050305198
C	1.56099622107118	-1.78058124965517	-2.97311350406999
C	1.34891663209680	-1.04747293851467	-4.13503907838385
C	1.17765796797718	0.33500260244705	-4.06581985126500
C	1.19179224801753	0.97502462053736	-2.83518694979415
N	1.82977932902756	-1.86624388825350	-0.55461099368343
C	2.14717922468241	-3.25495103618372	-0.64106675904409
C	1.12384293600001	-4.19802829656677	-0.73246849075323
C	1.43781666642995	-5.55372886454547	-0.81030286701102
C	2.77036404036668	-5.96459179716493	-0.79896793087916
C	3.79192105302598	-5.01732563087950	-0.71731654347605
C	3.48338270440028	-3.66088124691294	-0.64233677089853
C	-1.83684215386720	-1.42593185212949	-0.27649998116214
C	-2.10407474188732	-2.42890762674764	-1.21556221554748
C	-2.19529602027288	-2.13192182758379	-2.57343235128582
C	-2.03535159114308	-0.82036549495534	-3.01146060638901
C	-1.77347218358623	0.18838507447413	-2.09127858574995
C	-1.65445619640641	-0.09131941560043	-0.72438500624939
N	-1.36770980722666	0.91315240514306	0.19189358770376
C	-1.37529041364000	0.64532974039075	1.55434121170407
C	-1.53471968905151	-0.68862517073787	2.01332794112876

C	-1.50067259560908	-0.94901645810351	3.38742994528667
C	-1.32092166071145	0.08154868288470	4.30329438108899
C	-1.19851475908948	1.39719954430473	3.85730546040063
C	-1.22843896403718	1.67442398521607	2.49817629306439
N	-1.75374943291088	-1.70413250287522	1.08615518137744
C	-2.02673982740551	-3.02554517966463	1.55014887563449
C	-0.97482095698756	-3.87049242868530	1.90331691665654
C	-1.24543746585774	-5.16420833871386	2.34567040467494
C	-2.56339908269732	-5.61077451290952	2.43602055247464
C	-3.61398878104041	-4.75905107359964	2.09180154742098
C	-3.34883224626332	-3.46379229119342	1.65273985212781
H	3.36166863049748	2.52205473343657	-0.51345290983727
H	3.27899289875198	5.02451237669398	-0.79228535271354
H	-3.44370248298203	2.43658838273225	-0.15348332943809
H	-3.46397267517934	4.90797426972367	-0.65202449383498
H	0.82399794253102	8.93838036548572	-1.37555053500051
H	-0.74639681104441	9.05385431944565	-0.49188256705760
H	-0.75123432268448	8.77039768050197	-2.24050617159559
H	2.38264257182431	-2.99353280037602	1.80202971743219
H	2.49283779121686	-1.83017698471983	3.98314203051531
H	2.12175226418730	0.64386728209501	4.09464146194843
H	1.61548207383061	1.90138022610201	2.01277817704385
H	1.71989248841902	-2.85702680360686	-3.02923446331348
H	1.33478322766094	-1.56101419340285	-5.09846395573116
H	1.02892946382700	0.92211740652422	-4.97400549022057
H	1.05525088237225	2.05325739299017	-2.77208277618172
H	0.08896433128085	-3.85488846607995	-0.75261518092971
H	0.63412068156774	-6.29069975473654	-0.87883106261686
H	3.01555686285882	-7.02754020386876	-0.85901854920220
H	4.83681741936665	-5.33595866147640	-0.71542101192817
H	4.27081654818787	-2.90668005273544	-0.57841999616478
H	-2.25881023620515	-3.45152634715031	-0.87031532704794
H	-2.40073598527349	-2.93398789043838	-3.28519028802386
H	-2.11398914457492	-0.57323905331743	-4.07128817459541
H	-1.65887132210376	1.22130571463623	-2.41611877209744
H	-1.62303201570299	-1.97352448501494	3.73748722075250
H	-1.29443071348728	-0.14770641169734	5.37047979867827
H	-1.07607869460810	2.21547721535455	4.56946873325130
H	-1.13029728892564	2.69810640587739	2.14052448124979
H	0.04790071748700	-3.49796770356891	1.83574091356933
H	-0.41937168520857	-5.82522324996168	2.61823519063620
H	-2.77451450542090	-6.62572094027855	2.78096889713025
H	-4.64765891408401	-5.10404906861917	2.16872113302088
H	-4.15924688652196	-2.78462729198847	1.37914536762714

### XYZ coordinates of p2npp at T<sub>1</sub>

O	-2.37055470299637	7.08977318383700	-1.23210582698485
C	-1.34061684908243	6.45729717151104	-1.04094931233491
C	-1.30871141091838	5.01146846169567	-0.83320277513462
C	-0.07554432502580	4.34503374822873	-0.63256303145723
C	-0.05509503314314	2.91666822623303	-0.43423591860390
C	1.21624565345836	2.29553416031584	-0.31966982334457
C	2.40614243662977	3.04726628550935	-0.32102725505705

C	2.37029469732954	4.42100847994145	-0.44946608399737
C	1.13741585820666	5.07745967213055	-0.62508251783607
C	-1.30860097416721	2.25127082116402	-0.36902803750701
C	-2.51869345227980	2.94042934707446	-0.57282542008789
C	-2.52202841297629	4.29785993230868	-0.82475568168655
N	-0.11430637426077	7.12416017804114	-1.00376483470977
C	-0.17168945997076	8.55989266605975	-1.19253152791708
C	1.13635405740193	6.52881864357527	-0.80502999044597
O	2.15943989200320	7.20041035460186	-0.79022105258987
C	1.90213384309954	-1.25373454094889	0.66721381799538
C	2.22544234285064	-1.97071364320765	1.82572640678774
C	2.30877890068957	-1.33362810909119	3.06141425842547
C	2.08388572103219	0.03726485048641	3.15653012825600
C	1.77373011605254	0.76622610155656	2.01465202371687
C	1.66768198085400	0.14181500287113	0.76518491337590
N	1.33174306496608	0.86869501709204	-0.37168674814564
C	1.34153645604178	0.26085894312036	-1.62293685074985
C	1.54189014437162	-1.13911927889921	-1.72716807249423
C	1.50593081517746	-1.74180048593026	-2.98931004776626
C	1.29192156040323	-0.98266625028164	-4.13469122470162
C	1.13713628077563	0.39967225372009	-4.03855759894382
C	1.16440799988321	1.01411398067120	-2.79442679730321
N	1.80687809425457	-1.87594334406715	-0.57514361535917
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