

## Electronic Supporting Information(ESI)

### **Spin-orbit charge transfer intersystem crossing and thermal activation delayed fluorescence (TADF) studies of compact orthogonal anthraquinone phenothiazine derivatives**

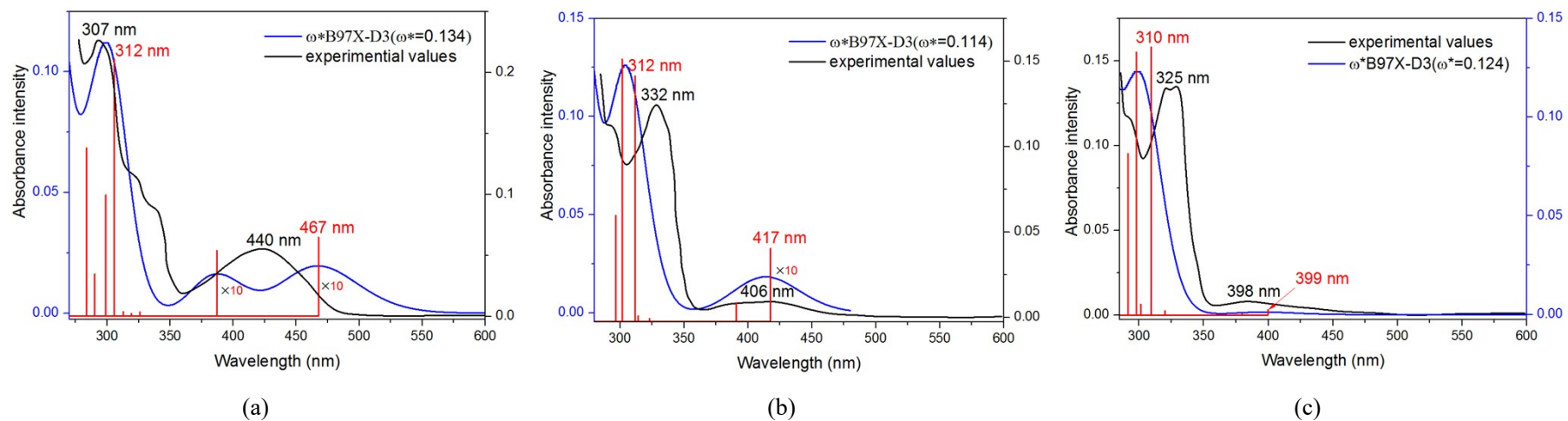
LingLing Lv,<sup>\*</sup> <sup>a</sup> Kun Yuan,<sup>a</sup> TianYu Zhao<sup>a</sup>, HuiXue Li<sup>a</sup> and DongMei Wang<sup>b</sup>

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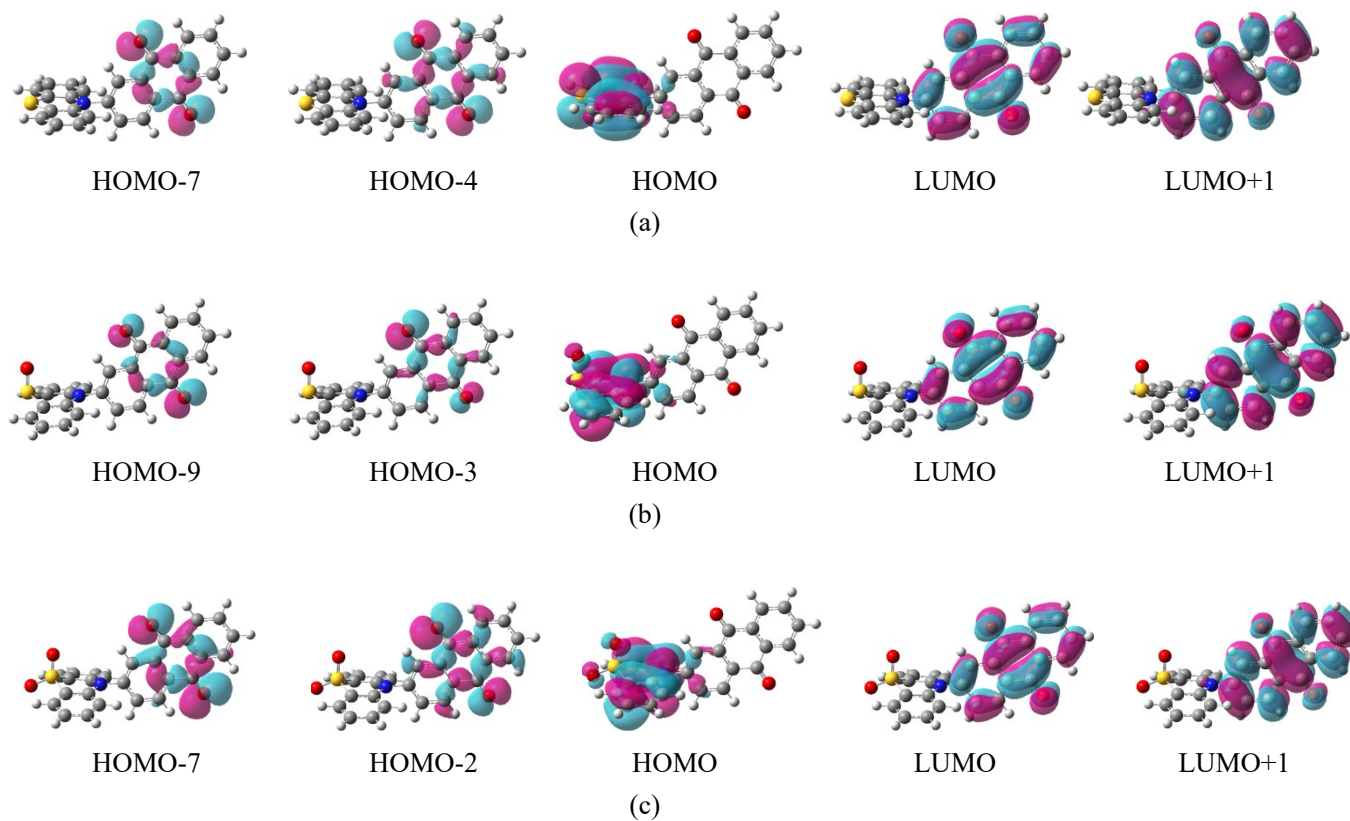
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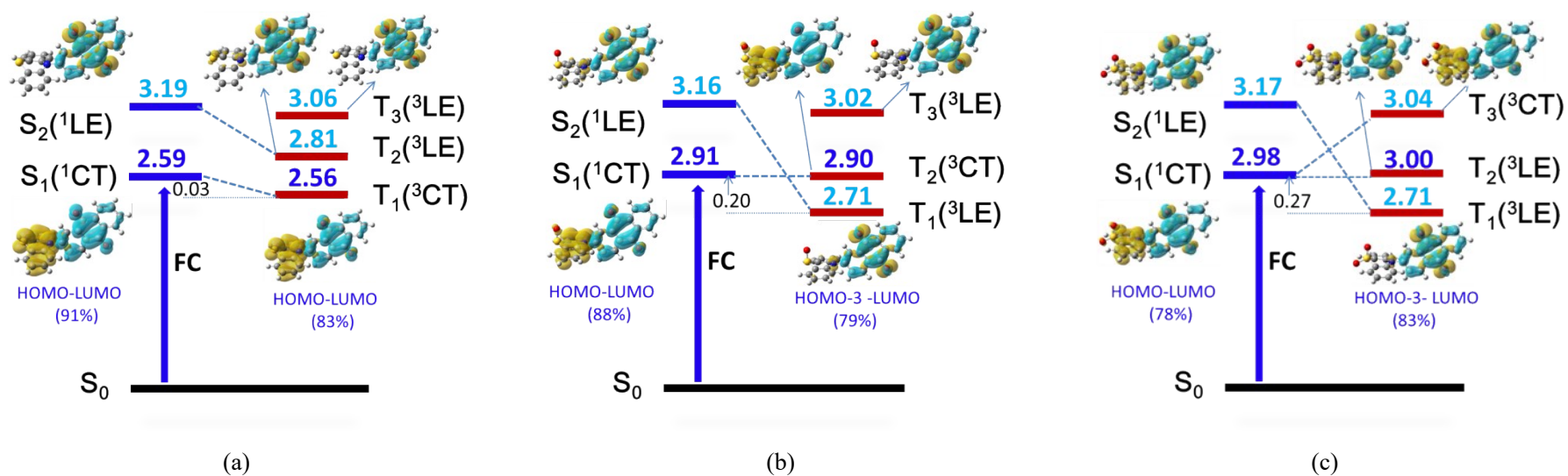
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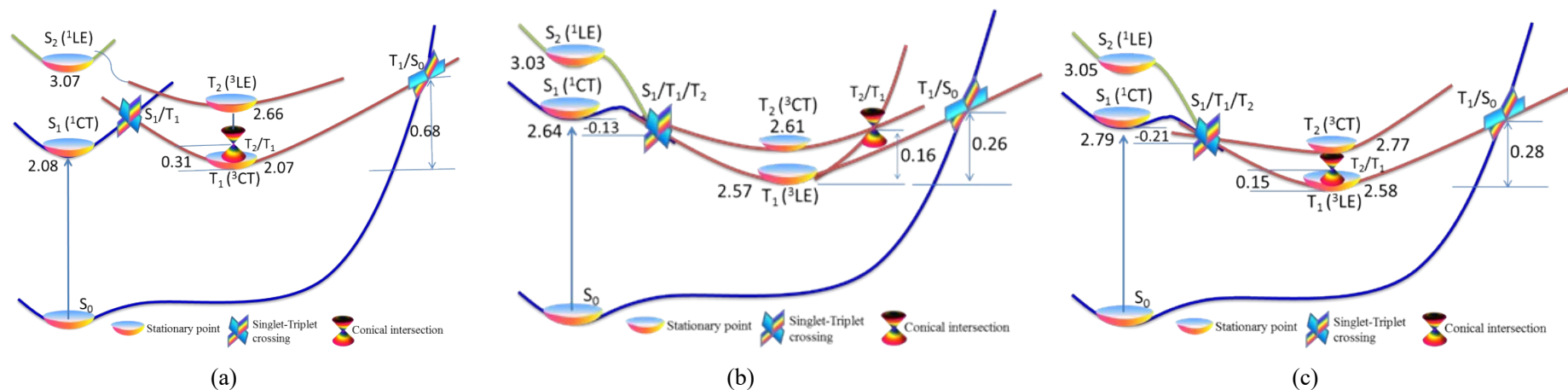
**Fig. S1** Comparison of the calculated and the experimental absorption spectra of (a) AQ-PTZ, (b) AQ-PTZ-O and (c) AQ-PTZ-O<sub>2</sub> in cyclohexane (with PCM mode), and calculated at the TD-DFT at the tuned- $\omega^*$ B97X-D3 level.



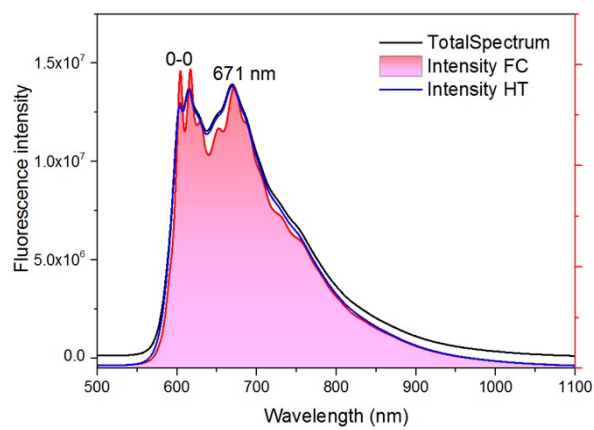
**Fig. S2** Key transition active orbitals of (a) AQ-PTZ, (b) AQ-PTZ-O, and (c) AQ-PTZ-O<sub>2</sub> compounds from the tuned- $\omega$ \*B97X-D3 level of theory in cyclohexane (with PCM mode).



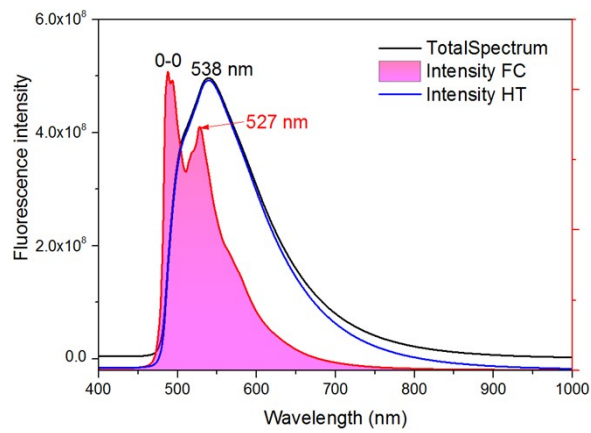
**Fig. S3** Adiabatic energy transition diagrams of (a) AQ-PTZ, (b) AQ-PTZ-O and (c) AQ-PTZ-O<sub>2</sub> are from calculation by the tuned- $\omega$ \*B97X-D3 level of theory in cyclohexane (with PCM mode). The density difference distributions of the excited states are inserted into the diagrams. CT: charge transfer. LE: Local excitation. FC: Franck-Condon.



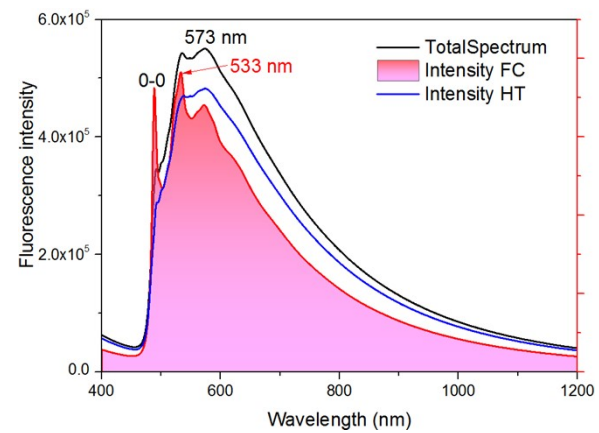
**Fig. S4** Nonabatic potential energy surface diagrams of (a) AQ-PTZ, (b) AQ-PTZ-O and (c) AQ-PTZ-O<sub>2</sub> are from single-point calculation at the tuned- $\omega$ \*B97X-D3 level of theory in cyclohexane (with PCM mode). Minimum energy crossing point (MECP) of different spin states (S<sub>1</sub>/T<sub>1</sub>, T<sub>1</sub>/S<sub>0</sub> and S<sub>1</sub>/T<sub>1</sub>/T<sub>2</sub>) and conical intersection of the same spin states (T<sub>2</sub>/T<sub>1</sub>) were also obtained.



(a)

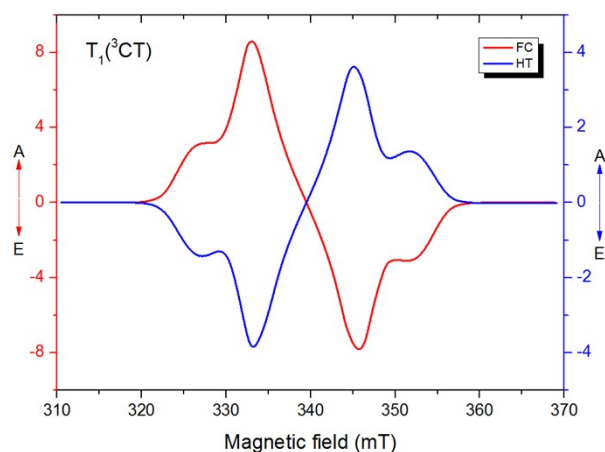


(b)

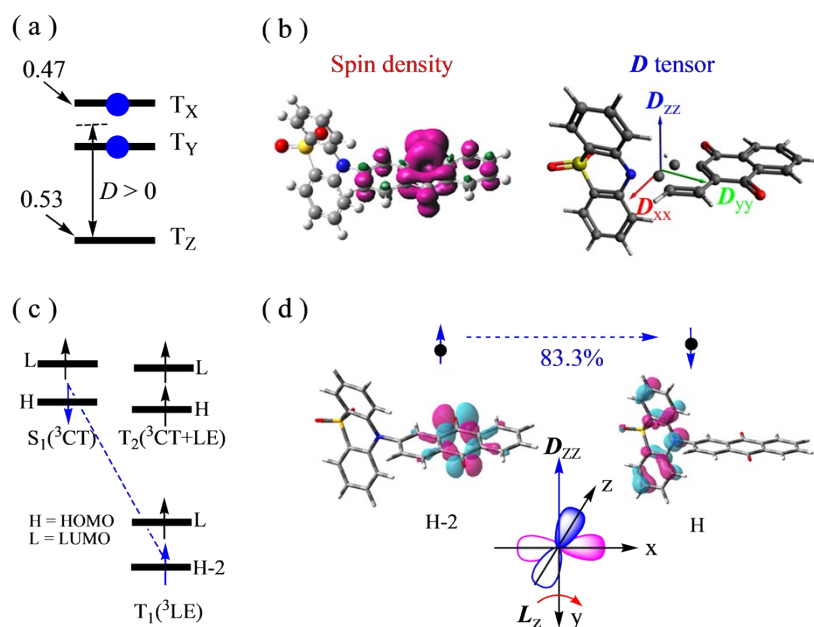


(c)

**Fig. S5** Calculated fluorescence emission spectrum of compounds (a) AQ-PTZ, (b) AQ-PTZ-O and (c) AQ-PTZ-O2 including FC and HT contributions from the tuned-TD- $\omega$ \*B97X-D3/ def2-tzvp(-f) //def2/J level at T = 300 K.



**Fig. S6** Simulated EPR spectra of the charge-transfer triplet  $T_1(^3CT)$  of the AQ-PTZ-O compound.



**Fig. S7** (a) Relative populations in the zero-field  $T_1(^3LE)$  spin sublevels obtained for  $D > 0$  of AQ-PTZ-O<sub>2</sub>; (b) Spin density and the ZFS tensor ( $D$ ) orientations of AQ-PTZ-O<sub>2</sub>; (c) Schematic representation of the  $S_1 \leftrightarrow T_1$  allowed ISC in AQ-PTZ-O<sub>2</sub>; (d) Representative topologies of the spin-flip orbitals are depicted between the H-2 and L orbitals, demonstrating that SOC is effective as the angular momentum change ( $L_z$ ) along the z-axis to cause the spin-flip.

**Table S1** Optimized coordinate parameters of (a) AQ-PTZ, (b) AQ-PTZ-O, and (c) AQ-PTZ-O<sub>2</sub> compounds from the CAM-B3LYP level of theory in cyclohexane (with PCM mode) for the S<sub>0</sub>, S<sub>1</sub>, S<sub>2</sub>, T<sub>1</sub> and T<sub>2</sub> states.

AQ-PTZ							
Coordinates from S <sub>0</sub> state				Coordinates from S <sub>1</sub> state			
C	-2.44887600167903	3.57457507364198	-0.83092559612766	C	-2.21569661538571	3.63193022476594	-0.41425085435792
C	-1.76812620302903	2.36933982558048	-0.78351736581714	C	-1.62263384643194	2.40528065468759	-0.54092985529014
C	-2.36584092362406	1.23061589010157	-0.25150367671612	C	-2.36274856801322	1.22442438821502	-0.35174798325480
C	-3.66691804839773	1.34194046568377	0.24374914027786	C	-3.72938205767901	1.34698245950966	-0.03157293166504
C	-4.35449353289686	2.54021036543743	0.15692930941200	C	-4.31530614661516	2.60692799561493	0.09736517924591
C	-3.74859603979579	3.66666088874441	-0.37164368147638	C	-3.57017626608303	3.74129182814680	-0.09065719425134
C	-3.66694636994721	-1.34186740720896	0.24369919556419	C	-3.72943111734470	-1.34697072173835	-0.03187175357863
C	-2.36587322116853	-1.23054425877383	-0.25155875264085	C	-2.36278978885336	-1.22439111544302	-0.35199983605474
C	-1.76819280717088	-2.36924471429521	-0.78366274604843	C	-1.62271931482403	-2.40523023287789	-0.54145831079088
H	-0.75621033258494	-2.32688517883775	-1.15391712222300	H	-0.57668496001281	-2.33663929824127	-0.78563158467562
C	-2.44896584892927	-3.57446456372112	-0.83112662156764	C	-2.21583478175326	-3.63188671337955	-0.41509351725585
C	-3.74867653728928	-3.66655284761896	-0.37181741684600	C	-3.57032381095596	-3.74127134662101	-0.09155222631483
C	-4.35454483976918	-2.54012022080317	0.15682763290776	C	-4.31541076127291	-2.60692381707030	0.09674237358423
H	-1.95130021583249	4.44313753635149	-1.24063637680484	H	-1.62271313577316	4.52246552843743	-0.56510824687505
H	-0.75612946373942	2.32699149285957	-1.15373212514640	H	-0.57660402317088	2.33670708442956	-0.78512617927176
H	-5.36835054985791	2.58920365395509	0.53229040718389	H	-5.36539418659674	2.67322222783822	0.34913842728270
H	-4.28731453823973	4.60277127151599	-0.41654666386038	H	-4.03023254115238	4.71352238383772	0.01184665260769
H	-1.95141806844868	-4.44301251542922	-1.24090251349261	H	-1.62288765412823	-4.52240943592900	-0.56616883254783
H	-4.28741205855825	-4.60265159733714	-0.41675942685772	H	-4.03042455364327	-4.71350814046899	0.01069000329341
H	-5.36839908359279	-2.58911501495701	0.53219635118194	H	-5.36550758070040	-2.67323860654269	0.34847535838726
N	-1.67985060054993	0.00002496937653	-0.18419786549254	N	-1.73719775688421	0.00001829081795	-0.47493755764584
S	-4.40968714911097	0.00002854876758	1.10244783806594	S	-4.76161029717248	-0.00000488421030	0.23392728893957
C	7.12239822135522	0.00021106422615	0.41990214585117	C	6.98886570227391	0.00006187247373	0.43181155788545
C	6.19696187101204	0.00015452653201	-0.60542986821521	C	6.10370756270815	-0.00008695986501	-0.61754012470327
C	4.83918549598783	-0.00007811549311	-0.31796139719227	C	4.72250271886886	-0.00010144559799	-0.39248900637962
C	4.41143018895660	-0.00025669555675	1.00977797184350	C	4.24396020611374	-0.00000569750560	0.92963759051361
C	5.34689433975361	-0.00020055399307	2.03493602556655	C	5.16127155593764	0.00016971460281	1.98719545512275
C	6.69675926934023	0.00003035804314	1.74126776673394	C	6.51267249106917	0.00020171402855	1.74673018042030
C	3.86612914840582	-0.00015921271419	-1.43838337571829	C	3.81726551999572	-0.00009649707861	-1.54931989424519
C	2.96687642757023	-0.00050517327808	1.35147817617101	C	2.80991072698162	-0.00019710040132	1.23298215887855
C	1.99278601829144	-0.00025296968669	0.22846824020353	C	1.92355017758634	-0.00006789121413	0.09260469959440
C	2.41983978899692	-0.00010431170918	-1.09669271920945	C	2.40051902337861	-0.00011635093143	-1.24961007699619
C	1.48323826494047	0.00008107607375	-2.12227928003856	C	1.47760559193871	-0.00009974106467	-2.30223756474745
H	1.83034864036051	0.00018444590823	-3.14543317844960	H	1.86770778217623	-0.00012139705802	-3.31061178013123
C	0.13661268473501	0.00012171146480	-1.82909268446768	C	0.12588255635738	-0.00002523832050	-2.07506647361042
C	-0.28913595047564	-0.00000459192863	-0.50499661269964	C	-0.31972615118874	0.00001311598298	-0.73925537069056
C	0.63517244926693	-0.00019850327771	0.51805155692829	C	0.54344333909411	0.00000187963640	0.31499629534851
H	8.17970536084109	0.00039425395946	0.19186262759890	H	8.05433875752093	0.00009096044047	0.24294558507403
H	6.50910326944847	0.00028894109516	-1.63995332754116	H	6.44820368725534	-0.00014900506620	-1.64195518707262



H	4.99726603682659	-0.00033873589567	3.05743020438257	H	4.77068781287683	0.00022628630278	2.99487788499517
H	7.42247408180908	0.00007582335867	2.54327901605533	H	7.21064319385528	0.00031653292994	2.57372475766546
H	-0.59917794488485	0.00025149177721	-2.62219333701304	H	-0.58593456931785	-0.00001641718364	-2.88843510335699
H	0.30822056880639	-0.00030935044762	1.54793296528117	H	0.18545925674342	-0.00000327709460	1.33571937647787
O	2.59070937822864	-0.00042324014146	2.50283676782227	O	2.38543342582227	0.00062201552816	2.40358400386194
O	4.23442582463936	0.00029409865002	-2.59283660736919	O	4.24984039639923	-0.00061782732262	-2.71270438341496
<b>Coordinates from S<sub>2</sub> state</b>				<b>Coordinates from T<sub>1</sub> state</b>			
C	-2.46535326130228	3.56339220455097	-0.86380988328287	C	-2.21890357759309	3.63510466930525	-0.445057923267842
C	-1.77945311644409	2.36125114892768	-0.82635780206611	C	-1.62717693565310	2.40629828346279	-0.57010499655796
C	-2.35532833192397	1.22829350855035	-0.25902048195686	C	-2.36251609244147	1.22647227697318	-0.35371077935866
C	-3.63897279420766	1.34078679754725	0.28000898295064	C	-3.72312711539195	1.34971319520315	-0.00606869335561
C	-4.33257971786023	2.53676258579656	0.20544447308864	C	-4.30699525004476	2.61192452979075	0.12155166850655
C	-3.74825189198107	3.65752754886130	-0.35774013274641	C	-3.56735632405198	3.74610279712217	-0.09451832395105
C	-3.63853266197891	-1.34078214473708	0.28020464436575	C	-3.72298102250454	-1.34973121336853	-0.00615322546205
C	-2.35494051840395	-1.22792330783455	-0.25887763443261	C	-2.36238792975557	-1.22632112906342	-0.35381316605451
C	-1.77870780968526	-2.36077278667958	-0.82608828690852	C	-1.62694224174739	-2.40605652207321	-0.57034887016779
H	-0.78142805876021	-2.31240103155677	-1.23403646429093	H	-0.58525026451447	-2.33601560250096	-0.83592220929839
C	-2.46420528680245	-3.56314892695356	-0.86335657442995	C	-2.21854044751156	-3.63493251775028	-0.44538252936259
C	-3.74704911456151	-3.65764978737394	-0.35721965826916	C	-3.56696613799742	-3.74609684894926	-0.09479480519089
C	-4.33173126593774	-2.53700699990065	0.20583499212330	C	-4.30671547619069	-2.61201272754689	0.12138847300040
H	-1.98691798340298	4.42818741699408	-1.30317874536080	H	-1.62971478088636	4.52481881282517	-0.61952347228165
H	-0.78213574924900	2.31315120871855	-1.23426965967010	H	-0.58546241510356	2.33637875690608	-0.83562631942707
H	-5.33285448971745	2.58794200730940	0.61530053970493	H	-5.35250398585960	2.68116648741861	0.39339185019979
H	-4.29075591393787	4.59180095819080	-0.39532645401855	H	-4.02760532741965	4.71937559561591	0.00579588865917
H	-1.98549767888341	-4.42784233045926	-1.30262962508035	H	-1.62927033243364	-4.52457107124957	-0.61995880021816
H	-4.28923232562455	-4.59211611870712	-0.39464087134849	H	-4.02711200823660	-4.71942482027022	0.00545631311342
H	-5.33197488933342	-2.58847186440293	0.61573304112472	H	-5.35221029209528	-2.68138455550940	0.39324903580529
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S	-4.34528133200413	-0.00004891360649	1.17066094753512	S	-4.74795690753391	-0.00007410251418	0.29724270357080
C	7.10072394472639	-0.00075201256879	0.44241116332637	C	6.98509380207270	-0.00023644844687	0.44092949221837
C	6.18733941306224	-0.00030500164730	-0.58545062043253	C	6.10198685104631	-0.00009339106847	-0.61022929654653
C	4.81709843628047	-0.00010244693472	-0.32149002674761	C	4.72235486223442	-0.00005944652978	-0.38634946920667
C	4.38069752045251	-0.00035778443133	1.00604967314608	C	4.24191571039223	-0.00016907996981	0.93304382329398
C	5.31651802261293	-0.00081553561248	2.05073935715052	C	5.15502347975250	-0.00031537691539	1.99184417832358
C	6.65975096727097	-0.00099756241117	1.76685957681192	C	6.50684745244725	-0.00035212112748	1.75365865866614
C	3.87617592476161	0.00052440027113	-1.44946813632724	C	3.81745424840379	0.00005510154692	-1.54313051224524
C	2.96402651754840	-0.00019366393305	1.31025581142172	C	2.80711149302266	-0.00011557447899	1.23354789545759
C	2.01071901620475	0.00026100546719	0.22305766048963	C	1.92066214248416	0.00002774888900	0.09358832116817
C	2.44956048064016	0.00053892732735	-1.10401433087097	C	2.39925380675893	0.00014729227996	-1.24592244540411
C	1.50371769007422	0.00087449523357	-2.13061763845896	C	1.48075012206124	0.00032289440169	-2.29841942894893
H	1.86291866739788	0.00110344471736	-3.15036321071708	H	1.87283805171790	0.00041937649782	-3.30551807979082
C	0.16005278258080	0.00086323264570	-1.84969992073489	C	0.12808812851541	0.00035019826377	-2.07250600143543
C	-0.27421692522034	0.00049998029850	-0.51945821353191	C	-0.32059920961070	0.00018829257903	-0.73955773879334
C	0.63666762482484	0.00024432853991	0.50473548172096	C	0.54179748989280	0.00003832798258	0.31564450268893

H	8.15982977102801	-0.00090818574596	0.22406290867050	H	8.05024524234775	-0.00026667935819	0.25413078278243
H	6.50171002402728	-0.00008320210008	-1.62005799078359	H	6.44737933431262	-0.00001291198602	-1.63372031125141
H	4.96332836793718	-0.00100941052335	3.07265398535550	H	4.76169351039079	-0.00039602291353	2.99776857307117
H	7.37750830728868	-0.00132459698941	2.57620837874200	H	7.20262538006429	-0.00046490647484	2.58165021726969
H	-0.56999540569725	0.00107073983738	-2.64763566108282	H	-0.58052503088187	0.00047267150653	-2.88748567197221
H	0.29391259588056	-0.00006069240184	1.52984529406843	H	0.18489999079454	-0.00008592117301	1.33598574661612
O	2.56581611534504	-0.00024107757330	2.50777608797369	O	2.38394730777850	-0.00028918785383	2.40229263284654
O	4.25983283731496	0.00022822450765	-2.61432734996612	O	4.25027762818321	0.00028452258763	-2.70384000083861
<b>Coordinates from T<sub>2</sub> state</b>				<b>Coordinates from the T<sub>1</sub>/S<sub>0</sub> MECP</b>			
C	-2.41828432722647	3.58983493689270	-0.79824450650328	C	-2.20473136634032	3.56452833249018	-0.37208990018192
C	-1.75240990375603	2.37849002545867	-0.77975499443925	C	-1.58174716596238	2.38540486905475	-0.48657175171635
C	-2.36376882238267	1.23205712018199	-0.27382952413339	C	-2.34524072397084	1.18261692299228	-0.33454403426823
C	-3.66532411762202	1.34563057807087	0.22623459029399	C	-3.74499183412990	1.30444261690914	-0.06813994108043
C	-4.33453966501280	2.55818789033982	0.17704236650825	C	-4.37216497644063	2.58422599776549	0.05515709642213
C	-3.71633687821872	3.68690166258293	-0.32766978065000	C	-3.61121541713072	3.67537975991787	-0.09396959844886
C	-3.66084343456395	-1.34553527403916	0.23043651133295	C	-3.74514898460383	-1.30436960871835	-0.06832378220607
C	-2.35994141399757	-1.22865943549308	-0.27044903082872	C	-2.34538225716868	-1.18267813838756	-0.33472274837288
C	-1.74565704777868	-2.37377668186691	-0.77597270351156	C	-1.58205814958881	-2.38554336901240	-0.48699997981743
H	-0.73819555581271	-2.31892980627642	-1.15666958773298	H	-0.52786924080407	-2.30170052270018	-0.68416549114276
C	-2.40768353000814	-3.58720573876419	-0.79218012288795	C	-2.20519828821542	-3.56460370346196	-0.37271955152680
C	-3.70490235340428	-3.68775288350512	-0.31995675009169	C	-3.61169129496785	-3.67532018172463	-0.09458956133497
C	-4.32625277697383	-2.56030456824355	0.18362224259399	C	-4.37249312838991	-2.58409244661533	0.05474088561466
H	-1.91399960216742	4.46118224239582	-1.19346574457808	H	-1.63134453477028	4.47276619120057	-0.48677805791711
H	-0.74403782091563	2.32658457163280	-1.15843576720746	H	-0.52756387576034	2.30145567017911	-0.68373062772325
H	-5.34643278046931	2.61255648853792	0.55713244668060	H	-5.43073627571342	2.64098088459430	0.26496895715909
H	-4.24348158335834	4.63042752860745	-0.34965950420752	H	-4.04988418367463	4.65825103017608	-0.00469404408399
H	-1.90125358567706	-4.45735903411965	-1.18731038348159	H	-1.63193579887856	-4.47289743442903	-0.48758745654759
H	-4.22908989365488	-4.63297131912325	-0.34019225164581	H	-4.05048916448448	-4.65814930665668	-0.00548658368895
H	-5.33778620595442	-2.61723252604118	0.56420758060172	H	-5.43107147137775	-2.64074392607733	0.26454499793279
N	-1.68678140914430	0.00290501576084	-0.24680489971069	N	-1.74236725272828	-0.00005689560685	-0.44153506994453
S	-4.44160514962835	-0.00001754021523	1.03941146931845	S	-4.72125020874811	0.00008081378918	0.12435239691737
C	7.08466394379758	-0.00604589022166	0.43041279706145	C	6.97653949048969	0.00039593939712	0.38269049296939
C	6.16844769097523	-0.00356579724773	-0.59399784239323	C	6.09899619453622	0.00026107116433	-0.64078573064239
C	4.79952210041197	-0.00146482419012	-0.32713299901224	C	4.67876919395209	-0.00001500914573	-0.42902486922423
C	4.36126693268675	-0.00292361013332	1.00161469025034	C	4.20097515057940	-0.00014962084425	0.91673634073972
C	5.30119458598408	-0.00512736481491	2.04120124691472	C	5.17129874192473	-0.00000442405894	1.97510032891856
C	6.64448147309979	-0.00681678766315	1.75430245730138	C	6.49742928828875	0.00024727840691	1.73019388208901
C	3.85847924612611	0.00214077127954	-1.45605270127597	C	3.81297459375638	-0.00023497141261	-1.55634459648084
C	2.94299777925102	-0.00241090051922	1.29532389217378	C	2.81858733540270	-0.00041898906714	1.23421073462998
C	1.99042026582002	-0.0002604106161	0.21405869147959	C	1.99005327216433	-0.00026259615526	0.13595221449603
C	2.43159902164376	0.00271831263144	-1.11679140534564	C	2.46108293707264	-0.00013289859876	-1.24452789404868
C	1.49237358635508	0.00559451426638	-2.14750349913207	C	1.47768578875757	-0.00003551206522	-2.30372092783489
H	1.85640444679835	0.00737638278868	-3.16515171589588	H	1.87725542657181	-0.00002569831612	-3.30901548259477
C	0.14699862900608	0.00677279896573	-1.87560204999293	C	0.14995217895509	0.00000008725017	-2.08914339104440

C	-0.28812219484839	0.00380985036523	-0.54644016665205	C	-0.24689868886761	-0.00010193141798	-0.70670295202189
C	0.61465574588257	0.00054782359412	0.48431723449282	C	0.55955246969534	-0.00018123491016	0.34317955892921
H	8.14333327695376	-0.00731864087363	0.21096080996409	H	8.04343570528136	0.00059874174312	0.19306761079947
H	6.47953855000644	-0.00276250242252	-1.62932813472101	H	6.42623847444501	0.00032591052249	-1.67140602059647
H	4.95517754009577	-0.00634153772173	3.06511367361320	H	4.77970274521264	-0.00009286393564	2.98297866066236
H	7.36434596617953	-0.00906973619566	2.56156448347802	H	7.20689631677441	0.00035130551589	2.54958390428210
H	-0.58105029792108	0.00905069085593	-2.67487320632701	H	-0.57457280801496	0.00004416043686	-2.89194537629481
H	0.26284325498299	-0.00143706150698	1.50599319353245	H	0.23110930681235	-0.00021804619047	1.37578714963799
O	2.53928045635349	-0.00173442465783	2.49684087626940	O	2.34717752179017	-0.00055830358330	2.48429033662395
O	4.24585685808669	0.00431872170888	-2.61865898150314	O	4.25843595826909	0.00052804958595	-2.80060712803831

**Coordinates from the  $T_2/T_1$  MECP**

C	-2.22269505975029	3.64561890267326	-0.10998776899961
C	-1.61940732548972	2.42085400113088	-0.15564647015196
C	-2.36884955534251	1.23185288437784	-0.22824922217927
C	-3.80244167204461	1.34716385688986	-0.25909648577194
C	-4.39621491491827	2.62391749562878	-0.23099954026236
C	-3.63985273248332	3.75333514631244	-0.15511421643310
C	-3.80250448724045	-1.34843410735546	-0.28956875362625
C	-2.36862311359674	-1.23029554068327	-0.24417037085142
C	-1.61735134162609	-2.41914627355546	-0.17662262880028
H	-0.54090715778522	-2.36190475436194	-0.13485044064108
C	-2.21818445047425	-3.64524491563504	-0.15723673162406
C	-3.63512399382725	-3.75549146961306	-0.22424716402106
C	-4.39327044564219	-2.62652277251882	-0.28998784494010
H	-1.61492634266749	4.53588013912172	-0.03541017880227
H	-0.54240544885850	2.36619806512824	-0.13106681590401
H	-5.47658471798895	2.69026522924263	-0.26424157329808
H	-4.11300420394439	4.72442623294487	-0.12694947489742
H	-1.60972870678654	-4.53532193115243	-0.08593720043202
H	-4.10601785934481	-4.72802503772584	-0.21859276963266
H	-5.47306512077318	-2.69482666914204	-0.33597522023622
N	-1.74436821722276	0.00101818673823	-0.30475707217457
S	-4.83934999601985	0.00001943233180	-0.36046762236840
C	7.06157838347400	-0.00525034218292	0.27461112340908
C	6.12812745482054	-0.02218384089311	-0.74268811717792
C	4.77166610832914	-0.00971756923728	-0.44594829968954
C	4.35696501508341	0.02041735215443	0.88655988080026
C	5.30145590964679	0.03764672394275	1.90406867544551
C	6.64855468188543	0.02479606650070	1.60012359255576
C	3.79229423582208	-0.02841482047900	-1.56004220965155
C	2.91738748953812	0.03588594562648	1.23840403577920
C	1.93657752397711	0.01297102808996	0.11727530262366
C	2.35852305568263	-0.01594833055949	-1.21117671300536
C	1.40766913138738	-0.03429785188877	-2.23283526009219

H	1.74790540271447	-0.05529963823461	-3.25771552532466
C	0.06707289405231	-0.02639858419475	-1.93326510589182
C	-0.34340471079821	0.00045607170167	-0.60496856080059
C	0.58455821418763	0.01987809069608	0.41775793270210
H	8.11688522310251	-0.01504973491811	0.03725889899408
H	6.43068160403338	-0.04512809927971	-1.77970445762926
H	4.96037617013890	0.06120236531410	2.92916846347408
H	7.38163111688724	0.03822675804930	2.39514848851188
H	-0.67746836938567	-0.04209970585661	-2.71765377819110
H	0.26802106681265	0.03989238025324	1.45109751581132
O	2.54492330449211	0.06838508483674	2.39094204657200
O	4.15899695794351	-0.05500745021833	-2.71957936317680

**AQ-PTZ-O**

Coordinates from $S_0$ state				Coordinates from $S_1$ state			
C	-2.20374207115075	3.60104045520105	-0.74189532564533	C	-2.12540502045231	3.60736413345078	-0.69382199120342
C	-1.52956474749874	2.40097686250822	-0.67354695867892	C	-1.48248175963713	2.38895481968400	-0.68963865042764
C	-2.19948246762174	1.22283621430891	-0.32380100432037	C	-2.18429333398257	1.21643434609242	-0.36141163318453
C	-3.55614466147737	1.31805982559180	-0.00266657754648	C	-3.53840623896423	1.32457243693001	0.00131638136045
C	-4.22519397953424	2.53314724535411	-0.09223488093734	C	-4.16549496810732	2.54956371508341	-0.01602396172131
C	-3.56292946247977	3.67912192550432	-0.47060809952966	C	-3.46886050097505	3.69789851768377	-0.37265773228377
C	-3.55625873342792	-1.31820241138409	-0.00220752462626	C	-3.53812919161505	-1.32473069149987	0.00228793264169
C	-2.19958112935177	-1.22321690206612	-0.32334560943740	C	-2.18405504164462	-1.21656622669178	-0.36057161498866
C	-1.52976301843390	-2.40154390823465	-0.67265528649238	C	-1.48203656830858	-2.38916230482839	-0.68808397987583
H	-0.47597462016622	-2.37890955369432	-0.90020132142444	H	-0.43985259195052	-2.33088910241921	-0.95312096291397
C	-2.20405664084488	-3.60156340803037	-0.74062927458528	C	-2.12469777767073	-3.60770934586388	-0.69135612834484
C	-3.56326117081510	-3.67942024684098	-0.46936298777890	C	-3.46810498873446	-3.69830561226196	-0.37000586392875
C	-4.22542215850921	-2.53325621223424	-0.09138271338379	C	-4.16496327561791	-2.54986665983803	-0.01415135197086
H	-1.65593860538523	4.49165297948903	-1.01965213841490	H	-1.56782367264996	4.49504043090299	-0.95619194255719
H	-0.47578645896867	2.37815770910451	-0.90112196076737	H	-0.44025275146129	2.33072466936027	-0.95450475539337
H	-5.27614097635487	2.56503109500877	0.16669865228579	H	-5.20608938451832	2.61281956810123	0.27476611496031
H	-4.08675248349128	4.62206865160893	-0.53432654809279	H	-3.97302265536838	4.65347042683112	-0.38347191804817
H	-1.65633133280911	-4.49232166211199	-1.01807393105434	H	-1.56695426485556	-4.49544775721061	-0.95316908213900
H	-4.08717730581143	-4.62233449116083	-0.53279431382499	H	-3.97206443695625	-4.65399137677814	-0.38010989995626
H	-5.27637859052270	-2.56495157282116	0.16753492061763	H	-5.20553320107377	-2.61313379355362	0.27672756005565
N	-1.53241229813736	-0.00021735782331	-0.32221578703717	N	-1.53788130576804	-0.00002969643168	-0.43914396594864
S	-4.44738874555735	0.00009959350260	0.75767393514170	S	-4.46592226212149	0.00008874143152	0.72819212362125
C	7.25850034019874	0.00056499492213	0.47481891662364	C	7.17521260870629	-0.00000376775617	0.51501217914905
C	6.35283077696725	-0.00011981327814	-0.56787211144188	C	6.29665481479409	-0.00006005860047	-0.54041173082461
C	4.98973467774359	-0.00012131052540	-0.30601049444590	C	4.91513531798911	0.00005232066809	-0.32186061513257
C	4.53643575799806	0.00064767669305	1.01340960597260	C	4.43008106118268	0.00021687070212	0.99483180972661
C	5.45243920037312	0.00129089546900	2.05615463906458	C	5.33845479676304	0.00028686901159	2.05927221050536
C	6.80762295043030	0.00125892150553	1.78788020754846	C	6.69162088867090	0.00017469369569	1.82624807625575
C	4.03900027691923	-0.00105067328674	-1.44415131024730	C	4.01429779789173	0.00003286109592	-1.48324172101706
C	3.08595287659760	0.00100257910172	1.32789286507851	C	2.99223448885251	0.00024268639807	1.29216255606849

C	2.13251620255047	0.00010380319177	0.18613648978780	C	2.10957434885265	0.00016101164800	0.14401194481600
C	2.58537666345858	-0.00060078864468	-1.13047952862216	C	2.59706194294566	-0.00001066724460	-1.19101925922565
C	1.67100639703692	-0.00104734353410	-2.17589226850878	C	1.68321802620410	-0.00018496347499	-2.25235170221059
H	2.04012402513569	-0.00156934008453	-3.19123999211424	H	2.08580709628438	-0.00031958990465	-3.25637154530261
C	0.31876114659961	-0.00088584796727	-1.91047150047102	C	0.33152817827398	-0.00018153098855	-2.03744774027981
C	-0.12840664231830	-0.00032569563390	-0.59547100402383	C	-0.12439274231190	0.00000607433205	-0.70262447544640
C	0.76929927143883	0.00015485146501	0.44998884260659	C	0.72940467767217	0.00017288200339	0.36133504331808
H	8.31995848791779	0.00054385908084	0.26703689698841	H	8.24168776462478	-0.00009220739245	0.33237880870198
H	6.68397484062530	-0.00070460432879	-1.59647517975633	H	6.64655697997251	-0.00018139155805	-1.56305537485292
H	5.08332982839578	0.00188865511346	3.07177320825346	H	4.94156701132875	0.00040370775023	3.06450845847445
H	7.51807443104639	0.00180533062731	2.60341259436708	H	7.38416742482487	0.00021799099971	2.65763271238087
H	-0.40357355523923	-0.00124203599005	-2.71578153746137	H	-0.37535135718037	-0.00033434332371	-2.85509347641955
H	0.42132156373676	0.00066656411622	1.47335482441430	H	0.36059626691383	0.00028282186873	1.37828279590663
O	2.68657111054145	0.00108198396458	2.47090221345278	O	2.56614889761172	0.00064646937705	2.45775288746309
O	4.42735871079593	-0.0011434725500	-2.59180321598452	O	4.45134891529459	-0.00045148260166	-2.64365681736257
O	-4.07964268060028	0.00033685449782	2.19945657445214	O	-4.13740501372854	0.00064350512033	2.17360529755487

Coordinates from S <sub>2</sub> state				Coordinates from T <sub>1</sub> state			
C	-2.16771974444425	3.60519530758636	-0.71688140686372	C	-2.23608238972217	3.58592630425325	-0.82022696181508
C	-1.50689296085164	2.39693042222942	-0.67861571299320	C	-1.54941681021784	2.39227003488222	-0.76130130510406
C	-2.19219102154330	1.21951893297204	-0.34419106864070	C	-2.19069538896533	1.22097289037609	-0.34400213036885
C	-3.54850286975175	1.32030755018442	-0.00498004678108	C	-3.52657892362565	1.31554451491955	0.05402072806362
C	-4.19858046766088	2.54084402567928	-0.05900024118743	C	-4.20924539705101	2.52339386024828	-0.02385608292801
C	-3.52102681797766	3.68870829596044	-0.42567137392203	C	-3.57753177281623	3.66269927212448	-0.47011187542675
C	-3.54759481158080	-1.32050362787405	-0.00367639630775	C	-3.52645464215323	-1.31547048706018	0.05490853569110
C	-2.19137891114962	-1.21908834376830	-0.34306685141109	C	-2.19058133712524	-1.22104246240488	-0.34316926106481
C	-1.50531573098916	-2.39631879303063	-0.67657041194385	C	-1.54915805895196	-2.39255130592675	-0.75962481759202
H	-0.45679865141725	-2.35622099149451	-0.92247997285713	H	-0.51121101860036	-2.36689399351634	-1.05144042323185
C	-2.16529075608669	-3.60508309724852	-0.71361453857548	C	-2.23566076969595	-3.58634442783625	-0.81763288503075
C	-3.51849326942528	-3.68928050507724	-0.42211975172104	C	-3.57708920481211	-3.66303400035476	-0.46741915635315
C	-4.19682099593861	-2.54154509252791	-0.05648064434748	C	-4.20895848088912	-2.52346961912390	-0.02204135319481
H	-1.61530346095337	4.49516018775835	-0.98533598175507	H	-1.71331672763641	4.47216150993726	-1.15457707397914
H	-0.45829425577509	2.35734949515064	-0.92426224937792	H	-0.51147151411499	2.36654094664901	-1.05308591748981
H	-5.24464701234839	2.58678151362752	0.21614907437007	H	-5.24269995901626	2.55619549682022	0.29758192759655
H	-4.03632801528549	4.63760820012921	-0.46531585796030	H	-4.11050025105660	4.60101723640925	-0.52641668045591
H	-1.61229235884048	-4.49490243851684	-0.98135128559470	H	-1.71277784908317	-4.47276546995436	-1.15130615577427
H	-4.03312823100315	-4.63858129097113	-0.46079808358380	H	-4.10992878813222	-4.60146885273346	-0.52298961683533
H	-5.24283510879466	-2.58795095671487	0.21879051474901	H	-5.24240224458847	-2.55616904651593	0.29944661827042
N	-1.53595622737607	0.00041643604647	-0.38271632554523	N	-1.52049457735855	-0.00001908615786	-0.35183583807483
S	-4.44831644110654	-0.00004166839889	0.74910529759985	S	-4.34768978117164	0.00028063705414	0.89340922493141
C	7.21049205946569	-0.00105140793441	0.49386434903793	C	7.23524660172943	0.00058672960851	0.50806648364672
C	6.32103362697925	-0.00064521663510	-0.55353151997223	C	6.33782543041439	0.00033443583162	-0.53325349295028
C	4.94340445969650	-0.00014694792024	-0.31915044482571	C	4.96475965308926	-0.00009940336652	-0.29090272390349
C	4.47595844543925	-0.00009795843815	0.99944065455964	C	4.50141272070397	-0.00017421212403	1.02828853728263
C	5.39080856952924	-0.00049426058852	2.06011964936217	C	5.42157099910003	0.00007910031121	2.08623492889135

C	6.74072813332860	-0.00097417583753	1.80917189675227	C	6.77007734094876	0.00047361466945	1.82274565853523
C	4.02960863515039	0.00026344905605	-1.46957358271987	C	4.04554925945019	-0.00040624343213	-1.43589366945812
C	3.04707533881271	0.00030040156845	1.28585979756154	C	3.07860078731782	-0.00043051018021	1.29337374976279
C	2.13575410478044	0.00050987683806	0.16733738661068	C	2.13988674256087	-0.00031588213300	0.19437346563346
C	2.60268180692335	0.00047319759810	-1.16177623036323	C	2.60974650206894	-0.00033062811497	-1.12247276155505
C	1.67957342262223	0.00054408041051	-2.21017084936149	C	1.69595348316121	-0.00022510744694	-2.17589975028643
H	2.05769687199781	0.00047434671758	-3.22265313986278	H	2.08726149084450	-0.00025961409920	-3.18360023660419
C	0.32918083014023	0.00064172166424	-1.96348447050760	C	0.34515579281079	-0.00017561118492	-1.93611526088729
C	-0.12111802719244	0.00068068691111	-0.63632050335513	C	-0.11608596265863	-0.00008846441462	-0.61940350620290
C	0.75661665675927	0.00064669903851	0.41176828953229	C	0.75822741708114	-0.00020422827444	0.43682735529322
H	8.27455711273404	-0.00143330871022	0.29953276185053	H	8.29773507044344	0.00089141446142	0.30803379030583
H	6.65919152150687	-0.00068887379282	-1.58042687780145	H	6.66805444815251	0.00042401182963	-1.56278700796143
H	5.00902497647540	-0.00045057725058	3.07152629623179	H	5.06053929024303	0.00005901464883	3.10506907624402
H	7.44143124490581	-0.00130593612897	2.63344515847548	H	7.47436798234098	0.00073392245876	2.64365369698288
H	-0.38717302345543	0.00061933739899	-2.77345920105411	H	-0.36633650310775	-0.00014594142084	-2.75016587870583
H	0.39822457709930	0.00061610622786	1.43209826936597	H	0.37630354433464	-0.00020320233268	1.44810258876500
O	2.62291742354552	0.00031572012243	2.46556152433205	O	2.65519654842921	-0.00042445796440	2.48892348452745
O	4.44932697294616	-0.00005962518825	-2.62902105294288	O	4.44906833010161	0.00018767870668	-2.59089785107866
O	-4.08040261989011	0.00077910317167	2.18868015374421	O	-3.84728608277586	0.00075963187376	2.29512482388942

Coordinates from T <sub>2</sub> state				Coordinates from the T <sub>1</sub> /S <sub>0</sub> MECP			
C	-2.22520923682948	3.59323853027772	-0.78905976349452	C	0.79370247704893	3.56040080769621	0.35439667320137
C	-1.54359007353396	2.39676592513159	-0.73371389160873	C	0.24604376553565	2.54563504575484	1.09902599724878
C	-2.19452136063061	1.22137335074392	-0.34238900163332	C	-0.54125943951248	1.54183401458587	0.49883827874998
C	-3.53657115062768	1.31613459486957	0.03499791141012	C	-0.75698023399967	1.62019391928643	-0.89356573224099
C	-4.21420059200583	2.52738364109471	-0.04053289030422	C	-0.18893819414119	2.63848524248456	-1.63520886176920
C	-3.57251694126928	3.67014227263166	-0.46192952709890	C	0.58385733060596	3.60896202025769	-1.02056521629054
C	-3.53631269964102	-1.31625639901057	0.03590859476020	C	-2.16557267033417	-0.62240334568355	-0.49236553232347
C	-2.19428445019319	-1.22148991984740	-0.34155904421073	C	-1.75159000782814	-0.44921485829426	0.84638051512779
C	-1.54311427160449	-2.39703941035250	-0.73202493211467	C	-2.13644384312317	-1.42835737428646	1.78509983646419
H	-0.49983211380319	-2.37251503384957	-1.00383852748248	H	-1.80339025811300	-1.29265629168845	2.80451406528708
C	-2.22448475527575	-3.59369486441547	-0.78647501654547	C	-2.89358095742193	-2.51239052409897	1.41369773917177
C	-3.57177111779944	-3.67063881323406	-0.45927198763428	C	-3.29585826882879	-2.66141874012491	0.09005857870179
C	-4.21368921204445	-2.52770175055402	-0.03872193379249	C	-2.92563275782308	-1.71698629549024	-0.85368520283939
H	-1.69339767759788	4.48213830281190	-1.10130975469968	H	1.39901328423243	4.31594773848526	0.83586654048604
H	-0.50030044318083	2.37225026365272	-1.00551353120802	H	0.40763972528813	2.47472678409308	2.16534481720278
H	-5.25288752430293	2.55910172630715	0.26383052768871	H	-0.35900410812429	2.67798051111437	-2.70351198798540
H	-4.10188603944103	4.61062079645680	-0.51577116553877	H	1.02375767156828	4.39938641751104	-1.61260008557382
H	-1.69248945976921	-4.48271682661587	-1.09806246112083	H	-3.17435729777945	-3.25237568116339	2.15068285996068
H	-4.10094244123066	-4.61126964232348	-0.51239560092645	H	-3.89119104813503	-3.51340596599555	-0.20737985731675
H	-5.25236521562890	-2.55941238194556	0.26568320351124	H	-3.23619184389670	-1.83215798455867	-1.88439468043897
N	-1.52576160402516	0.00000545480907	-0.35544501785972	N	-1.00871866554120	0.57491844070735	1.31947958324194
S	-4.37909638581440	0.00013713741173	0.85082191226239	S	-1.80559926792254	0.51600159357209	-1.80654290849730
C	7.24149528805683	-0.00001970115376	0.50554551799261	C	4.19249290482108	2.25255346035785	0.35316567430346
C	6.35305460615874	-0.00000677980376	-0.54459672129448	C	3.57979260655376	1.63736568802977	-0.72102261492451

C	4.97602259523668	0.00010533702025	-0.30547875552379	C	2.82594876312239	0.48905464499330	-0.52901652473547
C	4.50503942509634	0.00018591505064	1.02596798421006	C	2.68746207097321	-0.04151476564181	0.75355373037542
C	5.42593547590713	0.00018382685015	2.07665950949412	C	3.29838148904950	0.58577476856406	1.82948442613389
C	6.77726338137117	0.00007601791028	1.81867850630164	C	4.04942176138836	1.72793728234986	1.62984823849858
C	4.03441005241299	0.00016443981385	-1.40822847837520	C	2.17173171153231	-0.14577180261059	-1.70077225686649
C	3.07817977486498	0.00020925479877	1.29478793632684	C	1.89116182959967	-1.26989428791833	0.99396262865885
C	2.13852095801131	0.00018512817176	0.18828680906040	C	1.25492234578818	-1.91745378358323	-0.18324737900602
C	2.60902760944265	0.00007382641684	-1.14270264066144	C	1.38177885011214	-1.38014170174031	-1.46564840476643
C	1.68728619125579	-0.00008032859809	-2.19492806979870	C	0.76624407191123	-1.99560550873332	-2.55007039513757
H	2.04773617449191	-0.00017091304009	-3.21257742097165	H	0.87567422199188	-1.55383551779347	-3.53042624828049
C	0.33857704493101	-0.00010750575820	-1.93893389617707	C	0.02243224237703	-3.15163749575793	-2.36853767844236
C	-0.12085091920979	0.00004755188131	-0.62336789735014	C	-0.06244086429361	-3.63044689754388	-1.08844870463470
C	0.76174238945343	0.00021117174512	0.42776058155602	C	0.51021309651146	-3.07904514507272	0.01586266309807
H	8.30473795502342	-0.00010454381523	0.30873143345710	H	4.77965006443293	3.14781318908992	0.19880280068753
H	6.71034104025157	-0.00006807784460	-1.56363440997158	H	3.67066091200629	2.03571695108334	-1.72118601442960
H	5.06201182897140	0.00023560458978	3.09339559345570	H	3.17339238874396	0.16299533440966	2.81603162198740
H	7.48056795805375	0.00005494095201	2.63994168417694	H	4.52578781214240	2.21354570079932	2.47085031128800
H	-0.37621577137662	-0.00023493682008	-2.75041925669928	H	-0.46476893509547	-3.63660187241491	-3.20369376332400
H	0.38760539661350	0.00029883687642	1.44106552421971	H	0.41013769267749	-3.48478706525582	1.01270443448646
O	2.65814236564379	0.00049727877102	2.47170553685356	O	1.76337355263149	-1.73540490127636	2.10496264039461
O	4.44917283127995	-0.00012203884752	-2.59084606810212	O	2.27723025709457	0.32891785490809	-2.81156546519130
O	-3.91769388569260	0.00064874078311	2.26571389546135	O	-3.05750123782700	1.24618039659325	-2.14340413974168

Coordinates from the $S_1/T_1/T_2$ MECP				Coordinates from the $T_2/T_1$ MECP			
C	-2.41330778463294	3.52300573353979	-1.02482034457834	C	-2.21889325481205	3.59118129937919	-0.78067088931501
C	-1.67044133545189	2.36126523834851	-0.95618437890057	C	-1.53671016003238	2.39497026735308	-0.72403245232759
C	-2.19544958036165	1.21395115729229	-0.36568925159437	C	-2.18749230021730	1.21999859224588	-0.33137117255406
C	-3.47093209645134	1.30531163407113	0.18351302733460	C	-3.53000027934380	1.31445173128417	0.04480726284629
C	-4.22637994740734	2.47524207872534	0.08358915557171	C	-4.20791039365864	2.52527720143943	-0.03158980340882
C	-3.70854831999656	3.58920793617013	-0.52552710083089	C	-3.56612915484006	3.66795928261993	-0.45343320865103
C	-3.47535163187847	-1.30326943355955	0.18381988470179	C	-3.53203809544931	-1.31685633048780	0.03220556494009
C	-2.19959055270860	-1.21634473891382	-0.36547920294531	C	-2.18873489773542	-1.22191466992435	-0.34128457548870
C	-1.67864101451022	-2.36543891667674	-0.95608502618832	C	-1.53908102404467	-2.39578201046825	-0.73936277649271
H	-0.68268535441909	-2.36270673946306	-1.37151192255977	H	-0.49499016670293	-2.37176205752383	-1.00795161338944
C	-2.42547613644229	-3.52464706446530	-1.02450530030359	C	-2.22356857116515	-3.59004159789967	-0.80675911380240
C	-3.72083479283556	-3.58641347742866	-0.52493141376699	C	-3.57204420022733	-3.66634858152568	-0.48444911452581
C	-4.23478362905094	-2.47063271819495	0.08413517454301	C	-4.21224348735889	-2.52569984031606	-0.05507805605115
H	-1.97383385228753	4.39338368555031	-1.49516698575020	H	-1.68772781527975	4.47984969413305	-1.09466001808231
H	-0.67437986496253	2.35521902241819	-1.37126750523232	H	-0.49374782555737	2.36991167874413	-0.99717292560530
H	-5.21752729798181	2.48974696803389	0.51978695538889	H	-5.24691367174810	2.55677433465068	0.27172240111108
H	-4.28426375395375	4.50078462205401	-0.59757270006989	H	-4.09582159540030	4.60820703628969	-0.50839991975569
H	-1.98909414834435	-4.39654469249693	-1.49491282717618	H	-1.69314505268105	-4.47758545132324	-1.12514519075111
H	-4.29966124913968	-4.49603490607250	-0.59676966868939	H	-4.10355502889653	-4.60503837973613	-0.54791716846271
H	-5.22592011636159	-2.48170404176743	0.52046162982515	H	-5.25185038251041	-2.55748595261775	0.24614013530110
N	-1.49460268141643	-0.00238114678079	-0.31334258611528	N	-1.51870354407648	-0.00106537019319	-0.34394073588996

S	-4.09170985385263	0.00218473704257	1.18810216165080	S	-4.37374082489200	-0.00434097538575	0.85468603089598
C	7.30674135276489	0.01534399432815	0.58939891669534	C	7.22296688565875	-0.00526731533813	0.49342364754021
C	6.41046856773095	0.01009029171077	-0.46662921097919	C	6.33803966195724	-0.01910352509867	-0.56016793216440
C	5.04830335571440	0.00095466341092	-0.22942176568752	C	4.96936816646767	-0.00868036255176	-0.33316976311402
C	4.58548873010673	-0.00219015501244	1.08530614631355	C	4.47912511119757	0.00862812711192	1.03850206483324
C	5.47840466006725	0.00176410364235	2.15063274395259	C	5.41851946036338	0.02429771331677	2.10798586824099
C	6.83807161328977	0.01122941623822	1.89295898255141	C	6.74748370230515	0.01663740643229	1.84639363000599
C	4.11010456717728	-0.00535292167160	-1.38283958119406	C	4.04568871184060	-0.01203484147881	-1.45587976679080
C	3.14250841854945	-0.00904181531430	1.31760457809471	C	3.07727612200992	0.00970385231982	1.31288387198965
C	2.14687204768307	-0.00698671587692	0.19953547846938	C	2.14678189510879	0.00219425340242	0.18191694886152
C	2.63474677542139	-0.00638129829972	-1.09155541753250	C	2.60806183745360	-0.00502958065805	-1.13781395226215
C	1.74076591200403	-0.00483182955036	-2.14737124143396	C	1.68854202473624	-0.00736564947381	-2.18825982875837
H	2.13218126373167	-0.00376374224514	-3.15446749624762	H	2.06701652103317	-0.01064707305697	-3.20019600829121
C	0.37840601471189	-0.00441881555200	-1.90401463971452	C	0.34000768549411	-0.00417299668516	-1.93489536908288
C	-0.10577794951909	-0.00446019228161	-0.61003424554605	C	-0.11386639690898	-0.00068490042876	-0.61609014688691
C	0.78955807757478	-0.00616586984283	0.45402460504569	C	0.77230271186983	0.00374014793629	0.43138619146408
H	8.36970133884722	0.02247843405750	0.39445534034498	H	8.28801353148382	-0.00768905296564	0.30682783295597
H	6.75269037137540	0.01273639947797	-1.49191503641266	H	6.68516877914214	-0.03341842646564	-1.58358861999422
H	5.11553482307636	-0.00097619844805	3.16838157397269	H	5.03792177322551	0.04061663028853	3.11847591678471
H	7.53412850912987	0.01525446978562	2.72028647567980	H	7.46406404758058	0.02603570207228	2.65600794172254
H	-0.31987264329525	-0.00370471101905	-2.72963109772399	H	-0.37778147569573	-0.00392516072304	-2.74385000548962
H	0.39645612417571	-0.00592447434814	1.46027745959356	H	0.41230339731755	0.00850265684226	1.45028420742119
O	2.70450253176366	-0.02256041820514	2.47417899825729	O	2.66342112713684	0.02095924845933	2.49719540881321
O	4.50825728041948	-0.00845870630738	-2.51886096851776	O	4.45057027540458	-0.02749829875503	-2.61769517449182
O	-3.30194174805373	0.00100115389680	2.45581262770431	O	-3.91306882955248	-0.01163845523991	2.26973537615239

**AQ-PTZ-O<sub>2</sub>**

<b>Coordinates from S<sub>0</sub> state</b>				<b>Coordinates from S<sub>1</sub> state</b>			
C	-2.22798230126872	3.59941912101636	-0.76443705503928	C	-2.21946818660530	3.59669488478793	-0.79178656128822
C	-1.55140132891170	2.40011832424920	-0.70539162968844	C	-1.54665894871908	2.39442838279046	-0.76186979749026
C	-2.20688007890842	1.22851989298799	-0.31223082181894	C	-2.19332463595693	1.22698641463317	-0.33982396066950
C	-3.55008041555183	1.34208903889537	0.05389598638768	C	-3.52083252442553	1.34330410139933	0.08438706401086
C	-4.23269653542707	2.54762586160008	-0.03237007053698	C	-4.19750393916163	2.55080743310152	0.03170287784159
C	-3.57708882084781	3.68411731812434	-0.44713857119948	C	-3.55172035903197	3.68516839039721	-0.41258261596719
C	-3.54998699840500	-1.34225436626617	0.05448152802708	C	-3.52069897759173	-1.34337024797851	0.08506857805624
C	-2.20679078824269	-1.22875794408248	-0.31168485755374	C	-2.19319393860806	-1.22713616106814	-0.33916529731567
C	-1.55122867624984	-2.40049012338563	-0.70430817093614	C	-1.54641056523807	-2.39471862143808	-0.76064274186588
H	-0.50772343395380	-2.37249065182266	-0.97356279111360	H	-0.51658797928466	-2.35583367738395	-1.07664207347832
C	-2.22772735042925	-3.59986077126496	-0.76283769389692	C	-2.21909270411158	-3.59707046645408	-0.78994567152623
C	-3.57683150430640	-3.68451093459075	-0.44551790737059	C	-3.55133492734052	-3.68549038749397	-0.41069313184562
C	-4.23251804114013	-2.54788017277267	-0.03125208998777	C	-4.19724476541217	-2.55096921318370	0.03299688086251
H	-1.69064987229294	4.48496029242302	-1.07630717852851	H	-1.69395104294239	4.47998917785165	-1.12827468532999
H	-0.50789896256248	2.37206126781482	-0.97465898073448	H	-0.51682117731156	2.35550285062913	-1.07781039044191
H	-5.27684551564650	2.57395127485500	0.24770540091427	H	-5.22784471219875	2.58573662286775	0.35803596012143
H	-4.10145477039459	4.62668988523049	-0.50975570686656	H	-4.07420005710794	4.63009351542532	-0.45118518962501



H	-1.69032980310252	-4.48550163681418	-1.07431179726471	H	-1.69348851400092	-4.48047860329361	-1.12599954304423
H	-4.10113406812620	-4.62714543702904	-0.50772921113031	H	-4.07371926613619	-4.63048762173263	-0.44882123698509
H	-5.27666736786022	-2.57415226059280	0.24882910521259	H	-5.22758440185612	-2.58583213787295	0.35933335032549
N	-1.54252536464871	-0.00009449257618	-0.30956469450725	N	-1.53307724198335	-0.00005060764263	-0.37603472266174
C	7.24739748341068	0.00009749417813	0.48165196028617	C	7.19544627012999	0.00032507272330	0.52043465180989
C	6.34185607865424	-0.00027214218769	-0.56114727721770	C	6.31240975760056	-0.00011655063473	-0.53076039824614
C	4.97876187614087	-0.00001874902168	-0.29942314537123	C	4.93249781892595	-0.00016555667823	-0.29742740316523
C	4.52554480765852	0.00065551283315	1.02013392242898	C	4.45842167071739	0.00025677162043	1.01502175260350
C	5.44141535312042	0.00101113744302	2.06296592860584	C	5.36945066850067	0.00072553425269	2.07899063914657
C	6.79654744847652	0.00073071024413	1.79471581468924	C	6.72014252203549	0.00076465756118	1.83423713409163
C	4.02829170802063	-0.00059568840685	-1.43769991020527	C	4.02153532214501	-0.00055108096932	-1.44317930981011
C	3.07547443896965	0.00104469587050	1.33451168671014	C	3.02626676737456	0.00007860727865	1.31445937773141
C	2.12213650578772	0.00032931824294	0.19244957020462	C	2.11989010350704	-0.00001348670000	0.17191741054471
C	2.57423119782047	-0.00028411886312	-1.12411352523975	C	2.59671834641706	-0.00042197141837	-1.14303107108199
C	1.65953666621384	-0.00072181778709	-2.16933874954318	C	1.68363912313014	-0.00061149635520	-2.20689785734588
H	2.02850169193794	-0.00117680569914	-3.18474654391867	H	2.08117883755721	-0.00090465528670	-3.21306775422907
C	0.3072776051448	-0.00061670734546	-1.90364513263231	C	0.33552739798943	-0.00046190757215	-1.97387932932833
C	-0.13864226266230	-0.00011065995943	-0.58817712714952	C	-0.12997135487608	-0.00008409760335	-0.65065283835370
C	0.75920835296477	0.00037055345972	0.45676623686154	C	0.73924550274266	0.00014472313052	0.40606158832681
H	8.30885615900680	-0.00012497557262	0.27397574005244	H	8.26012495067504	0.00034260931957	0.32955947932615
H	6.67299147795628	-0.00079726273765	-1.58975199947745	H	6.65584868118817	-0.00042681193230	-1.55598759045164
H	5.07207984015629	0.00152224237336	3.07851208997003	H	4.97993246644022	0.00102934801407	3.08751134460502
H	7.50699547508990	0.00101054348325	2.61023304584479	H	7.41640625275785	0.00112272640639	2.66207280862659
H	-0.41529197364097	-0.00096690283389	-2.70881003661761	H	-0.37280584566804	-0.00067458532985	-2.79103998997406
H	0.41234543555263	0.00081153573985	1.48049285599228	H	0.37270959883797	0.00040092023447	1.42359030544603
O	2.67497494474663	0.00122828155504	2.47711482039331	O	2.60637344574380	0.00137563145765	2.48092121585319
O	4.41598144391415	-0.00107563958326	-2.58539497624289	O	4.43944571948857	-0.00115701126373	-2.60858396585569
O	-3.99689308155276	0.00037800810091	2.21261506406807	O	-3.89163619389032	0.00047085887037	2.25524789057730
S	-4.35342899720210	0.00005723008310	0.81752548227261	S	-4.29953043224472	0.00012451781655	0.87540554123670
O	-5.75201008277847	-0.00006870960842	0.48409475286760	O	-5.70681078220115	-0.00001172528318	0.58619261623311
<b>Coordinates from S<sub>2</sub> state</b>				<b>Coordinates from T<sub>1</sub> state</b>			
C	-2.15596516175630	3.61176123030890	-0.67973389402616	C	-2.26244946378411	3.58121273529292	-0.85036461252570
C	-1.50675723461696	2.39754729643311	-0.65715381315851	C	-1.57291727631539	2.38908882975563	-0.79171668660654
C	-2.19900981461491	1.22426962748047	-0.31822665160741	C	-2.19973349948521	1.22626371075201	-0.33372231241706
C	-3.55164544323912	1.34736992778913	0.03379332658117	C	-3.52358464155254	1.33944223060167	0.09679721705302
C	-4.19774727911216	2.56640265362673	-0.00700845202180	C	-4.22031477434112	2.53662008887777	0.01282701217207
C	-3.50490640665626	3.70698383996293	-0.37232324066453	C	-3.59460542665401	3.66498643663691	-0.46668866851329
C	-3.55099375275056	-1.34745644288093	0.03537199005421	C	-3.52355963537566	-1.33947898440295	0.09749904915988
C	-2.19845091866454	-1.22409029270636	-0.31693083481836	C	-2.19969685697543	-1.22650243828248	-0.33303686103652
C	-1.50567204230746	-2.39741252967961	-0.65465252794837	C	-1.57283039138769	-2.38954854214137	-0.79038712339071
H	-0.46196861946018	-2.34557763433706	-0.91607432984246	H	-0.54485599594230	-2.35774994540140	-1.11418585213845
C	-2.15426750088989	-3.61197679722549	-0.67573063588231	C	-2.26231431543561	-3.58173365207896	-0.84837379922241
C	-3.50311427004502	-3.70751973223020	-0.36801410242193	C	-3.59446971916102	-3.66534673745006	-0.46466326672331
C	-4.19648612150440	-2.56685937198832	-0.00395845838125	C	-4.22023953366152	-2.53673122870263	0.01419647184749

H	-1.59877580148214	4.49744197982282	-0.95128411543409	H	-1.75040629888109	4.46102478971169	-1.21638977501054
H	-0.46297779471830	2.34593042013026	-0.91833062461950	H	-0.54494363935840	2.35716655212489	-1.11549100983442
H	-5.24367856717841	2.61533653393852	0.26306394397196	H	-5.24902905782610	2.56389042634914	0.34484588806972
H	-4.01100339270187	4.66095881440849	-0.40407248137191	H	-4.12896875650808	4.60193192516716	-0.52968462578882
H	-1.59667528922750	-4.49768876205551	-0.94634989746494	H	-1.75023002510241	-4.46173039028617	-1.21389699897020
H	-4.00873434594113	-4.66178540010168	-0.39858576236335	H	-4.12879512983354	-4.60234781867084	-0.52714358001456
H	-5.24236863225970	-2.61600603598914	0.26627004055494	H	-5.24895672845784	-2.56385426845611	0.34621518864767
N	-1.55222118169235	0.00021358405006	-0.37134126753679	N	-1.53105438099626	-0.00012114991747	-0.33252898834054
C	7.19375680352430	-0.00046433396536	0.47531215553885	C	7.22661796354646	0.00051119741830	0.51373303649032
C	6.30191712576450	0.00015313760693	-0.56885817225108	C	6.32817940236596	0.00012615100079	-0.52658383287331
C	4.92353124369832	0.00023278177321	-0.32448122410394	C	4.95534322134312	0.00000327050288	-0.28281813521629
C	4.45890168444462	-0.00031268712632	0.99565460490494	C	4.49361243300496	0.00031035825227	1.03685119687144
C	5.38076154081953	-0.00096086823925	2.04685448146973	C	5.41473581430716	0.00067914855617	2.09393734269193
C	6.73066202234888	-0.00105118671261	1.79331512245278	C	6.76287698128197	0.00078511682899	1.82907169067949
C	4.00209872825899	0.00060230701163	-1.46369400618688	C	4.03464740644743	-0.00046945851285	-1.42678289552608
C	3.02630183982268	-0.00001492433897	1.30449780013608	C	3.07106109113920	0.00033045694095	1.30299962822170
C	2.11989666076503	0.00016834942749	0.17161659888992	C	2.13094861189068	0.00001988534951	0.20563002286081
C	2.58328665731333	0.00061205009328	-1.16377759592285	C	2.59875788587307	-0.00035137153383	-1.11176737443407
C	1.65562232820208	0.00087306860619	-2.21286392700411	C	1.68347165211837	-0.00065236808701	-2.16387750928728
H	2.02440090840473	0.00114509874673	-3.22839069666199	H	2.07354113356617	-0.00096759574977	-3.17207585630701
C	0.30702747692251	0.00075203254747	-1.96311041137749	C	0.33292830311377	-0.00059416785038	-1.92257054373204
C	-0.13606207219834	0.00038828644038	-0.63157078694051	C	-0.12631872763194	-0.00018727205313	-0.60480678002164
C	0.74579854434776	0.00010942166018	0.41327179894269	C	0.74949419921984	0.00009022190072	0.44984045826259
H	8.25703660887811	-0.00052840460095	0.27555152646291	H	8.28886339949462	0.00058818795341	0.31252113249471
H	6.64006504779887	0.00053662203227	-1.59552165936452	H	6.65716933107161	-0.00010781028304	-1.55652933853036
H	4.99728951783933	-0.00134337540699	3.05769519837806	H	5.05453315319330	0.00093046362924	3.11307736418784
H	7.43508235489103	-0.00155083390009	2.61428598329807	H	7.46800211527016	0.00110270315615	2.64923705011375
H	-0.41073093642822	0.00094379656581	-2.77197029569578	H	-0.37916380328038	-0.00088209410433	-2.73612461687427
H	0.39809807775347	-0.00015837218872	1.43759393072833	H	0.36985597665266	0.00039023381083	1.46194033737093
O	2.61051190559632	-0.00169232526242	2.47191870141325	O	2.64840463893741	0.00038814304431	2.49897652314447
O	4.42738366187831	0.00175210935142	-2.63342992764304	O	4.43621562247579	-0.00053554864801	-2.58205969186570
O	-4.17044876217877	0.00106163679605	2.14535819250881	O	-3.79128376744908	0.00053269641658	2.28613636346463
S	-4.41521790312056	0.00016043105306	0.72915216396117	S	-4.26477645702160	0.00018930721482	0.92607676814848
O	-5.77585374998764	-0.00042165672759	0.27422557246801	O	-5.68606428389536	0.00012264536704	0.70922433324821
<b>Coordinates from T<sub>2</sub> state</b>				<b>Coordinates from the T<sub>2</sub>/T<sub>1</sub> MECP</b>			
C	-2.24952854642434	3.59049007522015	-0.81439797028226	C	-2.22977366917476	3.58770772648976	-0.80164495469494
C	-1.56593070609968	2.39497899342309	-0.76203988446691	C	-1.55098254662630	2.38963301207506	-0.74624317142584
C	-2.20333451952690	1.22709164599325	-0.33075884666825	C	-2.19578161314204	1.22311358688567	-0.32192892838318
C	-3.53339379030308	1.34024240088010	0.08057032741855	C	-3.52860645853486	1.34077107174920	0.07953043773815
C	-4.22407342813609	2.54177187236663	0.00217011200483	C	-4.21416203915853	2.54499716609361	-0.00177994231792
C	-3.58757527646374	3.67434411457060	-0.45142816094974	C	-3.57015783698011	3.67603641895138	-0.44851518113141
C	-3.53257387967124	-1.34040455152661	0.08173677444831	C	-3.53829579703863	-1.33942542833501	0.07436620632643
C	-2.20259003957077	-1.22679464088315	-0.32969975979042	C	-2.20446766285112	-1.23005004187976	-0.32621272310116
C	-1.56447544692344	-2.39466620232033	-0.75998205166104	C	-1.56784434560584	-2.39981923614708	-0.75394991487194

H	-0.53100929918779	-2.36372333009405	-1.06548595004920	H	-0.53164597215100	-2.37263985905101	-1.05032012698116
C	-2.24732391982757	-3.59065219558931	-0.81124526586256	C	-2.25541750700508	-3.59261346057915	-0.81444466992540
C	-3.58529962892464	-3.67502105916813	-0.44814290496195	C	-3.59674346984585	-3.67227888834304	-0.46282444219471
C	-4.22249764633303	-2.54243774712504	0.00444042090957	C	-4.23259243958419	-2.53828378456200	-0.01193626647436
H	-1.72764493025056	4.47361634916109	-1.15780405048403	H	-1.70210858887885	4.46944507447784	-1.13972844604591
H	-0.53242901130743	2.36441022745578	-1.06746686903797	H	-0.51535831055769	2.35595304972862	-1.04396519892983
H	-5.25774648379544	2.56826979942910	0.31860064189955	H	-5.25018445677889	2.57456326283635	0.30660525873564
H	-4.11752158853503	4.61409966865226	-0.50938835313254	H	-4.09625445613615	4.6178085860711	-0.50890344193708
H	-1.72490105571462	-4.47375774620289	-1.15388276726060	H	-1.73400117143818	-4.47698138607613	-1.15534114108402
H	-4.11465806532210	-4.61516125452400	-0.50522914922968	H	-4.12984565883252	-4.60982372997246	-0.52740235037118
H	-5.25614612879039	-2.56929410239149	0.32092094609585	H	-5.26895838018055	-2.56153120589189	0.29582834769123
N	-1.53641975179628	0.00035016268053	-0.33740512792579	N	-1.53340690017492	-0.00588490139203	-0.32720405248203
C	7.23187627866985	-0.00130043321400	0.50988219753387	C	7.22555801412711	0.01872635409472	0.46785175297712
C	6.34220603988073	-0.00067131032475	-0.53933407136744	C	6.35224476356142	0.00836253011911	-0.56812980031735
C	4.96571283267288	0.00014297384267	-0.29855242738960	C	4.95356948048528	-0.00065800629526	-0.32314295751635
C	4.49631534904516	0.00032794368440	1.03350138777617	C	4.47592820139210	0.00218269808945	1.05581346550127
C	5.41813665151048	-0.00031411037457	2.08327921662187	C	5.40251826829739	0.01231380068462	2.09245504830927
C	6.76916805023598	-0.00112356175072	1.82349353647775	C	6.74900258186591	0.02120607323726	1.82371341838769
C	4.02281427732192	0.00067835223250	-1.40063313950212	C	4.03232972510074	-0.00963401179491	-1.41822020411086
C	3.06991343630040	0.00116285329030	1.30317830506055	C	3.05424284788262	-0.00251633558080	1.35074722536460
C	2.12884876791638	0.00093926344141	0.19829139996979	C	2.13243824776657	-0.00667398039725	0.20276636993165
C	2.59744697988627	0.00073830239015	-1.13326385700342	C	2.59824695555737	-0.01076502379552	-1.11481289533407
C	1.67445631695046	0.00050668255711	-2.18422879605123	C	1.68052488612386	-0.01512986434523	-2.16912601741433
H	2.03363458768570	0.00032679495027	-3.20232383355328	H	2.05558887943294	-0.01857576896683	-3.18213092236643
C	0.32595070692950	0.00041919379392	-1.92673616939707	C	0.33209814944514	-0.01408860676790	-1.91557564775197
C	-0.13136020322879	0.00060721588976	-0.61028432233025	C	-0.12745137772323	-0.00948693712419	-0.59807375945469
C	0.75244248955807	0.00088975839774	0.43967889659005	C	0.75860662549536	-0.00664752133703	0.44848321234078
H	8.29489239390180	-0.00198114756964	0.31194851847422	H	8.29127950059649	0.02578635341646	0.28545126069496
H	6.69828972611563	-0.00085231592238	-1.55878806216281	H	6.68680657634093	0.00739802276543	-1.59501046957728
H	5.05574712341459	-0.00018834523276	3.10055763476797	H	5.03271219810305	0.01541552102917	3.10790594990915
H	7.47350996711083	-0.00165068915546	2.64385985208303	H	7.46449306040635	0.03109033488105	2.63433844397772
H	-0.38961484439630	0.00016267754905	-2.73757765360310	H	-0.38312472303092	-0.01658879751173	-2.72715947088763
H	0.37997578933588	0.00101550525499	1.45355395764256	H	0.40448199071828	-0.00333313749477	1.46971920300569
O	2.65037050738009	0.00071424519870	2.48066566123418	O	2.64184215290105	-0.00325002192059	2.51140778330093
O	4.43558363249794	0.00027024052034	-2.58322872255386	O	4.44689489867450	-0.01448285250713	-2.59865091242375
O	-3.86374570256375	0.00073608294199	2.26044823355189	O	-3.88558305085268	-0.00198539137203	2.25348685277485
S	-4.29655274855364	0.00003260205618	0.88687461158031	S	-4.30440168813859	0.00195076650505	0.87567627345708
O	-5.71124751267392	-0.00050618445487	0.62901887453626	O	-5.71656013385310	0.00752186672379	0.60359483908262
<b>Coordinates from the S<sub>1</sub>/ T<sub>1</sub>/T<sub>2</sub> MECP</b>							
C	-2.33834384176855	3.53828361569689	-0.95160023102935				
C	-1.61881668266893	2.36645288556689	-0.83295988061218				
C	-2.20587331185188	1.21980228042471	-0.30070501152200				
C	-3.52418087814724	1.33267432044685	0.13223074789999				
C	-4.26064170359131	2.50521447001155	-0.02192096247994				

C	-3.67080288448209	3.61710332059679	-0.56625707625122
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