

Multi-Resonance Thermally Activated Delayed Fluorescence Molecules with Intramolecular-lock: Theoretical Design and Performance Prediction

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To confirm that the O3LYP function is suitable for the simulation of MR-TADF systems, the energy gap between S₁ and T₁, FWHM, k_r and k_{IC} are compared with experimental values of 8 MR-TADF molecules as shown in Table S1 and S2. Calculating the mean average deviation (MAD), which was determined according to the equation

$$MAD = \frac{1}{n} \sum_{i=1}^n |x_i| \#(1)$$

where $x_i = y_i^{Experiment} - y_i^{Calculated}$, with $y_i^{Experiment}$ being emission energy of S₁, ΔE_{ST} obtained from the peak maxima (or the difference thereof) of the fluorescence and phosphorescence spectra to measure the six functionals for the eight molecules with experimental data, and we can find that the results O3LYP fits the experimental data better for S₁ and energy gap (ΔE_{ST}). Although it is proved that the TD-DFT method could overestimate the energy gap between S₁ and T₁, we find that the general rule obtained from TD-DFT is similar to the results of the SCS-CC2 method which has been proven to provide better S-T energy gap (as shown in Fig. S1) [1]. The reason why the SCS-CC2 method is not used here is because it is time consuming and the cost performance is not high. Considering the computational cost and the prediction precision, we choose to use O3LYP here.

The formula of RMSD is shown as:

$$RMSD = \sqrt{\frac{1}{N} \sum_i^{natom} [(x_i - x'_i)^2 + (y_i - y'_i)^2 + (z_i - z'_i)^2]} \#(2)$$

where i is the atomic ordinal number, x_i and x'_i are the x coordinates of the i th atom, y and z have the same meaning. Which is used to compare the structure, when one has two similar structures. The first figure out how to compare two structures, which usually means that you must find the root mean square deviation (RMSD). VMD using an algorithm computes the transformation, needed to move one structure onto another in order to minimize the RMSD to get the difference in the molecule structures.

To quantitatively categorize the transition property, the S_r^{index} , which is the full

space integral to the $S_r(r)$ functions is defined as:

$$S_{r,index} = \int S_r(r) dr \equiv \int \sqrt{\rho^{hole}(r)\rho^{ele}(r)} dr \#(3)$$

Here ρ^{hole} is the hole density and ρ^{ele} is the electron density. $S_{r,index}$ which represents the particle-hole overlap, using this formula we can clearly understand which regions of the electron and hole overlap compare significantly.

In order to show that O3LYP is a suitable functional, we calculated different other physical quantities for eight molecules for which experimental data are available. Calculating the mean average deviation (MAD), which was determined according to the equation

In order to describe the process of intersystem crossing (ISC) and reverse intersystem crossing (RISC), the spin-orbit coupling (SOC) of the singlet and triplet states in the compounds was studied. [2] SOC is a relativistic effect, which arises naturally in Dirac theory, a fully relativistic one-particle theory for spin 1/2 systems. [3] The SOC matrix elements $\langle S_1 | H_{SO} | T_1 \rangle$ between excited states can be evaluated as residues of quadratic response functions [4,5]. The electronic spin-orbit interaction operator, referred to as the Breit-Pauli spin-orbit Hamiltonian, is given by

$$H_{SO} = \frac{\alpha^2}{2} \left[\sum_{iA} Z_A \frac{l_{iA} \cdot s_i}{r_{iA}^3} - \sum_{ij} \frac{l_{ij} \cdot (s_i + 2s_j)}{r_{ij}^3} \right] \#(4)$$

where i, j refers to electrons and A to nuclei. Note that the relative orbital angular momentum between two particles, e.g. $l_{ij} = (r_i - r_j) \times p_i$ is asymmetric, i.e. $l_{ij} \neq l_{ji}$. This means that the two-electron integrals over this operator do not have the permutation symmetry as do the electron repulsion integrals. They could have been symmetrized, had it not been the asymmetry in the spin part, which has its origin in the Thomas precession [6]. This formalism is implemented in the powerful molecular electronic structure program DALTON to exploit the structure of the excited states that need to be calculated based on the spin-orbit operators, to obtain three components of the transition dipole moment. Getting the square root of the three components is the total transition dipole moment and the conversion unit is given in cm^{-1} which are the values of SOC.

[7,8]

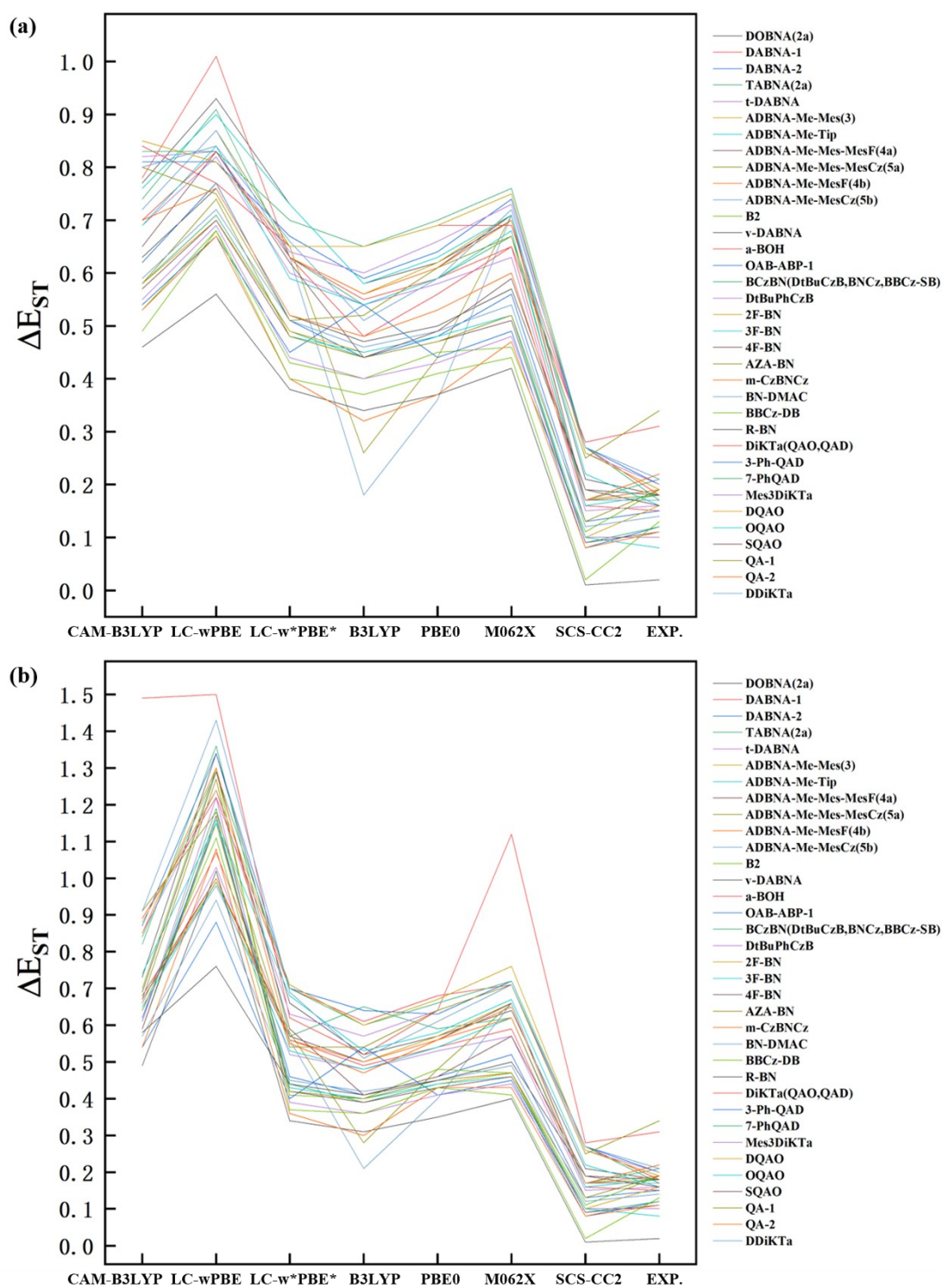


Fig. S1. The diagram of ΔE_{ST} for theoretical and experimental structures by time-dependent density functional theory (TD-DFT) (a) and consider the Tamm-Dancoff approximation (TDA) (b). DFT functionals used 6-31G(d,p) basis set, SCS-CC2 used cc-pVDZ, calculations are in the gas phase[1].

Table S1. Energy gap (ΔE_{ST}) between S_1 and T_1 was calculated using different functionals for the eight molecules in toluene. The full width at half maximum (FWHM) from S_1 to S_0 was calculated using different functionals for the eight molecules in toluene. And the radiation rates (k_r) and the internal conversion rate (k_{IC}) between S_1 and S_0 was calculated using different functionals for the eight molecules in toluene. Experimental values are also listed.

		O3LYP	B3LYP	PBE0	PBE33	BMK	M062X	EXP.
2PXZBN	$\Delta E_{ST}(\text{eV})$	0.31	0.37	0.40	0.43	0.43	0.43	0.19 ^a
	FWHM(nm)	86	32	30	27	23	22	34 ^a
	$k_r(\text{s}^{-1})$	2.55×10^7	6.92×10^7	8.10×10^7	1.04×10^8	1.23×10^8	1.50×10^8	1.33×10^8 ^a
	$k_{IC}(\text{s}^{-1})$	2.04×10^8	1.08×10^8	1.05×10^8	9.76×10^7	9.29×10^7	9.74×10^7	3.82×10^7 ^a
2DMACBN	$\Delta E_{ST}(\text{eV})$	0.30	0.33	0.36	0.40	0.40	0.40	0.14 ^a
	FWHM(nm)	37	27	25	22	20	18	29 ^a
	$k_r(\text{s}^{-1})$	6.68×10^7	9.75×10^7	1.16×10^8	1.50×10^8	1.73×10^8	2.09×10^8	9.20×10^7 ^b
	$k_{IC}(\text{s}^{-1})$	1.10×10^8	9.84×10^7	9.61×10^7	8.96×10^7	8.79×10^7	9.04×10^7	5.44×10^7 ^b
2DPABN	$\Delta E_{ST}(\text{eV})$	0.36	0.41	0.45	0.49	0.49	0.49	0.15 ^c
	FWHM(nm)	17	13	13	11	8	8	33 ^d
	$k_r(\text{s}^{-1})$	5.44×10^7	7.68×10^7	9.57×10^7	1.32×10^8	1.61×10^8	1.97×10^8	9.60×10^7 ^b
	$k_{IC}(\text{s}^{-1})$	8.46×10^7	8.48×10^7	8.36×10^7	8.04×10^7	8.12×10^7	8.37×10^7	1.30×10^7 ^b
2PTZBN	$\Delta E_{ST}(\text{eV})$	0.25	0.32	0.35	0.38	0.38	0.39	0.15 ^a
	FWHM(nm)	122	44	41	35	31	27	39 ^a
	$k_r(\text{s}^{-1})$	2.09×10^7	6.70×10^7	7.96×10^7	1.04×10^8	1.27×10^8	1.54×10^8	9.98×10^7 ^a
	$k_{IC}(\text{s}^{-1})$	1.83×10^8	1.05×10^8	1.03×10^8	9.47×10^7	9.35×10^7	9.28×10^7	7.17×10^7 ^a
2CzBN	$\Delta E_{ST}(\text{eV})$	0.33	0.33	0.36	0.40	0.38	0.39	0.14 ^a
	FWHM(nm)	21	8	8	7	5	7	25 ^a
	$k_r(\text{s}^{-1})$	7.82×10^7	1.35×10^8	1.61×10^8	2.09×10^8	2.43×10^8	2.91×10^8	1.30×10^8 ^a
	$k_{IC}(\text{s}^{-1})$	1.07×10^8	9.08×10^7	1.04×10^8	9.04×10^7	8.33×10^7	7.88×10^7	/
2TMCzBN	$\Delta E_{ST}(\text{eV})$	0.34	0.33	0.37	0.41	0.39	0.39	0.09 ^a
	FWHM(nm)	32	14	14	12	12	18	27 ^a
	$k_r(\text{s}^{-1})$	8.43×10^7	1.44×10^8	1.70×10^8	2.19×10^8	2.52×10^8	3.00×10^8	1.60×10^8 ^a
	$k_{IC}(\text{s}^{-1})$	8.96×10^{10}	1.12×10^8	1.09×10^8	1.03×10^8	1.02×10^8	1.09×10^8	/
PTZDMACBN	$\Delta E_{ST}(\text{eV})$	0.30	0.32	0.35	0.39	0.39	0.39	0.14 ^e
	FWHM(nm)	66	42	39	32	47	24	48 ^e
	$k_r(\text{s}^{-1})$	4.60×10^7	7.66×10^7	9.05×10^7	1.20×10^8	1.47×10^8	1.76×10^8	1.00×10^8 ^e
	$k_{IC}(\text{s}^{-1})$	1.17×10^8	1.02×10^8	9.96×10^7	9.23×10^7	7.84×10^8	9.16×10^7	1.50×10^7 ^e
DPACzBN	$\Delta E_{ST}(\text{eV})$	0.39	0.38	0.42	0.46	0.45	0.45	0.11 ^a
	FWHM(nm)	23	12	12	10	10	9	23 ^a
	$k_r(\text{s}^{-1})$	5.01×10^7	1.08×10^8	1.30×10^8	1.72×10^8	2.01×10^8	2.42×10^8	1.50×10^8 ^f
	$k_{IC}(\text{s}^{-1})$	8.43×10^7	9.46×10^7	9.31×10^7	8.88×10^7	8.93×10^7	9.23×10^7	2.00×10^2 ^f

- a Measured in 1×10^{-5} M toluene solution at 300K.
 b Measured in 1 wt% doped films of emitters in mCBP at 300 K.
 c Measured in the saturated in EtOH at 300K.
 d Measured in 2×10^{-5} M in CH_2Cl_2 at 300K.
 e Measured in 1×10^{-5} M toluene solution at 298K.
 f Measured in 3 wt % doped 26DCzPPy film at 326K.

Table S2. Mean average deviation (MAD) of S_1 , energy gap (ΔE_{ST}), full width at half maximum (FWHM), radiation rates (k_r) and internal conversion rate (k_{IC}) between computed and experimental data.

	O3LYP	B3LYP	PBE0	PBE33	BMK	M062X
MAD- S_1 (eV)	0.22	0.16	0.20	0.38	0.41	0.59
MAD- ΔE_{ST} (eV)	0.18	0.21	0.24	0.28	0.28	0.28
MAD-FWHM(nm)	23	10	10	13	13	16
MAD- k_r (s^{-1})	6.68×10^7	2.61×10^7	2.08×10^7	3.84×10^7	6.08×10^7	9.48×10^7
MAD- k_{IC} (s^{-1})	9.84×10^7	6.68×10^7	6.46×10^7	5.85×10^7	1.73×10^8	5.93×10^7

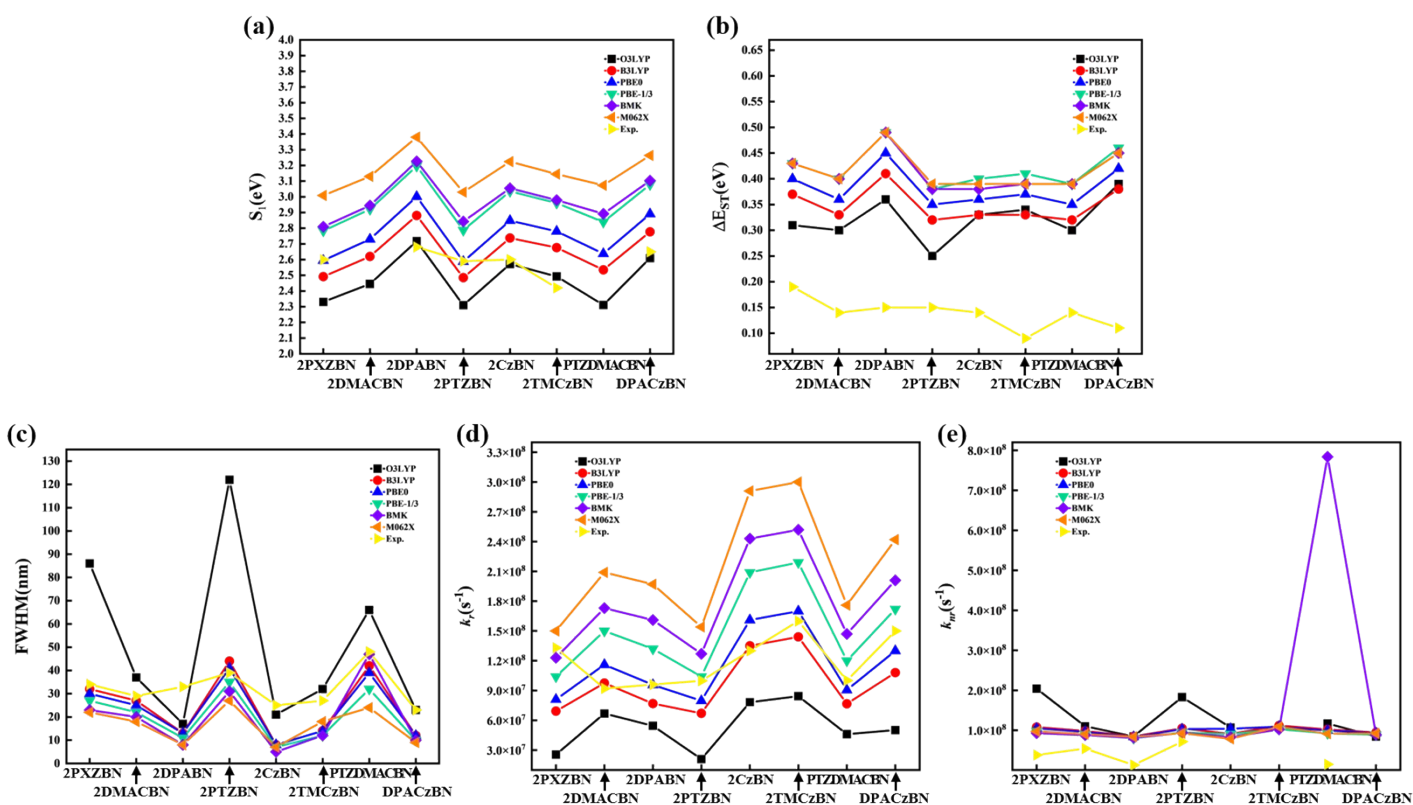


Fig. S2. The energy of S_1 (a), energy gap (ΔE_{ST}) (b), full width at half maximum (FWHM) (c), radiation rates (k_r) (d) and internal conversion rate (k_{IC}) (e) for calculated using different functionals for the eight molecules in toluene and experimental data.

Table S3. The cartesian coordinates of the studied 36 molecules by O3LYP/6-31G(d) in toluene.

2PXZBN	S₀			S₁			T₁		
C	-1.532651	-2.192185	-0.084041	1.498206	-2.201589	-0.025126	1.497184	-2.194328	-0.019397
C	-0.407842	-2.993005	0.067807	0.361250	-3.010359	-0.090162	0.362283	-3.008894	-0.111816
C	0.868273	-2.432658	0.140107	-0.894557	-2.422668	-0.101053	-0.892986	-2.414113	-0.139559
C	1.021742	-1.041174	0.062411	-1.021776	-1.011388	-0.030455	-1.021671	-1.009909	-0.047658
C	-0.122966	-0.207600	-0.048528	0.121587	-0.183786	0.014442	0.119867	-0.171370	0.011377
C	-1.399233	-0.801224	-0.126167	1.375672	-0.794231	0.045034	1.378763	-0.793134	0.050837
H	-0.538464	-4.069433	0.125057	0.481645	-4.084801	-0.176200	0.484868	-4.081692	-0.206441
H	1.721582	-3.084179	0.281744	-1.768993	-3.051594	-0.213581	-1.767434	-3.040242	-0.270181
B	-0.016497	1.308506	-0.050376	0.018722	1.358344	-0.003274	0.018266	1.351116	-0.006089
N	2.280704	-0.422676	0.129453	-2.271741	-0.394601	-0.068840	-2.277990	-0.391807	-0.074634
N	-2.558337	-0.021058	-0.235450	2.542173	-0.024298	0.157112	2.547533	-0.020224	0.158531
C	2.405108	0.920347	0.535659	-2.416972	0.943944	-0.552273	-2.424585	0.947048	-0.542382
C	3.651631	1.320142	1.055025	-3.658738	1.296909	-1.080894	-3.672538	1.308917	-1.058402
C	1.337505	1.849710	0.464932	-1.342658	1.878492	-0.498138	-1.346431	1.878058	-0.492248
C	3.855540	2.610240	1.516951	-3.905007	2.579552	-1.575248	-3.915631	2.592309	-1.548722
C	1.569810	3.151402	0.967242	-1.623237	3.168589	-1.011836	-1.625794	3.169056	-1.001234
C	2.799517	3.530517	1.484966	-2.867224	3.512489	-1.535796	-2.872105	3.518764	-1.516315
H	4.827807	2.871086	1.923848	-4.887106	2.816419	-1.970380	-4.899557	2.835637	-1.935150
H	0.749798	3.862274	0.974908	-0.827665	3.906893	-1.025378	-0.828143	3.904960	-1.019096
H	2.950860	4.533853	1.873410	-3.036122	4.514978	-1.921523	-3.038843	4.522574	-1.899658
C	3.480556	-1.049172	-0.303994	-3.455667	-1.021400	0.369053	-3.457557	-1.027144	0.362182
C	3.540800	-2.021314	-1.310555	-3.499909	-1.980386	1.395237	-3.492018	-2.003746	1.371922
C	4.687499	-0.605799	0.259438	-4.672660	-0.614324	-0.214248	-4.679287	-0.612600	-0.204488
C	4.761061	-2.596860	-1.668232	-4.703952	-2.583834	1.748747	-4.692824	-2.612094	1.726521
H	2.630973	-2.334208	-1.808896	-2.587530	-2.245070	1.917290	-2.574622	-2.276918	1.880206
C	5.907644	-1.170223	-0.097997	-5.877429	-1.218155	0.138351	-5.880956	-1.223756	0.146625
C	5.943830	-2.187723	-1.052053	-5.891717	-2.219595	1.107797	-5.886309	-2.239268	1.100675
H	4.779796	-3.363058	-2.438062	-4.713468	-3.330054	2.537911	-4.695565	-3.370199	2.504244
H	6.810971	-0.797627	0.374996	-6.787195	-0.882488	-0.349416	-6.794760	-0.881353	-0.328645
H	6.893569	-2.639122	-1.324108	-6.831011	-2.692170	1.380074	-6.822841	-2.716924	1.373416
O	4.689549	0.418662	1.176887	-4.702657	0.388051	-1.141388	-4.718831	0.406333	-1.113051
C	-2.491763	1.311326	-0.686740	2.473912	1.307374	0.697024	2.481582	1.312104	0.684465
C	-3.613692	1.896368	-1.308020	3.553848	1.799803	1.433083	3.567534	1.814758	1.409834
C	-1.273299	2.042746	-0.574246	1.278642	2.072630	0.508079	1.283238	2.071350	0.503082
C	-3.552476	3.198489	-1.784447	3.544200	3.115541	1.910254	3.552901	3.128463	1.884524
C	-1.259816	3.360184	-1.084664	1.325635	3.405269	0.998324	1.323543	3.400868	0.995236
C	-2.373659	3.946205	-1.669414	2.429330	3.924474	1.665355	2.429539	3.928839	1.652222
H	-4.425138	3.623999	-2.274002	4.395903	3.491747	2.469852	4.406489	3.510959	2.437096
H	-0.330698	3.920560	-1.044126	0.443044	4.027509	0.885302	0.435139	4.016378	0.891718
H	-2.326269	4.960893	-2.055401	2.412421	4.951334	2.024178	2.407756	4.954802	2.013172
C	-3.747894	-0.630952	0.254082	3.732118	-0.615278	-0.280237	3.738468	-0.617992	-0.274069
C	-4.806838	0.077628	0.835463	4.867500	0.103286	-0.704869	4.869809	0.096538	-0.712389
C	-3.826217	-2.034842	0.232080	3.801601	-2.027135	-0.353436	3.803067	-2.028199	-0.333093
C	-5.949106	-0.588773	1.282577	6.020008	-0.559923	-1.107551	6.022302	-0.570675	-1.110340

C	-4.959548	-2.703596	0.683480	4.960980	-2.693187	-0.742520	4.961045	-2.698559	-0.719344
C	-6.037592	-1.977331	1.190671	6.084216	-1.959933	-1.109840	6.084034	-1.969556	-1.096599
H	-6.764992	-0.012996	1.710086	6.876740	0.024143	-1.431401	6.878299	0.009117	-1.443431
H	-4.973822	-3.788073	0.635615	4.951295	-3.778396	-0.764392	4.950897	-3.783853	-0.731283
H	-6.927407	-2.498780	1.531425	6.991268	-2.472164	-1.415378	6.989595	-2.486348	-1.399174
O	-2.770363	-2.791305	-0.223992	2.711969	-2.807328	-0.054872	2.711758	-2.804118	-0.027291
H	-4.520122	1.319437	-1.449879	4.409597	1.166310	1.640179	4.426950	1.185548	1.614214
H	-4.741549	1.154896	0.931329	4.832835	1.185117	-0.721199	4.833410	1.178045	-0.743772
PTZPXZBN		S₀			S₁			T₁	
C	-1.674826	-2.182629	-0.014474	-1.633474	-2.187422	-0.101880	-1.635124	-2.181140	-0.109717
C	-0.549517	-2.982520	-0.173374	-0.494596	-2.998816	-0.163246	-0.498185	-2.997603	-0.198438
C	0.727550	-2.420420	-0.227532	0.759167	-2.411428	-0.150791	0.755048	-2.402552	-0.201164
C	0.878658	-1.031895	-0.126685	0.882087	-0.997934	-0.070786	0.881950	-0.996344	-0.096356
C	-0.261830	-0.202988	0.009342	-0.257762	-0.174822	-0.005784	-0.255774	-0.162664	-0.014030
C	-1.538892	-0.793584	0.068810	-1.512158	-0.784677	0.001978	-1.515699	-0.783931	-0.000617
H	-0.681179	-4.057530	-0.250731	-0.615929	-4.071707	-0.265677	-0.621142	-4.068574	-0.311651
H	1.587751	-3.066115	-0.361047	1.640966	-3.033629	-0.248288	1.637011	-3.022363	-0.316209
B	-0.138505	1.308284	0.090241	-0.140770	1.363759	0.044809	-0.139748	1.356002	0.041790
N	2.150892	-0.426690	-0.180227	2.138570	-0.391496	-0.108463	2.144890	-0.391189	-0.118728
N	-2.692375	-0.011720	0.213446	-2.676425	-0.013788	0.132184	-2.680612	-0.010451	0.130885
C	2.282952	0.926278	-0.568549	2.284982	0.953775	-0.587176	2.295219	0.955913	-0.577022
C	3.504640	1.337144	-1.143020	3.495248	1.313638	-1.186041	3.513415	1.325175	-1.161780
C	1.219460	1.856987	-0.413318	1.215325	1.892944	-0.438180	1.223868	1.891418	-0.433617
C	3.691689	2.663086	-1.528466	3.723185	2.635330	-1.605941	3.737784	2.647329	-1.572762
C	1.436487	3.177948	-0.861650	1.485161	3.211229	-0.890688	1.488828	3.208693	-0.883164
C	2.649792	3.586338	-1.398622	2.705093	3.577544	-1.447527	2.712884	3.583423	-1.426638
H	4.641732	2.962318	-1.962268	4.677807	2.906365	-2.045226	4.695548	2.925144	-2.001245
H	0.617685	3.888436	-0.806120	0.694941	3.952835	-0.826935	0.693895	3.945887	-0.827263
H	2.791625	4.610941	-1.731437	2.868692	4.602020	-1.774134	2.874208	4.608947	-1.750903
C	3.267767	-1.051839	0.452044	3.248802	-1.016688	0.511453	3.248557	-1.026614	0.504087
C	3.119333	-1.789931	1.636400	3.095685	-1.744700	1.705439	3.083086	-1.769824	1.686484
C	4.558769	-0.873778	-0.071230	4.540576	-0.869329	-0.031086	4.545199	-0.873840	-0.023459
C	4.219387	-2.402925	2.232086	4.184490	-2.380817	2.292679	4.166340	-2.412362	2.277378
H	2.136121	-1.893969	2.081365	2.117302	-1.803439	2.169925	2.099376	-1.836705	2.138123
C	5.664595	-1.468897	0.544657	5.633695	-1.497049	0.576647	5.632676	-1.508752	0.587075
C	5.494460	-2.255854	1.681783	5.455720	-2.270547	1.721461	5.443377	-2.295603	1.720758
H	4.077380	-2.984075	3.139145	4.042152	-2.944919	3.210190	4.014417	-2.988054	3.186118
H	6.654593	-1.309682	0.127012	6.623401	-1.369882	0.147580	6.626484	-1.376717	0.169064
H	6.354371	-2.730600	2.145874	6.309798	-2.760447	2.180567	6.292639	-2.791639	2.182185
C	-2.614849	1.297972	0.724416	-2.606156	1.295549	0.728519	-2.610568	1.298819	0.718119
C	-3.734240	1.864252	1.368014	-3.690570	1.759959	1.476521	-3.698290	1.769145	1.461820
C	-1.388645	2.024301	0.652033	-1.405350	2.059725	0.589074	-1.406284	2.057742	0.581982
C	-3.663004	3.140657	1.907750	-3.674801	3.050097	2.019224	-3.678883	3.056681	2.003942
C	-1.365944	3.314909	1.227346	-1.443207	3.361261	1.150172	-1.441858	3.358640	1.142533
C	-2.476594	3.882003	1.835576	-2.550663	3.858181	1.831596	-2.549320	3.859401	1.820016
H	-4.534036	3.549721	2.413922	-4.530746	3.405562	2.585946	-4.533601	3.415589	2.570204

H	-0.431384	3.867697	1.219008	-0.552993	3.978800	1.080595	-0.549229	3.973040	1.077315
H	-2.421534	4.875657	2.271883	-2.527471	4.864583	2.243661	-2.522517	4.864944	2.234010
C	-3.886995	-0.599048	-0.290938	-3.864795	-0.589705	-0.324442	-3.871820	-0.589612	-0.318861
C	-4.946372	0.134085	-0.840129	-4.999455	0.142887	-0.727110	-5.003860	0.143519	-0.726170
C	-3.969449	-2.002767	-0.320963	-3.933560	-1.999516	-0.443887	-3.938140	-1.998320	-0.429556
C	-6.092972	-0.511483	-1.306072	-6.150183	-0.506875	-1.154646	-6.156908	-0.506885	-1.145591
C	-5.107492	-2.650370	-0.791110	-5.092626	-2.651993	-0.857555	-5.100286	-2.651714	-0.834809
C	-6.185450	-1.902273	-1.265476	-6.213836	-1.906403	-1.203686	-6.220952	-1.906467	-1.182049
H	-6.908944	0.082304	-1.707957	-7.006162	0.087033	-1.461893	-7.012452	0.085185	-1.457096
H	-5.125179	-3.735814	-0.783961	-5.083434	-3.735825	-0.914850	-5.093131	-3.735760	-0.886095
H	-7.078472	-2.407961	-1.621198	-7.119906	-2.407763	-1.529338	-7.128322	-2.409363	-1.501864
S	4.755770	0.132814	-1.514371	4.757054	0.098746	-1.490118	4.776950	0.113966	-1.467652
H	-4.646618	1.290102	1.479029	-4.553224	1.124667	1.644940	-4.561658	1.135147	1.631087
H	-4.877486	1.213946	-0.896631	-4.964148	1.224648	-0.709053	-4.964228	1.225273	-0.719864
O	-2.914579	-2.781189	0.099799	-2.847652	-2.790130	-0.165262	-2.850924	-2.786499	-0.154737
DPAPXZBN		S₀			S₁			T₁	
C	1.252351	-2.141083	0.418690	1.231133	-2.167840	0.327281	1.234072	-2.159373	0.344042
C	0.067937	-2.864591	0.469598	0.046028	-2.888948	0.488216	0.052635	-2.887145	0.498489
C	-1.167549	-2.232388	0.334374	-1.167116	-2.227520	0.409702	-1.164326	-2.220687	0.400798
C	-1.223608	-0.842396	0.127922	-1.215285	-0.823809	0.153120	-1.215126	-0.824063	0.145306
C	-0.020416	-0.088060	0.096423	-0.018427	-0.077743	0.066112	-0.019759	-0.064837	0.059061
C	1.212188	-0.757855	0.234791	1.192177	-0.764041	0.163710	1.196659	-0.761348	0.165208
H	0.118900	-3.937546	0.629295	0.093370	-3.962563	0.635708	0.100097	-3.959946	0.646590
H	-2.066819	-2.832128	0.379986	-2.078375	-2.800825	0.515006	-2.075823	-2.795460	0.498019
B	-0.033110	1.423527	-0.038570	-0.030674	1.453292	-0.124671	-0.034885	1.446196	-0.122154
N	-2.445415	-0.176872	-0.038208	-2.429034	-0.180654	-0.016140	-2.434226	-0.179027	-0.019767
N	2.426540	-0.057864	0.185885	2.408964	-0.069082	0.106997	2.414813	-0.063122	0.095895
C	-2.546692	1.176824	-0.396278	-2.558693	1.189928	-0.406140	-2.566261	1.190282	-0.394464
C	-3.818137	1.713836	-0.708106	-3.836749	1.687335	-0.693590	-3.847216	1.690560	-0.676908
C	-1.393923	2.018988	-0.454322	-1.400947	2.031735	-0.495117	-1.411360	2.034157	-0.479821
C	-3.946965	3.029149	-1.126585	-4.013548	3.013726	-1.107841	-4.023783	3.016788	-1.081878
C	-1.579747	3.341692	-0.918877	-1.634933	3.356147	-0.953282	-1.645180	3.358218	-0.928234
C	-2.822356	3.853998	-1.257802	-2.902557	3.845403	-1.251302	-2.913638	3.849759	-1.222516
H	-4.936388	3.409399	-1.369950	-5.014904	3.375716	-1.324892	-5.025391	3.380380	-1.295448
H	-0.705112	3.973804	-1.034375	-0.779539	4.007670	-1.099500	-0.790810	4.011954	-1.070376
H	-2.923803	4.874772	-1.616366	-3.023957	4.870029	-1.596328	-3.035820	4.876289	-1.561178
C	-3.653241	-0.946846	0.113598	-3.634064	-0.954851	0.141049	-3.636569	-0.959025	0.132599
C	-4.203572	-1.617443	-0.983756	-4.175425	-1.644274	-0.949059	-4.175349	-1.642591	-0.962217
C	-4.268288	-1.027896	1.366499	-4.257504	-1.014459	1.390977	-4.258352	-1.030613	1.382566
C	-5.370943	-2.366206	-0.825111	-5.338594	-2.397973	-0.783719	-5.336757	-2.400018	-0.802316
H	-3.716122	-1.547617	-1.951743	-3.684512	-1.585002	-1.915963	-3.684308	-1.575466	-1.928495
C	-5.435740	-1.777706	1.519544	-5.421030	-1.769325	1.549950	-5.420100	-1.789239	1.535977
C	-5.988252	-2.447215	0.425309	-5.962522	-2.461678	0.464485	-5.960368	-2.474459	0.445451
H	-5.796966	-2.885634	-1.679432	-5.756619	-2.934256	-1.631553	-5.753693	-2.930792	-1.654117
H	-5.912222	-1.838185	2.494436	-5.902902	-1.815557	2.522959	-5.901608	-1.843880	2.508713
H	-6.897160	-3.030625	0.546546	-6.868363	-3.048782	0.590563	-6.864932	-3.064405	0.567248

C	2.477703	1.318694	0.475034	2.454878	1.320763	0.483301	2.461804	1.323643	0.463349
C	3.675298	1.883196	0.959943	3.601896	1.808687	1.112432	3.617436	1.820257	1.076324
C	1.302246	2.116619	0.354271	1.299885	2.136063	0.261648	1.300543	2.133438	0.259396
C	3.730334	3.226125	1.305013	3.702552	3.163813	1.448332	3.712032	3.171729	1.416076
C	1.407430	3.470985	0.743551	1.457443	3.502848	0.617132	1.451255	3.496644	0.623464
C	2.592455	4.034225	1.197267	2.625160	4.011868	1.176239	2.622905	4.012340	1.167697
H	4.660480	3.636141	1.691232	4.605761	3.537469	1.922210	4.618508	3.550399	1.879698
H	0.515716	4.088367	0.717926	0.613271	4.171472	0.490070	0.599865	4.159200	0.514483
H	2.630336	5.080444	1.488886	2.686529	5.068247	1.429297	2.678851	5.067116	1.428341
C	3.543596	-0.819865	-0.254831	3.532826	-0.793605	-0.283989	3.540009	-0.793940	-0.286100
C	4.612245	-0.287327	-0.986828	4.689974	-0.221567	-0.854180	4.690177	-0.228934	-0.874562
C	3.529945	-2.205965	-0.016982	3.514788	-2.204841	-0.140456	3.519483	-2.199774	-0.119385
C	5.680954	-1.096487	-1.377049	5.777035	-1.012541	-1.195749	5.777060	-1.023627	-1.209603
C	4.588802	-3.017475	-0.412156	4.615698	-2.996191	-0.465014	4.618988	-2.995088	-0.439123
C	5.681705	-2.458012	-1.075652	5.757810	-2.400967	-0.985149	5.757845	-2.407209	-0.975446
H	6.508239	-0.654357	-1.924964	6.650064	-0.543722	-1.640573	6.646730	-0.562266	-1.668399
H	4.535313	-4.080121	-0.196184	4.542820	-4.069010	-0.317302	4.548501	-4.065575	-0.274676
H	6.514287	-3.089560	-1.372121	6.617424	-3.010621	-1.245339	6.615541	-3.021557	-1.231299
H	-4.705052	1.096951	-0.641254	-4.709021	1.052735	-0.603074	-4.718673	1.054323	-0.590172
H	-3.829921	-0.503757	2.210687	-3.828959	-0.470101	2.227301	-3.830577	-0.492086	2.223005
H	4.550713	1.261117	1.104877	4.422555	1.140467	1.349952	4.444457	1.156398	1.303033
H	4.612531	0.765698	-1.242933	4.717465	0.845941	-1.032312	4.712714	0.835123	-1.073712
O	2.455772	-2.799843	0.604953	2.402551	-2.853061	0.322067	2.409267	-2.841344	0.359656

CzPXZBN

	S₀			S₁			T₁		
C	-1.504536	-2.171882	0.354284	1.471968	-2.192066	-0.264477	-1.475502	-2.189878	0.254080
C	-0.409879	-3.019119	0.311240	0.364680	-3.047787	-0.299948	-0.370945	-3.051948	0.274316
C	0.887462	-2.510389	0.209157	-0.906099	-2.512513	-0.241154	0.900679	-2.509400	0.202318
C	1.091117	-1.128109	0.158724	-1.093122	-1.102999	-0.172304	1.092611	-1.106998	0.150363
C	-0.026485	-0.240710	0.146799	0.021469	-0.228675	-0.114382	-0.019280	-0.219630	0.099001
C	-1.323558	-0.786255	0.246751	1.299999	-0.798383	-0.181977	-1.303703	-0.798704	0.173724
H	-0.575874	-4.090720	0.363630	0.526228	-4.120148	-0.315919	-0.532631	-4.123680	0.283330
H	1.704690	-3.209665	0.120753	-1.745139	-3.187404	-0.170954	1.739354	-3.184654	0.122495
B	0.110210	1.274536	-0.022314	-0.113540	1.301641	0.099376	0.114938	1.293614	-0.101925
N	2.367506	-0.545071	0.067234	-2.356583	-0.537319	-0.077641	2.363089	-0.538952	0.069587
N	-2.466686	0.024787	0.224614	2.448877	0.012298	-0.139499	-2.452309	0.013757	0.136915
C	2.532195	0.778619	-0.338176	-2.535593	0.793818	0.366092	2.545220	0.792894	-0.359296
C	3.900320	1.037076	-0.578155	-3.898384	1.026663	0.601009	3.911216	1.029648	-0.584172
C	1.515626	1.744016	-0.462450	-1.508833	1.756179	0.505483	1.522094	1.757322	-0.496466
C	4.275920	2.298706	-1.039270	-4.307491	2.290532	1.070868	4.319442	2.295766	-1.042208
C	1.945621	2.998340	-0.946527	-1.973610	3.015153	0.995197	1.984600	3.013455	-0.976285
C	3.286154	3.268079	-1.237825	-3.320520	3.261829	1.270348	3.335069	3.265911	-1.243980
H	5.318073	2.527460	-1.247040	-5.353205	2.505332	1.269449	5.366518	2.514039	-1.231151
H	1.211708	3.781399	-1.112167	-1.253193	3.806923	1.177384	1.265246	3.806713	-1.156106
H	3.566996	4.249001	-1.612215	-3.611867	4.241982	1.642864	3.626642	4.248707	-1.608676
C	3.649687	-1.122836	0.190525	-3.636639	-1.120498	-0.224642	3.639270	-1.121775	0.220553
C	4.058684	-2.357117	0.708137	-4.041033	-2.330428	-0.796643	4.038736	-2.340258	0.781772

C	4.616126	-0.172017	-0.236657	-4.602114	-0.177733	0.228185	4.611632	-0.178005	-0.216735
C	5.423594	-2.648568	0.727580	-5.405846	-2.629030	-0.830660	5.401285	-2.640468	0.822001
H	3.362420	-3.068289	1.130716	-3.344590	-3.019315	-1.256167	3.336946	-3.032798	1.227448
C	5.977654	-0.488199	-0.213133	-5.963215	-0.500384	0.187666	5.971678	-0.504079	-0.171049
C	6.377644	-1.736119	0.257244	-6.358850	-1.733061	-0.327078	6.361161	-1.742129	0.333227
H	5.746839	-3.604942	1.130122	-5.726190	-3.568535	-1.272649	5.717303	-3.584594	1.257462
H	6.714022	0.239208	-0.544447	-6.703823	0.213528	0.538070	6.715942	0.211476	-0.510443
H	7.432467	-1.995440	0.281526	-7.414087	-1.990859	-0.363963	7.415265	-2.003558	0.374275
C	-2.386586	1.399078	0.516072	2.371415	1.397420	-0.520668	-2.373083	1.396801	0.509238
C	-3.516065	2.073886	1.022459	3.463081	1.991868	-1.159390	-3.467974	1.996587	1.142440
C	-1.149532	2.086262	0.360019	1.157957	2.103378	-0.288308	-1.154372	2.098247	0.278624
C	-3.442138	3.422728	1.338833	3.427702	3.351329	-1.488493	-3.431313	3.353810	1.468065
C	-1.123987	3.456258	0.707268	1.172237	3.474066	-0.633078	-1.172055	3.472321	0.615540
C	-2.243397	4.129209	1.174914	2.283549	4.096416	-1.201026	-2.282811	4.095652	1.178326
H	-4.320297	3.920635	1.742724	4.286764	3.809876	-1.970227	-4.287920	3.815600	1.950637
H	-0.182071	3.990567	0.636726	0.267664	4.054572	-0.485111	-0.267439	4.052808	0.468925
H	-2.185996	5.182316	1.436614	2.245882	5.155306	-1.446138	-2.243586	5.154892	1.422107
C	-3.654585	-0.606645	-0.242552	3.636274	-0.591364	0.273869	-3.644955	-0.590779	-0.266349
C	-4.665531	0.055888	-0.950095	4.729934	0.105661	0.827729	-4.736468	0.107696	-0.822174
C	-3.779331	-1.993768	-0.057126	3.752920	-2.000449	0.173789	-3.760674	-1.997162	-0.157189
C	-5.809549	-0.628733	-1.363664	5.889406	-0.566782	1.187499	-5.899870	-0.562432	-1.170944
C	-4.914070	-2.682403	-0.473407	4.924623	-2.672937	0.517201	-4.938098	-2.667439	-0.487787
C	-5.946728	-1.993228	-1.110076	6.004195	-1.954597	1.015261	-6.017101	-1.948267	-0.984381
H	-6.588653	-0.087065	-1.892376	6.713057	-0.003538	1.616261	-6.722942	-0.001052	-1.602886
H	-4.964894	-3.752373	-0.297023	4.954754	-3.751685	0.402866	-4.971849	-3.745253	-0.366761
H	-6.838724	-2.527236	-1.424657	6.918841	-2.470506	1.290062	-6.934810	-2.463498	-1.250332
H	-4.438796	1.534069	1.200741	4.341526	1.406642	-1.408389	-4.345410	1.411367	1.394844
H	-4.562347	1.111766	-1.170181	4.654551	1.174695	0.979273	-4.654734	1.174414	-0.986257
O	-2.763430	-2.712961	0.529979	2.705513	-2.764711	-0.257428	-2.711369	-2.760399	0.265972

DMACPXZBN

	S_0			S_1			T_1		
C	0.516859	-2.438261	0.004078	0.544461	-2.425860	0.066577	0.539556	-2.419981	0.018742
C	-0.766842	-2.987307	0.014390	-0.713104	-3.003313	0.020398	-0.719168	-3.004134	-0.010876
C	-1.890360	-2.174011	0.098098	-1.845420	-2.180926	0.006246	-1.849724	-2.174669	0.000170
C	-1.744002	-0.784705	0.145150	-1.713304	-0.776279	0.066652	-1.718852	-0.775562	0.063136
C	-0.460414	-0.206479	0.127405	-0.454562	-0.176380	0.088730	-0.453557	-0.165089	0.078662
C	0.679144	-1.047412	0.073109	0.681003	-1.010132	0.105710	0.680009	-1.011331	0.079808
H	1.373526	-3.097252	-0.073090	1.421777	-3.060359	0.026758	1.417255	-3.053550	-0.037192
H	-0.905020	-4.063059	-0.038536	-0.839923	-4.078041	-0.052103	-0.847910	-4.077294	-0.092448
B	-0.325341	1.305984	0.155804	-0.323411	1.360971	0.087561	-0.322350	1.351978	0.084062
N	-2.895958	0.011281	0.205154	-2.874195	0.008703	0.120115	-2.880051	0.013278	0.116660
N	1.951186	-0.447736	0.052915	1.938390	-0.413620	0.099653	1.943356	-0.415650	0.087841
C	-2.830384	1.337295	0.675871	-2.814621	1.337205	0.675432	-2.819683	1.340806	0.662834
C	-3.973377	1.931546	1.248471	-3.922569	1.833096	1.365482	-3.931066	1.843936	1.347300
C	-1.595541	2.050672	0.636870	-1.601219	2.086322	0.555055	-1.602150	2.083406	0.548773
C	-3.916538	3.224034	1.750817	-3.918251	3.141449	1.864307	-3.921301	3.148560	1.847692
C	-1.588195	3.357267	1.174698	-1.652726	3.408603	1.068195	-1.648940	3.403332	1.064781

C	-2.720992	3.952396	1.712135	-2.781015	3.934794	1.690059	-2.776992	3.934661	1.681713
H	-4.806687	3.655657	2.202106	-4.792069	3.521982	2.385607	-4.794011	3.533268	2.367677
H	-0.649241	3.901866	1.195522	-0.756793	4.018750	1.011590	-0.749293	4.008485	1.015722
H	-2.676292	4.958510	2.120344	-2.765430	4.955064	2.067283	-2.756371	4.953189	2.063335
C	-4.069366	-0.581719	-0.338896	-4.048075	-0.571243	-0.364770	-4.057634	-0.569718	-0.360209
C	-4.164908	-1.985168	-0.328013	-4.126881	-1.984053	-0.439921	-4.135113	-1.981087	-0.424159
C	-5.093536	0.142089	-0.962435	-5.158990	0.157382	-0.836726	-5.165007	0.159229	-0.838069
C	-5.285059	-2.637575	-0.833298	-5.275125	-2.639605	-0.878337	-5.287236	-2.637133	-0.853387
C	-6.222609	-0.508201	-1.463523	-6.297569	-0.496133	-1.289296	-6.306876	-0.494521	-1.281415
C	-6.331046	-1.896092	-1.383801	-6.373701	-1.896261	-1.294633	-6.384738	-1.894135	-1.271940
H	-5.314308	-3.722043	-0.791998	-5.274881	-3.724828	-0.898655	-5.290025	-3.722363	-0.866025
H	-7.012116	0.079508	-1.923176	-7.134384	0.094668	-1.650677	-7.142703	0.094257	-1.647946
H	-7.210802	-2.405328	-1.766597	-7.271094	-2.400125	-1.639876	-7.284000	-2.399305	-1.610550
C	2.124363	0.883899	-0.377642	2.133866	0.914562	-0.406936	2.141978	0.913782	-0.399383
C	3.398746	1.239387	-0.882959	3.402808	1.215939	-0.923632	3.416960	1.223302	-0.904118
C	1.058903	1.823294	-0.298238	1.064165	1.859705	-0.339877	1.072774	1.857610	-0.333263
C	3.605281	2.568215	-1.251080	3.650472	2.540334	-1.326923	3.663834	2.549017	-1.293511
C	1.325027	3.139387	-0.730346	1.379068	3.169849	-0.781586	1.385815	3.168055	-0.766481
C	2.580096	3.518658	-1.180030	2.644132	3.506085	-1.244789	2.654303	3.511538	-1.216453
H	4.570604	2.876770	-1.636652	4.621492	2.822168	-1.715584	4.637507	2.836409	-1.671774
H	0.519263	3.866992	-0.726135	0.599054	3.925050	-0.779087	0.603906	3.921302	-0.767090
H	2.768122	4.540047	-1.500765	2.852827	4.524301	-1.566684	2.862906	4.531971	-1.531058
C	3.084899	-1.072093	0.645609	3.057415	-1.032427	0.703717	3.057612	-1.043532	0.693490
C	4.361244	-0.778025	0.128883	4.338530	-0.777173	0.171303	4.342868	-0.783517	0.174657
C	2.950407	-1.874043	1.788996	2.908305	-1.797013	1.873938	2.898467	-1.822723	1.852148
C	5.476189	-1.332374	0.769259	5.440445	-1.340102	0.824625	5.439614	-1.355081	0.829512
C	4.074224	-2.427386	2.395272	4.020629	-2.358505	2.491266	4.005802	-2.391442	2.472147
H	1.967667	-2.050898	2.210800	1.924496	-1.921171	2.313072	1.910459	-1.954684	2.279084
C	5.343774	-2.161093	1.883152	5.292645	-2.134052	1.963141	5.282321	-2.161976	1.957364
H	6.471532	-1.119849	0.395830	6.439680	-1.162620	0.443707	6.441865	-1.174032	0.458229
H	3.953729	-3.048140	3.279324	3.893179	-2.944818	3.397353	3.870421	-2.989143	3.369624
H	6.228133	-2.584493	2.351753	6.170227	-2.559698	2.442348	6.155621	-2.594589	2.438154
C	4.436754	0.130263	-1.099448	4.427621	0.083884	-1.088694	4.442641	0.093029	-1.074092
C	5.851309	0.684991	-1.329327	5.852103	0.609447	-1.329059	5.868868	0.621268	-1.297103
H	5.881335	1.309622	-2.225947	5.892507	1.204222	-2.245003	5.917175	1.226178	-2.206038
H	6.203606	1.280528	-0.481251	6.207867	1.228759	-0.499871	6.217863	1.231086	-0.458029
H	6.561706	-0.128799	-1.497782	6.552595	-0.218774	-1.467560	6.570376	-0.205462	-1.438988
C	4.037890	-0.687534	-2.361996	4.029674	-0.778577	-2.321975	4.053534	-0.754171	-2.320636
H	4.053435	-0.043625	-3.247892	4.055372	-0.166538	-3.229701	4.087965	-0.132052	-3.221228
H	4.747094	-1.507881	-2.517620	4.730447	-1.611953	-2.445726	4.754233	-1.587055	-2.447567
H	3.037056	-1.115913	-2.272671	3.022903	-1.191309	-2.223485	3.045472	-1.166563	-2.235260
H	-4.894785	1.367509	1.334606	-4.795495	1.208789	1.522253	-4.806011	1.222327	1.502956
H	-5.011266	1.219035	-1.048924	-5.113498	1.238805	-0.851880	-5.113847	1.240152	-0.866856
O	-3.140977	-2.758376	0.170733	-3.061803	-2.774561	-0.090291	-3.069218	-2.769524	-0.076944
TMCzPXZBN		S₀		S₁		T₁			
C	-1.903796	-2.282757	0.252717	-1.873135	-2.296620	0.147337	-1.876175	-2.293163	0.141243

C	-0.808797	-3.127429	0.173347	-0.767647	-3.154557	0.139305	-0.772910	-3.156439	0.118055
C	0.489319	-2.614912	0.115179	0.504590	-2.618424	0.126456	0.500147	-2.612408	0.090870
C	0.693880	-1.231593	0.145413	0.693762	-1.208290	0.147477	0.693565	-1.210087	0.125155
C	-0.423459	-0.343379	0.175217	-0.419508	-0.328516	0.136038	-0.417504	-0.318213	0.120591
C	-1.721377	-0.893762	0.228896	-1.698797	-0.899497	0.155897	-1.702585	-0.899014	0.148956
H	-0.975885	-4.200115	0.162106	-0.930428	-4.225573	0.087270	-0.935841	-4.226500	0.060948
H	1.307875	-3.308243	-0.002920	1.343776	-3.288952	0.023812	1.339117	-3.282710	-0.020927
B	-0.284745	1.180121	0.104953	-0.281115	1.212978	0.029869	-0.280481	1.205071	0.023229
N	1.969447	-0.645897	0.100185	1.957716	-0.640537	0.101018	1.964020	-0.640714	0.089772
N	-2.864803	-0.082078	0.241824	-2.846863	-0.087463	0.160481	-2.850611	-0.085500	0.157995
C	2.136014	0.701752	-0.213718	2.140857	0.718381	-0.244893	2.149653	0.716905	-0.243275
C	3.504795	0.979887	-0.421417	3.504295	0.970340	-0.446818	3.515478	0.971896	-0.435963
C	1.126024	1.675756	-0.285205	1.121557	1.692129	-0.327204	1.132898	1.692815	-0.323855
C	3.881771	2.268874	-0.789760	3.916363	2.263300	-0.817751	3.925903	2.266707	-0.797611
C	1.564530	2.959454	-0.677664	1.595083	2.979915	-0.718655	1.603175	2.976397	-0.707075
C	2.906201	3.270990	-0.941134	2.944600	3.267062	-0.968046	2.957119	3.268470	-0.950065
H	4.928960	2.504446	-0.967142	4.966973	2.485314	-0.984219	4.977281	2.491300	-0.956381
H	0.826714	3.748042	-0.795866	0.872069	3.780334	-0.848226	0.881104	3.778307	-0.833794
C	3.253182	-1.227944	0.191024	3.237426	-1.231129	0.214956	3.240612	-1.230975	0.208193
C	3.671015	-2.491497	0.622441	3.648307	-2.476885	0.698378	3.647164	-2.483378	0.682043
C	4.220433	-0.250102	-0.158007	4.205973	-0.258831	-0.154724	4.214865	-0.258933	-0.147995
C	5.036372	-2.773197	0.632395	5.012720	-2.768072	0.723471	5.009562	-2.776141	0.712959
H	2.980421	-3.238110	0.990090	2.955693	-3.204713	1.100435	2.949832	-3.213560	1.071400
C	5.582871	-0.562388	-0.143366	5.566996	-0.579988	-0.122836	5.575199	-0.583294	-0.111452
C	6.010512	-1.836248	0.237349	5.987877	-1.844348	0.299136	5.990611	-1.851217	0.302005
H	5.355577	-3.755865	0.972215	5.327392	-3.737884	1.101372	5.320491	-3.749552	1.084961
H	6.312980	0.195890	-0.416016	6.302974	0.166312	-0.411818	6.314288	0.163625	-0.390969
C	-2.789232	1.271410	0.619298	-2.771347	1.268623	0.632637	-2.773414	1.269530	0.619862
C	-3.925755	1.913630	1.151619	-3.868730	1.821532	1.298531	-3.873531	1.829171	1.280354
C	-1.550373	1.966155	0.523391	-1.554496	1.987150	0.458567	-1.551686	1.983185	0.446462
C	-3.856683	3.239761	1.553783	-3.836286	3.156163	1.716665	-3.838819	3.162072	1.694284
C	-1.529939	3.310993	0.957860	-1.573025	3.333634	0.891622	-1.571814	3.333005	0.872465
C	-2.655767	3.953952	1.452059	-2.688837	3.917699	1.488932	-2.686669	3.919677	1.464710
H	-4.740615	3.711725	1.975890	-4.699478	3.582838	2.219844	-4.699638	3.592598	2.197905
H	-0.587158	3.847848	0.934029	-0.667050	3.921880	0.790416	-0.665289	3.920331	0.772462
H	-2.601947	4.988268	1.780995	-2.653361	4.958217	1.803547	-2.648822	4.960648	1.777813
C	-4.046133	-0.683592	-0.277549	-4.031773	-0.661133	-0.302515	-4.040788	-0.662047	-0.293896
C	-5.047938	0.020518	-0.957460	-5.119141	0.071941	-0.820594	-5.126079	0.071063	-0.815292
C	-4.173177	-2.079307	-0.176489	-4.150541	-2.072871	-0.295776	-4.158094	-2.071619	-0.275712
C	-6.186400	-0.637497	-1.426033	-6.275745	-0.573867	-1.235259	-6.286439	-0.574405	-1.218360
C	-5.302247	-2.741115	-0.648125	-5.318675	-2.720078	-0.694621	-5.331249	-2.718764	-0.661820
C	-6.326619	-2.014607	-1.256150	-6.393158	-1.969517	-1.155604	-6.405574	-1.968816	-1.122819
H	-6.958718	-0.064751	-1.931472	-7.094625	0.017574	-1.634261	-7.105053	0.014482	-1.621303
H	-5.355350	-3.819650	-0.536282	-5.350382	-3.804006	-0.651560	-5.365982	-3.802155	-0.610581
H	-7.214358	-2.528389	-1.613587	-7.305252	-2.465436	-1.472543	-7.320323	-2.465652	-1.430770
H	-4.850740	1.364162	1.282416	-4.749758	1.221988	1.499892	-4.754161	1.230317	1.485239

H	-4.942007	1.087610	-1.112665	-5.041610	1.148579	-0.900651	-5.042886	1.146179	-0.909197
O	-3.165417	-2.832309	0.381105	-3.107125	-2.865168	0.095272	-3.112420	-2.861482	0.109719
C	3.310510	4.659045	-1.379428	3.358173	4.649557	-1.417635	3.362835	4.655392	-1.392082
H	3.680020	4.660447	-2.412799	3.497828	4.689083	-2.506375	3.239571	4.778669	-2.476576
H	2.468821	5.355945	-1.330002	2.604840	5.399996	-1.158335	2.751946	5.426348	-0.910231
H	4.114542	5.060806	-0.751471	4.307361	4.953181	-0.961971	4.412370	4.862026	-1.159087
C	7.473875	-2.205984	0.236653	7.450238	-2.215933	0.315675	7.451864	-2.227127	0.326819
H	7.712757	-2.887408	-0.590205	7.690555	-2.922946	-0.489309	7.689899	-2.954518	-0.460309
H	8.110577	-1.322928	0.128311	8.089355	-1.337995	0.183070	8.093565	-1.354559	0.173068
H	7.760398	-2.715240	1.163875	7.731849	-2.698550	1.258708	7.732521	-2.687110	1.281550
PXZPTZBN		S₀			S₁			T₁	
C	-1.424699	-2.175514	0.201400	-1.387893	-2.196722	0.092764	-1.386088	-2.187326	0.097406
C	-0.288807	-2.960821	-0.016241	-0.228214	-2.986660	0.000347	-0.231877	-2.982070	-0.035736
C	0.975557	-2.395045	-0.143023	1.018105	-2.390969	-0.064755	1.015193	-2.380188	-0.118754
C	1.124054	-1.001453	-0.050957	1.133211	-0.979142	-0.008979	1.131718	-0.976820	-0.030357
C	-0.021216	-0.175172	0.098367	-0.017250	-0.161644	0.057992	-0.015806	-0.148528	0.055880
C	-1.295097	-0.779558	0.215118	-1.274192	-0.782963	0.123070	-1.277015	-0.778131	0.128351
H	-0.395856	-4.040122	-0.079474	-0.317293	-4.066135	-0.068486	-0.324639	-4.059635	-0.117056
H	1.826422	-3.037791	-0.331861	1.893728	-3.012955	-0.203662	1.888788	-2.999189	-0.284360
B	0.098507	1.341211	0.143557	0.096543	1.380594	0.057345	0.096842	1.376197	0.062526
N	2.379101	-0.385680	-0.145312	2.379821	-0.358759	-0.084751	2.386753	-0.353817	-0.089327
N	-2.445939	0.021551	0.329960	-2.422573	0.025255	0.234293	-2.428144	0.027482	0.244159
C	2.497678	0.965646	-0.524408	2.510515	0.978425	-0.570653	2.519877	0.985065	-0.555833
C	3.726859	1.372599	-1.077673	3.732977	1.334511	-1.140988	3.750014	1.352907	-1.109159
C	1.437065	1.894719	-0.394035	1.439815	1.909325	-0.476365	1.444047	1.911994	-0.462568
C	3.919913	2.673816	-1.512369	3.959572	2.620626	-1.634463	3.974016	2.641352	-1.596647
C	1.657561	3.209683	-0.866027	1.698683	3.204264	-0.987548	1.703287	3.208697	-0.964040
C	2.870494	3.597354	-1.416025	2.923749	3.553311	-1.551447	2.931916	3.565814	-1.518079
H	4.877986	2.942182	-1.947012	4.926586	2.861523	-2.063152	4.944197	2.890436	-2.012981
H	0.841307	3.923692	-0.823558	0.901501	3.940961	-0.965109	0.904907	3.943941	-0.942645
H	3.013841	4.610746	-1.780666	3.079578	4.558779	-1.934876	3.084897	4.574184	-1.894984
C	3.592706	-1.025923	0.231169	3.580567	-0.984330	0.312316	3.579956	-0.991334	0.303160
C	3.685224	-2.015252	1.218237	3.662942	-1.937219	1.341316	3.648557	-1.973803	1.306162
C	4.779761	-0.575979	-0.367618	4.775696	-0.577227	-0.313812	4.783225	-0.573232	-0.301021
C	4.914657	-2.603301	1.518887	4.879779	-2.537300	1.655529	4.859988	-2.584201	1.616218
H	2.793415	-2.331702	1.746006	2.769865	-2.201580	1.895856	2.748916	-2.248826	1.844083
C	6.009330	-1.153939	-0.067843	5.993305	-1.177217	-0.000824	5.995471	-1.188576	0.004157
C	6.075294	-2.189297	0.864723	6.043565	-2.174488	0.971683	6.032016	-2.209387	0.951199
H	4.958470	-3.382677	2.274249	4.917886	-3.279926	2.447246	4.888964	-3.345740	2.389990
H	6.896479	-0.776266	-0.566644	6.884905	-0.841267	-0.520905	6.892876	-0.843619	-0.499558
H	7.032043	-2.650368	1.092316	6.992679	-2.644479	1.212646	6.976707	-2.689451	1.189233
C	-2.352285	1.345741	0.818388	-2.314038	1.329446	0.840003	-2.325183	1.335897	0.826885
C	-3.477720	1.920239	1.440417	-3.375519	1.791398	1.620683	-3.399434	1.816186	1.584154
C	-1.132420	2.069237	0.729963	-1.125245	2.094892	0.649463	-1.130459	2.094179	0.649735
C	-3.407913	3.203389	1.964861	-3.343564	3.082493	2.158193	-3.364258	3.106730	2.115240
C	-1.104878	3.366180	1.290722	-1.144346	3.402631	1.203488	-1.144883	3.400800	1.202338

C	-2.216675	3.938063	1.893148	-2.226187	3.893796	1.925323	-2.233582	3.905622	1.903771
H	-4.281486	3.624078	2.456815	-4.178746	3.440687	2.753462	-4.206307	3.475444	2.694395
H	-0.171281	3.920604	1.270646	-0.262115	4.025984	1.089907	-0.254265	4.014644	1.103554
H	-2.161210	4.935864	2.320161	-2.192793	4.901867	2.333083	-2.196461	4.913498	2.311551
C	-3.625566	-0.411085	-0.351351	-3.630953	-0.377910	-0.346950	-3.637269	-0.385490	-0.342875
C	-4.386380	0.481201	-1.122459	-4.527408	0.560371	-0.905917	-4.516255	0.543569	-0.937841
C	-4.002829	-1.764860	-0.325226	-3.987251	-1.747798	-0.429148	-3.992465	-1.752253	-0.397917
C	-5.540874	0.052417	-1.773962	-5.729410	0.157235	-1.464988	-5.716136	0.133844	-1.501021
C	-5.147721	-2.195720	-1.003180	-5.210299	-2.144482	-0.991214	-5.207052	-2.157838	-0.969140
C	-5.934229	-1.285193	-1.706024	-6.089381	-1.198890	-1.498471	-6.078439	-1.219673	-1.506555
H	-6.122791	0.767317	-2.349182	-6.388813	0.906079	-1.894903	-6.367793	0.875181	-1.955033
H	-5.414622	-3.248292	-0.975903	-5.453305	-3.202392	-1.036676	-5.452168	-3.215815	-0.997050
H	-6.832290	-1.623954	-2.214871	-7.032493	-1.511328	-1.936309	-7.017775	-1.539960	-1.947269
H	-4.394764	1.348580	1.533834	-4.237270	1.155548	1.798839	-4.268328	1.187897	1.753341
H	-4.077467	1.517515	-1.199616	-4.259060	1.609438	-0.898978	-4.241029	1.590980	-0.953597
O	4.754455	0.469888	-1.259748	4.772883	0.424998	-1.242730	4.795628	0.454146	-1.200201
S	-2.993097	-2.919295	0.565035	-2.928709	-2.997237	0.200403	-2.927468	-2.989788	0.258804
2PTZBN		S₀			S₁			T₁	
C	1.563069	-2.173997	-0.104902	1.523186	-2.189344	-0.022480	-1.524724	-2.180283	0.004944
C	0.423996	-2.954195	0.118060	0.360047	-2.980872	0.061938	-0.365265	-2.976016	-0.111010
C	-0.840770	-2.382991	0.222536	-0.884413	-2.383859	0.103911	0.879931	-2.372867	-0.165794
C	-0.983245	-0.992206	0.106851	-0.993839	-0.970030	0.042849	0.993910	-0.966699	-0.073671
C	0.159580	-0.174181	-0.067076	0.153272	-0.157785	-0.044240	-0.150887	-0.144006	0.031029
C	1.433490	-0.779280	-0.163713	1.411019	-0.779688	-0.087789	-1.414041	-0.773922	0.076017
H	0.529222	-4.032170	0.202815	0.449321	-4.059322	0.145404	-0.457298	-4.052422	-0.208060
H	-1.701056	-3.017335	0.401910	-1.768698	-2.998342	0.225236	1.762912	-2.985510	-0.307933
B	0.024560	1.334902	-0.194579	0.025198	1.380451	-0.107771	-0.021803	1.375598	0.107389
N	-2.249898	-0.385659	0.188899	-2.246669	-0.358820	0.122658	2.253765	-0.356427	-0.131049
N	2.579523	0.022072	-0.315408	2.556118	0.031640	-0.215859	-2.559538	0.036388	0.210830
C	-2.372699	0.975957	0.547330	-2.376257	0.984884	0.604293	2.390485	0.990428	-0.589714
C	-3.572992	1.400164	1.155744	-3.564066	1.349174	1.244775	3.587859	1.365211	-1.212628
C	-1.316838	1.900570	0.328963	-1.312800	1.918891	0.415352	1.324866	1.920900	-0.404275
C	-3.747578	2.736594	1.509250	-3.773456	2.673527	1.663531	3.795152	2.691512	-1.619291
C	-1.520054	3.235216	0.742232	-1.561266	3.240857	0.866087	1.570810	3.243297	-0.846252
C	-2.713954	3.657368	1.310697	-2.760814	3.613652	1.462412	2.775818	3.625285	-1.427493
H	-4.680672	3.047689	1.970568	-4.710765	2.949256	2.136134	4.736994	2.975028	-2.078345
H	-0.705462	3.944473	0.633741	-0.771394	3.979359	0.766965	0.777009	3.978169	-0.752272
H	-2.846800	4.691627	1.616196	-2.911990	4.640561	1.787275	2.925822	4.654354	-1.745779
C	-3.391278	-1.029508	-0.381011	-3.380979	-0.978603	-0.461244	3.379295	-0.991722	0.452364
C	-3.288325	-1.791832	-1.554495	-3.274071	-1.695443	-1.666440	3.255710	-1.734136	1.640426
C	-4.659880	-0.842577	0.190951	-4.651606	-0.830841	0.127887	4.657251	-0.836425	-0.118554
C	-4.408864	-2.423609	-2.089192	-4.385915	-2.322740	-2.219671	4.359283	-2.375041	2.194060
H	-2.324320	-1.900070	-2.038797	-2.313021	-1.754773	-2.165761	2.288095	-1.802046	2.125387
C	-5.786992	-1.458288	-0.363339	-5.768794	-1.448436	-0.445573	5.765755	-1.470460	0.454198
C	-5.659952	-2.270964	-1.487788	-5.635306	-2.213000	-1.602380	5.616308	-2.257451	1.593551
H	-4.302205	-3.023797	-2.988600	-4.278627	-2.879572	-3.146391	4.239407	-2.950108	3.107969

H	-6.759709	-1.293190	0.090930	-6.741996	-1.320168	0.019437	6.744615	-1.336663	0.002847
H	-6.535893	-2.760493	-1.904067	-6.507238	-2.696033	-2.034478	6.481482	-2.752414	2.025654
C	2.476771	1.320932	-0.865059	2.444483	1.310966	-0.877257	-2.450245	1.316528	0.860000
C	3.600890	1.874926	-1.508527	3.507603	1.742079	-1.673208	-3.521700	1.758958	1.643367
C	1.249785	2.038929	-0.819429	1.250020	2.074518	-0.732123	-1.249594	2.073190	0.725711
C	3.522960	3.128921	-2.097764	3.468031	3.004534	-2.275051	-3.478343	3.017848	2.245815
C	1.214872	3.305141	-1.446660	1.258790	3.348320	-1.354752	-1.256436	3.346106	1.349138
C	2.324849	3.855613	-2.071275	2.342160	3.814228	-2.093951	-2.342895	3.818806	2.077776
H	4.395932	3.531639	-2.605568	4.305472	3.340256	-2.880205	-4.317943	3.359121	2.844766
H	0.276322	3.851462	-1.460605	0.369276	3.967069	-1.280736	-0.361852	3.958554	1.285582
H	2.263245	4.829502	-2.549480	2.301352	4.799446	-2.553313	-2.298565	4.802296	2.540501
C	3.763465	-0.379053	0.377110	3.763115	-0.350403	0.376633	-3.773142	-0.352525	-0.373334
C	4.525430	0.545688	1.107602	4.663015	0.608055	0.895556	-4.664786	0.603120	-0.907903
C	4.142422	-1.732406	0.405365	4.117446	-1.717837	0.512636	-4.128803	-1.718240	-0.487092
C	5.683192	0.146086	1.771672	5.864093	0.225032	1.469216	-5.871564	0.218496	-1.469921
C	5.290692	-2.132798	1.096290	5.341547	-2.093251	1.088196	-5.357148	-2.096149	-1.051203
C	6.078271	-1.192635	1.757653	6.221712	-1.129668	1.556678	-6.235227	-1.134919	-1.529811
H	6.266243	0.884948	2.314532	6.525298	0.988911	1.868636	-6.529737	0.978577	-1.881138
H	5.559384	-3.185128	1.112031	5.583615	-3.148691	1.175166	-5.604388	-3.151459	-1.122914
H	6.978640	-1.508784	2.276856	7.164592	-1.425672	2.006102	-7.181830	-1.434372	-1.969303
S	-4.805047	0.205137	1.610506	-4.811907	0.132793	1.598522	4.841203	0.156886	-1.566190
H	4.523401	1.307766	-1.568929	4.375412	1.105744	-1.815995	-4.393543	1.127183	1.780596
H	4.214474	1.583672	1.143092	4.395966	1.656336	0.848134	-4.388588	1.649876	-0.881792
S	3.134872	-2.927057	-0.432795	3.064753	-2.992658	-0.068840	-3.064888	-2.988687	0.089697
DPAPTZBN		S₀			S₁			T₁	
C	1.158204	-2.098211	0.554530	-1.130323	-2.133772	-0.464402	1.133432	-2.123463	0.476696
C	-0.038844	-2.819891	0.542635	0.078800	-2.836107	-0.611251	-0.070667	-2.832313	0.617936
C	-1.265559	-2.197614	0.345246	1.286100	-2.180129	-0.472623	-1.282666	-2.174299	0.461836
C	-1.318228	-0.804545	0.142402	1.321856	-0.785506	-0.183054	-1.322050	-0.785287	0.174634
C	-0.116679	-0.047524	0.150370	0.119005	-0.043773	-0.116074	-0.121442	-0.030800	0.109029
C	1.116247	-0.716065	0.334592	-1.096748	-0.732797	-0.251223	1.100646	-0.726732	0.247274
H	-0.011239	-3.893685	0.706149	0.063086	-3.906728	-0.790524	-0.053350	-3.901839	0.799427
H	-2.163781	-2.800616	0.346722	2.200611	-2.751335	-0.559471	-2.196219	-2.748366	0.541351
B	-0.147521	1.467999	0.043090	0.146141	1.487246	0.068158	-0.153016	1.483806	-0.061525
N	-2.537646	-0.151556	-0.062656	2.532311	-0.149665	0.038874	-2.537875	-0.149304	-0.041681
N	2.321735	0.009722	0.281326	-2.295408	0.005500	-0.173039	2.299423	0.012051	0.159929
C	-2.642959	1.206625	-0.404884	2.657445	1.214062	0.447178	-2.668199	1.215468	-0.429548
C	-3.907229	1.734593	-0.756882	3.924077	1.702830	0.795865	-3.939044	1.706035	-0.769416
C	-1.498484	2.059504	-0.403915	1.504330	2.060914	0.488883	-1.518591	2.065826	-0.466038
C	-4.033839	3.056783	-1.153915	4.087336	3.027227	1.219637	-4.105383	3.032157	-1.178385
C	-1.679828	3.390463	-0.846541	1.721632	3.384560	0.952740	-1.739130	3.390822	-0.915436
C	-2.914243	3.896209	-1.222495	2.976906	3.867272	1.309142	-2.996886	3.875043	-1.263723
H	-5.016831	3.431789	-1.429143	5.079317	3.383106	1.484953	-5.098692	3.389333	-1.437016
H	-0.808189	4.033607	-0.913488	0.862807	4.040612	1.054144	-0.882666	4.050416	-1.012999
H	-3.013764	4.923480	-1.562561	3.089276	4.891792	1.657327	-3.112235	4.902539	-1.601704
C	-3.744447	-0.933053	0.039639	3.738943	-0.927902	-0.082513	-3.740826	-0.935517	0.071105

C	-4.249605	-1.597440	-1.082720	4.232654	-1.638423	1.016622	-4.228836	-1.637457	-1.035749
C	-4.403512	-1.028034	1.268765	4.414123	-0.967891	-1.306095	-4.415767	-0.992039	1.293968
C	-5.416351	-2.355732	-0.972353	5.399859	-2.392812	0.886826	-5.392647	-2.398457	-0.914971
H	-3.727888	-1.516185	-2.031761	3.701802	-1.594832	1.963048	-3.696754	-1.581993	-1.980812
C	-5.570117	-1.787409	1.373210	5.581527	-1.723306	-1.429680	-5.579698	-1.754188	1.408264
C	-6.077706	-2.451609	0.254282	6.075501	-2.436477	-0.335038	-6.069289	-2.457972	0.305671
H	-5.807337	-2.871028	-1.845677	5.780887	-2.944967	1.741901	-5.770120	-2.943471	-1.776136
H	-6.080907	-1.859477	2.329736	6.103703	-1.753669	-2.382330	-6.102521	-1.797105	2.360043
H	-6.985982	-3.042521	0.337876	6.984559	-3.023923	-0.433479	-6.975679	-3.050623	0.397024
C	2.342237	1.388216	0.592020	-2.300149	1.378303	-0.618127	2.308180	1.383671	0.591227
C	3.540801	1.953364	1.070552	-3.426932	1.848024	-1.296007	3.448467	1.865228	1.244147
C	1.162109	2.173591	0.490252	-1.147906	2.187995	-0.395144	1.147095	2.186994	0.391941
C	3.583596	3.287224	1.450416	-3.500200	3.186832	-1.694171	3.517031	3.200193	1.645527
C	1.249569	3.518102	0.917883	-1.272320	3.538880	-0.816450	1.267132	3.534863	0.819581
C	2.431173	4.080337	1.381380	-2.416996	4.033397	-1.432907	2.419100	4.037423	1.414494
H	4.513000	3.701827	1.833298	-4.385724	3.552097	-2.206576	4.409162	3.571730	2.141736
H	0.351096	4.126584	0.909878	-0.424212	4.203379	-0.689258	0.410265	4.191885	0.714837
H	2.458203	5.117624	1.704717	-2.458351	5.077384	-1.736531	2.456137	5.079481	1.725025
C	3.431000	-0.603658	-0.375158	-3.443040	-0.556453	0.381284	3.450523	-0.559540	-0.387813
C	4.202487	0.102707	-1.310798	-4.378613	0.231807	1.092917	4.371298	0.216857	-1.127457
C	3.722736	-1.960533	-0.151116	-3.709582	-1.949477	0.274411	3.719297	-1.945118	-0.248166
C	5.288172	-0.503675	-1.939293	-5.525520	-0.327928	1.626397	5.519447	-0.348616	-1.655171
C	4.796340	-2.572463	-0.805984	-4.886570	-2.501463	0.808317	4.893936	-2.504115	-0.777993
C	5.597310	-1.840248	-1.680405	-5.798255	-1.699409	1.474754	5.798033	-1.713037	-1.469574
H	5.881938	0.070043	-2.645707	-6.212363	0.303964	2.182418	6.198821	0.272200	-2.232307
H	4.997761	-3.624316	-0.624299	-5.064156	-3.568346	0.705770	5.077314	-3.567548	-0.652958
H	6.441133	-2.317329	-2.171006	-6.700986	-2.133121	1.893768	6.699870	-2.153772	-1.883529
H	-4.789023	1.107234	-0.737265	4.796368	1.063825	0.744289	-4.809229	1.063839	-0.722923
H	-3.999819	-0.508054	2.132576	4.022271	-0.407583	-2.149854	-4.027025	-0.439312	2.144093
H	4.426393	1.335545	1.172588	-4.254608	1.177820	-1.506504	4.284630	1.201148	1.438804
H	3.956502	1.134979	-1.533677	-4.176059	1.287092	1.227216	4.158769	1.266687	-1.288239
S	2.697601	-2.879797	0.966539	-2.619932	-3.018407	-0.576450	2.628050	-3.000830	0.625177
CzPTZBN		S₀			S₁			T₁	
C	1.406186	-2.135916	-0.465243	1.367115	-2.168319	-0.388205	1.371099	-2.165107	-0.363374
C	0.303563	-2.980575	-0.353194	0.238207	-3.012120	-0.394673	0.245462	-3.014748	-0.354775
C	-0.985561	-2.478146	-0.191350	-1.025357	-2.476456	-0.275388	-1.020040	-2.474421	-0.227386
C	-1.191740	-1.093449	-0.158783	-1.204131	-1.069886	-0.191889	-1.205050	-1.074115	-0.163364
C	-0.076948	-0.203808	-0.188388	-0.084139	-0.199141	-0.157339	-0.087667	-0.190488	-0.135942
C	1.221587	-0.749616	-0.325925	1.199533	-0.773741	-0.260982	1.202087	-0.770845	-0.240150
H	0.450668	-4.055669	-0.401997	0.370818	-4.088571	-0.432385	0.379737	-4.090601	-0.383554
H	-1.796087	-3.176883	-0.051874	-1.862311	-3.150270	-0.176206	-1.855489	-3.149409	-0.118362
B	-0.231201	1.315947	-0.061520	-0.230022	1.332763	0.040230	-0.236110	1.326586	0.043580
N	-2.468329	-0.521951	-0.042568	-2.467566	-0.507084	-0.060154	-2.475315	-0.510106	-0.049593
N	2.353034	0.086255	-0.303123	2.327040	0.075798	-0.205727	2.328726	0.078813	-0.194791
C	-2.636562	0.809839	0.334404	-2.639651	0.821810	0.388104	-2.653356	0.821469	0.379172
C	-3.999068	1.061182	0.607550	-3.994976	1.051679	0.665488	-4.012697	1.054085	0.643056

C	-1.626915	1.786091	0.402095	-1.614419	1.787361	0.487693	-1.632495	1.789892	0.475902
C	-4.373540	2.331525	1.043934	-4.391196	2.317257	1.140866	-4.411149	2.323031	1.101719
C	-2.054325	3.051246	0.860716	-2.064085	3.048083	0.979478	-2.082879	3.049777	0.953453
C	-3.388071	3.316249	1.183687	-3.402841	3.293532	1.298588	-3.425933	3.299919	1.261034
H	-5.411261	2.556638	1.276193	-5.430602	2.530778	1.371905	-5.452834	2.539424	1.320538
H	-1.323254	3.845398	0.979683	-1.339792	3.844147	1.125346	-1.360579	3.847977	1.097332
H	-3.668471	4.305085	1.536933	-3.685311	4.276123	1.671351	-3.710823	4.285707	1.622822
C	-3.749816	-1.115020	-0.116219	-3.749802	-1.094618	-0.166736	-3.753542	-1.099282	-0.161417
C	-4.162399	-2.362772	-0.596453	-4.169837	-2.305182	-0.727507	-4.165648	-2.319877	-0.709332
C	-4.712058	-0.163286	0.317046	-4.705092	-0.155830	0.316168	-4.717446	-0.158648	0.301522
C	-5.524797	-2.666117	-0.570188	-5.533775	-2.607555	-0.719081	-5.527596	-2.625364	-0.708957
H	-3.472909	-3.076924	-1.024820	-3.487048	-2.991436	-1.210572	-3.475596	-3.010319	-1.175799
C	-6.070738	-0.490879	0.339824	-6.065824	-0.482537	0.317897	-6.076916	-0.489915	0.296382
C	-6.472868	-1.752129	-0.091692	-6.473972	-1.715781	-0.184654	-6.476462	-1.730469	-0.193482
H	-5.850645	-3.633414	-0.943305	-5.864767	-3.547338	-1.152684	-5.852296	-3.571289	-1.134035
H	-6.803573	0.237728	0.676116	-6.796997	0.229502	0.691295	-6.813471	0.223993	0.655504
H	-7.525571	-2.020666	-0.079935	-7.528977	-1.977028	-0.188830	-7.530260	-1.996101	-0.203116
C	2.243982	1.455971	-0.632397	2.212816	1.440689	-0.658826	2.213791	1.441663	-0.636960
C	3.376441	2.125715	-1.135569	3.288554	2.009606	-1.344588	3.296539	2.020047	-1.309581
C	1.003230	2.133450	-0.504460	1.003480	2.144755	-0.427145	0.996744	2.140034	-0.415133
C	3.291815	3.461563	-1.500987	3.232336	3.350130	-1.739644	3.237271	3.357181	-1.704397
C	0.961732	3.488955	-0.904071	0.992498	3.497298	-0.839707	0.987589	3.495179	-0.823427
C	2.079136	4.155141	-1.386236	2.083948	4.097043	-1.466251	2.080605	4.098546	-1.439114
H	4.170648	3.958970	-1.903893	4.076643	3.795091	-2.258797	4.081641	3.806410	-2.219436
H	0.013738	4.015643	-0.857987	0.087340	4.078091	-0.693259	0.079358	4.072954	-0.685490
H	2.012365	5.196342	-1.690279	2.030694	5.141642	-1.764513	2.024682	5.142638	-1.738829
C	3.521327	-0.393274	0.367939	3.519633	-0.361052	0.373094	3.533122	-0.361745	0.366283
C	4.219129	0.418066	1.275934	4.364004	0.531594	1.073410	4.372394	0.527820	1.074774
C	3.949806	-1.718940	0.186676	3.922603	-1.721127	0.302768	3.940030	-1.716001	0.271807
C	5.364614	-0.052424	1.914164	5.559167	0.101095	1.622946	5.578177	0.100817	1.603840
C	5.085620	-2.195442	0.849202	5.144077	-2.142433	0.853432	5.173035	-2.133670	0.799198
C	5.811057	-1.356521	1.692557	5.968240	-1.237405	1.502844	5.997178	-1.230687	1.451776
H	5.897765	0.601311	2.598932	6.176394	0.810889	2.166207	6.193852	0.805719	2.154894
H	5.392865	-3.226507	0.699775	5.425043	-3.188967	0.778948	5.462146	-3.176495	0.707034
H	6.702800	-1.727336	2.190060	6.907706	-1.568847	1.934153	6.945057	-1.561287	1.865236
H	4.310574	1.589330	-1.262256	4.173312	1.419707	-1.562550	4.183836	1.432992	-1.524102
H	3.868598	1.425310	1.470695	4.056572	1.563560	1.186104	4.053053	1.553402	1.210892
S	3.006995	-2.779018	-0.875753	2.935149	-2.914648	-0.506654	2.937323	-2.909629	-0.519845

DMACPTZBN

	S_0			S_1			T_1		
C	0.630255	-2.407885	0.006809	0.671518	-2.399084	0.110987	0.666281	-2.392645	0.054739
C	-0.645104	-2.961325	0.065111	-0.579910	-2.983156	0.116419	-0.587472	-2.981463	0.074587
C	-1.783482	-2.162890	0.213650	-1.736878	-2.178669	0.126317	-1.741028	-2.170335	0.111811
C	-1.638398	-0.768958	0.240451	-1.610960	-0.768415	0.151021	-1.615628	-0.763482	0.139253
C	-0.354391	-0.180878	0.189075	-0.346546	-0.159205	0.140912	-0.344848	-0.147277	0.126639
C	0.787309	-1.015011	0.095298	0.796871	-0.984010	0.136068	0.796208	-0.984585	0.105414
H	1.487475	-3.058842	-0.117763	1.551695	-3.027585	0.046017	1.545454	-3.021144	-0.028187

H	-0.759783	-4.039910	0.002256	-0.676687	-4.062750	0.060459	-0.687372	-4.059498	0.008410
B	-0.206300	1.330576	0.268964	-0.203352	1.377698	0.155216	-0.199735	1.371174	0.155106
N	-2.781218	0.049393	0.307770	-2.751384	0.058057	0.202337	-2.756128	0.063678	0.195340
N	2.056869	-0.418489	0.050515	2.053173	-0.384997	0.093715	2.058636	-0.386823	0.081789
C	-2.689702	1.364146	0.822269	-2.652506	1.356316	0.828415	-2.658397	1.362007	0.809469
C	-3.837041	1.947480	1.394472	-3.741382	1.820085	1.568586	-3.755302	1.837930	1.535584
C	-1.453644	2.066965	0.814029	-1.444559	2.103948	0.704815	-1.443675	2.101207	0.699862
C	-3.773843	3.217735	1.950095	-3.714802	3.101410	2.130709	-3.723088	3.114407	2.100839
C	-1.434490	3.349209	1.408025	-1.468476	3.399154	1.284276	-1.463227	3.393656	1.283587
C	-2.567054	3.929696	1.961775	-2.575300	3.896119	1.965509	-2.572556	3.898371	1.953385
H	-4.665704	3.644338	2.402629	-4.571696	3.463027	2.692099	-4.581960	3.482138	2.655133
H	-0.491327	3.885332	1.454585	-0.572128	4.009252	1.225588	-0.560773	3.995706	1.238527
H	-2.516290	4.916019	2.415305	-2.543526	4.895792	2.393602	-2.535715	4.895293	2.387371
C	-3.931262	-0.358039	-0.434915	-3.936662	-0.330559	-0.426196	-3.948595	-0.330956	-0.424467
C	-4.325867	-1.707455	-0.445203	-4.299984	-1.698675	-0.535420	-4.315075	-1.696472	-0.510629
C	-4.643042	0.553674	-1.229883	-4.805893	0.619932	-1.009527	-4.808335	0.616482	-1.023267
C	-5.440932	-2.114676	-1.184760	-5.503941	-2.079853	-1.148705	-5.524200	-2.079190	-1.112258
C	-5.769275	0.148092	-1.942816	-5.985967	0.230620	-1.620490	-5.994962	0.226496	-1.622457
C	-6.181032	-1.185358	-1.913013	-6.354080	-1.123183	-1.681934	-6.371096	-1.124909	-1.655952
H	-5.721676	-3.164005	-1.184777	-5.753601	-3.135185	-1.213095	-5.780555	-3.133687	-1.160685
H	-6.313937	0.877815	-2.535687	-6.622290	0.987997	-2.069685	-6.627351	0.979859	-2.083532
H	-7.056854	-1.506275	-2.469956	-7.280932	-1.424002	-2.160586	-7.302371	-1.428399	-2.124489
C	2.223191	0.924358	-0.346377	2.234828	0.941607	-0.415848	2.246215	0.943270	-0.404340
C	3.480639	1.289991	-0.884800	3.486771	1.246896	-0.971007	3.505124	1.256790	-0.945140
C	1.164881	1.861891	-0.202336	1.169249	1.883466	-0.311503	1.181534	1.884301	-0.297278
C	3.680152	2.629604	-1.215293	3.719202	2.573857	-1.372965	3.738969	2.586508	-1.328539
C	1.421815	3.192079	-0.595760	1.465675	3.197045	-0.752079	1.478695	3.199894	-0.722932
C	2.662819	3.581276	-1.074486	2.715579	3.538507	-1.252459	2.733030	3.548555	-1.208776
H	4.632441	2.947639	-1.624758	4.677105	2.859380	-1.790785	4.700342	2.878075	-1.734327
H	0.619820	3.921608	-0.537939	0.684175	3.950301	-0.716284	0.696461	3.952321	-0.686901
H	2.845575	4.612569	-1.365135	2.913819	4.559189	-1.573037	2.932718	4.572500	-1.517578
C	3.210364	-1.064183	0.583115	3.192565	-1.002504	0.662947	3.191521	-1.017379	0.650426
C	4.467324	-0.762679	0.025642	4.455868	-0.746639	0.090172	4.460473	-0.755947	0.093236
C	3.114256	-1.891723	1.711682	3.082751	-1.762163	1.840339	3.068475	-1.797611	1.812759
C	5.602073	-1.341889	0.606591	5.579287	-1.305493	0.710033	5.576668	-1.329792	0.712432
C	4.256522	-2.468640	2.258725	4.215097	-2.319934	2.424013	4.194116	-2.368199	2.396983
H	2.147637	-2.071267	2.168195	2.113559	-1.887335	2.310554	2.094163	-1.929797	2.269949
C	5.506600	-2.198937	1.702620	5.469357	-2.096072	1.854899	5.454061	-2.139172	1.842711
H	6.583735	-1.125533	0.200695	6.565531	-1.126919	0.297005	6.567003	-1.148069	0.310767
H	4.166168	-3.110147	3.131401	4.117227	-2.903241	3.335740	4.086316	-2.967054	3.297416
H	6.405306	-2.640634	2.124695	6.362377	-2.519272	2.307037	6.341620	-2.573525	2.294991
C	4.503179	0.183610	-1.175557	4.505286	0.115258	-1.171798	4.524022	0.127244	-1.153469
C	5.911486	0.738956	-1.439694	5.921064	0.641311	-1.457543	5.943088	0.656381	-1.416226
H	5.911495	1.392710	-2.315827	5.931263	1.237856	-2.373249	5.963544	1.268037	-2.321732
H	6.298578	1.304508	-0.586312	6.303639	1.259362	-0.639401	6.317985	1.260017	-0.583879
H	6.610309	-0.072074	-1.661393	6.616944	-0.186436	-1.620205	6.639608	-0.169373	-1.585719

C	4.052994	-0.590940	-2.448019	4.067154	-0.745357	-2.392453	4.096534	-0.712184	-2.392593
H	4.039169	0.081338	-3.312569	4.064584	-0.132639	-3.300127	4.104556	-0.084885	-3.290214
H	4.751434	-1.408759	-2.656411	4.762676	-1.579406	-2.539211	4.792153	-1.544969	-2.545404
H	3.053880	-1.017908	-2.335558	3.063633	-1.157119	-2.262113	3.091066	-1.124174	-2.279237
S	-3.380218	-2.887470	0.481444	-3.287216	-2.964790	0.129144	-3.292561	-2.958974	0.150737
H	-4.767569	1.391077	1.426526	-4.619129	1.194437	1.697840	-4.638133	1.218174	1.657006
H	-4.318262	1.586951	-1.277268	-4.530211	1.666666	-0.981981	-4.521852	1.660768	-1.017275
TMCzPTZBN		S₀			S₁			T₁	
C	-1.804739	-2.247901	0.373949	-1.766643	-2.276937	0.271749	-1.770211	-2.270820	0.254474
C	-0.701453	-3.088138	0.233937	-0.640312	-3.122862	0.239587	-0.646881	-3.121845	0.207614
C	0.590114	-2.580676	0.117811	0.626263	-2.584602	0.170867	0.621593	-2.578673	0.128378
C	0.798550	-1.195953	0.159841	0.809406	-1.176501	0.177866	0.810155	-1.177808	0.150037
C	-0.315451	-0.306129	0.223204	-0.308299	-0.300181	0.184814	-0.305273	-0.289438	0.163902
C	-1.616252	-0.856829	0.312912	-1.594061	-0.876330	0.235575	-1.596918	-0.871207	0.217729
H	-0.851029	-4.163990	0.223832	-0.776013	-4.199135	0.208641	-0.784239	-4.197051	0.170670
H	1.402290	-3.272477	-0.044966	1.463294	-3.253279	0.041937	1.457194	-3.248211	-0.009414
B	-0.157258	1.218724	0.187637	-0.156092	1.241316	0.095424	-0.151409	1.235823	0.087359
N	2.075461	-0.622223	0.090738	2.074709	-0.611356	0.099729	2.081691	-0.612430	0.085905
N	-2.746862	-0.018634	0.319086	-2.719584	-0.023205	0.225642	-2.721988	-0.018817	0.215960
C	2.248454	0.729890	-0.200274	2.255185	0.745371	-0.249918	2.267097	0.744259	-0.247559
C	3.613446	0.999970	-0.437251	3.612912	0.994857	-0.487799	3.627913	0.995027	-0.474456
C	1.246204	1.712263	-0.223897	1.238533	1.721311	-0.297690	1.253807	1.723062	-0.293174
C	3.992185	2.293383	-0.786225	4.016232	2.289855	-0.862178	4.032312	2.291727	-0.836843
C	1.685129	3.002269	-0.596043	1.700797	3.009807	-0.689216	1.715606	3.008625	-0.674223
C	3.021922	3.307886	-0.887210	3.045135	3.296567	-0.975989	3.064398	3.298557	-0.951828
H	5.036282	2.524285	-0.986300	5.062281	2.510950	-1.056561	5.079740	2.514327	-1.022378
H	0.951035	3.799286	-0.674456	0.975650	3.813457	-0.785451	0.992180	3.814089	-0.769015
C	3.357812	-1.217671	0.139785	3.355603	-1.205797	0.178836	3.359127	-1.208673	0.170117
C	3.775878	-2.490492	0.541501	3.777495	-2.452255	0.652410	3.773982	-2.462422	0.633676
C	4.324031	-0.241818	-0.216230	4.317926	-0.236863	-0.216346	4.328605	-0.240137	-0.209145
C	5.138885	-2.783125	0.512616	5.141041	-2.746773	0.640855	5.135604	-2.760392	0.629166
H	3.089289	-3.237429	0.915621	3.094954	-3.177934	1.074754	3.085030	-3.189810	1.042370
C	5.683671	-0.564432	-0.240683	5.678496	-0.561627	-0.220957	5.688086	-0.569601	-0.207961
C	6.110303	-1.847958	0.107957	6.107424	-1.826758	0.189321	6.109372	-1.839614	0.192971
H	5.458135	-3.773444	0.829179	5.462979	-3.717038	1.011558	5.452082	-3.734985	0.993324
H	6.412825	0.192987	-0.518020	6.408158	0.183186	-0.529294	6.422410	0.175270	-0.504980
C	-2.641979	1.329959	0.727643	-2.608225	1.308336	0.767342	-2.609926	1.312566	0.743465
C	-3.781888	1.971623	1.250129	-3.692947	1.835783	1.472206	-3.700983	1.852145	1.434961
C	-1.398653	2.011032	0.659100	-1.393240	2.022457	0.599575	-1.387676	2.019970	0.583544
C	-3.702055	3.283751	1.694287	-3.639942	3.147292	1.954704	-3.644021	3.161075	1.914945
C	-1.362304	3.340445	1.138534	-1.386386	3.346035	1.099880	-1.380983	3.346551	1.078657
C	-2.486725	3.979911	1.640626	-2.485306	3.906766	1.747842	-2.480832	3.913372	1.715551
H	-4.587067	3.758658	2.110651	-4.490893	3.560113	2.489364	-4.494922	3.579814	2.444799
H	-0.412975	3.866714	1.138599	-0.477776	3.932132	1.005418	-0.468940	3.928168	0.991532
H	-2.423519	5.001367	2.006311	-2.434100	4.929410	2.114859	-2.426302	4.935808	2.082785
C	-3.903913	-0.457372	-0.397019	-3.906787	-0.418716	-0.394841	-3.920673	-0.421058	-0.387496

C	-4.586121	0.404597	-1.269596	-4.738709	0.518477	-1.049825	-4.746935	0.511146	-1.054235
C	-4.336613	-1.790384	-0.297162	-4.314113	-1.778380	-0.414435	-4.331614	-1.776410	-0.379438
C	-5.721205	-0.027689	-1.952061	-5.927948	0.127383	-1.640877	-5.946289	0.120060	-1.625338
C	-5.461231	-2.227378	-1.004430	-5.528650	-2.160717	-1.006589	-5.556456	-2.159120	-0.949711
C	-6.171999	-1.341492	-1.811597	-6.342071	-1.214281	-1.609505	-6.369712	-1.216613	-1.559527
H	-6.242634	0.664389	-2.607610	-6.535844	0.871901	-2.147004	-6.552599	0.858675	-2.141640
H	-5.771515	-3.264728	-0.917929	-5.813244	-3.208961	-1.000841	-5.848624	-3.204901	-0.924039
H	-7.055459	-1.682564	-2.343956	-7.276652	-1.515360	-2.072623	-7.312061	-1.519707	-2.005538
H	-4.718578	1.430616	1.329947	-4.582213	1.235716	1.637907	-4.593196	1.256097	1.598244
H	-4.232102	1.420781	-1.401546	-4.427053	1.554427	-1.093671	-4.423920	1.542307	-1.123575
S	-3.413516	-2.908464	0.722291	-3.337988	-3.023009	0.331459	-3.340282	-3.017411	0.354774
C	3.429014	4.703007	-1.299443	3.444764	4.682520	-1.427704	3.462140	4.689984	-1.386787
H	3.799593	4.722680	-2.332096	3.401122	4.772766	-2.521613	3.244188	4.851281	-2.451109
H	2.588619	5.400355	-1.237311	2.780268	5.448131	-1.013958	2.915075	5.457743	-0.828536
H	4.233309	5.091366	-0.663280	4.468866	4.925241	-1.124760	4.532653	4.867184	-1.242799
C	7.569946	-2.229080	0.062890	7.568565	-2.202957	0.165833	7.569153	-2.221570	0.178087
H	7.784494	-2.883474	-0.792009	7.785761	-2.906302	-0.648894	7.785626	-2.937604	-0.625568
H	8.211954	-1.348057	-0.029386	8.206806	-1.326248	0.021169	8.210894	-1.349327	0.022528
H	7.871637	-2.772333	0.965526	7.873221	-2.691354	1.098647	7.869955	-2.697332	1.118762
PXZDPABN		S₀			S₁			T₁	
C	1.506847	2.299829	-0.479467	-1.475762	-2.256891	-0.633519	-1.469960	-2.249305	-0.624731
C	0.336746	3.025486	-0.677501	-0.314236	-2.975100	-0.891950	-0.303875	-2.970332	-0.895148
C	-0.926064	2.447864	-0.572349	0.942968	-2.381385	-0.734502	0.947086	-2.376558	-0.735725
C	-1.020528	1.082551	-0.271410	1.003179	-1.049963	-0.301536	1.007567	-1.045547	-0.295880
C	0.150904	0.291160	-0.112336	-0.148008	-0.258484	-0.123719	-0.144785	-0.248237	-0.114794
C	1.422763	0.925113	-0.188353	-1.404449	-0.892611	-0.247360	-1.402655	-0.892037	-0.237162
H	0.411861	4.080900	-0.928368	-0.384047	-4.009505	-1.215384	-0.375920	-4.000507	-1.230226
H	-1.811613	3.044314	-0.754057	1.842664	-2.941115	-0.962483	1.848009	-2.932127	-0.969850
B	0.055799	-1.215132	0.063078	-0.053848	1.261525	0.077637	-0.055203	1.264009	0.069329
N	-2.270565	0.453746	-0.153957	2.270345	-0.422853	-0.099467	2.275582	-0.418195	-0.097926
N	2.582886	0.167731	0.013469	-2.567242	-0.160379	-0.001458	-2.569945	-0.160283	0.001944
C	-2.412030	-0.926974	-0.386863	2.437360	0.958756	-0.380707	2.437968	0.961169	-0.368657
C	-3.687677	-1.388244	-0.764218	3.720488	1.400892	-0.716115	3.725384	1.409489	-0.694061
C	-1.325366	-1.827803	-0.295906	1.338302	1.857240	-0.301559	1.328224	1.859069	-0.295630
C	-3.904658	-2.721152	-1.072503	3.974843	2.733099	-1.059301	3.979073	2.742406	-1.031885
C	-1.572037	-3.174885	-0.650677	1.624903	3.187534	-0.662988	1.622238	3.194481	-0.648261
C	-2.830485	-3.618973	-1.030778	2.905095	3.619302	-1.040236	2.902596	3.624678	-1.013638
H	-4.899945	-3.033243	-1.374049	4.986320	3.037081	-1.306254	4.990332	3.051036	-1.272046
H	-0.744213	-3.875367	-0.659174	0.819343	3.913540	-0.660039	0.816867	3.920493	-0.654866
H	-2.989439	-4.658183	-1.305597	3.067481	4.661314	-1.303243	3.064808	4.667846	-1.273648
C	-3.440601	1.128492	0.287015	3.387645	-1.119368	0.339462	3.395566	-1.121307	0.332806
C	-3.433420	2.219416	1.165829	3.332166	-2.294540	1.121219	3.336957	-2.299996	1.107569
C	-4.682975	0.615335	-0.118089	4.670050	-0.610002	0.000850	4.674450	-0.610086	-0.002269
C	-4.628192	2.832138	1.546416	4.497651	-2.955505	1.480783	4.501117	-2.964525	1.462746
H	-2.490024	2.596607	1.542389	2.368854	-2.665324	1.448992	2.373045	-2.669063	1.435133
C	-5.877944	1.216892	0.264291	5.836296	-1.285899	0.353404	5.840771	-1.290981	0.341759

C	-5.851252	2.345174	1.084457	5.752128	-2.466561	1.085135	5.755330	-2.475641	1.065565
H	-4.595200	3.689247	2.213081	4.431750	-3.854040	2.087225	4.434979	-3.864965	2.066097
H	-6.811242	0.785812	-0.084650	6.790112	-0.863527	0.054365	6.794929	-0.867604	0.045411
H	-6.782095	2.824093	1.374365	6.659377	-2.992238	1.366915	6.662234	-3.004713	1.341973
C	2.576691	-1.176035	0.420815	-2.577008	1.195396	0.428846	-2.584885	1.197677	0.414605
C	3.797070	-1.802941	0.764803	-3.797343	1.783792	0.792996	-3.809343	1.787761	0.772276
C	1.359697	-1.915285	0.492254	-1.356216	1.952067	0.468877	-1.369925	1.957630	0.452756
C	3.812787	-3.112669	1.219859	-3.855456	3.120105	1.210206	-3.868902	3.121700	1.182156
C	1.429611	-3.236950	0.989661	-1.471582	3.296424	0.923102	-1.485963	3.298106	0.901752
C	2.623193	-3.839748	1.355459	-2.683346	3.875457	1.281535	-2.698375	3.879571	1.255930
H	4.764760	-3.565559	1.487015	-4.814671	3.551324	1.484496	-4.829455	3.553399	1.451587
H	0.504533	-3.791550	1.109557	-0.565153	3.885575	1.021063	-0.580278	3.888596	0.998047
H	2.637449	-4.856264	1.739383	-2.715254	4.908330	1.622266	-2.732103	4.913170	1.593412
C	3.853797	0.823454	-0.164930	-3.830540	-0.833760	-0.142921	-3.830192	-0.840569	-0.137246
C	4.481382	0.786857	-1.413553	-4.525080	-0.759813	-1.354752	-4.520863	-0.781680	-1.351996
C	4.454835	1.495660	0.904252	-4.363628	-1.563474	0.925282	-4.363279	-1.561812	0.936451
C	5.711482	1.422479	-1.590778	-5.747508	-1.418299	-1.497466	-5.741501	-1.444360	-1.490955
C	5.684787	2.129884	0.721491	-5.585987	-2.221379	0.777339	-5.583755	-2.223815	0.792283
C	6.314407	2.094241	-0.524925	-6.279508	-2.149968	-0.432952	-6.274488	-2.166180	-0.420424
H	6.197326	1.392287	-2.562443	-6.282929	-1.359877	-2.441555	-6.274822	-1.396532	-2.436807
H	6.150090	2.651148	1.553904	-5.996188	-2.787991	1.609298	-5.994772	-2.782758	1.628974
H	7.272130	2.588511	-0.665011	-7.231391	-2.662285	-0.546097	-7.225068	-2.681529	-0.530582
H	4.732051	-1.262351	0.693201	-4.716171	1.212467	0.754034	-4.726995	1.214354	0.735264
H	4.003507	0.262245	-2.235693	-4.102974	-0.187320	-2.175459	-4.098001	-0.216788	-2.177556
H	2.462196	2.801117	-0.557116	-2.433740	-2.747582	-0.749313	-2.427203	-2.740695	-0.744153
H	3.957186	1.516983	1.869315	-3.818437	-1.609579	1.863489	-3.819977	-1.597634	1.876188
O	-4.747147	-0.513452	-0.899979	4.799757	0.545425	-0.704840	4.803306	0.556339	-0.689784
PTZDPABN		S₀			S₁			T₁	
C	-1.648223	-2.268243	-0.591227	-1.620233	-2.199518	-0.789347	-1.607252	-2.199769	-0.757094
C	-0.478309	-2.991078	-0.803014	-0.457155	-2.906166	-1.084277	-0.437001	-2.911516	-1.043183
C	0.785080	-2.416452	-0.677926	0.801033	-2.326763	-0.888923	0.811483	-2.326594	-0.845336
C	0.876744	-1.060515	-0.344351	0.858492	-1.021055	-0.387036	0.867776	-1.008829	-0.359158
C	-0.290848	-0.278414	-0.150610	-0.288510	-0.243276	-0.158148	-0.284943	-0.226842	-0.144464
C	-1.563439	-0.904936	-0.249483	-1.547841	-0.864062	-0.321158	-1.541857	-0.862251	-0.304575
H	-0.554499	-4.039345	-1.081742	-0.530056	-3.921275	-1.463631	-0.507064	-3.927546	-1.419315
H	1.675918	-3.006834	-0.858693	1.704860	-2.877153	-1.126893	1.718869	-2.873457	-1.077950
B	-0.181339	1.211921	0.117524	-0.174505	1.254209	0.140051	-0.182561	1.265439	0.136734
N	2.140656	-0.448450	-0.215141	2.134967	-0.413600	-0.144022	2.138225	-0.400681	-0.131805
N	-2.718706	-0.151536	-0.010963	-2.704763	-0.138638	-0.025710	-2.706117	-0.141220	-0.027314
C	2.288849	0.941278	-0.417436	2.314676	0.971512	-0.424320	2.311546	0.984416	-0.391983
C	3.542330	1.422952	-0.849809	3.570291	1.441144	-0.830933	3.573187	1.458329	-0.791618
C	1.201581	1.833232	-0.228782	1.207656	1.859610	-0.246866	1.195835	1.871949	-0.223107
C	3.736087	2.785462	-1.066975	3.779774	2.805697	-1.115032	3.780757	2.822979	-1.060367
C	1.427524	3.196816	-0.517202	1.462378	3.211222	-0.550355	1.455727	3.229509	-0.515259
C	2.669217	3.675348	-0.914535	2.711238	3.680026	-0.974960	2.706278	3.696494	-0.921392
H	4.709770	3.141066	-1.392372	4.764396	3.155402	-1.408468	4.765073	3.177405	-1.348208

H	0.596295	3.890597	-0.452407	0.650222	3.924342	-0.459613	0.640764	3.940880	-0.439483
H	2.813567	4.732153	-1.122583	2.850667	4.737792	-1.183576	2.848357	4.755363	-1.124292
C	3.213206	-1.153147	0.407974	3.150937	-1.157702	0.440813	3.167793	-1.155767	0.435444
C	2.983479	-2.043999	1.468020	2.863212	-2.208633	1.346546	2.884623	-2.190228	1.357146
C	4.538497	-0.905638	0.014376	4.518086	-0.878225	0.156227	4.524807	-0.889795	0.119270
C	4.041597	-2.729571	2.060322	3.880349	-2.961747	1.905370	3.903826	-2.957946	1.895534
H	1.969874	-2.208905	1.815699	1.831349	-2.398796	1.615095	1.856628	-2.359993	1.653700
C	5.600835	-1.575849	0.629990	5.535285	-1.655358	0.728653	5.544571	-1.680043	0.667394
C	5.353499	-2.507559	1.635921	5.223893	-2.698003	1.590763	5.239836	-2.716790	1.540454
H	3.837327	-3.427586	2.867674	3.631533	-3.750747	2.609248	3.661618	-3.737509	2.611959
H	6.617991	-1.361225	0.314868	6.570841	-1.426143	0.495173	6.577465	-1.464756	0.409978
H	6.180922	-3.038291	2.098493	6.018906	-3.289794	2.034329	6.038404	-3.318531	1.964140
C	-2.701757	1.166700	0.472434	-2.699357	1.184274	0.495069	-2.714935	1.188110	0.470730
C	-3.919089	1.783874	0.844714	-3.914298	1.758477	0.902026	-3.939435	1.759845	0.858948
C	-1.478725	1.891257	0.595059	-1.473818	1.927531	0.586685	-1.496357	1.938105	0.566980
C	-3.926578	3.062758	1.379832	-3.958560	3.059787	1.414790	-3.994495	3.061498	1.360791
C	-1.540979	3.179640	1.174818	-1.574946	3.233255	1.137924	-1.608209	3.242924	1.108861
C	-2.731524	3.768759	1.570371	-2.780366	3.797632	1.540829	-2.820170	3.804781	1.496370
H	-4.876589	3.507270	1.667197	-4.913787	3.478876	1.720489	-4.954494	3.479400	1.652750
H	-0.611893	3.717363	1.334948	-0.662147	3.804844	1.275432	-0.700029	3.820255	1.251158
H	-2.739944	4.758968	2.017848	-2.802106	4.802728	1.956646	-2.850507	4.811883	1.906309
C	-3.993570	-0.788144	-0.227428	-3.972784	-0.792673	-0.207165	-3.968824	-0.808491	-0.207756
C	-4.611318	-0.689480	-1.477480	-4.666846	-0.640083	-1.411939	-4.652699	-0.682057	-1.420984
C	-4.606927	-1.504786	0.805303	-4.510517	-1.584149	0.813756	-4.508372	-1.584529	0.823515
C	-5.844450	-1.307357	-1.692631	-5.893916	-1.279971	-1.594280	-5.874450	-1.332783	-1.600827
C	-5.839887	-2.120798	0.584687	-5.737381	-2.223145	0.626376	-5.729959	-2.233963	0.638177
C	-6.459951	-2.023051	-0.663238	-6.430767	-2.072281	-0.576762	-6.414519	-2.109279	-0.573021
H	-6.322708	-1.228861	-2.665336	-6.429178	-1.159533	-2.532572	-6.402930	-1.232788	-2.545265
H	-6.314913	-2.676665	1.388730	-6.151307	-2.837317	1.421958	-6.146470	-2.835893	1.441618
H	-7.420009	-2.503340	-0.832754	-7.386232	-2.569991	-0.720705	-7.365871	-2.615204	-0.715184
S	4.834843	0.278856	-1.267408	4.952303	0.363213	-0.995533	4.942384	0.374623	-1.017887
H	-4.858390	1.257865	0.732687	-4.838914	1.200678	0.823086	-4.859877	1.195969	0.775448
H	-4.123727	-0.131070	-2.271166	-4.240881	-0.021096	-2.196100	-4.224140	-0.075131	-2.213065
H	-2.604377	-2.764720	-0.689539	-2.578588	-2.681503	-0.936349	-2.563589	-2.684520	-0.907323
H	-4.116758	-1.574181	1.771908	-3.965357	-1.692249	1.746885	-3.969701	-1.672478	1.762455
2DPABN		S₀		S₁			T₁		
C	1.219238	-2.334665	0.017327	-1.206083	2.332529	0.024915	-1.206217	2.324817	0.012945
C	-0.000032	-3.003315	0.000003	-0.000004	3.021409	0.000003	-0.000001	3.021946	0.000000
C	-1.219311	-2.334647	-0.017297	1.206076	2.332531	-0.024911	1.206215	2.324817	-0.012945
C	-1.226109	-0.928716	0.000675	1.207014	0.901654	-0.010251	1.208431	0.906366	-0.003159
C	-0.000021	-0.204028	-0.000009	-0.000001	0.177222	0.000000	0.000000	0.168234	-0.000002
C	1.226040	-0.928713	-0.000660	-1.207017	0.901652	0.010253	-1.208431	0.906365	0.003156
H	2.138859	-2.903811	0.027463	-2.134283	2.886860	0.047729	-2.135497	2.878861	0.026650
H	-0.000050	-4.090946	0.000027	-0.000005	4.107015	0.000004	-0.000001	4.106952	0.000001
H	-2.138896	-2.903842	-0.027518	2.134275	2.886865	-0.047724	2.135495	2.878862	-0.026649
B	-0.000004	1.312943	0.000011	0.000000	-1.366010	0.000001	0.000000	-1.354943	-0.000003

N	-2.439602	-0.228874	0.009178	2.419954	0.228283	-0.002077	2.429035	0.223569	0.002154
N	2.439564	-0.228940	-0.009205	-2.419956	0.228280	0.002077	-2.429035	0.223569	-0.002156
C	-2.539864	1.156382	0.211526	2.551756	-1.182304	0.158062	2.555865	-1.178421	0.161324
C	-3.818647	1.740872	0.369176	3.840306	-1.725631	0.268794	3.845296	-1.728652	0.276804
C	-1.373673	1.974208	0.273063	1.380473	-2.010982	0.211091	1.382359	-2.007075	0.211298
C	-3.947288	3.090748	0.657823	4.021111	-3.099342	0.485777	4.021064	-3.098313	0.497293
C	-1.562480	3.333269	0.615182	1.624319	-3.384584	0.486234	1.622450	-3.377101	0.489632
C	-2.813897	3.897870	0.811730	2.903347	-3.922282	0.616322	2.899730	-3.917838	0.626682
H	-4.942467	3.510701	0.784808	5.027244	-3.501512	0.565182	5.025344	-3.503977	0.581712
H	-0.686925	3.957441	0.754556	0.775144	-4.042644	0.626051	0.772512	-4.034935	0.625020
H	-2.913181	4.946813	1.078178	3.025160	-4.984681	0.817692	3.018003	-4.979905	0.831360
C	-3.654248	-0.990704	-0.130933	3.631497	1.004664	-0.104061	3.638537	1.002586	-0.104583
C	-4.301802	-1.501038	0.999158	4.259386	1.481488	1.050986	4.269043	1.483037	1.047456
C	-4.181839	-1.220762	-1.404868	4.171685	1.274630	-1.364587	4.172957	1.273384	-1.367258
C	-5.477126	-2.239361	0.851738	5.425386	2.240846	0.939995	5.435479	2.240517	0.931619
H	-3.882056	-1.316495	1.983628	3.831730	1.257574	2.023685	3.844270	1.261219	2.021884
C	-5.357656	-1.959728	-1.547062	5.338585	2.034456	-1.468152	5.340223	2.031301	-1.475659
C	-6.006544	-2.469667	-0.420319	5.965865	2.518255	-0.318050	5.972355	2.515574	-0.328367
H	-5.978304	-2.634143	1.731652	5.909795	2.615534	1.837750	5.923637	2.615090	1.827382
H	-5.765493	-2.136089	-2.538919	5.755210	2.247648	-2.448934	5.753983	2.242329	-2.458109
H	-6.921931	-3.044705	-0.532857	6.873648	3.109878	-0.401458	6.880938	3.105378	-0.415542
C	2.539859	1.156318	-0.211608	-2.551757	-1.182308	-0.158065	-2.555866	-1.178422	-0.161325
C	3.818639	1.740750	-0.369424	-3.840306	-1.725637	-0.268802	-3.845297	-1.728653	-0.276801
C	1.373700	1.974175	-0.273076	-1.380472	-2.010984	-0.211089	-1.382360	-2.007075	-0.211302
C	3.947312	3.090628	-0.658044	-4.021107	-3.099349	-0.485784	-4.021065	-3.098315	-0.497289
C	1.562513	3.333240	-0.615197	-1.624315	-3.384588	-0.486230	-1.622451	-3.377102	-0.489634
C	2.813932	3.897802	-0.811833	-2.903342	-3.922288	-0.616322	-2.899730	-3.917839	-0.626681
H	4.942490	3.510536	-0.785171	-5.027239	-3.501520	-0.565193	-5.025344	-3.503979	-0.581704
H	0.686940	3.957394	-0.754514	-0.775139	-4.042647	-0.626042	-0.772513	-4.034936	-0.625024
H	2.913259	4.946747	-1.078255	-3.025152	-4.984687	-0.817691	-3.018004	-4.979906	-0.831357
C	3.654212	-0.990760	0.131079	-3.631499	1.004662	0.104061	-3.638537	1.002586	0.104582
C	4.182065	-1.220410	1.404984	-4.171691	1.274619	1.364587	-4.172956	1.273383	1.367258
C	4.301509	-1.501495	-0.998980	-4.259380	1.481498	-1.050985	-4.269043	1.483039	-1.047456
C	5.357966	-1.959235	1.547116	-5.338590	2.034447	1.468152	-5.340221	2.031301	1.475660
C	5.476916	-2.239711	-0.851608	-5.425379	2.240858	-0.939993	-5.435478	2.240520	-0.931618
H	3.881375	-1.317458	-1.983381	-3.831719	1.257592	-2.023683	-3.844270	1.261222	-2.021884
C	6.006664	-2.469496	0.420398	-5.965864	2.518257	0.318052	-5.972354	2.515576	0.328370
H	5.766065	-2.135287	2.538924	-5.755219	2.247633	2.448934	-5.753980	2.242328	2.458111
H	5.977887	-2.634751	-1.731525	-5.909783	2.615555	-1.837747	-5.923636	2.615095	-1.827380
H	6.922106	-3.044429	0.532992	-6.873646	3.109882	0.401460	-6.880936	3.105381	0.415545
H	4.712573	1.136265	-0.286432	-4.714862	-1.092644	-0.196614	-4.720996	-1.096993	-0.206359
H	3.669409	-0.819324	2.274383	-3.676268	0.891317	2.251644	-3.673842	0.890205	2.252276
H	-4.712558	1.136389	0.286010	4.714861	-1.092636	0.196601	4.720995	-1.096990	0.206365
H	-3.669003	-0.819898	-2.274267	3.676257	0.891336	-2.251645	3.673843	0.890207	-2.252277
CzDPABN		S₀		S₁			T₁		
C	0.950671	-2.579674	0.236436	0.950643	-2.565083	0.323432	0.944080	-2.556054	0.363844

C	-0.331349	-3.125325	0.296367	-0.312813	-3.126897	0.392827	-0.319512	-3.122102	0.438333
C	-1.472282	-2.345719	0.184792	-1.449948	-2.330100	0.256685	-1.456132	-2.322602	0.284425
C	-1.344611	-0.948063	0.046209	-1.320537	-0.923821	0.092870	-1.322699	-0.924168	0.105617
C	-0.054279	-0.346588	0.008762	-0.045079	-0.313215	0.040597	-0.044646	-0.306534	0.054530
C	1.090773	-1.200895	0.056980	1.084130	-1.164433	0.089725	1.083470	-1.168440	0.109522
H	1.805073	-3.222156	0.386732	1.819652	-3.177302	0.514825	1.812734	-3.169957	0.556107
H	-0.439128	-4.197604	0.440347	-0.423335	-4.190874	0.577543	-0.430292	-4.183231	0.636476
H	-2.443955	-2.818800	0.223119	-2.425592	-2.792987	0.314627	-2.433198	-2.782785	0.341757
B	0.067980	1.178385	0.019477	0.085525	1.226075	0.023578	0.082074	1.219064	0.032561
N	-2.491827	-0.149947	-0.030203	-2.472976	-0.144634	0.000854	-2.475964	-0.140998	-0.000190
N	2.354470	-0.592470	-0.029881	2.339961	-0.584863	-0.007460	2.347164	-0.586228	-0.001096
C	-2.468875	1.236679	-0.240426	-2.475954	1.257536	-0.199357	-2.477105	1.256796	-0.195970
C	-3.685578	1.928370	-0.447553	-3.706787	1.913677	-0.394396	-3.708865	1.913772	-0.396217
C	-1.237550	1.952832	-0.247069	-1.245445	1.985835	-0.206066	-1.241799	1.984311	-0.191550
C	-3.686289	3.291240	-0.699895	-3.747664	3.290080	-0.621860	-3.750473	3.289001	-0.613949
C	-1.294554	3.335775	-0.538636	-1.343002	3.368225	-0.468501	-1.343128	3.370504	-0.443561
C	-2.484678	4.008594	-0.765068	-2.560590	4.020319	-0.670434	-2.559469	4.018919	-0.647906
H	-4.635419	3.796177	-0.863779	-4.707725	3.777552	-0.768115	-4.708504	3.778479	-0.764591
H	-0.363143	3.885982	-0.612721	-0.428712	3.946161	-0.536470	-0.431384	3.952743	-0.503801
H	-2.487233	5.071504	-0.991142	-2.580342	5.090039	-0.864439	-2.579235	5.089962	-0.835446
C	-3.774187	-0.798782	0.086127	-3.750842	-0.813668	0.067288	-3.754906	-0.811954	0.056089
C	-4.409254	-1.307928	-1.051030	-4.331173	-1.328777	-1.095747	-4.321826	-1.329463	-1.111830
C	-4.379550	-0.915241	1.340809	-4.400246	-0.938412	1.298750	-4.414338	-0.935161	1.281842
C	-5.651108	-1.933792	-0.929904	-5.565545	-1.976147	-1.021607	-5.556646	-1.976989	-1.048386
H	-3.928637	-1.210701	-2.020069	-3.816471	-1.219482	-2.045686	-3.797437	-1.222077	-2.056577
C	-5.621626	-1.541615	1.456142	-5.634451	-1.586971	1.364523	-5.648737	-1.584256	1.336448
C	-6.258581	-2.051450	0.322404	-6.218010	-2.106176	0.206542	-6.220794	-2.105329	0.173632
H	-6.143012	-2.328313	-1.815063	-6.015977	-2.377657	-1.925315	-5.998065	-2.380061	-1.955759
H	-6.090268	-1.630819	2.432615	-6.137954	-1.686184	2.322326	-6.161401	-1.682120	2.289453
H	-7.225593	-2.538859	0.414393	-7.178923	-2.610640	0.260988	-7.181972	-2.610064	0.219586
C	2.523841	0.769458	0.207669	2.531905	0.798315	0.197023	2.538484	0.792444	0.197410
C	3.900339	1.067641	0.316126	3.908332	1.066320	0.286623	3.916294	1.066812	0.272398
C	1.494718	1.720957	0.306517	1.497312	1.756730	0.268386	1.503874	1.753189	0.268726
C	4.282742	2.374321	0.618553	4.328943	2.389580	0.533496	4.333495	2.389805	0.510835
C	1.934046	3.021128	0.638581	1.977510	3.078511	0.547180	1.981621	3.071234	0.543391
C	3.286695	3.339852	0.798613	3.337498	3.368569	0.674346	3.342087	3.367126	0.660554
H	5.331943	2.638731	0.722996	5.381906	2.641608	0.614287	5.386509	2.645995	0.579697
H	1.202336	3.807237	0.793201	1.265494	3.884022	0.688735	1.269500	3.876559	0.684514
H	3.569431	4.357243	1.056452	3.637525	4.393759	0.883634	3.640850	4.393443	0.864786
C	3.634484	-1.166956	-0.188006	3.609675	-1.183496	-0.173621	3.610723	-1.181319	-0.176160
C	4.611888	-0.163566	0.053110	4.595942	-0.178308	0.048649	4.602763	-0.177423	0.031573
C	4.025660	-2.444923	-0.603153	3.974029	-2.464190	-0.596524	3.972993	-2.469305	-0.588378
C	5.973420	-0.465174	-0.046102	5.952156	-0.508651	-0.058349	5.958104	-0.509651	-0.083271
C	5.390282	-2.721290	-0.702225	5.334896	-2.769127	-0.701702	5.329666	-2.772919	-0.702647
H	3.309979	-3.204277	-0.887361	3.243259	-3.207765	-0.888518	3.238739	-3.215819	-0.863534
C	6.359896	-1.752297	-0.410526	6.314542	-1.806428	-0.417791	6.315664	-1.808970	-0.433853

H	6.719003	0.302511	0.143578	6.714171	0.245566	0.118682	6.721882	0.245476	0.082490
H	5.699986	-3.711711	-1.025411	5.628498	-3.763027	-1.027275	5.621128	-3.768998	-1.024046
H	7.414595	-2.000422	-0.492273	7.366135	-2.067022	-0.506357	7.365703	-2.073203	-0.528485
H	-4.629553	1.399532	-0.425895	-4.636937	1.361243	-0.375238	-4.637381	1.358445	-0.388366
H	-3.875431	-0.515668	2.215860	-3.937743	-0.529691	2.192189	-3.960401	-0.525175	2.178991
DMACDPABN		S₀			S₁			T₁	
C	-0.564448	-2.467723	0.462832	-0.580636	-2.415670	0.588412	-0.578957	-2.403877	0.614657
C	0.701460	-3.027008	0.622280	0.672654	-2.989016	0.795300	0.669406	-2.979826	0.824240
C	1.867954	-2.282264	0.477613	1.831265	-2.237216	0.618502	1.832614	-2.225466	0.626284
C	1.774322	-0.910932	0.173385	1.747922	-0.864571	0.247803	1.749999	-0.863225	0.246823
C	0.497620	-0.299671	0.041782	0.490132	-0.250945	0.076455	0.489941	-0.238380	0.077138
C	-0.666503	-1.102957	0.162023	-0.652932	-1.056605	0.196983	-0.655638	-1.052376	0.206649
H	-1.450223	-3.078259	0.592909	-1.483483	-2.991130	0.757847	-1.482766	-2.978243	0.786172
H	0.782424	-4.081846	0.874024	0.749156	-4.027765	1.101995	0.747270	-4.014079	1.143728
B	0.374356	1.197859	-0.177540	0.362456	1.259541	-0.181965	0.368138	1.256793	-0.173972
N	2.926894	-0.133294	0.007818	2.905112	-0.117894	0.047801	2.910528	-0.116329	0.042836
N	-1.926777	-0.497905	0.006666	-1.912694	-0.466378	-0.011761	-1.918370	-0.463549	-0.011005
C	2.909266	1.198843	-0.437318	2.911595	1.231725	-0.408894	2.919154	1.232006	-0.401288
C	4.130935	1.841965	-0.745314	4.142394	1.833681	-0.713273	4.152574	1.834471	-0.705782
C	1.681127	1.909355	-0.585704	1.680503	1.957845	-0.545771	1.688485	1.961113	-0.531588
C	4.141057	3.135203	-1.245367	4.198951	3.152400	-1.181500	4.210366	3.151770	-1.166245
C	1.747730	3.212713	-1.129743	1.796233	3.278551	-1.053937	1.806530	3.281995	-1.033113
C	2.944013	3.828847	-1.463658	3.017607	3.871462	-1.363476	3.027709	3.873365	-1.342334
H	5.094957	3.599936	-1.483888	5.164364	3.596844	-1.408363	5.175164	3.596747	-1.394068
H	0.818265	3.741695	-1.313687	0.886606	3.841830	-1.233159	0.898748	3.849338	-1.208039
H	2.954297	4.830442	-1.885180	3.047216	4.888881	-1.747714	3.058305	4.892147	-1.722696
C	4.201191	-0.757429	0.258192	4.174081	-0.770954	0.242939	4.178454	-0.775235	0.234018
C	4.867255	-1.435930	-0.767772	4.768431	-1.480932	-0.805635	4.766996	-1.483524	-0.818353
C	4.767021	-0.685157	1.534477	4.807226	-0.693888	1.487271	4.812915	-0.704513	1.477674
C	6.099917	-2.039861	-0.514247	5.993767	-2.118459	-0.604365	5.991689	-2.123666	-0.622259
C	6.000116	-1.290549	1.782669	6.032917	-1.332842	1.682249	6.037840	-1.346475	1.667133
C	6.667810	-1.968062	0.759961	6.627394	-2.045576	0.638344	6.628449	-2.056271	0.619175
H	6.615604	-2.565873	-1.313359	6.452593	-2.671000	-1.420080	6.447473	-2.673970	-1.441097
H	6.437693	-1.232248	2.775780	6.521620	-1.273473	2.651152	6.529019	-1.291351	2.634976
H	7.627815	-2.438698	0.955124	7.581612	-2.542369	0.792619	7.582214	-2.555137	0.769241
C	-2.114817	0.876900	0.250068	-2.136543	0.921406	0.256598	-2.138663	0.918661	0.244247
C	-3.414271	1.297696	0.622863	-3.440689	1.303874	0.603658	-3.448094	1.308607	0.582569
C	-1.029858	1.784775	0.128724	-1.044975	1.832043	0.110212	-1.043919	1.830174	0.105810
C	-3.623089	2.661783	0.821904	-3.692478	2.676329	0.790684	-3.696337	2.677437	0.761829
C	-1.300931	3.142408	0.399081	-1.367354	3.191675	0.339394	-1.365655	3.189221	0.333144
C	-2.576200	3.584091	0.717847	-2.658396	3.603266	0.656974	-2.657023	3.603438	0.637068
H	-4.606319	3.022906	1.102434	-4.686423	3.024097	1.043754	-4.690307	3.029487	1.008993
H	-0.486143	3.858275	0.377060	-0.580943	3.936033	0.283648	-0.577220	3.932072	0.287575
H	-2.763565	4.637137	0.912150	-2.866062	4.660270	0.810788	-2.864101	4.660632	0.790135
C	-3.023988	-1.193603	-0.573516	-2.962382	-1.192717	-0.586207	-2.970546	-1.198261	-0.581570
C	-4.329965	-0.829439	-0.193440	-4.293448	-0.846013	-0.246368	-4.300104	-0.852096	-0.244963

C	-2.819640	-2.141738	-1.587679	-2.702069	-2.193191	-1.547433	-2.707420	-2.202052	-1.535162
C	-5.403884	-1.459593	-0.834158	-5.324845	-1.545345	-0.876626	-5.331614	-1.557114	-0.870314
C	-3.904503	-2.767109	-2.194529	-3.751805	-2.877269	-2.144906	-3.756208	-2.891006	-2.130505
H	-1.811344	-2.378263	-1.907608	-1.679735	-2.390992	-1.848514	-1.683984	-2.403940	-1.829495
C	-5.203785	-2.429410	-1.816142	-5.068787	-2.555599	-1.808608	-5.073873	-2.571641	-1.796139
H	-6.420348	-1.195641	-0.564874	-6.356486	-1.310875	-0.641180	-6.363515	-1.321874	-0.636535
H	-3.729786	-3.501156	-2.976947	-3.542143	-3.637256	-2.892493	-3.544102	-3.655608	-2.872750
H	-6.058184	-2.907716	-2.287599	-5.898193	-3.076777	-2.278765	-5.902013	-3.098455	-2.262257
C	-4.481003	0.229928	0.899299	-4.503361	0.220852	0.827035	-4.511581	0.227881	0.815434
C	-5.900557	0.816410	0.951402	-5.933345	0.786341	0.803756	-5.940856	0.794288	0.783733
H	-5.987194	1.549836	1.757308	-6.066382	1.526965	1.595831	-6.075841	1.542904	1.567994
H	-6.180563	1.301725	0.011127	-6.172260	1.258292	-0.154213	-6.177629	1.256274	-0.179627
H	-6.633474	0.034399	1.167498	-6.666160	-0.002303	0.994546	-6.674220	0.007785	0.980750
C	-4.186606	-0.422065	2.281435	-4.273418	-0.425869	2.226339	-4.282573	-0.401327	2.222365
H	-4.257976	0.329568	3.074989	-4.391387	0.330565	3.008990	-4.402285	0.363543	2.996589
H	-4.915851	-1.213407	2.487169	-5.002583	-1.224736	2.401653	-5.011646	-1.198474	2.405147
H	-3.187448	-0.861801	2.320962	-3.271003	-0.851016	2.318297	-3.280346	-0.825397	2.320704
H	5.072636	1.325268	-0.611784	5.068410	1.286589	-0.591612	5.076998	1.283328	-0.590509
H	4.239186	-0.156295	2.322660	4.336731	-0.135699	2.291280	4.345258	-0.148619	2.284853
H	2.827000	-2.767818	0.599572	2.792841	-2.707388	0.778776	2.794564	-2.695554	0.785233
H	4.417469	-1.485555	-1.755046	4.269238	-1.528019	-1.768972	4.264802	-1.526952	-1.780229
TMCzDPABN		S₀			S₁			T₁	
C	0.541340	-2.669320	0.328114	0.541419	-2.648348	0.420936	0.536333	-2.639515	0.450165
C	-0.741164	-3.209197	0.412374	-0.724440	-3.205282	0.510803	-0.729789	-3.200282	0.543657
C	-1.881012	-2.432268	0.269949	-1.858813	-2.413208	0.339609	-1.864069	-2.406671	0.357764
C	-1.750806	-1.042380	0.071284	-1.727971	-1.014458	0.117889	-1.730549	-1.015637	0.125047
C	-0.459643	-0.444659	0.006084	-0.451861	-0.408447	0.044549	-0.451676	-0.402939	0.053581
C	0.684136	-1.298817	0.091507	0.675960	-1.260864	0.132025	0.675554	-1.264334	0.146994
H	1.395120	-3.306305	0.503380	1.409205	-3.254394	0.636564	1.403671	-3.247868	0.664678
H	-0.851172	-4.274327	0.601155	-0.837090	-4.261086	0.736829	-0.842329	-4.253609	0.779459
H	-2.853517	-2.901374	0.329683	-2.835406	-2.872118	0.412682	-2.841694	-2.863828	0.429703
B	-0.334862	1.079455	-0.058190	-0.319888	1.128700	-0.039741	-0.323648	1.121224	-0.030782
N	-2.897416	-0.246439	-0.038638	-2.879312	-0.238716	-0.010303	-2.882672	-0.236555	-0.013692
N	1.947133	-0.697741	-0.021010	1.933630	-0.686648	0.012432	1.941021	-0.686567	0.019042
C	-2.873346	1.128606	-0.314419	-2.878874	1.153710	-0.271585	-2.880259	1.152163	-0.269505
C	-4.089839	1.811565	-0.549977	-4.107257	1.803482	-0.497670	-4.109056	1.803483	-0.500782
C	-1.640997	1.841452	-0.360017	-1.646435	1.878974	-0.305270	-1.644120	1.877208	-0.292027
C	-4.089647	3.160418	-0.869280	-4.145201	3.169428	-0.782487	-4.146520	3.168256	-0.776552
C	-1.697251	3.208155	-0.719697	-1.741708	3.251400	-0.625466	-1.741449	3.253232	-0.603343
C	-2.887221	3.871300	-0.974763	-2.956505	3.895707	-0.857803	-2.954101	3.894952	-0.838501
H	-5.038747	3.658299	-1.053810	-5.104144	3.651715	-0.952115	-5.103346	3.652617	-0.950753
H	-0.765215	3.752253	-0.824174	-0.826114	3.824269	-0.715360	-0.827487	3.829444	-0.685517
H	-2.888833	4.921721	-1.253307	-2.974321	4.956429	-1.096834	-2.971618	4.957030	-1.071936
C	-4.180137	-0.887541	0.109780	-4.157934	-0.901550	0.083533	-4.162234	-0.901016	0.073176
C	-4.819600	-1.445121	-1.002014	-4.739813	-1.463840	-1.056816	-4.734585	-1.465311	-1.070426
C	-4.781711	-0.948513	1.370200	-4.808510	-0.974047	1.318678	-4.819731	-0.972294	1.304287

C	-6.061767	-2.063465	-0.849832	-5.975404	-2.105371	-0.956298	-5.970850	-2.106577	-0.977428
H	-4.341839	-1.390919	-1.975807	-4.224790	-1.395096	-2.010403	-4.212517	-1.398365	-2.020217
C	-6.024135	-1.567712	1.516717	-6.044006	-1.616885	1.411369	-6.055724	-1.615143	1.389136
C	-6.665358	-2.125639	0.408356	-6.628470	-2.182878	0.275969	-6.632301	-2.182476	0.250435
H	-6.557033	-2.495648	-1.715330	-6.426442	-2.543429	-1.842622	-6.415694	-2.545755	-1.866259
H	-6.489707	-1.613727	2.497651	-6.547965	-1.675095	2.372348	-6.566255	-1.672056	2.346665
H	-7.632627	-2.607353	0.524574	-7.590413	-2.682789	0.351124	-7.594731	-2.682260	0.319614
C	2.116045	0.674304	0.145932	2.125299	0.703942	0.154301	2.130657	0.697883	0.158684
C	3.491093	0.980993	0.237878	3.499763	0.979412	0.228696	3.506674	0.979733	0.223494
C	1.093487	1.632884	0.196819	1.096426	1.667715	0.181459	1.099900	1.662908	0.186232
C	3.871794	2.300354	0.468723	3.918878	2.310546	0.411276	3.920649	2.309674	0.404663
C	1.538097	2.948083	0.457732	1.580092	2.996972	0.397185	1.579658	2.989918	0.405280
C	2.889322	3.296989	0.603322	2.940404	3.316196	0.515461	2.937854	3.314492	0.515977
H	4.924099	2.562440	0.555730	4.974475	2.559733	0.475227	4.975518	2.563904	0.462608
H	0.801697	3.737598	0.569702	0.863258	3.804897	0.497928	0.861261	3.795677	0.509375
C	3.229658	-1.276884	-0.144516	3.202161	-1.288822	-0.126025	3.205185	-1.285605	-0.126019
C	4.204657	-0.262794	0.041170	4.188478	-0.275973	0.045797	4.195477	-0.274022	0.037854
C	3.633537	-2.570752	-0.490589	3.577420	-2.585119	-0.489843	3.579770	-2.586765	-0.482116
C	5.566930	-0.564632	-0.043267	5.543675	-0.607590	-0.049168	5.551072	-0.607056	-0.060926
C	4.998692	-2.841664	-0.574113	4.937153	-2.885673	-0.583052	4.936176	-2.885594	-0.580822
H	2.926766	-3.351506	-0.737352	2.853115	-3.347414	-0.748082	2.853257	-3.350888	-0.728226
C	5.984616	-1.864965	-0.336136	5.935415	-1.918227	-0.347175	5.939142	-1.917069	-0.353491
H	6.303701	0.221472	0.104015	6.298680	0.161907	0.091485	6.306927	0.162718	0.073990
H	5.307299	-3.848393	-0.846744	5.228408	-3.893835	-0.866618	5.226929	-3.894765	-0.861923
H	-5.034570	1.286132	-0.498292	-5.038541	1.253888	-0.458489	-5.039216	1.251417	-0.472370
H	-4.274277	-0.511858	2.225384	-4.345357	-0.529342	2.194449	-4.362424	-0.526708	2.182602
C	3.294542	4.721841	0.901177	3.364503	4.742937	0.774802	3.364545	4.744174	0.748927
H	4.056993	5.078310	0.198395	4.254238	5.009007	0.192768	4.049529	5.088517	-0.035968
H	2.440529	5.402762	0.839844	2.570935	5.452710	0.521797	2.508052	5.424129	0.768180
H	3.719237	4.815335	1.908941	3.616987	4.896070	1.832809	3.897199	4.849657	1.702732
C	7.449758	-2.221219	-0.405616	7.393390	-2.294121	-0.431006	7.395500	-2.297797	-0.446928
H	7.673838	-2.831983	-1.287562	7.606187	-2.876655	-1.334989	7.611069	-2.832630	-1.379607
H	8.078516	-1.326778	-0.448120	8.037644	-1.410167	-0.439508	8.044995	-1.418652	-0.405378
H	7.761624	-2.800596	0.473255	7.693271	-2.913471	0.424779	7.685910	-2.963848	0.376088
PXZCzBN		S₀		S₁			T₁		
C	1.798115	-2.026721	0.252777	-1.776030	-2.033805	-0.294245	-1.768471	-2.032621	-0.279166
C	0.691920	-2.878661	0.386238	-0.672710	-2.880360	-0.496273	-0.658789	-2.883220	-0.485897
C	-0.604684	-2.372984	0.313100	0.619314	-2.344880	-0.413688	0.626428	-2.347125	-0.403571
C	-0.832081	-0.988499	0.122272	0.817837	-0.981487	-0.113857	0.822329	-0.980125	-0.106603
C	0.261666	-0.100546	0.007823	-0.261072	-0.093117	0.030813	-0.259360	-0.086182	0.036321
C	1.537520	-0.663977	0.048684	-1.523475	-0.668653	-0.023038	-1.521247	-0.669313	-0.009918
H	0.830713	-3.940883	0.570965	-0.803839	-3.930971	-0.736250	-0.791637	-3.931358	-0.734106
H	-1.438599	-3.049461	0.456103	1.466858	-2.991835	-0.611657	1.476020	-2.990614	-0.604637
B	0.141186	1.406903	-0.013198	-0.152578	1.428704	0.047373	-0.154769	1.428773	0.039091
N	-2.112299	-0.425810	0.098633	2.122233	-0.398512	-0.035596	2.122386	-0.392474	-0.033109
N	2.715331	0.060077	-0.047089	-2.702841	0.042536	0.106901	-2.704581	0.040924	0.108890

C	-2.308010	0.936711	0.415161	2.318198	0.955395	-0.430313	2.315895	0.961324	-0.424605
C	-3.601376	1.307672	0.837561	3.606372	1.320407	-0.845498	3.605921	1.329108	-0.833329
C	-1.271364	1.910133	0.377261	1.265877	1.914241	-0.406851	1.253018	1.919170	-0.405724
C	-3.888655	2.606046	1.224392	3.899912	2.604816	-1.319875	3.900564	2.616822	-1.300230
C	-1.594922	3.218742	0.808656	1.592419	3.190640	-0.896539	1.586690	3.200768	-0.884592
C	-2.871195	3.568100	1.221305	2.874483	3.536647	-1.353752	2.871008	3.545599	-1.329691
H	-4.895564	2.839459	1.556602	4.914601	2.835751	-1.626255	4.915513	2.852030	-1.601067
H	-0.808079	3.963807	0.851195	0.815384	3.946600	-0.932316	0.810156	3.956762	-0.926566
H	-3.087539	4.579381	1.554421	3.068605	4.541565	-1.718099	3.066483	4.552997	-1.687612
C	-3.261048	-1.134398	-0.349822	3.232192	-1.100715	0.409124	3.236532	-1.097968	0.403831
C	-3.220621	-2.174944	-1.286444	3.171476	-2.220874	1.267185	3.172173	-2.216625	1.263302
C	-4.514619	-0.710492	0.115161	4.517772	-0.663343	-0.008106	4.517347	-0.661389	-0.017957
C	-4.391858	-2.832986	-1.664287	4.329848	-2.893198	1.629413	4.327949	-2.893174	1.620502
H	-2.271687	-2.474871	-1.714808	2.211469	-2.540221	1.652892	2.211982	-2.527160	1.655306
C	-5.686905	-1.358113	-0.262145	5.676679	-1.350459	0.345904	5.675138	-1.356577	0.326846
C	-5.623838	-2.440070	-1.140397	5.584826	-2.475426	1.159026	5.581093	-2.480776	1.139004
H	-4.334106	-3.649972	-2.377774	4.258027	-3.747494	2.296251	4.257652	-3.744388	2.291032
H	-6.630905	-0.997531	0.134437	6.630108	-0.979445	-0.015999	6.628810	-0.989855	-0.038389
H	-6.535852	-2.954836	-1.428514	6.484614	-3.012285	1.443150	6.480162	-3.021810	1.417434
C	2.700236	1.418867	-0.423415	-2.696157	1.412400	0.495455	-2.703085	1.412281	0.484843
C	3.863458	2.039319	-0.912630	-3.850077	2.004068	1.015594	-3.861646	2.005021	0.999782
C	1.465664	2.146126	-0.368665	-1.462003	2.156332	0.384636	-1.475428	2.157715	0.377803
C	3.845744	3.375381	-1.294587	-3.871824	3.361633	1.351960	-3.883374	3.360160	1.333759
C	1.504436	3.495158	-0.783469	-1.548197	3.532501	0.738499	-1.558372	3.527822	0.734660
C	2.665023	4.119047	-1.222927	-2.715203	4.131487	1.191601	-2.727739	4.130582	1.181768
H	4.757985	3.827673	-1.675716	-4.782655	3.799791	1.750773	-4.796339	3.798446	1.728205
H	0.577304	4.058622	-0.793696	-0.643855	4.131929	0.696484	-0.652597	4.125316	0.696971
H	2.648381	5.159760	-1.535046	-2.720005	5.187571	1.452400	-2.733202	5.186159	1.443564
C	3.779873	-0.843746	0.179928	-3.756846	-0.853117	-0.153615	-3.753518	-0.858028	-0.152743
C	5.152248	-0.629192	0.346053	-5.131622	-0.642876	-0.303880	-5.128984	-0.654093	-0.309899
C	3.234331	-2.152590	0.335194	-3.207868	-2.157627	-0.369306	-3.195980	-2.161221	-0.361773
C	5.972302	-1.730767	0.595886	-5.945954	-1.738730	-0.597567	-5.936756	-1.753536	-0.603713
C	4.078901	-3.240862	0.580063	-4.049413	-3.240412	-0.655610	-4.033878	-3.249219	-0.649167
C	5.449520	-3.027445	0.695668	-5.420890	-3.030768	-0.754981	-5.403956	-3.044822	-0.755139
H	7.038917	-1.568719	0.726567	-7.014261	-1.576250	-0.715147	-7.005169	-1.596672	-0.727450
H	3.664127	-4.239009	0.693279	-3.628804	-4.230419	-0.812070	-3.608823	-4.238112	-0.800343
H	6.114880	-3.865164	0.886119	-6.084868	-3.861790	-0.976121	-6.063971	-3.878891	-0.977155
H	4.771769	1.471950	-1.053468	-4.733982	1.409714	1.202228	-4.745348	1.410237	1.185699
H	5.589621	0.359837	0.329351	-5.573526	0.341877	-0.236548	-5.575806	0.328911	-0.248003
O	-4.612150	0.374963	0.949848	4.657012	0.439987	-0.792877	4.655790	0.447855	-0.791380

PTZCzBN

	S₀			S₁			T₁		
C	-1.934953	-2.000576	-0.345229	-1.918790	-1.998346	-0.415229	-1.901545	-2.002065	-0.389125
C	-0.828941	-2.852793	-0.483303	-0.815874	-2.838106	-0.658113	-0.787641	-2.843813	-0.618482
C	0.468055	-2.348243	-0.392767	0.478084	-2.310945	-0.550516	0.495809	-2.310396	-0.506487
C	0.692319	-0.967983	-0.182774	0.676054	-0.964863	-0.187592	0.685850	-0.951848	-0.164734
C	-0.398048	-0.085393	-0.046365	-0.397630	-0.086410	0.009943	-0.396969	-0.071346	0.014957

C	-1.673950	-0.643897	-0.106242	-1.662914	-0.652591	-0.074517	-1.657482	-0.651292	-0.062181
H	-0.968082	-3.912415	-0.682001	-0.950805	-3.876751	-0.944165	-0.918022	-3.883447	-0.901703
H	1.308011	-3.020981	-0.524349	1.329169	-2.951014	-0.760500	1.352806	-2.945277	-0.707473
B	-0.264948	1.416557	0.052955	-0.270266	1.425186	0.107060	-0.280587	1.436050	0.101130
N	1.984738	-0.419588	-0.145908	1.991552	-0.395065	-0.074669	1.989074	-0.375508	-0.057043
N	-2.848796	0.079937	0.015401	-2.837414	0.058731	0.095871	-2.839229	0.053319	0.089520
C	2.188427	0.950419	-0.446087	2.196301	0.957830	-0.484664	2.191278	0.980358	-0.454486
C	3.461259	1.332259	-0.926435	3.451469	1.342254	-0.983892	3.451498	1.366328	-0.945689
C	1.152372	1.923767	-0.323650	1.136831	1.915137	-0.370822	1.121032	1.934570	-0.350689
C	3.732342	2.663199	-1.234378	3.697032	2.658947	-1.425462	3.696688	2.687908	-1.372856
C	1.461676	3.249938	-0.700590	1.427462	3.211677	-0.827820	1.418095	3.238155	-0.793335
C	2.725269	3.626934	-1.130575	2.673682	3.587852	-1.348064	2.669212	3.614467	-1.293826
H	4.720612	2.935317	-1.594207	4.681614	2.930864	-1.793022	4.682541	2.965548	-1.731644
H	0.673243	3.994551	-0.680472	0.644562	3.961336	-0.782214	0.632509	3.985312	-0.759776
H	2.932364	4.657368	-1.406194	2.841641	4.609521	-1.677705	2.840944	4.638893	-1.614110
C	3.043119	-1.139594	0.489134	3.008152	-1.117631	0.533414	3.018772	-1.111495	0.528234
C	2.798872	-1.946347	1.610949	2.730331	-2.086624	1.528812	2.743140	-2.067275	1.535030
C	4.364779	-0.994117	0.039953	4.372179	-0.908200	0.179345	4.371689	-0.918148	0.143718
C	3.835619	-2.657707	2.210911	3.749092	-2.820099	2.110158	3.759412	-2.822473	2.092376
H	1.791363	-2.025012	2.003668	1.705118	-2.231081	1.846133	1.723128	-2.183315	1.879995
C	5.407326	-1.690111	0.660489	5.392403	-1.665922	0.774027	5.389538	-1.700966	0.709177
C	5.141405	-2.543062	1.729570	5.088055	-2.624248	1.729492	5.088804	-2.655797	1.669671
H	3.620293	-3.290423	3.067521	3.505393	-3.543217	2.883315	3.522667	-3.535975	2.876196
H	6.423553	-1.556006	0.301162	6.423216	-1.486451	0.482919	6.416907	-1.540594	0.395881
H	5.952390	-3.094250	2.197205	5.882283	-3.202991	2.190909	5.883810	-3.251415	2.108016
C	-2.826814	1.420863	0.452021	-2.816724	1.405452	0.556136	-2.833276	1.404267	0.534294
C	-3.990499	2.026463	0.958717	-3.966843	1.980171	1.105898	-3.993575	1.974882	1.071002
C	-1.586656	2.143206	0.442675	-1.577012	2.144730	0.489911	-1.601904	2.150327	0.476474
C	-3.967472	3.341545	1.407031	-3.975459	3.315246	1.519008	-4.011560	3.308973	1.479824
C	-1.620933	3.469762	0.925374	-1.649144	3.495905	0.925004	-1.681239	3.497414	0.910847
C	-2.780991	4.079101	1.385541	-2.811390	4.081415	1.409121	-2.851068	4.080553	1.382557
H	-4.880720	3.780859	1.800693	-4.883645	3.738882	1.939304	-4.926051	3.729182	1.890163
H	-0.690280	4.025541	0.972936	-0.737681	4.086335	0.920878	-0.771981	4.090997	0.914368
H	-2.760161	5.102342	1.750563	-2.806048	5.120115	1.731911	-2.853393	5.119333	1.704509
C	-3.915493	-0.815568	-0.236918	-3.896551	-0.818286	-0.205585	-3.888257	-0.834366	-0.212273
C	-5.287527	-0.594139	-0.395489	-5.271595	-0.595733	-0.337223	-5.263438	-0.624828	-0.360376
C	-3.372307	-2.120566	-0.430951	-3.352549	-2.111789	-0.491633	-3.329163	-2.127072	-0.478673
C	-6.109701	-1.686763	-0.676240	-6.092056	-1.671297	-0.682658	-6.070933	-1.711041	-0.702047
C	-4.218853	-3.199666	-0.706368	-4.200706	-3.174383	-0.829505	-4.166800	-3.201656	-0.813527
C	-5.589360	-2.980741	-0.814131	-5.571842	-2.954846	-0.910266	-5.537186	-2.993659	-0.910303
H	-7.176102	-1.519092	-0.801391	-7.160382	-1.499299	-0.785719	-7.139467	-1.549554	-0.818417
H	-3.805739	-4.194634	-0.849477	-3.785145	-4.156564	-1.039899	-3.741167	-4.182612	-1.008435
H	-6.256292	-3.811379	-1.028467	-6.239874	-3.771126	-1.171045	-6.196525	-3.817650	-1.168965
S	4.680922	0.100405	-1.312055	4.799354	0.221900	-1.080274	4.791609	0.242099	-1.091682
H	-4.904689	1.460665	1.061784	-4.857569	1.385831	1.256053	-4.881914	1.375956	1.216520
H	-5.723414	0.394701	-0.350561	-5.709436	0.385839	-0.216741	-5.711184	0.354120	-0.255640

DPACzBN	S_0			S_1			T_1		
C	-1.500598	-2.064189	-0.019849	1.486825	-2.083655	0.048388	1.492327	-2.073850	0.024368
C	-0.331143	-2.835936	-0.081411	0.320474	-2.868080	0.106152	0.320905	-2.873338	0.067635
C	0.919433	-2.225625	-0.110163	-0.911586	-2.229215	0.129731	-0.912765	-2.234344	0.086584
C	1.040787	-0.812224	-0.054955	-1.022154	-0.792937	0.071108	-1.021521	-0.811772	0.043910
C	-0.120683	-0.005178	-0.027843	0.126025	0.014052	0.034335	0.132100	0.016869	0.013613
C	-1.347732	-0.671021	-0.028602	1.333725	-0.659287	0.052786	1.342943	-0.658704	0.038443
H	-0.385130	-3.921676	-0.098522	0.367986	-3.952164	0.120401	0.375936	-3.956320	0.072465
H	1.801877	-2.851194	-0.147492	-1.807726	-2.834909	0.170801	-1.808928	-2.841556	0.116163
B	-0.103678	1.501055	0.080432	0.118799	1.543406	-0.088081	0.119939	1.526588	-0.097860
N	2.281050	-0.177737	-0.014984	-2.260115	-0.173873	0.026147	-2.263518	-0.174135	0.010813
N	-2.580005	-0.036475	0.015313	2.560119	-0.042657	0.018281	2.574101	-0.034709	0.009527
C	2.432941	1.203019	0.215573	-2.436729	1.230767	-0.182934	-2.436757	1.222082	-0.200478
C	3.742318	1.723215	0.350954	-3.749586	1.717980	-0.282869	-3.752614	1.710804	-0.308326
C	1.307254	2.082509	0.331965	-1.307447	2.114660	-0.303523	-1.310278	2.107751	-0.319982
C	3.948709	3.057156	0.662049	-3.997499	3.070045	-0.557708	-3.998696	3.059830	-0.592604
C	1.580421	3.424235	0.691002	-1.619341	3.455096	-0.628123	-1.617768	3.440536	-0.651714
C	2.862902	3.919458	0.860863	-2.926513	3.935150	-0.752159	-2.928427	3.921721	-0.787081
H	4.967309	3.422670	0.768649	-5.023293	3.420998	-0.629021	-5.024011	3.410327	-0.670792
H	0.743542	4.091782	0.863597	-0.803706	4.145952	-0.806642	-0.802512	4.132722	-0.826934
H	3.024209	4.957159	1.140268	-3.099110	4.981299	-0.994815	-3.098589	4.966492	-1.036249
C	3.459776	-0.995728	-0.156949	-3.436771	-1.000001	0.138478	-3.440151	-0.999070	0.147034
C	4.068190	-1.553068	0.972225	-4.040334	-1.520164	-1.010970	-4.057486	-1.530838	-0.989022
C	3.981605	-1.239808	-1.430504	-3.961233	-1.284144	1.402802	-3.943129	-1.270997	1.422031
C	5.202248	-2.353101	0.823843	-5.169241	-2.331723	-0.890638	-5.186209	-2.338593	-0.843838
H	3.651720	-1.356880	1.955805	-3.623793	-1.287468	-1.986424	-3.653450	-1.310143	-1.972358
C	5.116059	-2.040737	-1.572716	-5.091051	-2.096531	1.515108	-5.072993	-2.079246	1.558087
C	5.727482	-2.597638	-0.447258	-5.695834	-2.620715	0.370723	-5.695292	-2.613251	0.427628
H	5.673998	-2.785179	1.702387	-5.635555	-2.738565	-1.783945	-5.665988	-2.753234	-1.726251
H	5.520601	-2.228783	-2.563682	-5.496744	-2.318591	2.498482	-5.464740	-2.290692	2.549312
H	6.610575	-3.220947	-0.560251	-6.575059	-3.252961	0.461125	-6.574503	-3.242405	0.536983
C	-2.684877	1.352938	-0.199479	2.689703	1.368266	0.213750	2.691994	1.368261	0.213089
C	-3.919991	1.922617	-0.558702	3.924769	1.904463	0.578732	3.923476	1.918778	0.584370
C	-1.505363	2.166227	-0.130181	1.505707	2.190448	0.092704	1.508005	2.184389	0.103287
C	-4.030180	3.286199	-0.799097	4.085746	3.285673	0.753096	4.063632	3.293821	0.777985
C	-1.676847	3.540411	-0.408162	1.736770	3.585150	0.284363	1.715367	3.573064	0.321809
C	-2.905565	4.110035	-0.716924	2.980160	4.123927	0.587407	2.951005	4.126123	0.630512
H	-4.996148	3.697659	-1.081510	5.057638	3.684004	1.029937	5.030599	3.698960	1.063759
H	-0.801471	4.179104	-0.420865	0.889802	4.259166	0.238237	0.857616	4.234475	0.289151
H	-2.983301	5.174150	-0.923445	3.084131	5.198408	0.724193	3.043406	5.198420	0.787531
C	-3.563656	-1.043777	0.151511	3.537282	-1.054751	-0.130643	3.548194	-1.043165	-0.132633
C	-4.937392	-0.965075	0.406109	4.898968	-0.984318	-0.408051	4.916671	-0.976859	-0.391669
C	-2.917408	-2.314325	0.094873	2.890620	-2.330699	-0.066556	2.892776	-2.319517	-0.081699
C	-5.662149	-2.152054	0.525021	5.619290	-2.183890	-0.537425	5.631307	-2.174153	-0.518248
C	-3.667743	-3.489689	0.211504	3.632455	-3.513490	-0.192111	3.637504	-3.505962	-0.204241
C	-5.042622	-3.404257	0.411394	5.006466	-3.435312	-0.413568	5.008828	-3.428911	-0.407214

H	-6.729306	-2.094878	0.722588	6.683717	-2.126391	-0.748182	6.698048	-2.122051	-0.719019
H	-3.176173	-4.457859	0.163046	3.135147	-4.477670	-0.133032	3.136938	-4.469143	-0.155596
H	-5.634915	-4.310661	0.503974	5.596058	-4.341691	-0.512524	5.598974	-4.335484	-0.504693
H	4.602049	1.077101	0.229930	-4.594165	1.053421	-0.156723	-4.597033	1.046401	-0.181643
H	3.497864	-0.802025	-2.298748	-3.484001	-0.869093	2.285543	-3.450940	-0.850117	2.293580
H	-4.788123	1.298902	-0.712132	4.767570	1.257990	0.779651	4.774824	1.280936	0.775844
H	-5.445159	-0.021765	0.555384	5.409068	-0.043640	-0.561974	5.432877	-0.037370	-0.534158
2CzBN		S₀			S₁			T₁	
C	-1.771064	-2.042482	-0.019929	-1.753508	-2.052667	-0.028377	-1.758170	-2.046317	-0.041285
C	-0.700799	-2.940850	-0.056201	-0.681663	-2.967992	-0.096374	-0.680053	-2.971773	-0.125743
C	0.614306	-2.476381	-0.011629	0.612829	-2.480234	-0.064283	0.612298	-2.483727	-0.096830
C	0.892247	-1.094852	0.065813	0.882835	-1.072806	0.050116	0.884112	-1.084876	0.029884
C	-0.168822	-0.150601	0.071751	-0.165572	-0.126400	0.054772	-0.170763	-0.121681	0.038164
C	-1.464018	-0.673257	0.056261	-1.446067	-0.661104	0.056674	-1.452053	-0.657162	0.051104
H	-0.876515	-4.009846	-0.144202	-0.857774	-4.031770	-0.218186	-0.861816	-4.032531	-0.259570
H	1.411364	-3.197975	-0.110996	1.428063	-3.175234	-0.205966	1.427042	-3.179922	-0.240874
B	-0.010674	1.358832	-0.064509	-0.005547	1.398918	-0.068941	-0.014501	1.387241	-0.082905
N	2.187582	-0.563049	0.069979	2.169514	-0.559957	0.062972	2.172251	-0.561018	0.054487
N	-2.622328	0.089350	0.045372	-2.601276	0.087294	0.069913	-2.609034	0.092808	0.074450
C	2.417744	0.783257	-0.227335	2.421031	0.811917	-0.239148	2.422232	0.806085	-0.244673
C	3.807936	1.000188	-0.366925	3.804552	0.997233	-0.379510	3.809244	0.996863	-0.376168
C	1.445018	1.797039	-0.364817	1.444123	1.827882	-0.357574	1.449580	1.823366	-0.369794
C	4.263200	2.267845	-0.723557	4.295564	2.274678	-0.720663	4.295066	2.270139	-0.718343
C	1.961079	3.055882	-0.747025	1.990532	3.091989	-0.727062	1.988828	3.079891	-0.739122
C	3.326529	3.287549	-0.927773	3.364374	3.298514	-0.901819	3.365076	3.291584	-0.910842
H	5.324951	2.462594	-0.850796	5.359609	2.455214	-0.839081	5.359468	2.454104	-0.830612
H	1.275224	3.878142	-0.923219	1.320918	3.928860	-0.894031	1.318617	3.915990	-0.907458
H	3.668318	4.275876	-1.223758	3.715809	4.290307	-1.179151	3.715576	4.282661	-1.190346
C	3.440388	-1.197869	0.223208	3.407742	-1.202477	0.229204	3.409565	-1.198889	0.233205
C	3.771357	-2.482087	0.667805	3.721592	-2.480152	0.709633	3.718572	-2.478479	0.714459
C	4.461052	-0.256814	-0.072719	4.437028	-0.265769	-0.081267	4.442917	-0.265812	-0.070080
C	5.121720	-2.827940	0.744319	5.065412	-2.848312	0.787844	5.060537	-2.844737	0.804609
H	3.024753	-3.194329	0.990944	2.963928	-3.166630	1.064683	2.955927	-3.164692	1.058616
C	5.806734	-0.626201	0.005841	5.775155	-0.659722	0.000546	5.779671	-0.658026	0.021996
C	6.133276	-1.920640	0.402415	6.083074	-1.954792	0.419837	6.083276	-1.952779	0.444371
H	5.386510	-3.823826	1.089520	5.320636	-3.836550	1.159503	5.313001	-3.832764	1.178826
H	6.587084	0.093810	-0.225642	6.568770	0.041170	-0.243319	6.575187	0.042513	-0.216610
H	7.175048	-2.221985	0.468486	7.122193	-2.265458	0.489462	7.121164	-2.264944	0.522241
C	-2.580387	1.480356	0.260430	-2.575667	1.494949	0.287045	-2.578300	1.495307	0.286740
C	-3.737372	2.181684	0.645111	-3.734277	2.165000	0.693947	-3.733100	2.174888	0.696411
C	-1.326637	2.163671	0.149617	-1.323940	2.186548	0.139352	-1.325199	2.182995	0.136369
C	-3.694203	3.554189	0.855589	-3.727064	3.549752	0.874677	-3.715265	3.556097	0.878171
C	-1.341100	3.555930	0.386646	-1.379439	3.589749	0.333370	-1.370011	3.585919	0.334400
C	-2.494479	4.256693	0.713271	-2.545473	4.266603	0.672501	-2.529316	4.269205	0.675967
H	-4.601462	4.071089	1.158396	-4.638000	4.052949	1.187087	-4.621603	4.064599	1.195860
H	-0.401868	4.096319	0.348697	-0.458599	4.156506	0.252409	-0.445562	4.146814	0.253238

H	-2.458358	5.328459	0.888717	-2.528661	5.345157	0.810550	-2.507038	5.346985	0.817949
C	-3.711154	-0.799041	-0.120984	-3.684547	-0.804915	-0.104849	-3.691435	-0.799260	-0.096153
C	-5.070219	-0.559927	-0.351937	-5.036183	-0.575877	-0.343246	-5.046192	-0.573041	-0.320688
C	-3.208307	-2.131945	-0.126882	-3.175801	-2.142513	-0.123274	-3.174677	-2.137483	-0.126158
C	-5.919983	-1.655528	-0.512763	-5.881982	-1.683717	-0.516889	-5.888586	-1.681043	-0.492882
C	-4.080976	-3.213706	-0.284582	-4.042595	-3.233259	-0.292877	-4.044286	-3.231648	-0.293832
C	-5.440023	-2.971346	-0.462614	-5.402800	-2.998392	-0.474788	-5.402516	-2.997904	-0.461708
H	-6.976398	-1.474407	-0.692200	-6.938108	-1.503342	-0.697420	-6.946876	-1.504725	-0.664572
H	-3.696749	-4.230307	-0.282954	-3.649882	-4.246190	-0.296243	-3.649156	-4.243547	-0.305232
H	-6.128267	-3.803050	-0.586061	-6.087706	-3.830516	-0.606553	-6.087994	-3.830063	-0.592144
H	-4.660974	1.656065	0.838669	-4.638770	1.617767	0.920065	-4.640105	1.632984	0.925247
H	-5.474324	0.438217	-0.450951	-5.447948	0.419523	-0.434404	-5.462158	0.421604	-0.401881
DMACCzBN		S₀			S₁			T₁	
C	0.254677	-2.372669	-0.192509	0.267278	-2.352857	-0.283651	0.272897	-2.352789	-0.303593
C	-1.042348	-2.866637	-0.324615	-1.019009	-2.875383	-0.417108	-1.007784	-2.875387	-0.437287
C	-2.144295	-2.000820	-0.255051	-2.119203	-2.004792	-0.299007	-2.117468	-1.998753	-0.301737
C	-1.877849	-0.640879	-0.041955	-1.858722	-0.628475	-0.048990	-1.862138	-0.627506	-0.042655
C	-0.600034	-0.092687	0.056636	-0.597365	-0.066961	0.046559	-0.600442	-0.059243	0.041023
C	0.487343	-0.988361	-0.007170	0.473654	-0.966029	-0.028163	0.478623	-0.969633	-0.041411
H	1.090024	-3.058597	-0.273844	1.121581	-3.008332	-0.414752	1.128802	-3.006786	-0.435159
H	-1.184033	-3.929705	-0.502505	-1.154815	-3.930408	-0.632903	-1.147146	-3.926570	-0.666489
B	-0.452825	1.410644	0.109533	-0.450155	1.452628	0.119028	-0.459179	1.445864	0.109287
N	-3.048976	0.098218	0.004392	-3.029769	0.091416	0.038922	-3.037099	0.092083	0.045902
N	1.776939	-0.445271	0.060634	1.765876	-0.420259	0.081594	1.766803	-0.415328	0.086531
C	-3.031223	1.451698	0.401736	-3.023127	1.459693	0.446401	-3.030515	1.457746	0.444368
C	-4.209282	2.080835	0.842092	-4.196886	2.053761	0.916273	-4.204532	2.057381	0.915102
C	-1.784321	2.161636	0.422960	-1.773683	2.185800	0.417523	-1.784791	2.183553	0.416329
C	-4.193096	3.408123	1.253372	-4.219621	3.402085	1.287862	-4.220768	3.401688	1.287373
C	-1.826917	3.501079	0.867608	-1.862536	3.550951	0.807705	-1.865143	3.543939	0.812076
C	-2.999356	4.133640	1.261200	-3.044669	4.155349	1.214778	-3.044559	4.153777	1.218958
H	-5.117691	3.866238	1.595905	-5.145673	3.843810	1.645383	-5.145070	3.845332	1.647804
H	-0.894282	4.050274	0.940764	-0.950407	4.137924	0.831925	-0.949987	4.126411	0.838079
H	-2.983008	5.166543	1.598407	-3.047579	5.203671	1.505241	-3.044868	5.200686	1.513479
C	-4.113246	-0.792391	-0.270786	-4.086046	-0.798076	-0.252084	-4.088907	-0.798890	-0.246698
C	-3.577290	-2.108367	-0.402757	-3.544490	-2.112736	-0.426956	-3.536415	-2.111460	-0.428405
C	-5.474015	-0.561230	-0.498580	-5.446338	-0.574794	-0.466937	-5.451597	-0.582243	-0.457458
C	-4.423627	-3.185677	-0.686311	-4.385071	-3.191900	-0.732249	-4.376437	-3.195341	-0.736632
C	-6.295697	-1.652472	-0.786128	-6.262343	-1.669367	-0.779023	-6.261247	-1.678408	-0.771769
C	-5.785081	-2.955390	-0.863424	-5.749526	-2.968636	-0.893693	-5.738797	-2.977068	-0.893078
H	-4.016601	-4.188896	-0.781737	-3.968967	-4.188169	-0.855729	-3.956070	-4.189231	-0.864613
H	-7.353243	-1.477042	-0.964710	-7.322311	-1.494974	-0.943874	-7.322485	-1.510542	-0.935026
H	-6.451435	-3.784778	-1.084533	-6.413515	-3.794939	-1.130277	-6.400237	-3.805070	-1.131847
C	2.018690	0.907026	-0.273613	2.032031	0.937855	-0.313035	2.029850	0.940399	-0.302896
C	3.335159	1.232978	-0.688245	3.342136	1.228188	-0.726768	3.343326	1.234537	-0.714929
C	0.984171	1.889153	-0.216619	0.992321	1.919392	-0.234242	0.987168	1.918705	-0.236825
C	3.620468	2.567740	-0.968448	3.653704	2.565511	-1.041019	3.646634	2.567424	-1.039523

C	1.337367	3.210560	-0.565933	1.372660	3.230289	-0.588835	1.361117	3.226322	-0.600608
C	2.633241	3.557848	-0.909105	2.675945	3.552198	-0.967778	2.663413	3.550604	-0.978748
H	4.619094	2.851539	-1.280633	4.656973	2.836688	-1.345370	4.648462	2.841907	-1.345482
H	0.565677	3.972653	-0.587266	0.624501	4.015295	-0.578362	0.608789	4.007479	-0.601788
H	2.882474	4.584938	-1.162917	2.930491	4.580247	-1.215902	2.913899	4.576814	-1.237919
C	2.855658	-1.159105	0.657984	2.802538	-1.134585	0.687191	2.807164	-1.135008	0.688975
C	4.166225	-0.890807	0.223055	4.136643	-0.873122	0.284612	4.139230	-0.874787	0.287111
C	2.628016	-2.028867	1.734815	2.532010	-2.045425	1.733075	2.531668	-2.047902	1.728892
C	5.222609	-1.541757	0.871588	5.158507	-1.558899	0.943730	5.159580	-1.570611	0.938980
C	3.694517	-2.677698	2.350052	3.571728	-2.717191	2.358829	3.569499	-2.725301	2.352629
H	1.618939	-2.184252	2.098910	1.511781	-2.178598	2.073833	1.509737	-2.181988	2.063419
C	4.997916	-2.438524	1.915866	4.890745	-2.476702	1.963875	4.888462	-2.490809	1.955383
H	6.243670	-1.351980	0.560798	6.191033	-1.388091	0.662192	6.192475	-1.403062	0.657272
H	3.503317	-3.351242	3.181318	3.355578	-3.403849	3.172520	3.351045	-3.414658	3.163267
H	5.838283	-2.935539	2.393019	5.712676	-2.990008	2.455228	5.708607	-3.010896	2.442471
C	4.338177	0.096028	-0.930648	4.352457	0.085174	-0.883737	4.359516	0.096275	-0.869815
C	5.784435	0.601109	-1.053914	5.804895	0.585770	-0.956510	5.810155	0.604484	-0.926138
H	5.887415	1.279597	-1.904665	5.942883	1.243259	-1.818039	5.953901	1.268185	-1.781799
H	6.117201	1.124112	-0.151849	6.097302	1.131445	-0.054129	6.091644	1.144632	-0.017044
H	6.467542	-0.231583	-1.241381	6.495532	-0.250158	-1.095406	6.505627	-0.227209	-1.064746
C	3.970269	-0.614471	-2.265790	4.047123	-0.670703	-2.213194	4.066284	-0.648107	-2.208377
H	4.054903	0.088344	-3.101486	4.169506	0.008538	-3.062983	4.192071	0.038753	-3.051430
H	4.653712	-1.451379	-2.446321	4.736972	-1.512530	-2.338207	4.760953	-1.485457	-2.335063
H	2.950251	-1.005176	-2.254324	3.025737	-1.058086	-2.235973	3.047031	-1.040380	-2.242039
H	-5.131849	1.525009	0.923163	-5.097484	1.468542	1.039998	-5.106287	1.474340	1.040521
H	-5.899531	0.433188	-0.501135	-5.880204	0.415168	-0.435761	-5.891215	0.405181	-0.421044
TMCzCzBN		S₀			S₁			T₁	
C	-2.170537	-2.133342	-0.092388	-2.152424	-2.141259	-0.107109	-2.154919	-2.135512	-0.116997
C	-1.097998	-3.027828	-0.161327	-1.080068	-3.050518	-0.214141	-1.076030	-3.051964	-0.238140
C	0.215410	-2.563407	-0.090881	0.215928	-2.562625	-0.157181	0.217391	-2.562846	-0.183374
C	0.490227	-1.185099	0.044947	0.481098	-1.165782	0.019626	0.483333	-1.173210	0.002667
C	-0.573114	-0.243381	0.087939	-0.569058	-0.219732	0.065808	-0.573245	-0.214264	0.053292
C	-1.866941	-0.768219	0.044267	-1.848460	-0.756088	0.042248	-1.853503	-0.753408	0.038684
H	-1.271506	-4.092523	-0.294647	-1.254104	-4.108343	-0.382413	-1.253992	-4.106941	-0.416536
B	-0.417476	1.271584	0.025282	-0.412746	1.309950	0.013765	-0.421452	1.300654	0.002322
N	1.782527	-0.651912	0.076757	1.768962	-0.648011	0.060013	1.772149	-0.645381	0.050495
N	-3.027504	-0.008423	0.062446	-3.007036	-0.010057	0.088228	-3.014061	-0.006908	0.092229
C	2.008349	0.708277	-0.150450	2.015846	0.737510	-0.173493	2.016361	0.732974	-0.178120
C	3.397013	0.940295	-0.272826	3.396321	0.939175	-0.294386	3.400548	0.940467	-0.292600
C	1.039022	1.726804	-0.242461	1.040885	1.757753	-0.249061	1.043405	1.755209	-0.258215
C	3.846854	2.224748	-0.560533	3.882059	2.233286	-0.569904	3.880388	2.230912	-0.568833
C	1.556823	3.004503	-0.555922	1.585282	3.034780	-0.552046	1.580768	3.026198	-0.560582
C	2.921786	3.272348	-0.722426	2.964498	3.279463	-0.712034	2.961563	3.275671	-0.719224
H	4.910986	2.421809	-0.670966	4.947997	2.416499	-0.671143	4.946100	2.418091	-0.666525
H	0.863480	3.828648	-0.692127	0.908217	3.873422	-0.680920	0.902987	3.864237	-0.689289
C	3.039635	-1.286930	0.197241	3.005801	-1.288748	0.200331	3.010821	-1.284673	0.199119

C	3.386285	-2.587931	0.574102	3.333119	-2.586801	0.617164	3.334638	-2.583277	0.615319
C	4.055624	-0.328746	-0.043285	4.034150	-0.335101	-0.054304	4.040797	-0.333907	-0.049302
C	4.738526	-2.922568	0.636772	4.676547	-2.945077	0.684861	4.677578	-2.939744	0.692354
H	2.649353	-3.326212	0.859399	2.581674	-3.298440	0.934064	2.580207	-3.295634	0.922742
C	5.403234	-0.692627	0.022587	5.371782	-0.724929	0.016512	5.378190	-0.721218	0.029272
C	5.764271	-2.002345	0.348615	5.711586	-2.038777	0.369475	5.715661	-2.034462	0.383974
H	5.004466	-3.934705	0.932897	4.931532	-3.949751	1.011904	4.930642	-3.944681	1.020237
H	6.173631	0.051016	-0.166357	6.157831	-0.002341	-0.187233	6.164819	0.002123	-0.169587
C	-2.990218	1.371271	0.342358	-2.982509	1.385266	0.370270	-2.986366	1.383969	0.370968
C	-4.151146	2.050889	0.753362	-4.141574	2.036457	0.805386	-4.142977	2.041545	0.809902
C	-1.737684	2.061863	0.270811	-1.730718	2.084411	0.256358	-1.734600	2.081191	0.255901
C	-4.112972	3.411919	1.029316	-4.135707	3.411644	1.049123	-4.129149	3.413110	1.056468
C	-1.757359	3.441075	0.574044	-1.787847	3.478398	0.514208	-1.783388	3.473420	0.519744
C	-2.914254	4.122966	0.927541	-2.954189	4.138209	0.882096	-2.944790	4.137689	0.890723
H	-5.023297	3.911661	1.351190	-5.047737	3.899418	1.382362	-5.037708	3.903801	1.395314
H	-0.819281	3.984685	0.566887	-0.867018	4.048456	0.461016	-0.859963	4.039408	0.467182
H	-2.881725	5.185249	1.154131	-2.938634	5.209387	1.069517	-2.925219	5.207722	1.083201
C	-4.113274	-0.890977	-0.147301	-4.086961	-0.894609	-0.126664	-4.092747	-0.892127	-0.119641
C	-5.472045	-0.645339	-0.373513	-5.441522	-0.658273	-0.350167	-5.449984	-0.659273	-0.332886
C	-3.606935	-2.221301	-0.209225	-3.575654	-2.229119	-0.207289	-3.573503	-2.225963	-0.209617
C	-6.318516	-1.734781	-0.585565	-6.283979	-1.757373	-0.573238	-6.288977	-1.758823	-0.555286
C	-4.476475	-3.297090	-0.417551	-4.440747	-3.312377	-0.425283	-4.440223	-3.312377	-0.426823
C	-5.835400	-3.050415	-0.590679	-5.801089	-3.072429	-0.593180	-5.799114	-3.074679	-0.584029
H	-7.374622	-1.548425	-0.761529	-7.341065	-1.572047	-0.743521	-7.347803	-1.577872	-0.719278
H	-4.089724	-4.311920	-0.458624	-4.045845	-4.323288	-0.476288	-4.042937	-4.321980	-0.484324
H	-5.074331	1.514329	0.916283	-5.046288	1.479139	1.004227	-5.049221	1.487464	1.010671
H	-5.878270	0.355244	-0.430702	-5.855475	0.339501	-0.393223	-5.867842	0.337311	-0.368423
H	1.014971	-3.278425	-0.215082	1.032042	-3.250952	-0.325428	1.033649	-3.251495	-0.353068
H	-6.521019	-3.877589	-0.753193	-6.484793	-3.898982	-0.762067	-6.482415	-3.901968	-0.752351
C	3.406465	4.660848	-1.067192	3.442329	4.678479	-1.020579	3.435360	4.673871	-1.031922
H	2.579064	5.374858	-1.110973	3.191349	5.373283	-0.209043	3.175575	5.370833	-0.225150
H	4.126437	5.029741	-0.326619	4.526093	4.713409	-1.165846	4.519581	4.713006	-1.171002
H	3.911530	4.678203	-2.040993	2.968850	5.068922	-1.929823	2.964391	5.056966	-1.945451
C	7.211699	-2.427054	0.398690	7.150891	-2.479874	0.427039	7.154625	-2.476891	0.450359
H	7.883176	-1.563364	0.409992	7.836100	-1.628198	0.392189	7.840489	-1.625545	0.419912
H	7.423178	-3.029672	1.289108	7.359719	-3.047826	1.340925	7.357292	-3.044349	1.365759
H	7.477585	-3.038740	-0.473301	7.396106	-3.136585	-0.418447	7.404559	-3.133375	-0.393631

PXZDMACBN

	S_0			S_1			T_1		
C	-1.499035	-1.925817	0.048764	-1.464818	-1.942336	-0.013025	-1.459476	-1.936043	0.011710
C	-0.398209	-2.759718	-0.176157	-0.365596	-2.767915	-0.256448	-0.360653	-2.765411	-0.253595
C	0.907842	-2.284232	-0.268743	0.935354	-2.254825	-0.317319	0.935995	-2.250711	-0.321346
C	1.158578	-0.913451	-0.115268	1.151373	-0.889172	-0.085178	1.150689	-0.887087	-0.082434
C	0.071684	-0.017781	0.050461	0.072778	0.000066	0.066455	0.073665	0.008647	0.079351
C	-1.241036	-0.544620	0.110507	-1.221835	-0.544728	0.093501	-1.222932	-0.544326	0.114807
H	-0.548246	-3.828840	-0.280394	-0.499928	-3.833686	-0.395608	-0.498760	-3.828658	-0.404988
H	1.712086	-2.981156	-0.470860	1.757562	-2.921936	-0.549485	1.757756	-2.914500	-0.564903

B	0.292010	1.484223	0.125629	0.282282	1.524155	0.117960	0.277702	1.523896	0.117240
N	2.457515	-0.385930	-0.167852	2.465999	-0.344076	-0.092624	2.468251	-0.340000	-0.094919
N	-2.330111	0.336251	0.201526	-2.316597	0.320211	0.213225	-2.322755	0.320682	0.221202
C	2.678110	0.964941	-0.498286	2.690007	0.994952	-0.517225	2.687894	0.997525	-0.509133
C	3.945960	1.304126	-1.008858	3.953666	1.312180	-1.023803	3.956413	1.322453	-1.007207
C	1.678965	1.959544	-0.365147	1.670939	1.980280	-0.413168	1.657694	1.981989	-0.403943
C	4.238020	2.601124	-1.397982	4.259500	2.594683	-1.491653	4.262443	2.607028	-1.470680
C	1.999828	3.269070	-0.793217	2.007962	3.260511	-0.891542	2.004210	3.267957	-0.870482
C	3.250170	3.590217	-1.300450	3.267817	3.566000	-1.424585	3.264666	3.573769	-1.396665
H	5.223195	2.815981	-1.800697	5.255040	2.798261	-1.871199	5.258494	2.816147	-1.844439
H	1.231941	4.034830	-0.751341	1.255280	4.041756	-0.858321	1.253149	4.050588	-0.837479
H	3.470090	4.601521	-1.631370	3.477386	4.571905	-1.778772	3.473271	4.582642	-1.743916
C	3.613095	-1.123673	0.209298	3.586844	-1.079401	0.282306	3.589071	-1.081871	0.272352
C	3.611682	-2.155397	1.156690	3.554968	-2.161028	1.188221	3.553485	-2.170881	1.168862
C	4.844274	-0.736451	-0.343123	4.846812	-0.701311	-0.249696	4.846972	-0.699640	-0.255270
C	4.789161	-2.839537	1.462495	4.710727	-2.872931	1.477500	4.707829	-2.885119	1.452852
H	2.685984	-2.429695	1.648282	2.619362	-2.421604	1.667517	2.617531	-2.432034	1.646589
C	6.022603	-1.410121	-0.037418	6.002199	-1.427272	0.032961	6.001744	-1.432189	0.016896
C	5.992775	-2.482745	0.854150	5.934088	-2.523483	0.887130	5.931149	-2.533809	0.861664
H	4.758705	-3.649274	2.186020	4.662478	-3.699268	2.180552	4.659970	-3.714900	2.151589
H	6.946392	-1.076807	-0.500105	6.937170	-1.107086	-0.415303	6.937165	-1.109296	-0.428206
H	6.909097	-3.018186	1.085433	6.833714	-3.087771	1.113351	6.829622	-3.101864	1.082703
C	-2.174802	1.640864	0.716797	-2.162545	1.623679	0.779563	-2.175812	1.630342	0.767523
C	-3.276625	2.277866	1.322733	-3.242544	2.192681	1.462351	-3.263376	2.208987	1.435345
C	-0.907307	2.285135	0.681491	-0.908959	2.308820	0.660961	-0.924686	2.312913	0.657424
C	-3.139107	3.544462	1.873538	-3.154802	3.489332	1.978616	-3.174459	3.504349	1.946793
C	-0.813213	3.567717	1.266677	-0.873560	3.628258	1.195094	-0.884193	3.626153	1.194679
C	-1.902338	4.202386	1.847468	-1.963620	4.211830	1.826021	-1.978121	4.219657	1.812134
H	-3.997631	4.011600	2.350076	-4.004629	3.920680	2.500568	-4.028834	3.941718	2.456685
H	0.155033	4.059214	1.285413	0.058607	4.183684	1.140067	0.052695	4.174618	1.151176
H	-1.794747	5.187426	2.293833	-1.885373	5.221933	2.222889	-1.898156	5.228810	2.210592
C	-3.530652	-0.085346	-0.438773	-3.520407	-0.084047	-0.412792	-3.518047	-0.092763	-0.417293
C	-4.323247	0.828792	-1.149851	-4.354704	0.852971	-1.048076	-4.345394	0.833746	-1.074744
C	-3.849171	-1.458537	-0.447778	-3.825916	-1.461996	-0.482944	-3.816858	-1.471628	-0.476913
C	-5.462154	0.399082	-1.824105	-5.502027	0.439158	-1.714839	-5.482464	0.408453	-1.752919
C	-4.990885	-1.865044	-1.149364	-4.982343	-1.849142	-1.169686	-4.960064	-1.871712	-1.179113
C	-5.803816	-0.952759	-1.821232	-5.825749	-0.917280	-1.774558	-5.798628	-0.949625	-1.804673
H	-6.066016	1.121307	-2.367316	-6.131250	1.179142	-2.202898	-6.108195	1.140819	-2.256743
H	-5.258733	-2.915273	-1.174507	-5.239093	-2.900310	-1.238148	-5.210378	-2.924840	-1.241287
H	-6.688794	-1.300175	-2.347573	-6.719236	-1.251289	-2.295057	-6.683267	-1.292553	-2.334517
C	-2.925260	-2.417130	0.308869	-2.886847	-2.447858	0.216802	-2.881085	-2.444829	0.245451
C	-3.224656	-2.313876	1.831973	-3.171121	-2.413516	1.749831	-3.173496	-2.388944	1.775086
H	-4.255445	-2.624055	2.036293	-4.198216	-2.740950	1.943126	-4.199937	-2.718500	1.968991
H	-2.548695	-2.967196	2.394367	-2.486368	-3.086104	2.277533	-2.488291	-3.050365	2.316325
H	-3.096678	-1.294440	2.203779	-3.049008	-1.409661	2.162795	-3.057947	-1.378696	2.173941
C	-3.125422	-3.881371	-0.111990	-3.080350	-3.894553	-0.264473	-3.068875	-3.898849	-0.214917

H	-4.142606	-4.214251	0.111376	-4.094601	-4.241044	-0.050353	-4.083028	-4.244837	0.001205
H	-2.939799	-4.032122	-1.180099	-2.900222	-3.997560	-1.339080	-2.885397	-4.018350	-1.287270
H	-2.455727	-4.537703	0.450469	-2.405042	-4.570866	0.266487	-2.392556	-4.564513	0.328205
H	-4.231518	1.767553	1.383764	-4.162255	1.629002	1.583273	-4.185951	1.648931	1.550534
H	-4.038008	1.873792	-1.187284	-4.089842	1.903307	-1.029027	-4.084510	1.885300	-1.064484
O	4.915422	0.339534	-1.195802	4.965934	0.378761	-1.068341	4.968346	0.393611	-1.053761
PTZDMACBN		S₀			S₁			T₁	
C	1.631699	-1.917280	0.032641	-1.595068	-1.930565	-0.106054	-1.585156	-1.925197	-0.084082
C	0.526867	-2.745624	0.261883	-0.489958	-2.746774	-0.368675	-0.475656	-2.743432	-0.351053
C	-0.779016	-2.264254	0.336159	0.809110	-2.229587	-0.401734	0.817396	-2.220575	-0.385470
C	-1.021669	-0.896005	0.163696	1.015630	-0.869368	-0.129380	1.021161	-0.857601	-0.117330
C	0.064234	-0.010488	-0.026888	-0.062681	0.006383	0.058262	-0.060958	0.021363	0.067532
C	1.375821	-0.538316	-0.070585	-1.356776	-0.540372	0.059499	-1.355134	-0.537215	0.071107
H	0.673837	-3.813286	0.383578	-0.622150	-3.807342	-0.544747	-0.606333	-3.803024	-0.531334
H	-1.593605	-2.953350	0.528294	1.641553	-2.884891	-0.634684	1.652419	-2.871994	-0.620316
B	-0.167478	1.482532	-0.178724	0.158599	1.520508	0.183385	0.150653	1.527172	0.183786
N	-2.330617	-0.377561	0.209160	2.335239	-0.328489	-0.117832	2.338052	-0.316035	-0.109628
N	2.461817	0.341179	-0.197287	-2.449785	0.321402	0.216802	-2.454660	0.321380	0.211589
C	-2.553189	0.981802	0.524268	2.558054	1.012699	-0.552891	2.558421	1.025883	-0.526247
C	-3.792745	1.340878	1.095138	3.784086	1.354324	-1.137645	3.791628	1.374475	-1.102435
C	-1.556064	1.969117	0.303458	1.534582	1.991388	-0.354522	1.524889	2.002374	-0.333040
C	-4.064940	2.671071	1.407614	4.048452	2.675315	-1.550192	4.053930	2.696993	-1.504806
C	-1.857462	3.296778	0.677684	1.842626	3.298325	-0.781564	1.838788	3.315055	-0.748606
C	-3.090026	3.653375	1.207382	3.067498	3.640523	-1.363101	3.065958	3.658780	-1.316962
H	-5.027396	2.930277	1.839842	5.011937	2.925121	-1.982859	5.018277	2.953272	-1.931042
H	-1.089039	4.055821	0.569833	1.088587	4.070505	-0.665586	1.081965	4.085350	-0.639865
H	-3.297777	4.683924	1.482354	3.257590	4.666757	-1.667311	3.256716	4.686974	-1.615066
C	-3.411601	-1.115859	-0.361487	3.382858	-1.074283	0.422958	3.391476	-1.076389	0.414139
C	-3.230191	-1.908976	-1.504955	3.161714	-1.975143	1.491421	3.172821	-1.974357	1.483083
C	-4.703786	-0.997894	0.175634	4.708815	-0.932923	-0.067167	4.708080	-0.942736	-0.091791
C	-4.292708	-2.631950	-2.042541	4.198103	-2.737104	2.004284	4.206846	-2.751840	1.979020
H	-2.249279	-1.968745	-1.962787	2.168791	-2.046876	1.918773	2.185108	-2.033735	1.924204
C	-5.773683	-1.705283	-0.382596	5.746802	-1.712571	0.461658	5.743444	-1.740667	0.415160
C	-5.565895	-2.543778	-1.475660	5.495483	-2.621037	1.481883	5.495279	-2.651674	1.433893
H	-4.124080	-3.253265	-2.917886	4.002355	-3.412649	2.832055	4.015564	-3.426345	2.808514
H	-6.765874	-1.591581	0.044619	6.752262	-1.590654	0.069683	6.745036	-1.627776	0.010849
H	-6.396982	-3.104312	-1.894400	6.307293	-3.217095	1.887959	6.305784	-3.260594	1.823325
C	2.301043	1.621105	-0.768996	-2.291761	1.597160	0.842702	-2.309985	1.603170	0.822520
C	3.403052	2.237613	-1.396159	-3.372744	2.137011	1.549163	-3.402381	2.146898	1.512554
C	1.028657	2.259757	-0.772474	-1.035802	2.281877	0.766326	-1.056742	2.289009	0.757575
C	3.261272	3.475205	-2.007908	-3.279924	3.403317	2.133187	-3.315610	3.412300	2.093583
C	0.931196	3.511968	-1.420101	-0.993921	3.566716	1.372782	-1.019693	3.570609	1.364340
C	2.020024	4.125207	-2.023375	-2.084229	4.124640	2.028434	-2.117654	4.131652	2.005532
H	4.120395	3.924497	-2.500254	-4.130627	3.811523	2.672216	-4.172765	3.822557	2.620870
H	-0.040094	3.995347	-1.469953	-0.057326	4.117122	1.353573	-0.082224	4.119624	1.356769
H	1.909375	5.086454	-2.518140	-2.001396	5.110879	2.480253	-2.039094	5.117674	2.458336

C	3.664538	-0.055079	0.455012	-3.654020	-0.054519	-0.424908	-3.652833	-0.068532	-0.435824
C	4.457762	0.885818	1.129273	-4.490262	0.910390	-1.014372	-4.485410	0.884835	-1.046930
C	3.982857	-1.427163	0.515534	-3.956416	-1.428465	-0.561110	-3.947058	-1.444659	-0.555078
C	5.598105	0.482494	1.817284	-5.637158	0.527137	-1.699874	-5.625836	0.487541	-1.735958
C	5.126116	-1.805906	1.230022	-5.112159	-1.783656	-1.266056	-5.095384	-1.814913	-1.264842
C	5.939958	-0.868381	1.865113	-5.957614	-0.825385	-1.825140	-5.939677	-0.867654	-1.843717
H	6.202738	1.224943	2.331564	-6.267985	1.288535	-2.151503	-6.255680	1.239646	-2.204067
H	5.394602	-2.854218	1.295164	-5.366996	-2.830640	-1.385683	-5.344712	-2.864462	-1.372517
H	6.825830	-1.195453	2.402843	-6.850274	-1.135889	-2.361370	-6.826687	-1.189275	-2.382783
S	-4.952104	0.078209	1.559076	5.053410	0.157045	-1.393258	5.051830	0.178361	-1.392704
C	3.059859	-2.415845	-0.203534	-3.018197	-2.447127	0.092205	-3.006012	-2.449009	0.115781
C	3.362040	-2.372112	-1.729084	-3.309261	-2.488648	1.623776	-3.302421	-2.473628	1.646404
H	4.393453	-2.689158	-1.919022	-4.336750	-2.826014	1.797014	-4.327338	-2.818518	1.820256
H	2.687779	-3.047668	-2.266697	-2.625805	-3.185616	2.120646	-2.614506	-3.158018	2.154400
H	3.234061	-1.368066	-2.140807	-3.189780	-1.506050	2.085963	-3.193574	-1.484362	2.096743
C	3.260704	-3.862067	0.275608	-3.209229	-3.868237	-0.461374	-3.187075	-3.878072	-0.420360
H	4.279066	-4.202077	0.069173	-4.224052	-4.225618	-0.268948	-4.200624	-4.238431	-0.226583
H	3.071029	-3.970438	1.348108	-3.024314	-3.917234	-1.538970	-2.998448	-3.940348	-1.496598
H	2.594365	-4.541468	-0.262783	-2.535888	-4.570153	0.037759	-2.511257	-4.569249	0.090155
H	4.361609	1.731646	-1.427321	-4.295777	1.572957	1.637776	-4.325554	1.582113	1.593599
H	4.171657	1.931284	1.127608	-4.226773	1.959030	-0.946285	-4.225015	1.935129	-0.993381
DPADMACBN		S₀			S₁			T₁	
C	1.247322	-1.887953	0.348376	1.223577	-1.912339	0.346190	1.225606	-1.900667	0.359332
C	0.086297	-2.668956	0.331645	0.059174	-2.688194	0.425565	0.067756	-2.683857	0.428314
C	-1.189797	-2.132818	0.189316	-1.202257	-2.117002	0.313057	-1.198526	-2.110080	0.297550
C	-1.352485	-0.741434	0.066155	-1.351654	-0.712964	0.133885	-1.350280	-0.714618	0.119347
C	-0.207631	0.095610	0.086095	-0.212353	0.110887	0.103312	-0.212770	0.123289	0.091734
C	1.070764	-0.503071	0.193976	1.044300	-0.511036	0.184047	1.047814	-0.504817	0.179026
H	0.163308	-3.745138	0.444395	0.121965	-3.760791	0.560248	0.130826	-3.755064	0.569272
H	-2.040317	-2.801815	0.179332	-2.069711	-2.762874	0.356649	-2.064729	-2.758308	0.335696
B	-0.344203	1.605862	0.026696	-0.338149	1.641008	-0.024752	-0.342941	1.637801	-0.017944
N	-2.621545	-0.168600	-0.075758	-2.615512	-0.154554	-0.033079	-2.619638	-0.155612	-0.041977
N	2.213659	0.309899	0.112508	2.186777	0.294635	0.081037	2.192851	0.301852	0.066998
C	-2.832238	1.192219	-0.349068	-2.843762	1.217431	-0.336653	-2.852139	1.214828	-0.325198
C	-4.142233	1.646231	-0.631218	-4.155417	1.642261	-0.600484	-4.167736	1.638419	-0.584974
C	-1.748233	2.120910	-0.350702	-1.747579	2.143333	-0.367766	-1.758794	2.145306	-0.345272
C	-4.373202	2.971624	-0.965720	-4.422588	2.975979	-0.934267	-4.439584	2.971704	-0.901740
C	-2.036358	3.452380	-0.730552	-2.072213	3.472131	-0.746753	-2.089350	3.474806	-0.707363
C	-3.315669	3.887435	-1.039689	-3.372181	3.889588	-1.021738	-3.390757	3.889923	-0.977583
H	-5.389344	3.289188	-1.188037	-5.446510	3.281172	-1.132872	-5.463957	3.276533	-1.097864
H	-1.213377	4.156134	-0.802847	-1.264627	4.189566	-0.848228	-1.286140	4.198091	-0.799994
H	-3.496523	4.918245	-1.332468	-3.564423	4.922571	-1.303891	-3.586697	4.925371	-1.247700
C	-3.765130	-1.040304	0.013513	-3.755972	-1.032511	0.026783	-3.756705	-1.039903	0.014008
C	-4.255484	-1.677656	-1.130951	-4.210358	-1.675185	-1.129650	-4.207430	-1.678209	-1.145781
C	-4.378768	-1.251185	1.251793	-4.404659	-1.240589	1.247789	-4.402663	-1.257123	1.234513
C	-5.361108	-2.524203	-1.033794	-5.310561	-2.531273	-1.059874	-5.305362	-2.537433	-1.080379

H	-3.769652	-1.506333	-2.087021	-3.700768	-1.500725	-2.072653	-3.698053	-1.497570	-2.087671
C	-5.484359	-2.098467	1.343399	-5.505183	-2.097257	1.311069	-5.500754	-2.117051	1.292963
C	-5.976763	-2.735575	0.202153	-5.959106	-2.743472	0.159068	-5.953166	-2.757931	0.137434
H	-5.740400	-3.017897	-1.924639	-5.660184	-3.031562	-1.959147	-5.653835	-3.033436	-1.982392
H	-5.959852	-2.259917	2.307255	-6.006381	-2.258869	2.261774	-6.001346	-2.285161	2.242800
H	-6.837652	-3.394900	0.275575	-6.815837	-3.410196	0.210732	-6.808230	-3.426994	0.185491
C	2.166781	1.673784	0.467618	2.156257	1.666007	0.498553	2.163444	1.669437	0.471697
C	3.342360	2.302321	0.927423	3.315255	2.214513	1.055954	3.332611	2.232145	1.003074
C	0.934905	2.384748	0.438608	0.940013	2.407762	0.377634	0.939137	2.405823	0.374106
C	3.313687	3.623495	1.350742	3.343386	3.558954	1.446121	3.356909	3.571241	1.395331
C	0.953204	3.718154	0.906633	1.021614	3.763579	0.790207	1.019189	3.759757	0.791956
C	2.112293	4.342911	1.346590	2.188515	4.331817	1.296852	2.189726	4.335091	1.275783
H	4.228381	4.084311	1.716158	4.251392	3.982150	1.866159	4.268586	4.001591	1.799832
H	0.017696	4.266091	0.952444	0.128258	4.376687	0.742955	0.120024	4.365651	0.767807
H	2.084756	5.369558	1.702382	2.192117	5.377845	1.596394	2.190548	5.379011	1.582574
C	3.352158	-0.278267	-0.505189	3.331947	-0.267137	-0.511474	3.338981	-0.271699	-0.520829
C	4.158179	0.466353	-1.380224	4.183157	0.521313	-1.312137	4.180059	0.499268	-1.344859
C	3.590089	-1.655234	-0.317822	3.571321	-1.654943	-0.364295	3.577227	-1.654031	-0.345527
C	5.232438	-0.132794	-2.030872	5.282454	-0.048518	-1.938073	5.277840	-0.082691	-1.964979
C	4.666313	-2.235961	-1.000094	4.691643	-2.195604	-1.002669	4.692582	-2.209091	-0.981433
C	5.493384	-1.489239	-1.838716	5.546605	-1.411527	-1.778745	5.542863	-1.441054	-1.778195
H	5.848251	0.459187	-2.703042	5.921969	0.568547	-2.563260	5.913112	0.521254	-2.607087
H	4.871295	-3.293504	-0.876905	4.909174	-3.252810	-0.904363	4.909636	-3.264419	-0.863910
H	6.326943	-1.968575	-2.345141	6.403481	-1.867688	-2.266651	6.397067	-1.907395	-2.261265
H	-4.978436	0.959319	-0.606507	-4.981313	0.944302	-0.551549	-4.989630	0.935129	-0.546645
H	-3.987492	-0.751056	2.132882	-4.044294	-0.731205	2.136658	-4.043295	-0.752031	2.126152
H	4.269868	1.743231	0.981215	4.199310	1.599089	1.187221	4.223161	1.622945	1.117267
H	3.932344	1.511094	-1.561262	3.958205	1.571301	-1.454823	3.951479	1.545359	-1.510272
C	2.655426	-2.423989	0.620806	2.630168	-2.468030	0.523430	2.635151	-2.448935	0.559374
C	3.043755	-2.108002	2.093574	3.047689	-2.250092	2.015444	3.042662	-2.195383	2.046222
H	2.994134	-1.037482	2.306517	3.015490	-1.194087	2.293581	3.007820	-1.133410	2.300164
H	2.363005	-2.621798	2.781080	2.372786	-2.799815	2.679068	2.364177	-2.729882	2.718685
H	4.064866	-2.449010	2.298126	4.067274	-2.617569	2.170502	4.061572	-2.557836	2.217668
C	2.749322	-3.945304	0.425048	2.703143	-3.976897	0.229560	2.714047	-3.963461	0.300782
H	2.078126	-4.463931	1.115020	2.042545	-4.533775	0.898165	2.051673	-4.505847	0.979485
H	2.493205	-4.245319	-0.595985	2.424665	-4.204570	-0.803785	2.440472	-4.216771	-0.727905
H	3.757773	-4.304656	0.647618	3.711062	-4.358201	0.409524	3.722444	-4.337505	0.493783

CzDMACBN

	S₀			S₁			T₁		
C	-1.471883	-1.907167	0.272809	1.443121	-1.932651	-0.255209	-1.445384	-1.928577	0.240955
C	-0.406739	-2.798085	0.144751	0.362671	-2.830631	-0.187641	-0.370713	-2.828013	0.158015
C	0.919491	-2.382344	0.024505	-0.943894	-2.383179	-0.088236	0.938933	-2.375379	0.047966
C	1.224775	-1.018965	0.067807	-1.235982	-0.994910	-0.113535	1.235614	-0.996387	0.086641
C	0.171788	-0.060587	0.119923	-0.183678	-0.052524	-0.127853	0.185729	-0.043466	0.108502
C	-1.161006	-0.534005	0.194374	1.132479	-0.556693	-0.182246	-1.133862	-0.552453	0.166360
H	-0.595779	-3.865933	0.143538	0.539706	-3.898605	-0.172611	-0.546293	-3.895816	0.143766
H	1.681525	-3.130472	-0.133813	-1.726958	-3.111007	0.065191	1.719987	-3.104923	-0.110423

B	0.427711	1.446742	0.040695	-0.429655	1.469341	0.001550	0.432820	1.468080	0.000753
N	2.540898	-0.531752	0.003846	-2.542286	-0.516107	-0.020641	2.548494	-0.517822	0.010563
N	-2.227032	0.378670	0.151534	2.201920	0.361294	-0.112271	-2.204141	0.363473	0.107985
C	2.807974	0.799534	-0.309609	-2.808751	0.820167	0.334519	2.820039	0.820231	-0.326234
C	4.191713	0.969393	-0.536686	-4.185383	0.976961	0.572243	4.198402	0.978419	-0.553371
C	1.865952	1.842024	-0.364469	-1.849480	1.857496	0.394337	1.863599	1.860576	-0.377709
C	4.661476	2.227968	-0.911105	-4.671298	2.241295	0.960515	4.688019	2.244219	-0.924223
C	2.389241	3.091814	-0.761264	-2.391583	3.113923	0.803314	2.408415	3.116041	-0.772429
C	3.746750	3.280163	-1.037269	-3.750397	3.287988	1.079248	3.769486	3.293040	-1.039519
H	5.717932	2.392398	-1.107270	-5.727253	2.401267	1.157620	5.745548	2.405303	-1.112214
H	1.716043	3.936997	-0.869535	-1.724530	3.962644	0.920509	1.744143	3.967546	-0.884171
H	4.100962	4.261080	-1.343389	-4.104708	4.269800	1.387409	4.125971	4.277493	-1.335891
C	3.775725	-1.213361	0.082047	-3.776090	-1.196400	-0.107968	3.778080	-1.199531	0.100015
C	4.088626	-2.507213	0.513364	-4.097772	-2.469967	-0.588665	4.093568	-2.481875	0.565886
C	4.812595	-0.311844	-0.282060	-4.804783	-0.294644	0.293706	4.813467	-0.298013	-0.284065
C	5.427371	-2.902681	0.508369	-5.436848	-2.868142	-0.581551	5.430208	-2.882148	0.562795
H	3.338484	-3.189912	0.887687	-3.355792	-3.136678	-1.007967	3.346539	-3.151768	0.970609
C	6.146012	-0.731582	-0.284511	-6.139218	-0.718312	0.295286	6.146395	-0.725162	-0.283088
C	6.448963	-2.035586	0.098368	-6.448496	-2.009188	-0.126954	6.448665	-2.021567	0.124707
H	5.675942	-3.906273	0.843414	-5.692456	-3.856995	-0.952477	5.681151	-3.875766	0.924239
H	6.936340	-0.041388	-0.567579	-6.927249	-0.037767	0.606932	6.938104	-0.043262	-0.582146
H	7.480985	-2.375401	0.101458	-7.482466	-2.344393	-0.130385	7.481143	-2.361003	0.130484
C	-2.054491	1.728495	0.519563	2.048532	1.711442	-0.556842	-2.050067	1.710312	0.542713
C	-3.158330	2.456796	1.008236	3.145102	2.355301	-1.145156	-3.152801	2.362918	1.116935
C	-0.769527	2.331079	0.455748	0.781703	2.343060	-0.427753	-0.775660	2.339438	0.418556
C	-3.003600	3.774863	1.413332	3.035410	3.687122	-1.555365	-3.045564	3.693040	1.519744
C	-0.658923	3.670814	0.892579	0.719646	3.686153	-0.852924	-0.722582	3.690786	0.830189
C	-1.748162	4.394952	1.355426	1.821084	4.355517	-1.392573	-1.825507	4.359812	1.356756
H	-3.863519	4.314887	1.802262	3.890901	4.185392	-2.002617	-3.900672	4.195112	1.962869
H	0.321240	4.137174	0.893795	-0.227634	4.210758	-0.783475	0.223942	4.216964	0.765033
H	-1.627311	5.422163	1.689103	1.724216	5.392801	-1.704551	-1.730456	5.398804	1.664216
C	-3.419971	-0.078519	-0.480779	3.394838	-0.067628	0.490379	-3.407306	-0.070583	-0.484462
C	-4.153667	0.769102	-1.324915	4.173312	0.830303	1.251997	-4.180214	0.820274	-1.255277
C	-3.788503	-1.430842	-0.338760	3.762162	-1.432898	0.396727	-3.776180	-1.430897	-0.372242
C	-5.284766	0.298542	-1.984984	5.325815	0.392424	1.886705	-5.341049	0.380815	-1.876163
C	-4.920529	-1.882380	-1.028196	4.932664	-1.838592	1.042741	-4.954376	-1.839548	-1.003586
C	-5.676423	-1.031193	-1.833458	5.715365	-0.945111	1.776845	-5.737915	-0.951378	-1.742559
H	-5.843226	0.969311	-2.632659	5.907810	1.090075	2.482144	-5.922414	1.073404	-2.478005
H	-5.225182	-2.918946	-0.937950	5.248645	-2.873413	0.984341	-5.273711	-2.872402	-0.931053
H	-6.555958	-1.409905	-2.347177	6.614582	-1.298678	2.273366	-6.643318	-1.306555	-2.226614
H	-4.128359	1.979656	1.093289	4.079782	1.823051	-1.287447	-4.087580	1.830524	1.257553
H	-3.829417	1.792343	-1.475398	3.847326	1.857074	1.363700	-3.847558	1.842903	-1.384443
C	-2.919088	-2.318021	0.554749	2.892412	-2.364088	-0.444137	-2.892898	-2.358494	0.458569
C	-3.161399	-3.815471	0.310914	3.115882	-3.846720	-0.099853	-3.122606	-3.841924	0.122830
H	-2.960207	-4.102618	-0.725941	2.883178	-4.063615	0.947050	-2.907657	-4.062423	-0.927081
H	-2.526753	-4.419079	0.965631	2.496836	-4.486195	-0.733606	-2.492542	-4.479045	0.747925

H	-4.194376	-4.084115	0.548048	4.151552	-4.136855	-0.291779	-4.154967	-4.131278	0.333350
C	-3.248098	-2.019867	2.045739	3.262894	-2.164168	-1.950495	-3.235485	-2.153272	1.969323
H	-4.293132	-2.270970	2.258266	4.309021	-2.442442	-2.114571	-4.277822	-2.432743	2.154537
H	-2.607623	-2.620633	2.700487	2.629706	-2.798233	-2.578922	-2.589766	-2.783532	2.588752
H	-3.094317	-0.967440	2.295368	3.128002	-1.127236	-2.266883	-3.097037	-1.115018	2.279924
2DMACBN		S₀			S₁			T₁	
C	-0.581905	-2.285371	-0.122308	-0.612975	-2.267943	-0.111444	-0.611729	-2.258502	-0.135545
C	0.730437	-2.753262	-0.097671	0.684716	-2.771304	-0.118725	0.685376	-2.767551	-0.133859
C	1.836920	-1.910266	0.058250	1.796914	-1.926398	0.005414	1.796347	-1.918737	0.008359
C	1.571908	-0.531527	0.135663	1.543421	-0.529721	0.100558	1.546224	-0.526601	0.099254
C	0.255245	-0.015703	0.139767	0.247593	0.009214	0.137883	0.247199	0.021594	0.130621
C	-0.832156	-0.914184	0.028146	-0.832945	-0.880029	0.063578	-0.833496	-0.877093	0.047889
H	-1.395333	-2.988181	-0.260833	-1.448330	-2.942604	-0.262063	-1.447220	-2.932649	-0.290152
H	0.881610	-3.822531	-0.199414	0.819244	-3.839331	-0.236539	0.820083	-3.834521	-0.255741
B	0.015666	1.480135	0.249548	0.015352	1.529480	0.213741	0.017957	1.526367	0.214383
N	2.654694	0.360720	0.181608	2.631159	0.348893	0.156265	2.637156	0.352236	0.152938
N	-2.140140	-0.400564	0.023917	-2.137824	-0.361770	0.067634	-2.141964	-0.359116	0.062981
C	2.509186	1.656435	0.722395	2.498228	1.642735	0.759360	2.507434	1.645806	0.744696
C	3.633753	2.297845	1.280371	3.609156	2.195367	1.405082	3.624717	2.207567	1.377855
C	1.232787	2.284661	0.765680	1.236175	2.315487	0.721231	1.241823	2.314651	0.716424
C	3.510429	3.551432	1.863234	3.537755	3.475034	1.965816	3.552815	3.483981	1.937183
C	1.154968	3.552519	1.384478	1.217740	3.612212	1.298027	1.224360	3.610560	1.293781
C	2.265330	4.191077	1.919195	2.335984	4.187400	1.894149	2.344837	4.190461	1.877865
H	4.387660	4.021031	2.301859	4.409506	3.898361	2.456973	4.426026	3.911898	2.421626
H	0.182925	4.029213	1.468555	0.281295	4.161584	1.306576	0.285826	4.155982	1.312964
H	2.168497	5.164526	2.392707	2.267818	5.184142	2.324895	2.276013	5.186158	2.310935
C	3.827199	-0.044050	-0.517039	3.815204	-0.042233	-0.504862	3.822485	-0.046619	-0.506547
C	4.156204	-1.414699	-0.553983	4.132280	-1.418093	-0.590344	4.136971	-1.422220	-0.577046
C	4.578691	0.883452	-1.255093	4.619736	0.910836	-1.158329	4.622318	0.898980	-1.173464
C	5.267277	-1.804275	-1.312150	5.277778	-1.784739	-1.304566	5.281941	-1.797176	-1.288586
C	5.688368	0.470003	-1.985875	5.750842	0.514421	-1.859695	5.754304	0.495433	-1.870650
C	6.040550	-0.878866	-2.012407	6.090278	-0.838236	-1.929757	6.093863	-0.857325	-1.924051
H	5.542780	-2.851754	-1.359910	5.549568	-2.831027	-1.383926	5.553055	-2.844308	-1.357643
H	6.260542	1.202528	-2.549275	6.355331	1.262704	-2.365331	6.357808	1.237820	-2.385939
H	6.902804	-1.213860	-2.582721	6.971964	-1.159241	-2.477571	6.975468	-1.184431	-2.468437
C	-2.399799	0.940218	-0.325261	-2.408822	0.974750	-0.364992	-2.414111	0.976378	-0.351812
C	-3.690270	1.242442	-0.824180	-3.691204	1.237506	-0.871986	-3.701797	1.244767	-0.851970
C	-1.397706	1.937267	-0.177268	-1.394995	1.971265	-0.222148	-1.398140	1.972540	-0.207057
C	-3.980680	2.575730	-1.109761	-4.006370	2.568170	-1.201088	-4.017047	2.574651	-1.167465
C	-1.746284	3.258837	-0.526625	-1.775673	3.283735	-0.590442	-1.781844	3.286610	-0.562900
C	-3.020460	3.584199	-0.964551	-3.054121	3.578304	-1.051963	-3.061799	3.584007	-1.014687
H	-4.960543	2.845114	-1.488047	-4.989119	2.821127	-1.579951	-5.000242	2.832177	-1.541965
H	-0.989539	4.035028	-0.467250	-1.040415	4.079843	-0.527128	-1.046835	4.082793	-0.499206
H	-3.272832	4.609960	-1.220902	-3.314785	4.601513	-1.314462	-3.323678	4.609018	-1.268852
C	-3.236577	-1.136767	0.556779	-3.209977	-1.092158	0.607561	-3.213861	-1.099905	0.598167
C	-4.524058	-0.896650	0.039934	-4.508913	-0.874141	0.091256	-4.512088	-0.882669	0.084303

C	-3.061413	-1.997995	1.650437	-3.011436	-1.952845	1.706077	-3.010380	-1.965858	1.689574
C	-5.605723	-1.565943	0.625356	-5.569439	-1.562315	0.686965	-5.570058	-1.581880	0.672653
C	-4.151494	-2.664312	2.202228	-4.085113	-2.633844	2.265520	-4.081461	-2.655255	2.244904
H	-2.073899	-2.133850	2.076055	-2.021802	-2.049162	2.138073	-2.019395	-2.063276	2.117847
C	-5.429983	-2.453422	1.686677	-5.369943	-2.442443	1.753606	-5.366462	-2.468194	1.732766
H	-6.608791	-1.397757	0.250018	-6.578316	-1.419988	0.317054	-6.579349	-1.441364	0.303282
H	-3.999258	-3.330150	3.047765	-3.921249	-3.288136	3.117475	-3.914419	-3.314765	3.092142
H	-6.288654	-2.965209	2.113000	-6.218723	-2.961870	2.190094	-6.212597	-2.995911	2.164394
C	-4.648479	0.083210	-1.127673	-4.653433	0.065395	-1.105191	-4.661872	0.073439	-1.098387
C	-4.181804	-0.621286	-2.434479	-4.216752	-0.691533	-2.394854	-4.226242	-0.663637	-2.399625
H	-4.231166	0.077014	-3.276862	-4.283247	-0.023295	-3.259712	-4.296498	0.016382	-3.254921
H	-3.155321	-0.986855	-2.357920	-3.187466	-1.051767	-2.326761	-3.196207	-1.023044	-2.339409
H	-4.832242	-1.475144	-2.653774	-4.870654	-1.553144	-2.570268	-4.879002	-1.523870	-2.585098
C	-6.094833	0.556079	-1.342038	-6.106379	0.526776	-1.305064	-6.116148	0.534802	-1.287874
H	-6.157132	1.235523	-2.196130	-6.185590	1.178202	-2.178809	-6.199510	1.197457	-2.152718
H	-6.746846	-0.290264	-1.574237	-6.761767	-0.327070	-1.497244	-6.770369	-0.317720	-1.489316
H	-6.495558	1.069361	-0.462276	-6.489021	1.068690	-0.434670	-6.497080	1.064236	-0.409113
H	4.283383	1.926291	-1.268584	4.338730	1.956528	-1.128814	4.338830	1.944371	-1.157902
H	4.596869	1.799473	1.280827	4.535694	1.633875	1.467817	4.552944	1.648397	1.434983
C	3.279597	-2.389627	0.238188	3.232919	-2.420901	0.133888	3.231595	-2.416682	0.151640
C	3.656500	-2.298743	1.744843	3.603857	-2.416682	1.652124	3.592695	-2.401764	1.670942
H	3.538664	-1.284115	2.132960	3.501146	-1.421693	2.091352	3.492564	-1.402782	2.101611
H	3.016167	-2.963684	2.334683	2.952069	-3.103140	2.202323	2.933330	-3.079803	2.222550
H	4.699200	-2.601166	1.892737	4.641280	-2.743335	1.778413	4.627286	-2.733429	1.807810
C	3.470963	-3.847503	-0.208449	3.408490	-3.856736	-0.388683	3.407476	-3.856675	-0.358843
H	3.231064	-3.988496	-1.267048	3.167668	-3.936897	-1.453132	3.173356	-3.945135	-1.424111
H	4.501218	-4.173341	-0.041827	4.435035	-4.199903	-0.239437	4.432308	-4.201049	-0.200147
H	2.837416	-4.516202	0.380582	2.770583	-4.550099	0.165001	2.763880	-4.543617	0.196140

TMCzDMACBN

	S₀			S₁			T₁		
C	-1.862369	-1.994404	0.207750	-1.834438	-2.016976	0.173681	-1.836779	-2.010757	0.167635
C	-0.794110	-2.878853	0.058123	-0.754983	-2.910343	0.070627	-0.762560	-2.905686	0.048858
C	0.532555	-2.457485	-0.027095	0.553446	-2.458608	0.007806	0.548581	-2.448976	-0.025917
C	0.835459	-1.096105	0.074914	0.843392	-1.073861	0.107158	0.842221	-1.073580	0.082872
C	-0.219544	-0.141019	0.154669	-0.208592	-0.130613	0.155122	-0.207518	-0.120397	0.138365
C	-1.552295	-0.619244	0.191540	-1.525029	-0.635398	0.169189	-1.527509	-0.629678	0.158031
H	-0.981917	-3.945906	0.010873	-0.931708	-3.976367	0.003233	-0.938536	-3.971558	-0.016389
H	1.298275	-3.197549	-0.204511	1.339098	-3.177587	-0.172261	1.332303	-3.169587	-0.210204
B	0.035259	1.369191	0.149814	0.039268	1.395985	0.112250	0.040484	1.394323	0.110376
N	2.149683	-0.605815	0.047386	2.150231	-0.593025	0.057982	2.155411	-0.593282	0.045488
N	-2.619562	0.293524	0.173509	-2.594579	0.279648	0.139483	-2.598219	0.283108	0.136013
C	2.416549	0.739761	-0.195236	2.421908	0.761062	-0.217909	2.430657	0.759752	-0.215733
C	3.801742	0.927557	-0.392867	3.800199	0.933087	-0.422474	3.810851	0.932805	-0.411916
C	1.478889	1.784200	-0.212759	1.468975	1.802908	-0.235994	1.479133	1.803955	-0.226398
C	4.271156	2.203519	-0.693506	4.290722	2.215756	-0.728274	4.303493	2.215128	-0.704120
C	2.008996	3.052454	-0.537159	2.020519	3.075954	-0.564199	2.032492	3.075984	-0.544191
C	3.369915	3.279998	-0.787189	3.385580	3.286799	-0.814194	3.397987	3.288730	-0.786716

H	5.332548	2.372574	-0.862246	5.352107	2.379508	-0.894452	5.365759	2.380500	-0.863093
H	1.329931	3.897258	-0.610781	1.350967	3.927971	-0.641169	1.364876	3.929552	-0.617182
C	3.387663	-1.285379	0.103420	3.383305	-1.275194	0.124884	3.384892	-1.277031	0.115336
C	3.711089	-2.596180	0.468975	3.708586	-2.571834	0.536655	3.704613	-2.579716	0.516510
C	4.424633	-0.364369	-0.196839	4.417012	-0.353605	-0.205016	4.424111	-0.357109	-0.201484
C	5.052191	-2.977766	0.461112	5.048002	-2.960841	0.528577	5.041726	-2.970887	0.512224
H	2.966225	-3.307257	0.798929	2.966943	-3.267544	0.906982	2.958616	-3.276479	0.875610
C	5.760337	-0.776101	-0.201446	5.751468	-0.773522	-0.206982	5.757350	-0.780536	-0.201337
C	6.092833	-2.096022	0.112142	6.083660	-2.085989	0.141924	6.083147	-2.096276	0.137363
H	5.297915	-3.997326	0.749457	5.296183	-3.969434	0.850268	5.286131	-3.982417	0.827646
H	6.544613	-0.060264	-0.435761	6.537515	-0.068117	-0.465537	6.546493	-0.075294	-0.450635
C	-2.455237	1.625406	0.605235	-2.446486	1.607456	0.646031	-2.449368	1.609944	0.628393
C	-3.567743	2.328811	1.110440	-3.551547	2.226512	1.245325	-3.559567	2.240848	1.212425
C	-1.170540	2.231527	0.588879	-1.176804	2.244706	0.565475	-1.172800	2.243644	0.551945
C	-3.421785	3.626567	1.579443	-3.448446	3.537546	1.717532	-3.456947	3.551280	1.675027
C	-1.069152	3.548945	1.090655	-1.122510	3.568847	1.053189	-1.124064	3.575835	1.026668
C	-2.166576	4.249547	1.570576	-2.230934	4.212710	1.605041	-2.233064	4.223038	1.563954
H	-4.288600	4.146888	1.979816	-4.310789	4.015151	2.174262	-4.318983	4.034758	2.125703
H	-0.089860	4.015490	1.128841	-0.173848	4.094703	1.023921	-0.175004	4.100913	1.002047
H	-2.052399	5.259917	1.954383	-2.139386	5.234358	1.966610	-2.142036	5.246766	1.920167
C	-3.802463	-0.136938	-0.494382	-3.783526	-0.123733	-0.495743	-3.795520	-0.128126	-0.490743
C	-4.526161	0.745538	-1.311050	-4.552551	0.803999	-1.227980	-4.558832	0.789963	-1.236422
C	-4.170890	-1.494540	-0.415757	-4.150188	-1.490408	-0.465560	-4.162841	-1.491156	-0.439474
C	-5.647194	0.302647	-2.006509	-5.697999	0.392918	-1.894427	-5.710303	0.373444	-1.891369
C	-5.292328	-1.917226	-1.139944	-5.311966	-1.870570	-1.143265	-5.329478	-1.878438	-1.105974
C	-6.038446	-1.032934	-1.918270	-6.087770	-0.947734	-1.847135	-6.105507	-0.963574	-1.819220
H	-6.197949	1.000182	-2.632172	-6.273993	1.115931	-2.465165	-6.285397	1.089635	-2.471486
H	-5.596577	-2.957052	-1.098711	-5.625691	-2.907812	-1.133640	-5.645054	-2.914829	-1.080723
H	-6.910050	-1.390166	-2.460157	-6.981163	-1.280292	-2.368219	-7.003172	-1.300724	-2.329992
H	-4.538054	1.847026	1.158115	-4.488922	1.689804	1.347437	-4.498083	1.706007	1.313119
H	-4.201666	1.774752	-1.412356	-4.228165	1.835535	-1.290259	-4.229304	1.818629	-1.317470
C	-3.312931	-2.417666	0.452015	-3.284175	-2.456191	0.340046	-3.285021	-2.449503	0.362605
C	3.873615	4.657007	-1.151337	3.882760	4.661203	-1.197913	3.900875	4.664974	-1.153612
H	4.236887	4.689370	-2.186467	3.912408	4.783068	-2.289315	4.041877	4.759356	-2.238868
H	3.086004	5.410042	-1.055445	3.234295	5.449403	-0.801916	3.198482	5.446146	-0.847063
H	4.708384	4.962713	-0.509527	4.897683	4.840385	-0.826815	4.868759	4.877321	-0.685862
C	7.525051	-2.571689	0.086440	7.515388	-2.561127	0.122623	7.512932	-2.577369	0.121100
H	7.721276	-3.198393	-0.793364	7.691084	-3.263430	-0.702978	7.688961	-3.274869	-0.708369
H	8.226122	-1.732362	0.053479	8.213917	-1.728178	-0.000007	8.215431	-1.746586	0.007003
H	7.764264	-3.175334	0.969205	7.777070	-3.086735	1.048545	7.768192	-3.110071	1.044681
C	-3.550074	-3.903715	0.142642	-3.506009	-3.923340	-0.065386	-3.512132	-3.919592	-0.027992
H	-3.333865	-4.147329	-0.902322	-3.269735	-4.097365	-1.119505	-3.291144	-4.102249	-1.083940
H	-2.923929	-4.533665	0.780504	-2.889525	-4.588665	0.543915	-2.885858	-4.579245	0.577437
H	-4.585984	-4.182617	0.353740	-4.542644	-4.220284	0.110407	-4.545988	-4.215677	0.165381
C	-3.663277	-2.182195	1.949384	-3.658141	-2.318714	1.852154	-3.634134	-2.300342	1.877986
H	-4.711009	-2.442054	2.136841	-4.704500	-2.604485	2.001207	-4.677017	-2.587721	2.047533

H	-3.031483	-2.809665	2.587354	-3.026389	-2.977501	2.456290	-2.990783	-2.952222	2.477404
H	-3.513585	-1.141120	2.244886	-3.525687	-1.295467	2.211133	-3.498985	-1.274036	2.227089
PXZTMCzBN		S₀			S₁			T₁	
C	1.859406	-1.577052	0.184464	1.836869	-1.588209	0.209054	-1.827813	-1.586579	-0.192352
C	0.888260	-2.552641	0.432107	0.864726	-2.553801	0.506751	-0.848215	-2.556197	-0.493442
C	-0.482939	-2.252830	0.464785	-0.506515	-2.217666	0.522698	0.514575	-2.220194	-0.506359
C	-0.884151	-0.908943	0.204873	-0.875109	-0.890301	0.172066	0.881385	-0.884955	-0.162123
C	0.075267	0.116552	0.027596	0.077003	0.133777	-0.010948	-0.075516	0.144831	0.012709
C	1.415375	-0.261413	-0.004313	1.404111	-0.265916	-0.032571	-1.401723	-0.263516	0.044464
H	1.193547	-3.571615	0.658339	1.156120	-3.564866	0.776161	-1.142076	-3.562583	-0.776137
B	-0.235102	1.600033	0.075659	-0.221594	1.629715	0.038561	0.215060	1.635179	-0.045762
N	-2.228012	-0.497754	0.202402	-2.236316	-0.447667	0.095539	2.234720	-0.435797	-0.085433
N	2.482332	0.609437	-0.156687	2.476287	0.590157	-0.213426	-2.479452	0.589705	0.214378
C	-2.581232	0.822823	0.562889	-2.592550	0.851079	0.557294	2.588585	0.864328	-0.541068
C	-3.919563	1.017255	0.958093	-3.921331	1.038756	0.955362	3.918965	1.053431	-0.938055
C	-1.671716	1.912508	0.566072	-1.663782	1.926971	0.574785	1.649654	1.939520	-0.566672
C	-4.359683	2.246679	1.419389	-4.364594	2.247157	1.505551	4.361199	2.264359	-1.484086
C	-2.146509	3.146467	1.070561	-2.137278	3.125691	1.136216	2.128520	3.142010	-1.122244
C	-3.455619	3.314546	1.497229	-3.449765	3.285052	1.611024	3.442318	3.300722	-1.585809
H	-5.393124	2.348255	1.736429	-5.403071	2.347536	1.802777	5.399480	2.368109	-1.779589
H	-1.456161	3.979452	1.151997	-1.460517	3.970797	1.207331	1.449967	3.984625	-1.203537
H	-3.789541	4.271189	1.889644	-3.761152	4.236341	2.033676	3.754850	4.253487	-2.005229
C	-3.261150	-1.221342	-0.451141	-3.238787	-1.174719	-0.523072	3.245271	-1.173746	0.515930
C	-3.050885	-2.095730	-1.522461	-3.013529	-2.150576	-1.515464	3.019031	-2.147213	1.509688
C	-4.578458	-0.970384	-0.039143	-4.582167	-0.912273	-0.139459	4.581978	-0.912994	0.123553
C	-4.129015	-2.770969	-2.099206	-4.078267	-2.860458	-2.050738	4.082069	-2.864409	2.035771
H	-2.044047	-2.252374	-1.893974	-2.000484	-2.328003	-1.856889	2.007244	-2.312858	1.860552
C	-5.656728	-1.633356	-0.613423	-5.645923	-1.642202	-0.665480	5.645362	-1.654154	0.636017
C	-5.427596	-2.556051	-1.636727	-5.394547	-2.623954	-1.618640	5.394574	-2.636471	1.587763
H	-3.946529	-3.461392	-2.917849	-3.887530	-3.601719	-2.821379	3.894764	-3.602083	2.810361
H	-6.657900	-1.412667	-0.256344	-6.651506	-1.414884	-0.326754	6.649995	-1.431892	0.291511
H	-6.265350	-3.084466	-2.082588	-6.219019	-3.190857	-2.039845	6.219462	-3.209541	1.999820
C	2.269815	1.961867	-0.483693	2.275403	1.957039	-0.544565	-2.286883	1.958885	0.533776
C	3.309312	2.746304	-1.014815	3.313176	2.712435	-1.098619	-3.330894	2.713938	1.081907
C	0.957365	2.517048	-0.325781	0.966645	2.531144	-0.335532	-0.984085	2.536978	0.329810
C	3.092913	4.080141	-1.338885	3.141866	4.072400	-1.374061	-3.162145	4.071695	1.356040
C	0.793383	3.873147	-0.683395	0.855449	3.918049	-0.631174	-0.872770	3.918494	0.628972
C	1.832582	4.658823	-1.165070	1.908575	4.680216	-1.118302	-1.929371	4.682167	1.109686
H	3.911922	4.662140	-1.754323	3.964862	4.639825	-1.800212	-3.988464	4.638097	1.777611
H	-0.197793	4.308990	-0.611828	-0.113802	4.392899	-0.512015	0.097294	4.392917	0.514958
H	1.661595	5.698489	-1.430949	1.764449	5.737288	-1.330732	-1.787577	5.738978	1.323878
C	3.664891	-0.152988	-0.003541	3.645615	-0.174030	-0.034970	-3.643437	-0.180469	0.034693
C	5.009194	0.223985	0.078467	4.993560	0.191495	0.036897	-4.993325	0.176848	-0.044446
C	3.303801	-1.517875	0.178116	3.276163	-1.535442	0.192956	-3.262985	-1.541459	-0.185404
C	5.969387	-0.767833	0.272629	5.945538	-0.802406	0.263089	-5.937871	-0.823234	-0.270642
C	4.291270	-2.490660	0.365945	4.258658	-2.510427	0.410601	-4.241140	-2.523936	-0.403910

C	5.639938	-2.131261	0.400073	5.608903	-2.161622	0.432640	-5.591201	-2.182350	-0.433922
H	7.012618	-0.467518	0.338345	6.991170	-0.507623	0.318837	-6.985113	-0.535632	-0.332454
H	4.003454	-3.530829	0.498597	3.962097	-3.543743	0.575365	-3.938159	-3.556353	-0.561999
H	4.273143	2.308923	-1.231355	4.253320	2.244613	-1.357062	-4.270577	2.244409	1.338719
H	5.325622	1.257598	0.040437	5.316775	1.220918	-0.038825	-5.323535	1.204489	0.025815
C	6.723601	-3.167123	0.576017	6.687161	-3.196933	0.640959	-6.663759	-3.222498	-0.647846
H	7.444204	-2.868097	1.345875	7.390679	-2.893299	1.425169	-7.335114	-2.945056	-1.469381
H	6.308180	-4.137333	0.864039	6.263707	-4.164131	0.927836	-6.232411	-4.199667	-0.884571
H	7.289818	-3.313710	-0.352891	7.275186	-3.352590	-0.272911	-7.287774	-3.344539	0.246861
C	-1.439571	-3.336580	0.902436	-1.481937	-3.265739	1.004945	1.492522	-3.265984	-0.992730
H	-2.234531	-2.935968	1.538905	-2.344293	-2.824060	1.511953	2.345579	-2.823638	-1.514754
H	-1.928497	-3.846103	0.064933	-1.870196	-3.893852	0.194800	1.894154	-3.886367	-0.183817
H	-0.901355	-4.094304	1.479435	-0.983260	-3.928905	1.717996	0.988437	-3.936326	-1.694921
O	-4.814959	-0.034911	0.943246	-4.861925	0.050598	0.782672	4.858768	0.062636	-0.784438
PTZTMCzBN		S₀			S₁			T₁	
C	1.979326	-1.566272	0.238141	1.961548	-1.573141	0.272912	-1.947308	-1.572325	-0.255032
C	0.997657	-2.536856	0.463948	0.979276	-2.529504	0.578681	-0.954183	-2.533008	-0.547644
C	-0.372643	-2.226822	0.467443	-0.389928	-2.188830	0.566255	0.404936	-2.188984	-0.529561
C	-0.758581	-0.878321	0.221279	-0.746494	-0.865772	0.197152	0.757471	-0.848606	-0.183014
C	0.208224	0.133723	0.039122	0.210005	0.142322	-0.019142	-0.209834	0.163827	0.009543
C	1.545620	-0.250909	0.026756	1.536863	-0.261372	-0.016579	-1.532909	-0.252622	0.016873
H	1.290939	-3.560676	0.684049	1.262616	-3.538761	0.863471	-1.235876	-3.541701	-0.834628
B	-0.102563	1.615667	0.031822	-0.092612	1.632234	-0.022260	0.081306	1.651090	0.014657
N	-2.111109	-0.470989	0.213875	-2.115984	-0.423493	0.105128	2.110948	-0.399840	-0.090748
N	2.616771	0.612426	-0.134299	2.611166	0.588568	-0.216812	-2.615521	0.589625	0.202594
C	-2.458776	0.853852	0.590670	-2.464093	0.868946	0.606396	2.460773	0.900494	-0.568489
C	-3.770466	1.067084	1.066175	-3.756312	1.083276	1.109303	3.758846	1.112928	-1.063863
C	-1.539008	1.939036	0.521125	-1.516945	1.938929	0.547069	1.506234	1.969699	-0.517863
C	-4.173744	2.333009	1.485812	-4.133547	2.327200	1.655626	4.139901	2.363843	-1.589098
C	-1.976662	3.191514	1.004884	-1.935014	3.159010	1.105117	1.934526	3.198254	-1.057782
C	-3.266238	3.395975	1.475962	-3.206653	3.356635	1.661582	3.212857	3.395984	-1.589905
H	-5.187826	2.476761	1.847999	-5.142474	2.471695	2.029230	5.150973	2.512284	-1.954460
H	-1.272559	4.016745	1.029707	-1.239989	3.992414	1.105035	1.236589	4.028847	-1.070885
H	-3.574342	4.372627	1.839332	-3.476416	4.325485	2.073242	3.490968	4.368380	-1.988409
C	-3.057079	-1.168457	-0.597020	-3.032684	-1.137771	-0.648763	3.041702	-1.138248	0.638935
C	-2.677106	-1.797367	-1.790987	-2.625128	-1.951003	-1.732791	2.636583	-1.928804	1.737786
C	-4.412660	-1.174510	-0.230086	-4.425344	-1.077908	-0.347446	4.421024	-1.103869	0.304189
C	-3.618738	-2.482516	-2.557771	-3.551651	-2.677215	-2.458981	3.558545	-2.684137	2.440943
H	-1.640443	-1.759044	-2.108090	-1.574695	-1.978484	-1.996753	1.593101	-1.917950	2.030148
C	-5.358146	-1.840319	-1.014969	-5.349819	-1.830308	-1.088447	5.341121	-1.886827	1.017293
C	-4.958884	-2.515752	-2.167760	-4.920479	-2.630638	-2.136458	4.915254	-2.679858	2.073557
H	-3.301640	-2.978604	-3.471067	-3.214091	-3.276766	-3.299647	3.228227	-3.268858	3.294559
H	-6.402959	-1.824974	-0.718301	-6.404724	-1.770060	-0.837508	6.391273	-1.853290	0.742697
H	-5.694441	-3.045280	-2.766743	-5.640582	-3.203412	-2.712627	5.635297	-3.274862	2.627210
C	2.410274	1.954470	-0.505586	2.410338	1.941668	-0.598286	-2.430207	1.946913	0.574279
C	3.459685	2.721669	-1.042683	3.453147	2.679139	-1.169328	-3.484887	2.679226	1.133562

C	1.095078	2.516342	-0.389113	1.099618	2.522428	-0.426353	-1.125401	2.535262	0.414733
C	3.249656	4.043143	-1.417215	3.281450	4.025514	-1.500180	-3.322449	4.024214	1.466463
C	0.938473	3.858808	-0.798456	0.987413	3.893206	-0.781169	-1.020652	3.901970	0.775193
C	1.986239	4.627067	-1.289009	2.044152	4.639848	-1.286090	-2.086062	4.644742	1.269488
H	4.076763	4.610589	-1.836693	4.108499	4.577797	-1.938484	-4.157035	4.572286	1.895953
H	-0.053744	4.296797	-0.761134	0.014716	4.368475	-0.693934	-0.048922	4.380714	0.698823
H	1.820410	5.656227	-1.595724	1.899559	5.686576	-1.544061	-1.948845	5.691277	1.531536
C	3.794346	-0.153365	0.043303	3.777446	-0.171024	-0.002725	-3.773673	-0.182561	-0.008995
C	5.139518	0.218483	0.131370	5.126172	0.193792	0.065226	-5.124446	0.168659	-0.091662
C	3.424714	-1.513352	0.245277	3.401768	-1.522997	0.269769	-3.382302	-1.535382	-0.262009
C	6.092980	-0.774583	0.351344	6.074216	-0.792907	0.333214	-6.060961	-0.830862	-0.353480
C	4.405443	-2.487272	0.458867	4.381250	-2.491058	0.528811	-4.352692	-2.517392	-0.515685
C	5.755697	-2.133869	0.499222	5.731911	-2.144252	0.548905	-5.704470	-2.182903	-0.549755
H	7.136994	-0.478159	0.421834	7.120262	-0.498994	0.386032	-7.109281	-0.547803	-0.417594
H	4.111074	-3.523417	0.607350	4.081577	-3.517459	0.727875	-4.041848	-3.543307	-0.698665
S	-4.880875	-0.308448	1.241396	-4.993970	-0.161330	1.025276	4.980447	-0.151801	-1.051159
H	4.427723	2.278273	-1.225118	4.397546	2.204503	-1.397929	-4.428653	2.199743	1.354103
H	5.461416	1.249813	0.078953	5.452407	1.219257	-0.044954	-5.461838	1.192069	0.002585
C	6.832354	-3.171854	0.703226	6.805825	-3.173939	0.803425	-6.768534	-3.222995	-0.802759
H	7.550040	-2.860849	1.470995	7.499698	-2.846862	1.586895	-7.431070	-2.928618	-1.625540
H	6.409729	-4.133536	1.008799	6.377158	-4.131162	1.115069	-6.328917	-4.191688	-1.058251
H	7.403087	-3.340858	-0.219084	7.405585	-3.358970	-0.097266	-7.402880	-3.370337	0.080760
C	-1.357940	-3.312361	0.825876	-1.389163	-3.236216	0.998133	1.408897	-3.234980	-0.956250
H	-2.158974	-2.928357	1.465118	-2.248990	-2.797215	1.511823	2.257585	-2.798431	-1.489990
H	-1.835087	-3.758351	-0.054035	-1.777576	-3.820412	0.155259	1.813445	-3.800949	-0.109362
H	-0.850667	-4.115440	1.368468	-0.914657	-3.939398	1.688881	0.929831	-3.952847	-1.628183
DPATMCzBN		S₀			S₁			T₁	
C	1.670623	-1.589139	-0.163188	1.667841	-1.581847	-0.242949	1.670517	-1.569147	-0.258126
C	0.666292	-2.544073	-0.343232	0.691490	-2.562370	-0.463002	0.689749	-2.560128	-0.511804
C	-0.694087	-2.211774	-0.413006	-0.663399	-2.220890	-0.536103	-0.661050	-2.221516	-0.580930
C	-1.068964	-0.833018	-0.273753	-1.058260	-0.824624	-0.342420	-1.055832	-0.839788	-0.372414
C	-0.066130	0.159429	-0.128042	-0.087128	0.181391	-0.201533	-0.080535	0.189907	-0.216968
C	1.263234	-0.256645	-0.055971	1.231437	-0.230665	-0.113927	1.236515	-0.224354	-0.108735
H	0.940061	-3.588135	-0.473320	0.980509	-3.595443	-0.628415	0.988588	-3.585477	-0.701567
B	-0.324378	1.648256	-0.190404	-0.379646	1.686881	-0.192151	-0.371416	1.673647	-0.211712
N	-2.405497	-0.382813	-0.313904	-2.397279	-0.418359	-0.361209	-2.397318	-0.417852	-0.351160
N	2.357829	0.586683	0.074839	2.300350	0.608038	0.088061	2.308010	0.616955	0.104937
C	-2.742882	0.970281	-0.573160	-2.782072	0.940429	-0.675985	-2.782407	0.934147	-0.671082
C	-4.098921	1.310998	-0.792387	-4.117936	1.197175	-1.011819	-4.123553	1.189103	-0.998466
C	-1.757421	2.005470	-0.626873	-1.824669	2.008541	-0.632043	-1.827151	2.000533	-0.650431
C	-4.462704	2.595911	-1.164332	-4.543551	2.486802	-1.354466	-4.545108	2.471339	-1.363933
C	-2.175577	3.288447	-1.052116	-2.297481	3.283327	-1.026444	-2.294049	3.264786	-1.062639
C	-3.496567	3.595618	-1.331680	-3.623391	3.531476	-1.378077	-3.622944	3.511069	-1.415648
H	-5.513099	2.812226	-1.344872	-5.587051	2.653125	-1.608085	-5.589823	2.637016	-1.612819
H	-1.421951	4.059523	-1.175169	-1.590504	4.105074	-1.063638	-1.586502	4.085475	-1.113620
H	-3.779890	4.591770	-1.660875	-3.934079	4.534563	-1.661770	-3.931638	4.509107	-1.717665

C	-3.436032	-1.212510	0.268430	-3.356229	-1.248641	0.323331	-3.352475	-1.247305	0.342893
C	-4.433474	-1.804823	-0.514305	-4.435387	-1.854334	-0.334904	-4.428805	-1.864155	-0.307822
C	-3.446515	-1.392863	1.655831	-3.197252	-1.436977	1.703802	-3.185324	-1.421535	1.723499
C	-5.431837	-2.571018	0.087957	-5.345623	-2.629415	0.383445	-5.332390	-2.637994	0.421091
H	-4.418476	-1.671585	-1.591632	-4.543833	-1.745478	-1.408937	-4.541652	-1.764685	-1.382295
C	-4.439441	-2.171053	2.253244	-4.107771	-2.217790	2.415311	-4.090614	-2.198899	2.444877
C	-5.436179	-2.759043	1.471945	-5.186767	-2.814116	1.758718	-5.168567	-2.807358	1.797200
H	-6.202159	-3.027486	-0.528061	-6.175489	-3.098685	-0.138376	-6.160869	-3.117087	-0.093820
H	-4.436470	-2.309805	3.331216	-3.977217	-2.350579	3.486102	-3.955474	-2.321638	3.516198
H	-6.211839	-3.360671	1.938279	-5.898009	-3.419662	2.313925	-5.874460	-3.411518	2.360599
C	2.188637	1.949810	0.378982	2.116784	1.980167	0.440217	2.117289	1.981746	0.442223
C	3.251870	2.706341	0.904283	3.162054	2.697980	1.022696	3.154904	2.716495	1.028821
C	0.893435	2.538854	0.214718	0.813596	2.565274	0.235221	0.816000	2.561626	0.231625
C	3.075098	4.046806	1.224207	3.006617	4.051993	1.347885	2.980885	4.062229	1.350177
C	0.768369	3.897709	0.578002	0.718131	3.941212	0.588427	0.699408	3.931213	0.587713
C	1.829464	4.656654	1.055932	1.777623	4.672790	1.111729	1.746589	4.675820	1.113305
H	3.911342	4.607131	1.635272	3.834440	4.596513	1.793168	3.799736	4.614703	1.803202
H	-0.210069	4.361336	0.517019	-0.243197	4.432658	0.487702	-0.268203	4.409898	0.483043
H	1.684698	5.699828	1.324045	1.638109	5.721907	1.364164	1.597038	5.722296	1.369124
C	3.516517	-0.218027	-0.024095	3.473555	-0.177623	-0.016040	3.477167	-0.169020	0.000356
C	4.872938	0.112485	-0.112864	4.818271	0.173032	-0.087083	4.825415	0.175394	-0.050977
C	3.114645	-1.578570	-0.139647	3.098944	-1.545488	-0.179776	3.092621	-1.536807	-0.185193
C	5.803696	-0.917187	-0.242414	5.771106	-0.845778	-0.235297	5.771864	-0.844442	-0.202134
C	4.073091	-2.590175	-0.263521	4.073618	-2.542145	-0.319489	4.070868	-2.538541	-0.327301
C	5.432641	-2.274783	-0.300000	5.431481	-2.206428	-0.331193	5.423064	-2.207624	-0.321007
H	6.856372	-0.653139	-0.313715	6.818748	-0.558787	-0.285778	6.822164	-0.564901	-0.238643
H	3.754313	-3.626612	-0.345831	3.768938	-3.579377	-0.434317	3.763173	-3.573139	-0.456386
H	-4.877498	0.567548	-0.694369	-4.852996	0.404948	-1.010164	-4.860151	0.398613	-0.974324
H	-2.675513	-0.924248	2.260272	-2.367443	-0.956850	2.213435	-2.352660	-0.936710	2.223567
H	4.202680	2.242071	1.121732	4.094356	2.210493	1.271734	4.090410	2.238996	1.285125
H	5.220555	1.136775	-0.129426	5.149909	1.202180	-0.070223	5.163267	1.202198	-0.014670
C	-1.640352	-3.344953	-0.742982	-1.614747	-3.319074	-0.930724	-1.615957	-3.322899	-0.968600
H	-2.296838	-3.621347	0.086884	-2.228354	-3.668917	-0.094772	-2.223617	-3.670681	-0.127809
H	-2.279639	-3.103983	-1.597193	-2.299561	-2.994411	-1.718948	-2.304219	-3.004257	-1.756432
H	-1.062571	-4.233706	-1.012442	-1.051743	-4.176225	-1.309234	-1.053161	-4.180549	-1.346157
C	6.484908	-3.351757	-0.407097	6.501973	-3.262791	-0.449834	6.495712	-3.260437	-0.453544
H	6.043343	-4.320282	-0.660074	6.084720	-4.221560	-0.771220	6.066740	-4.244337	-0.664143
H	7.229798	-3.111305	-1.174398	7.273991	-2.972674	-1.171020	7.196287	-3.019679	-1.261831
H	7.028150	-3.474681	0.538929	7.005330	-3.428524	0.511400	7.086431	-3.346330	0.467265
CzTMCzBN		S₀		S₁			T₁		
C	1.805838	-1.593075	0.038072	-1.793171	-1.595863	-0.054652	-1.796009	-1.588505	-0.065843
C	0.863526	-2.594977	0.265166	-0.859257	-2.618001	-0.287306	-0.856996	-2.618089	-0.323857
C	-0.516422	-2.330210	0.329762	0.504442	-2.329159	-0.378183	0.502269	-2.329852	-0.407070
C	-0.954526	-0.999447	0.078269	0.947706	-0.968979	-0.107758	0.946825	-0.978145	-0.123395
C	-0.018233	0.068074	-0.025757	0.022999	0.102722	-0.046893	0.018037	0.111141	-0.061925
C	1.331167	-0.276357	-0.071992	-1.313403	-0.256855	0.024917	-1.317865	-0.250219	0.025838

H	1.196136	-3.610569	0.467383	-1.196399	-3.626891	-0.506084	-1.201399	-3.617377	-0.571107
B	-0.345690	1.546847	0.166343	0.364024	1.596696	-0.190703	0.352320	1.587592	-0.208085
N	-2.301014	-0.590679	0.038345	2.279481	-0.581864	-0.029174	2.279553	-0.581424	-0.028373
N	2.384747	0.621108	-0.152717	-2.361930	0.628965	0.131922	-2.366584	0.634837	0.144538
C	-2.673493	0.704896	0.405734	2.691048	0.737881	-0.380352	2.690454	0.732916	-0.382323
C	-4.084156	0.785015	0.480739	4.093257	0.774654	-0.440561	4.096057	0.773572	-0.434426
C	-1.812130	1.805021	0.595807	1.836936	1.848494	-0.556035	1.841872	1.843790	-0.568670
C	-4.666594	1.975544	0.912453	4.727052	1.972210	-0.830373	4.725123	1.966084	-0.829016
C	-2.452607	2.980788	1.047094	2.523521	3.025685	-0.977180	2.521833	3.013231	-0.991423
C	-3.836509	3.059854	1.223213	3.915501	3.073020	-1.116458	3.916204	3.063763	-1.129509
H	-5.745967	2.066074	1.004203	5.808643	2.039772	-0.898861	5.807231	2.036363	-0.891068
H	-1.854475	3.859952	1.266161	1.952115	3.921470	-1.197716	1.950571	3.908723	-1.213652
H	-4.280040	3.987253	1.576134	4.381134	4.003860	-1.434049	4.381694	3.992699	-1.451451
C	-3.473681	-1.280693	-0.332850	3.427165	-1.299943	0.337248	3.424804	-1.294411	0.348586
C	-3.630904	-2.469280	-1.049020	3.547709	-2.502231	1.040141	3.540638	-2.498602	1.051656
C	-4.598013	-0.477637	-0.007566	4.570185	-0.505559	0.030886	4.571894	-0.505296	0.045775
C	-4.927013	-2.900643	-1.333470	4.828395	-2.972869	1.329353	4.818174	-2.967829	1.347570
H	-2.778253	-3.029054	-1.409871	2.675953	-3.042306	1.388262	2.665821	-3.037386	1.393597
C	-5.888916	-0.934364	-0.290914	5.844394	-1.004608	0.316516	5.844174	-1.004120	0.337284
C	-6.048983	-2.158070	-0.937415	5.966974	-2.243936	0.947624	5.961653	-2.241952	0.970270
H	-5.062883	-3.824878	-1.888988	4.940759	-3.905098	1.875563	4.927402	-3.898940	1.896438
H	-6.753855	-0.327120	-0.037371	6.729217	-0.420567	0.078530	6.730715	-0.421879	0.101222
H	-7.046182	-2.521928	-1.169421	6.954970	-2.632512	1.180400	6.947352	-2.632729	1.208244
C	2.155716	1.994380	-0.349349	-2.144526	2.019725	0.334781	-2.146426	2.020364	0.337276
C	3.182268	2.838809	-0.809253	-3.176642	2.834812	0.813178	-3.173767	2.844186	0.818555
C	0.839272	2.512835	-0.128359	-0.829812	2.545984	0.090980	-0.832052	2.543588	0.085314
C	2.950566	4.196799	-0.989069	-2.979711	4.207900	0.973810	-2.968619	4.212802	0.974303
C	0.659906	3.898041	-0.336858	-0.690902	3.944695	0.268508	-0.684821	3.941830	0.260834
C	1.687509	4.741141	-0.739166	-1.734469	4.767279	0.679037	-1.720956	4.769040	0.673321
H	3.758758	4.827479	-1.351207	-3.794851	4.825292	1.341438	-3.777825	4.834872	1.347537
H	-0.333853	4.314400	-0.212724	0.287112	4.387192	0.113964	0.294487	4.379726	0.101155
H	1.504588	5.801674	-0.889710	-1.571372	5.835678	0.799759	-1.553779	5.836701	0.793596
C	3.581957	-0.126520	-0.045257	-3.557777	-0.124578	0.046987	-3.562112	-0.120607	0.060377
C	4.918103	0.270128	0.070834	-4.889766	0.261005	-0.073366	-4.895272	0.261718	-0.046439
C	3.248709	-1.506390	0.039982	-3.222606	-1.509691	-0.027604	-3.218308	-1.506310	-0.029738
C	5.896879	-0.714191	0.200675	-5.869926	-0.735518	-0.182924	-5.872010	-0.736720	-0.158574
C	4.253203	-2.471192	0.165713	-4.225269	-2.483998	-0.133404	-4.223156	-2.484445	-0.137447
C	5.594607	-2.089265	0.231510	-5.570303	-2.109646	-0.194148	-5.565358	-2.112697	-0.185712
H	6.933646	-0.398654	0.292223	-6.907028	-0.420979	-0.271779	-6.911248	-0.426574	-0.237064
H	3.984921	-3.523336	0.224252	-3.950449	-3.534697	-0.180739	-3.945634	-3.533868	-0.194191
H	4.146398	2.434817	-1.082138	-4.125513	2.409198	1.108224	-4.122283	2.423011	1.121074
H	5.214733	1.309507	0.105897	-5.191966	1.297899	-0.123158	-5.202028	1.297937	-0.082355
C	6.697468	-3.114060	0.339084	-6.671069	-3.137759	-0.277532	-6.666538	-3.139978	-0.277437
H	7.417924	-2.848588	1.121161	-7.403761	-2.879127	-1.050006	-7.361480	-2.910769	-1.093485
H	6.301147	-4.107076	0.570911	-6.274954	-4.130793	-0.508471	-6.265152	-4.142662	-0.449971
H	7.259558	-3.195030	-0.600320	-7.216941	-3.212889	0.671612	-7.256939	-3.173937	0.646907

C	-1.396555	-3.447218	0.850582	1.388829	-3.405402	-0.963598	1.396086	-3.407536	-0.979642
H	-2.302939	-3.071871	1.328223	2.325502	-3.014267	-1.360479	2.330996	-3.013582	-1.379013
H	-1.703477	-4.162273	0.079402	1.636831	-4.190564	-0.240855	1.648139	-4.183188	-0.248536
H	-0.841297	-4.014428	1.604338	0.852991	-3.891675	-1.785131	0.865988	-3.905254	-1.797689
DMACTMCzBN		S₀			S₁			T₁	
C	0.185115	-2.235981	-0.287575	0.196218	-2.220052	-0.332729	0.198798	-2.219404	-0.360674
C	-1.184820	-2.544391	-0.317634	-1.168086	-2.555491	-0.373569	-1.157495	-2.554359	-0.401598
C	-2.174832	-1.569429	-0.162469	-2.153548	-1.574110	-0.197709	-2.152255	-1.566418	-0.201503
C	-1.747110	-0.248161	0.016747	-1.728960	-0.233198	-0.005605	-1.732344	-0.228275	-0.000713
C	-0.409790	0.137393	0.035427	-0.406574	0.170502	0.008541	-0.410181	0.182274	-0.005871
C	0.568900	-0.876403	-0.076624	0.560204	-0.847313	-0.079003	0.564079	-0.849246	-0.099786
H	-1.470451	-3.576496	-0.507029	-1.447097	-3.584195	-0.581470	-1.441496	-3.576384	-0.631619
B	-0.102917	1.619675	0.001897	-0.096959	1.668472	0.009883	-0.108607	1.665541	-0.007231
N	-2.824537	0.618607	0.109830	-2.807355	0.615996	0.122779	-2.814209	0.619509	0.132254
N	1.913435	-0.452207	-0.041248	1.899887	-0.410916	0.014731	1.898283	-0.405045	0.018514
C	-2.633483	1.971452	0.449124	-2.629055	1.984982	0.473370	-2.636562	1.986200	0.470577
C	-3.701810	2.748891	0.931247	-3.700658	2.727223	0.977171	-3.706691	2.734362	0.977041
C	-1.316188	2.531351	0.360385	-1.311064	2.559754	0.348078	-1.322386	2.561448	0.341425
C	-3.506923	4.080043	1.279021	-3.547991	4.081235	1.292244	-3.547565	4.083848	1.290341
C	-1.175624	3.883091	0.743703	-1.219724	3.937623	0.685896	-1.222699	3.934876	0.682510
C	-2.240245	4.661728	1.179630	-2.300755	4.689705	1.128378	-2.299178	4.691603	1.126593
H	-4.348375	4.656165	1.656118	-4.396275	4.640560	1.677293	-4.392621	4.645235	1.680125
H	-0.183526	4.322027	0.732191	-0.246219	4.414301	0.637818	-0.247068	4.407306	0.632755
H	-2.084837	5.698086	1.467255	-2.167808	5.740888	1.374755	-2.163451	5.741541	1.375576
C	-3.994535	-0.153520	-0.082895	-3.969877	-0.161309	-0.072850	-3.972828	-0.160919	-0.063548
C	-3.618426	-1.519466	-0.224269	-3.588625	-1.528464	-0.236939	-3.579799	-1.527658	-0.236039
C	-5.335509	0.214000	-0.233085	-5.310725	0.194526	-0.217811	-5.316357	0.187943	-0.200729
C	-4.591239	-2.500653	-0.441380	-4.556250	-2.517391	-0.458775	-4.548169	-2.522697	-0.457689
C	-6.280950	-0.786599	-0.453875	-6.251578	-0.815128	-0.445892	-6.251269	-0.825143	-0.429038
C	-5.938950	-2.149826	-0.543326	-5.907351	-2.176747	-0.549697	-5.896889	-2.187638	-0.541111
H	-4.292191	-3.540973	-0.545024	-4.247429	-3.553482	-0.574498	-4.235140	-3.557069	-0.576815
H	-7.321542	-0.493562	-0.572876	-7.294117	-0.525470	-0.556081	-7.296344	-0.542801	-0.533642
C	2.283005	0.858753	-0.435280	2.300396	0.896684	-0.444753	2.298399	0.901572	-0.430600
C	3.636172	1.050319	-0.813499	3.642733	1.048307	-0.828302	3.645818	1.055780	-0.808805
C	1.347295	1.933568	-0.436485	1.361494	1.974154	-0.424424	1.358135	1.976356	-0.427660
C	4.032678	2.330211	-1.197511	4.071471	2.326936	-1.234617	4.068101	2.329749	-1.223587
C	1.808189	3.189954	-0.884717	1.854364	3.219270	-0.869553	1.846083	3.217112	-0.880872
C	3.127818	3.396306	-1.250288	3.180274	3.395643	-1.260596	3.173011	3.395286	-1.266367
H	5.059262	2.508772	-1.496781	5.100335	2.490398	-1.530421	5.097219	2.495625	-1.517176
H	1.104391	4.012663	-0.957871	1.178423	4.066445	-0.914182	1.166123	4.060236	-0.940231
H	3.463585	4.373693	-1.587211	3.525876	4.375204	-1.583709	3.516696	4.371984	-1.599545
C	2.893526	-1.146983	0.723270	2.847281	-1.122019	0.755935	2.847373	-1.126399	0.757093
C	4.247614	-1.012141	0.361663	4.216004	-1.003541	0.402866	4.214469	-1.010250	0.408834
C	2.530890	-1.856981	1.876215	2.454814	-1.874871	1.882896	2.446305	-1.882567	1.876051
C	5.206707	-1.642859	1.162260	5.145964	-1.688888	1.188206	5.139357	-1.709687	1.188791
C	3.504615	-2.486901	2.647212	3.405226	-2.543768	2.639012	3.391315	-2.561442	2.631281

H	1.488688	-1.901242	2.173217	1.409774	-1.891112	2.171878	1.399248	-1.897508	2.157236
C	4.847548	-2.386802	2.287292	4.756518	-2.458172	2.288047	4.742849	-2.483856	2.282069
H	6.258119	-1.556721	0.912407	6.201323	-1.630755	0.948818	6.195526	-1.655866	0.952311
H	3.210169	-3.036765	3.537385	3.097773	-3.107456	3.515519	3.078109	-3.129309	3.502929
H	5.616223	-2.870683	2.883893	5.509607	-2.973840	2.877525	5.491614	-3.009242	2.868406
C	4.572151	-0.165558	-0.871500	4.572042	-0.171968	-0.829629	4.580487	-0.160912	-0.808723
C	6.055762	0.234996	-0.919955	6.060204	0.220420	-0.837208	6.066507	0.239797	-0.792756
H	6.272024	0.818694	-1.818368	6.303230	0.795468	-1.733557	6.319823	0.823895	-1.680253
H	6.353241	0.822375	-0.045718	6.332581	0.814994	0.040047	6.323599	0.826964	0.094017
H	6.691369	-0.653106	-0.971469	6.694230	-0.669798	-0.863843	6.705231	-0.646827	-0.819198
C	4.263352	-0.972860	-2.164293	4.303350	-1.003746	-2.119168	4.330526	-0.977628	-2.111276
H	4.497164	-0.367844	-3.046771	4.570598	-0.412903	-3.001199	4.604895	-0.375717	-2.983548
H	4.873170	-1.882296	-2.197736	4.906100	-1.918582	-2.119060	4.938335	-1.888887	-2.113875
H	3.212484	-1.261060	-2.226065	3.251423	-1.280601	-2.212700	3.281563	-1.260020	-2.220253
H	-4.674354	2.307168	1.093035	-4.654062	2.255276	1.170191	-4.660040	2.264600	1.175588
H	-5.658059	1.246516	-0.228116	-5.641117	1.224116	-0.197994	-5.653315	1.215349	-0.173098
C	1.158909	-3.355463	-0.570624	1.181357	-3.320192	-0.644516	1.189643	-3.315494	-0.676901
H	2.005517	-3.019139	-1.173658	2.098850	-2.947877	-1.101994	2.089135	-2.941661	-1.168526
H	1.575524	-3.795525	0.342292	1.474722	-3.877847	0.252192	1.514593	-3.851983	0.221218
H	0.655073	-4.155049	-1.121809	0.726248	-4.034506	-1.337055	0.724358	-4.047408	-1.343483
C	-7.007714	-3.195450	-0.750334	-6.972048	-3.224735	-0.761715	-6.959765	-3.235999	-0.761091
H	-7.709441	-2.902469	-1.539589	-7.665271	-2.937430	-1.560542	-7.595149	-2.989509	-1.620126
H	-6.575465	-4.161628	-1.027202	-6.534954	-4.191432	-1.028626	-6.519263	-4.220690	-0.942597
H	-7.598057	-3.348556	0.162482	-7.571930	-3.373449	0.145427	-7.620628	-3.324101	0.110589
2TMCzBN		S₀			S₁			T₁	
C	-2.196572	-1.656887	-0.117958	-2.182785	-1.656296	-0.135567	-2.184223	-1.649295	-0.144567
C	-1.251975	-2.640364	-0.409518	-1.246608	-2.658300	-0.434069	-1.242981	-2.655972	-0.466095
C	0.126388	-2.368128	-0.461902	0.118392	-2.361939	-0.505443	0.117505	-2.359478	-0.532491
C	0.562388	-1.053146	-0.132139	0.555120	-1.023064	-0.158486	0.555686	-1.028134	-0.174437
C	-0.377033	0.003353	0.041661	-0.372885	0.041951	-0.023648	-0.376740	0.050982	-0.036861
C	-1.725228	-0.348387	0.072308	-1.707543	-0.325387	0.031498	-1.711297	-0.320161	0.032237
H	-1.582690	-3.642547	-0.672732	-1.580999	-3.653704	-0.711333	-1.583309	-3.641615	-0.768151
B	-0.054873	1.493127	-0.052328	-0.039997	1.543616	-0.079024	-0.050725	1.537132	-0.094370
N	1.906195	-0.643317	-0.073419	1.888323	-0.631125	-0.065379	1.889516	-0.628348	-0.068621
N	-2.781646	0.538724	0.214033	-2.760229	0.549592	0.197706	-2.764553	0.553159	0.208261
C	2.269711	0.676013	-0.354353	2.288300	0.710192	-0.343071	2.287668	0.706741	-0.344341
C	3.678387	0.773316	-0.427005	3.686934	0.765587	-0.407647	3.690176	0.766431	-0.400870
C	1.408991	1.784269	-0.467269	1.431945	1.826228	-0.443234	1.434942	1.824260	-0.452664
C	4.250859	1.993202	-0.775827	4.308286	1.988922	-0.727072	4.306207	1.986014	-0.722621
C	2.045775	2.990129	-0.837950	2.108425	3.026965	-0.793958	2.105304	3.019635	-0.802968
C	3.430653	3.110730	-1.018921	3.505350	3.115286	-0.949378	3.503642	3.111327	-0.956173
H	5.331350	2.088932	-0.858572	5.390198	2.061304	-0.795144	5.388434	2.061890	-0.784621
H	1.436574	3.875998	-0.992461	1.524274	3.929241	-0.948314	1.520951	3.921618	-0.958038
C	3.087689	-1.347868	0.242418	3.040727	-1.356106	0.249164	3.041970	-1.351887	0.253634
C	3.268403	-2.578044	0.877259	3.186430	-2.597368	0.879481	3.183585	-2.594980	0.881383
C	4.203417	-0.516864	-0.027621	4.177180	-0.536769	-0.012640	4.180554	-0.536112	-0.002792

C	4.570200	-3.008873	1.126714	4.471683	-3.065469	1.132152	4.466882	-3.062101	1.139952
H	2.428197	-3.173994	1.208478	2.326264	-3.169658	1.203998	2.321114	-3.167621	1.198695
C	5.499458	-0.977784	0.222436	5.455372	-1.038647	0.236339	5.458196	-1.037575	0.250940
C	5.701301	-2.241834	0.783473	5.620275	-2.315862	0.792099	5.619230	-2.313806	0.806154
H	4.712097	-3.966803	1.621933	4.591905	-4.026360	1.625806	4.584432	-4.023398	1.633630
H	6.352051	-0.337763	0.008282	6.328897	-0.426437	0.027273	6.332632	-0.425536	0.045042
C	-2.556546	1.896722	0.500862	-2.545002	1.924206	0.487772	-2.547959	1.923742	0.489914
C	-3.584441	2.704822	1.019419	-3.575573	2.705588	1.022313	-3.575277	2.711439	1.027884
C	-1.242464	2.433010	0.311575	-1.232491	2.468619	0.270078	-1.236541	2.467129	0.266382
C	-3.356486	4.048295	1.290307	-3.380585	4.066276	1.268460	-3.374014	4.068185	1.271103
C	-1.066750	3.801286	0.613451	-1.095632	3.854754	0.535248	-1.092978	3.851829	0.531924
C	-2.095643	4.612050	1.074972	-2.137815	4.646662	1.003324	-2.129542	4.647140	1.002097
H	-0.074467	4.227897	0.515295	-0.119242	4.308297	0.403785	-0.115580	4.302241	0.397060
C	-3.976753	-0.204264	0.063291	-3.952019	-0.199951	0.066740	-3.956008	-0.198590	0.078591
C	-5.314452	0.194781	-0.024404	-5.287220	0.188024	-0.021441	-5.292383	0.185379	0.001747
C	-3.639507	-1.574973	-0.110062	-3.612904	-1.576598	-0.099956	-3.608533	-1.574293	-0.101168
C	-6.290714	-0.782105	-0.214683	-6.263220	-0.801391	-0.193547	-6.265291	-0.805803	-0.172040
C	-4.641770	-2.532824	-0.294559	-4.613488	-2.544962	-0.266105	-4.610500	-2.546107	-0.268638
C	-5.984354	-2.151569	-0.333167	-5.958672	-2.171841	-0.297239	-5.953749	-2.176496	-0.288952
C	4.045813	4.420556	-1.452027	4.133784	4.428819	-1.350994	4.130868	4.423207	-1.361692
H	4.359405	4.385109	-2.503565	4.003448	4.617835	-2.424987	4.010348	4.601164	-2.438662
H	3.339119	5.249410	-1.349520	3.676379	5.271832	-0.821057	3.664025	5.268658	-0.844438
H	4.935805	4.662757	-0.860191	5.208382	4.442732	-1.144087	5.203178	4.443140	-1.144424
C	7.091553	-2.771359	1.038723	6.994334	-2.878221	1.047822	6.991012	-2.878438	1.071746
H	7.373592	-3.526656	0.293357	7.234759	-3.674363	0.330382	7.220989	-3.699800	0.380275
H	7.839277	-1.973769	0.994636	7.768107	-2.110430	0.959053	7.769687	-2.119651	0.953553
H	7.166196	-3.248805	2.022181	7.066634	-3.320522	2.048150	7.066237	-3.286957	2.086218
H	-4.370777	-3.578360	-0.420444	-4.335781	-3.589490	-0.383478	-4.330201	-3.588943	-0.393898
C	1.008171	-3.449247	-1.051331	1.005328	-3.406312	-1.143792	1.011771	-3.404384	-1.163243
H	1.909898	-3.042652	-1.511918	1.939237	-2.992775	-1.524932	1.945231	-2.988815	-1.543910
H	1.323136	-4.205831	-0.324221	1.259212	-4.224605	-0.460881	1.266507	-4.218002	-0.475475
H	0.450903	-3.975200	-1.833014	0.469373	-3.854820	-1.986430	0.480573	-3.858601	-2.005577
H	-1.915287	5.660489	1.296752	-1.976422	5.705664	1.191154	-1.965102	5.705321	1.190918
H	-4.165643	4.650399	1.696325	-4.195054	4.657116	1.678934	-4.183882	4.661810	1.686956
H	-7.328611	-0.464528	-0.283973	-7.302002	-0.486011	-0.257860	-7.305976	-0.495264	-0.227762
H	-4.546577	2.280164	1.266872	-4.522112	2.259778	1.294394	-4.521279	2.268248	1.305983
H	-5.614062	1.233465	0.006857	-5.592655	1.224997	0.000037	-5.602010	1.220922	0.034260
C	-7.084806	-3.170535	-0.503154	-7.057580	-3.194687	-0.446573	-7.052107	-3.199329	-0.444120
H	-6.686087	-4.146695	-0.794685	-6.657345	-4.175423	-0.719375	-6.647770	-4.188794	-0.676230
H	-7.646990	-3.309617	0.429406	-7.618463	-3.315686	0.489001	-7.644147	-3.290870	0.475332
H	-7.805863	-2.859753	-1.267851	-7.778724	-2.899312	-1.217048	-7.746656	-2.923469	-1.246098

Table S4. Values of the dihedral angle (α_L), the dihedral angle (α_R) and the dihedral angle (α_A) of the studied 36 molecules by O3LYP/6-31G(d) in toluene.

Compound	State	$\alpha_L(^{\circ})$	$\alpha_R(^{\circ})$	$\alpha_A(^{\circ})$	Compound	State	$\alpha_L(^{\circ})$	$\alpha_R(^{\circ})$	$\alpha_A(^{\circ})$
2PXZBN	S ₀	28.34	26.20	36.22	PXZCzBN	S ₀	27.53	13.56	30.20
	S ₁	30.50	24.03	34.59		S ₁	24.48	10.63	29.26
	T ₁	30.05	24.45	34.74		T ₁	24.92	10.22	28.98
PTZPXZBN	S ₀	33.67	26.80	36.92	PTZCzBN	S ₀	33.51	14.76	30.86
	S ₁	35.50	24.72	35.13		S ₁	27.85	10.66	31.15
	T ₁	35.25	25.01	35.25		T ₁	30.00	10.67	30.68
DPAPXZBN	S ₀	91.49	28.65	30.66	DPACzBN	S ₀	89.72	15.93	23.14
	S ₁	92.23	25.73	28.26		S ₁	88.74	15.18	18.12
	T ₁	92.19	26.88	28.49		T ₁	88.74	15.06	19.52
CzPXZBN	S ₀	15.38	26.24	28.46	2CzBN	S ₀	14.08	12.51	21.54
	S ₁	16.81	24.11	27.92		S ₁	15.58	5.36	18.83
	T ₁	16.55	24.44	27.44		T ₁	15.35	11.67	19.10
DMACPXZBN	S ₀	32.77	26.66	34.94	DMACCzBN	S ₀	32.41	14.69	28.69
	S ₁	34.90	24.68	33.22		S ₁	31.13	13.09	25.82
	T ₁	34.68	25.12	33.25		T ₁	32.10	12.26	26.61
TMCzPXZBN	S ₀	15.23	26.41	28.22	TMCzCzBN	S ₀	14.08	12.73	21.32
	S ₁	16.61	24.21	27.46		S ₁	15.26	12.19	18.58
	T ₁	16.26	24.60	27.05		T ₁	15.06	11.68	18.88
PXZPTZBN	S ₀	28.89	31.74	36.70	PXZDMACBN	S ₀	28.28	30.77	36.20
	S ₁	31.18	29.01	36.59		S ₁	27.27	29.32	34.65
	T ₁	30.47	29.85	36.39		T ₁	26.96	28.98	34.40
2PTZBN	S ₀	34.40	32.09	37.37	PTZDMACBN	S ₀	33.82	31.16	36.89
	S ₁	36.06	29.15	37.18		S ₁	31.39	29.25	35.76
	T ₁	35.81	30.05	29.61		T ₁	32.43	29.51	35.48
DPAPTZBN	S ₀	91.49	33.28	30.88	DPADMACBN	S ₀	91.20	32.68	30.42
	S ₁	92.73	30.01	30.58		S ₁	91.85	32.24	27.31
	T ₁	92.74	31.45	30.55		T ₁	91.97	33.33	27.06
CzPTZBN	S ₀	15.46	32.33	28.88	CzDMACBN	S ₀	15.05	31.23	11.38
	S ₁	17.09	29.05	29.93		S ₁	15.76	31.15	27.56
	T ₁	16.85	30.06	29.44		T ₁	15.60	31.98	26.54
DMACPTZBN	S ₀	33.42	31.84	35.34	2DMACBN	S ₀	32.87	31.01	34.91
	S ₁	35.32	29.09	35.37		S ₁	32.87	30.70	32.57
	T ₁	35.15	30.05	35.23		T ₁	33.34	31.14	32.25
TMCzPTZBN	S ₀	15.26	32.37	28.68	TMCzDMACBN	S ₀	14.89	31.38	28.16
	S ₁	16.86	29.27	29.48		S ₁	15.63	31.40	26.95
	T ₁	16.61	30.30	29.09		T ₁	15.41	32.12	26.10
PXZDPABN	S ₀	28.96	90.08	30.48	PXZTMCzBN	S ₀	24.04	11.48	30.04
	S ₁	26.54	92.02	28.19		S ₁	22.83	3.88	29.15
	T ₁	26.51	92.18	27.75		T ₁	11.34	8.72	29.13
PTZDPABN	S ₀	34.07	89.40	31.35	PTZTMCzBN	S ₀	29.45	12.56	31.57
	S ₁	30.01	91.68	29.87		S ₁	25.38	9.06	31.54
	T ₁	31.57	91.56	29.25		T ₁	28.66	9.51	31.17
2DPABN	S ₀	89.15	87.79	24.79	DPATMCzBN	S ₀	67.67	14.47	11.19
	S ₁	89.59	87.81	19.43		S ₁	61.12	15.46	24.65
	T ₁	89.53	87.90	19.78		T ₁	63.14	13.69	25.79
CzDPABN	S ₀	16.54	89.29	21.44	CzTMCzBN	S ₀	16.14	9.39	21.67
	S ₁	17.11	88.77	18.11		S ₁	17.84	11.47	19.01
	T ₁	16.45	88.50	17.66		T ₁	17.96	10.29	19.15
DMACDPABN	S ₀	33.25	89.49	29.48	DMACTMCzBN	S ₀	28.29	13.06	29.51
	S ₁	32.36	90.21	25.75		S ₁	29.60	12.93	26.79
	T ₁	32.67	90.53	25.59		T ₁	30.83	11.86	27.50
TMCzDPABN	S ₀	16.49	89.55	8.78	2TMCzBN	S ₀	16.26	9.70	21.60
	S ₁	16.91	88.90	17.76		S ₁	17.84	11.14	19.04
	T ₁	16.33	88.61	17.63		T ₁	17.88	10.21	19.17

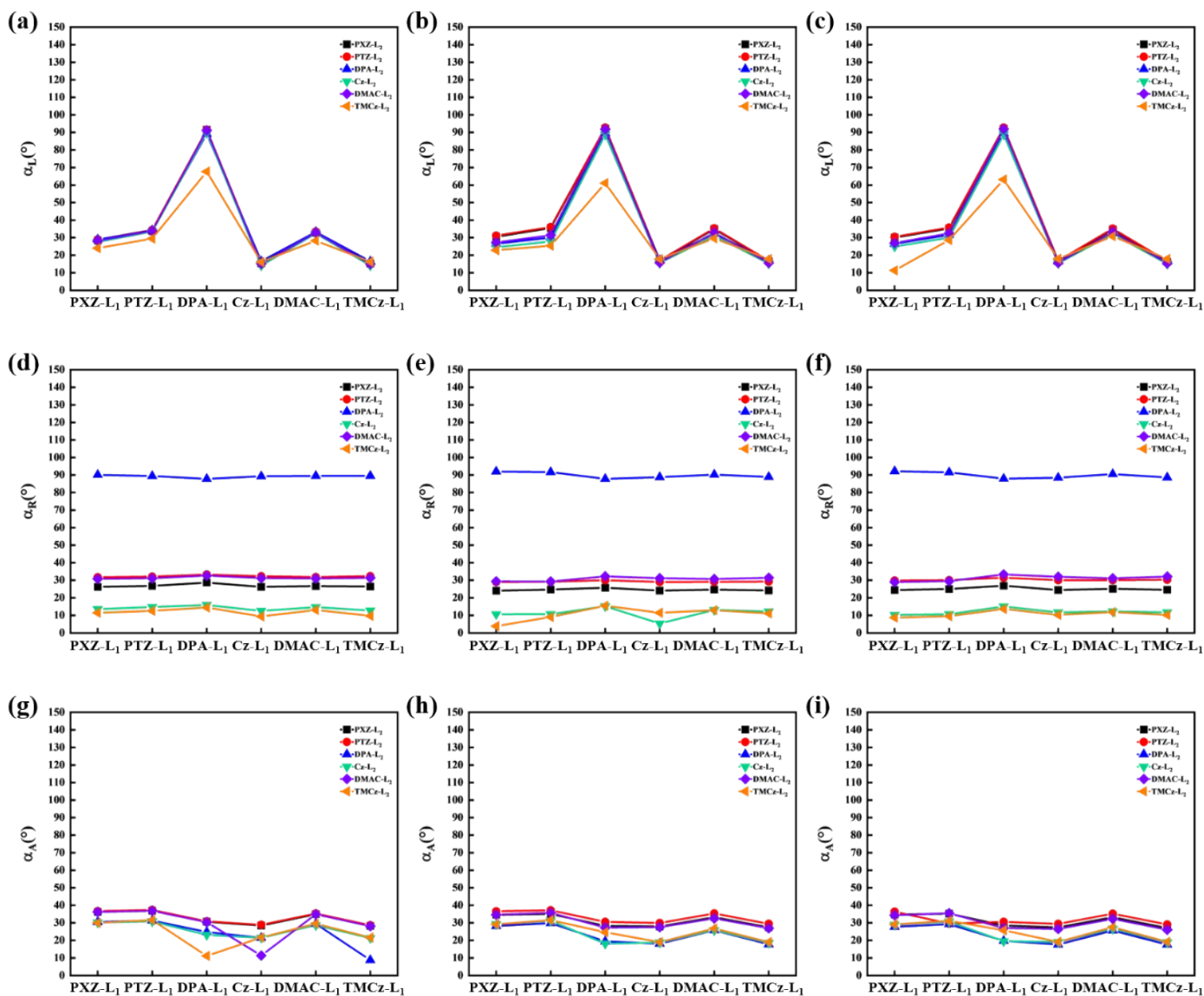


Fig. S3. Dihedral angle (α_L) (a-c), the dihedral angle (α_R) (d-f), and the dihedral angle (α_A) (g-i) of molecules in S₀, S₁ and T₁ by O3LYP/6-31G(d) in toluene.

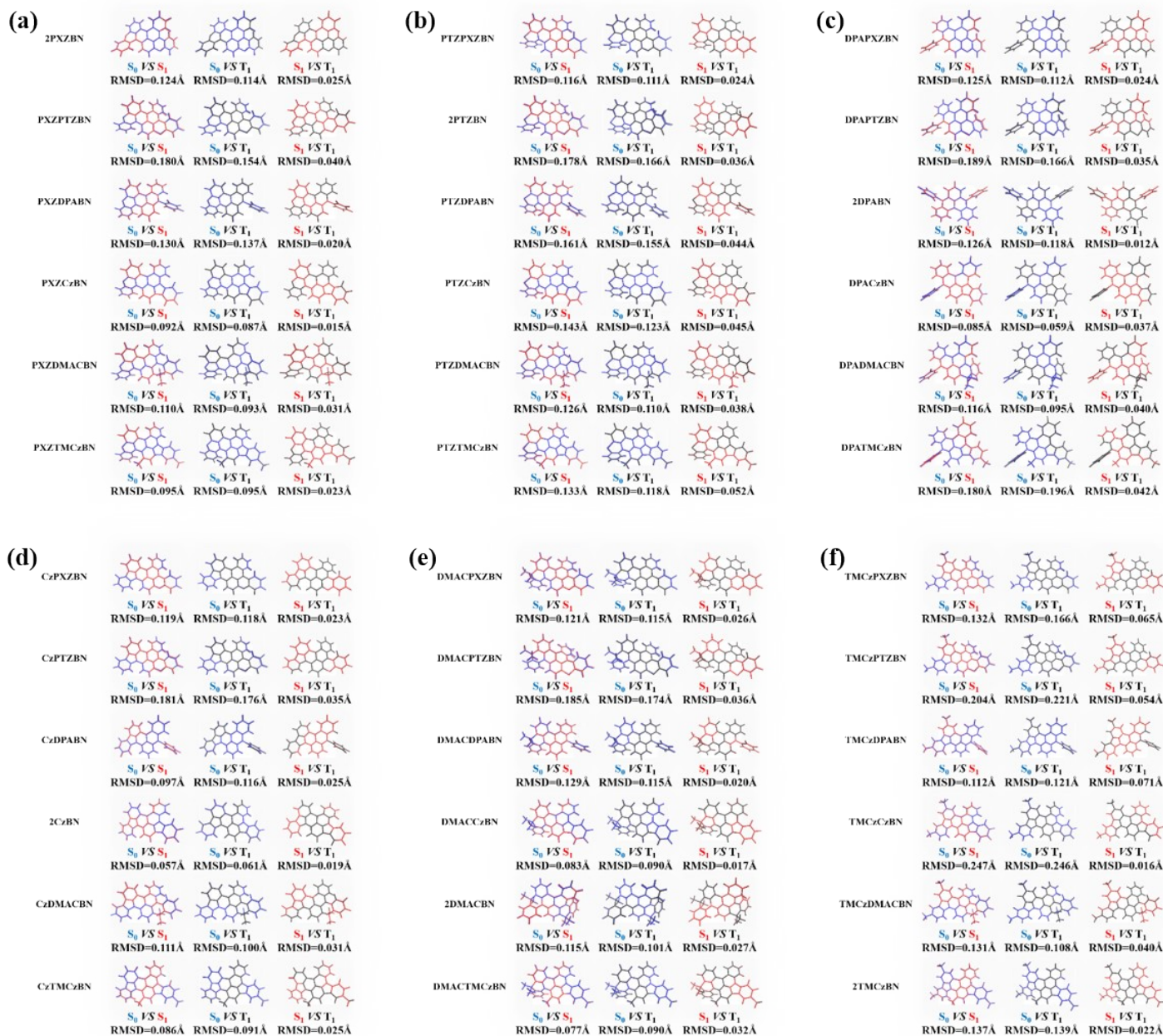


Fig. S4. Root mean square displacement (RMSD) for S_0 - S_1 , S_0 - T_1 or S_1 - T_1 of all studied molecules by O3LYP/6-31G(d) in toluene.

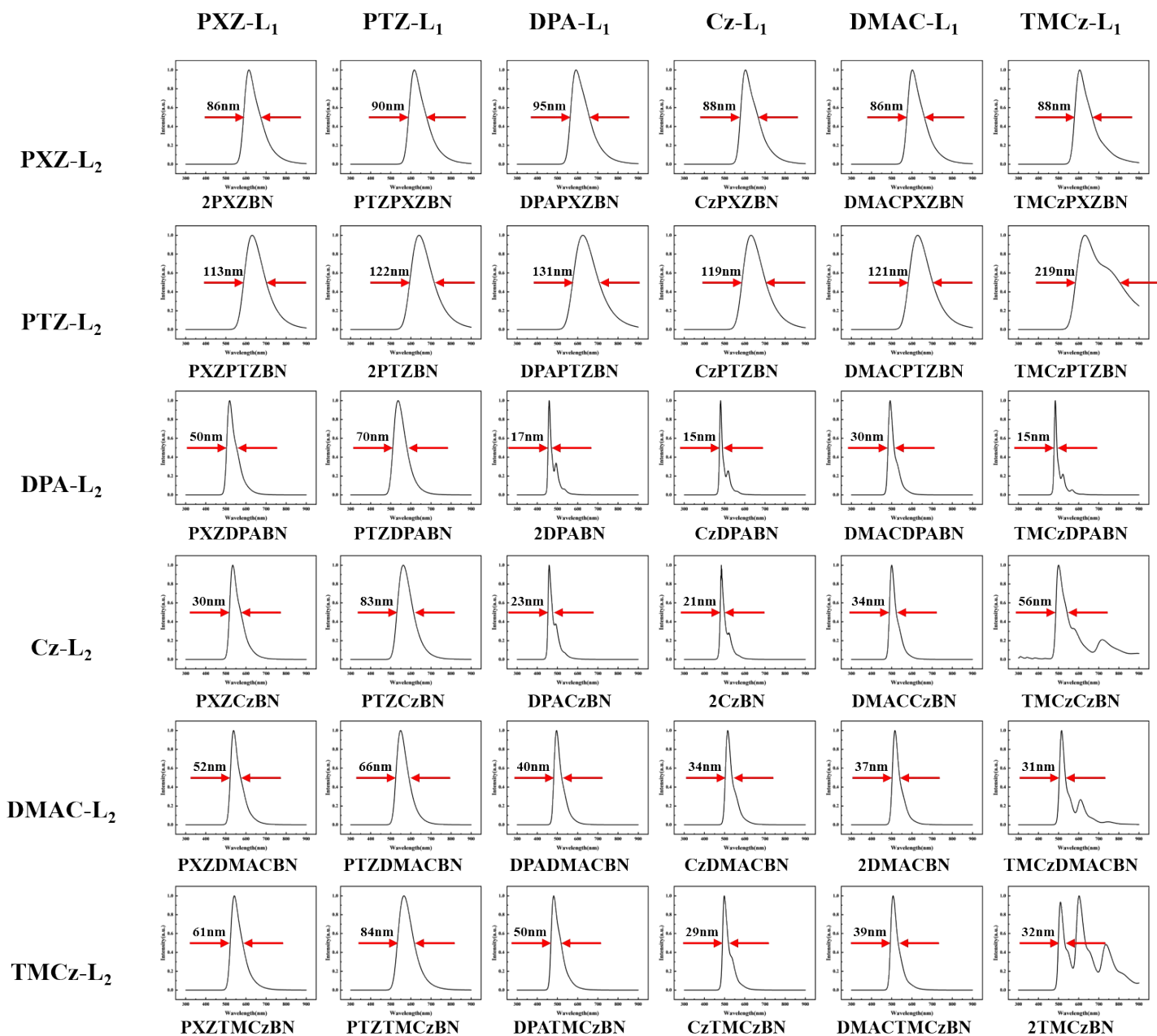


Fig. S5. Full width at half maximum (FWHM) of emission wavelength for all studied molecules by O3LYP/6-31G(d) in toluene.

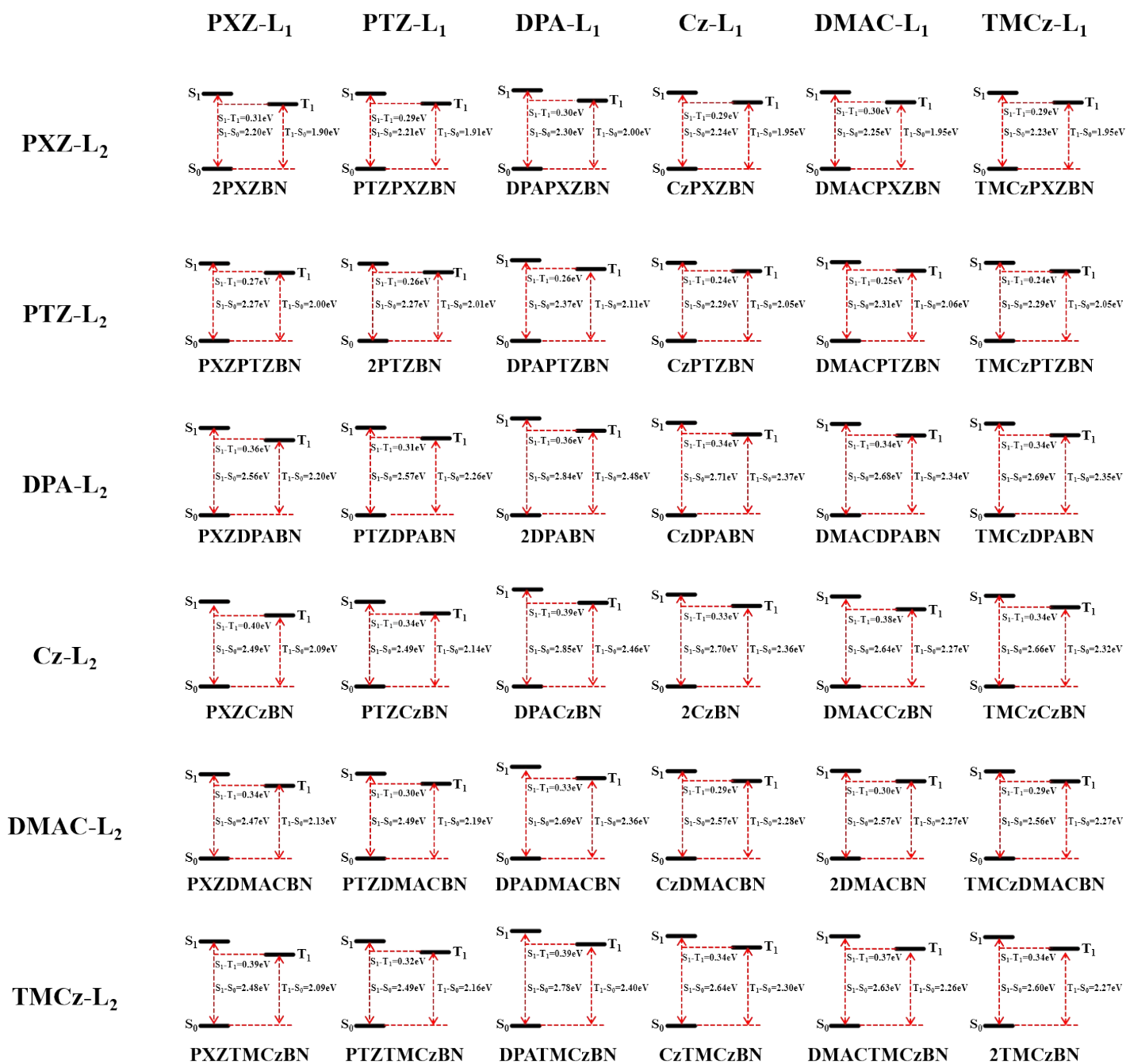


Fig. S6. Energy levels for all studied molecules by O3LYP/6-31G(d) in toluene.

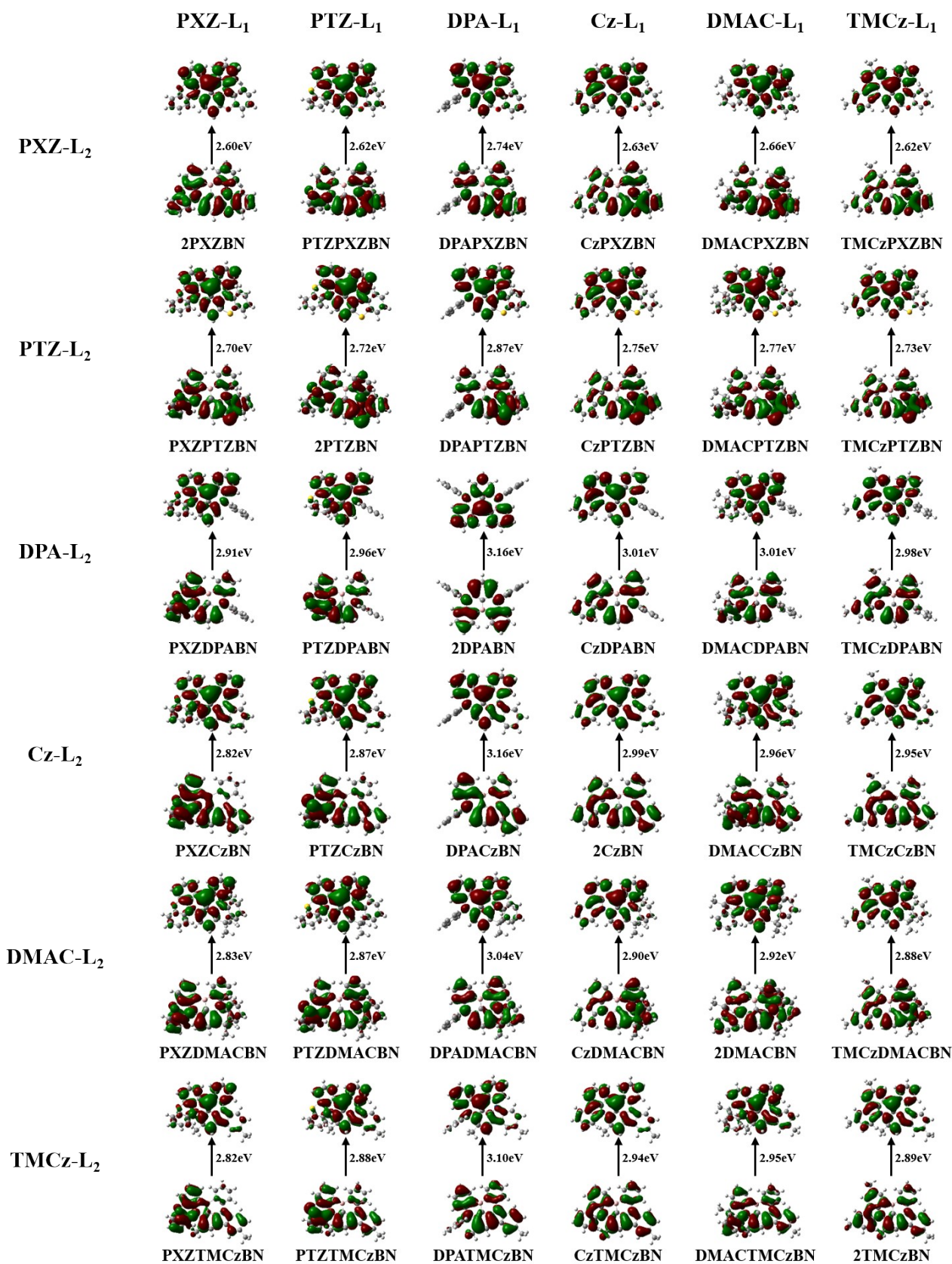


Fig. S7. Electron distributions of FMOs for all studied molecules by O3LYP/6-31G(d) in toluene. The value on the right side is the energy gap between the two orbitals.

Table S5. Molecule conformations and distributions of FMOs (HOMO and LUMO) for S_1 by S_0 for all studied molecules by O3LYP/6-31G(d) in toluene. The value of ΔE_{H-L} is the energy gap between the two orbitals.

Molecules	LUMO (eV)	HOMO (eV)	ΔE_{H-L} (eV)	Molecules	LUMO (eV)	HOMO (eV)	ΔE_{H-L} (eV)
2PXZBN	-1.83	-4.43	2.60	PXZCzBN	-1.88	-4.70	2.82
PTZPXZBN	-1.90	-4.52	2.62	PTZCzBN	-1.96	-4.83	2.87
DPAPXZBN	-1.64	-4.38	2.74	DPACzBN	-1.66	-4.81	3.16
CzPXZBN	-1.97	-4.60	2.63	2CzBN	-2.04	-5.03	2.99
DMACPXZBN	-1.78	-4.44	2.66	DMACCzBN	-1.84	-4.80	2.96
TMCzPXZBN	-1.92	-4.54	2.62	TMCzCzBN	-1.98	-4.93	2.95
PXZPTZBN	-1.88	-4.58	2.70	PXZDMACBN	-1.75	-4.58	2.83
2PTZBN	-1.95	-4.67	2.72	PTZDMACBN	-1.83	-4.69	2.87
DPAPTZBN	-1.69	-4.56	2.87	DPADMACBN	-1.55	-4.59	3.04
CzPTZBN	-2.02	-4.77	2.75	CzDMACBN	-1.91	-4.80	2.90
DMACPTZBN	-1.83	-4.60	2.77	2DMACBN	-1.71	-4.63	2.92
TMCzPTZBN	-1.97	-4.70	2.73	TMCzDMACBN	-1.85	-4.73	2.88
PXZDPABN	-1.61	-4.52	2.91	PXZTMCzBN	-1.88	-4.70	2.82
PTZDPABN	-1.69	-4.65	2.96	PTZTMCzBN	-1.96	-4.85	2.88
2DPABN	-1.39	-4.55	3.16	DPATMCzBN	-1.67	-4.77	3.10
CzDPABN	-1.78	-4.79	3.01	CzTMCzBN	-2.00	-4.94	2.94
DMACDPABN	-1.57	-4.58	3.01	DMACTMCzBN	-1.83	-4.78	2.95
TMCzDPABN	-1.73	-4.70	2.98	2TMCzBN	-1.95	-4.85	2.89

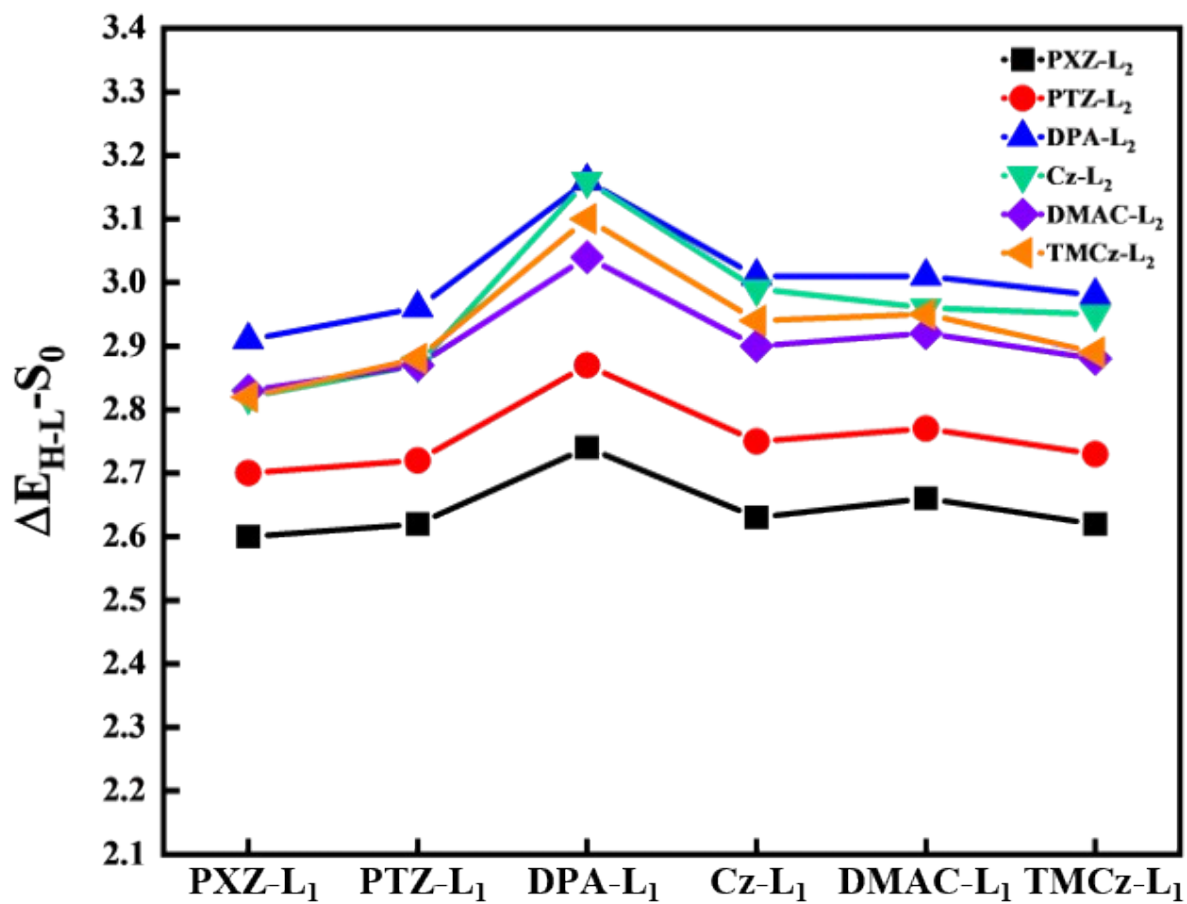


Fig. S8. The energy gap of FMOs for all studied molecules by O3LYP/6-31G(d) in toluene.

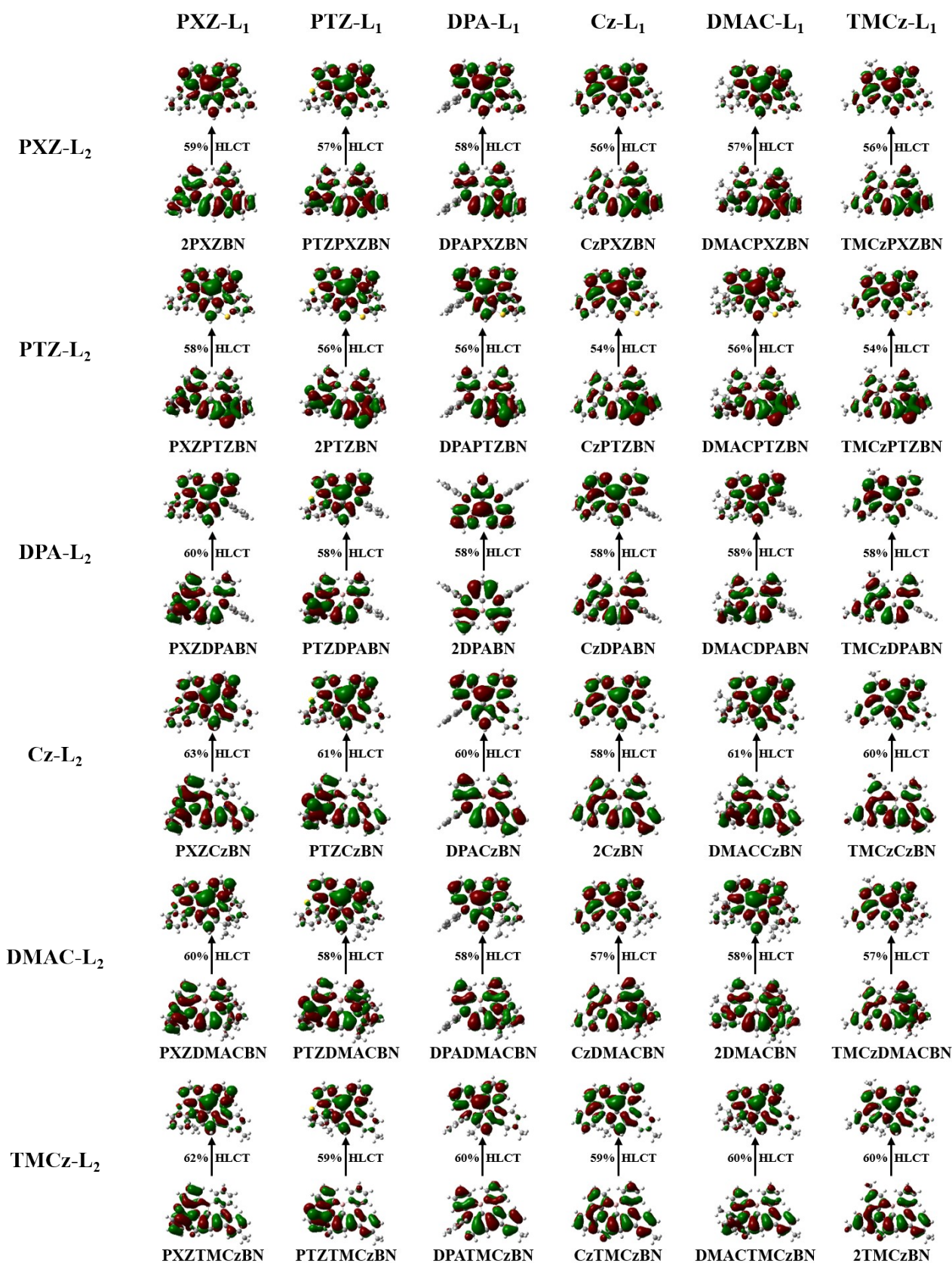


Fig. S9. Transition characteristics for S₁ state for all studied molecules by O3LYP/6-31G(d) in toluene. The value on the right side of each arrow represents the electron-hole overlap between the two orbitals.

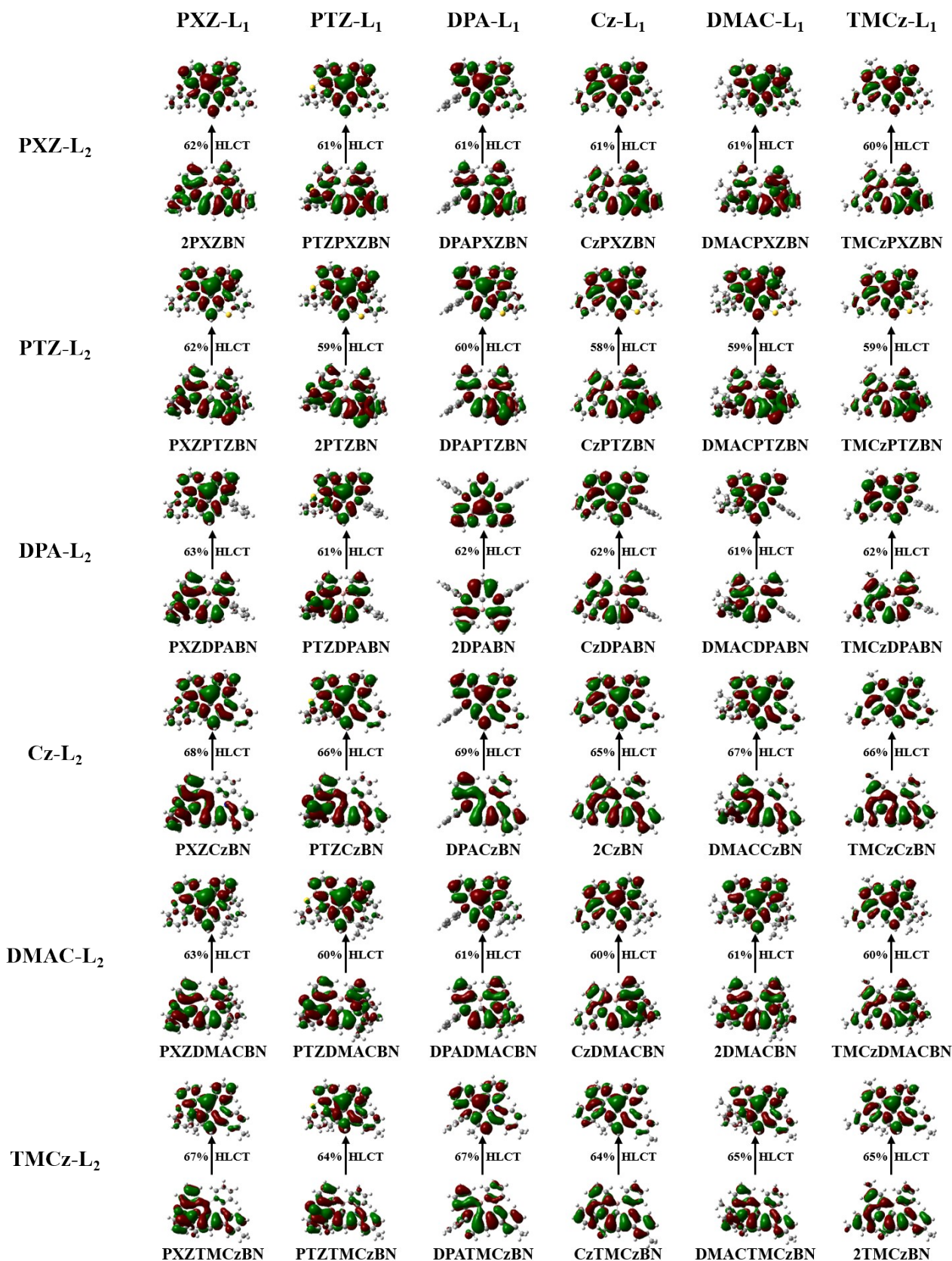


Fig. S10. Transition characteristics for T₁ state for all studied molecules by O3LYP/6-31G(d) in toluene. The value on the right side of each arrow represents the electron-hole overlap between the two orbitals.

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