

Electronic Supporting Information for:

Water Assisted Self-Photoredox of 2-(1-Hydroxyethyl)-9,10-Anthraquinone Through a Triplet Excited State Intra-Molecular Proton Transfer Pathway

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Contents

Section 1. Computational details

1.1 Simulation Model Setup

1.2 Molecular orbitals

Section 2. Figures (S2-1 to S2-3)

Section 3. Tables (S3-1 to S3-5)

Section 4. Cartesian Coordinates (S4-1 to S4-4)

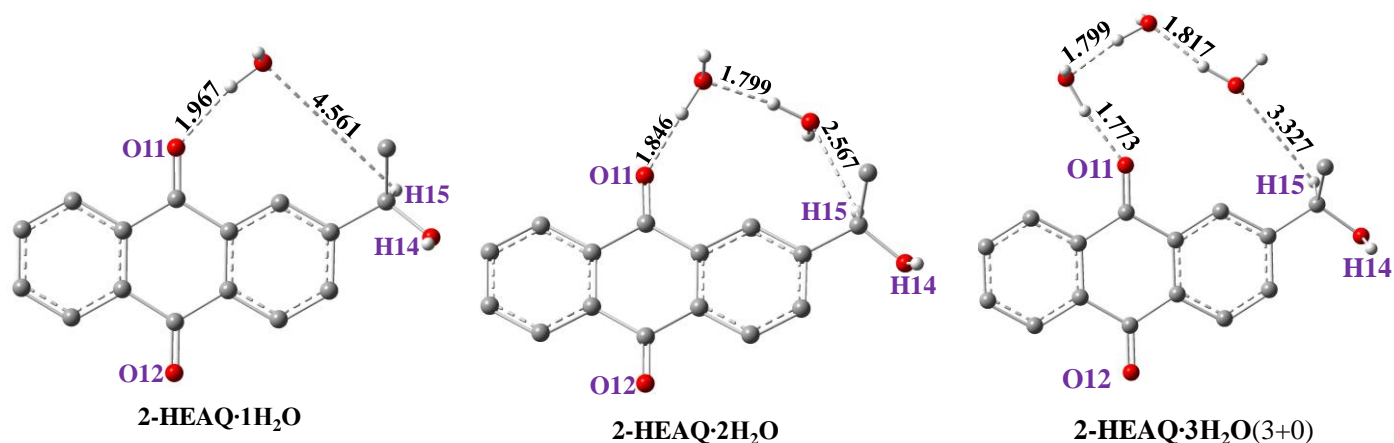
Section 1. Computational details

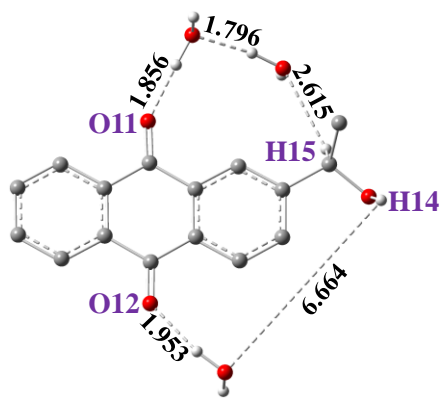
1.1 Simulation Model Setup

Table S1-1. The stabilization energies (S. E.) in kcal/mol for the energetic difference between hydrogen bonding and supra-molecular forms of 2-HEAQ· n H₂O ($n=1-6$) complexes (see Figure S1-1 for schematic structure) were obtained at the B3LYP/6-31G* level of theory. The $n(\text{O11} \dots \text{H15})/n(\text{O12} \dots \text{H14})$ represents the number of water molecules between O11 and H15 or O12 and H14, respectively, which can form the hydrogen bonds between water wires and 2-HEAQ.

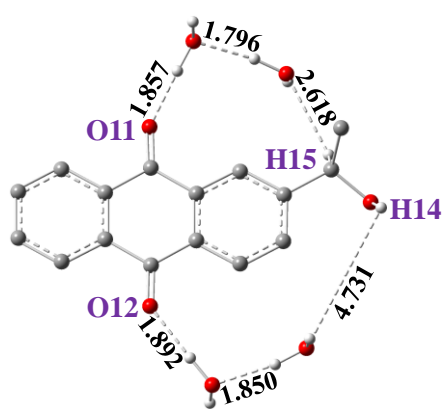
	n(O11 ... H15)	n(O12 ... H14)	S. E.
2-HEAQ·1H ₂ O	1	0	9.5
2-HEAQ·2H ₂ O	2	0	14.6
2-HEAQ·3H ₂ O	3	0	14.4
2-HEAQ·4H ₂ O	2	1	22.1
2-HEAQ·5H ₂ O	2	2	24.6
2-HEAQ·6H ₂ O	2	3	33.9
2-HEAQ·6H ₂ O	2	4	33.9

Figure S1-1. Schematic minimum structures for the 2-HEAQ· n H₂O ($n=1-6$) and 2-HEAQ·5H₂O·CH₃CN complexes in the S_0 state, along with selected bond parameters (bond lengths in Å) at the B3LYP/6-31G* level of theory. Some hydrogen atoms are omitted for clarity.





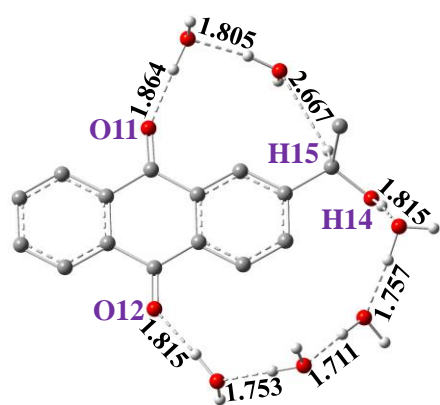
2-HEAQ·3H₂O(2+1)



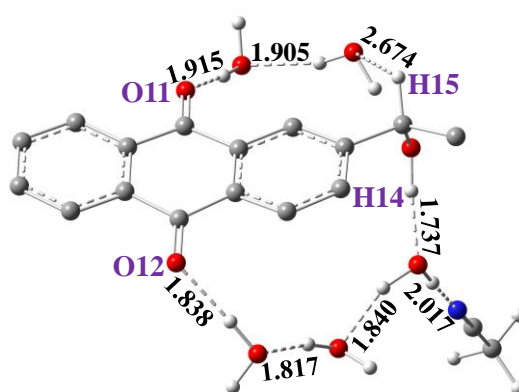
2-HEAQ·4H₂O



2-HEAQ·5H₂O



2-HEAQ·6H₂O



2-HEAQ·5H₂O·CH₃CN

1.2 Molecular orbitals

Figure S1-2. Molecular orbitals of 2-HEAQ·5H₂O used in defining the active space for the first step of ESIPT at the CASSCF(12e/10o) level of theory.

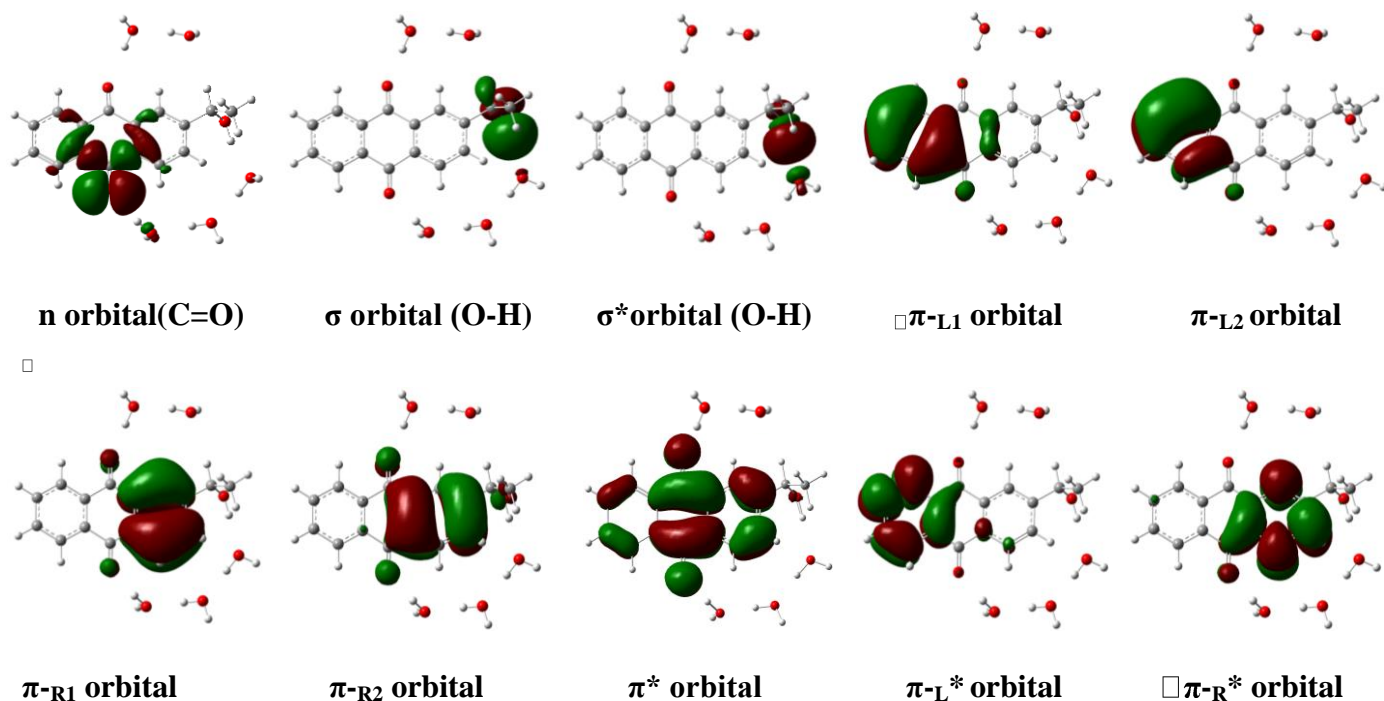
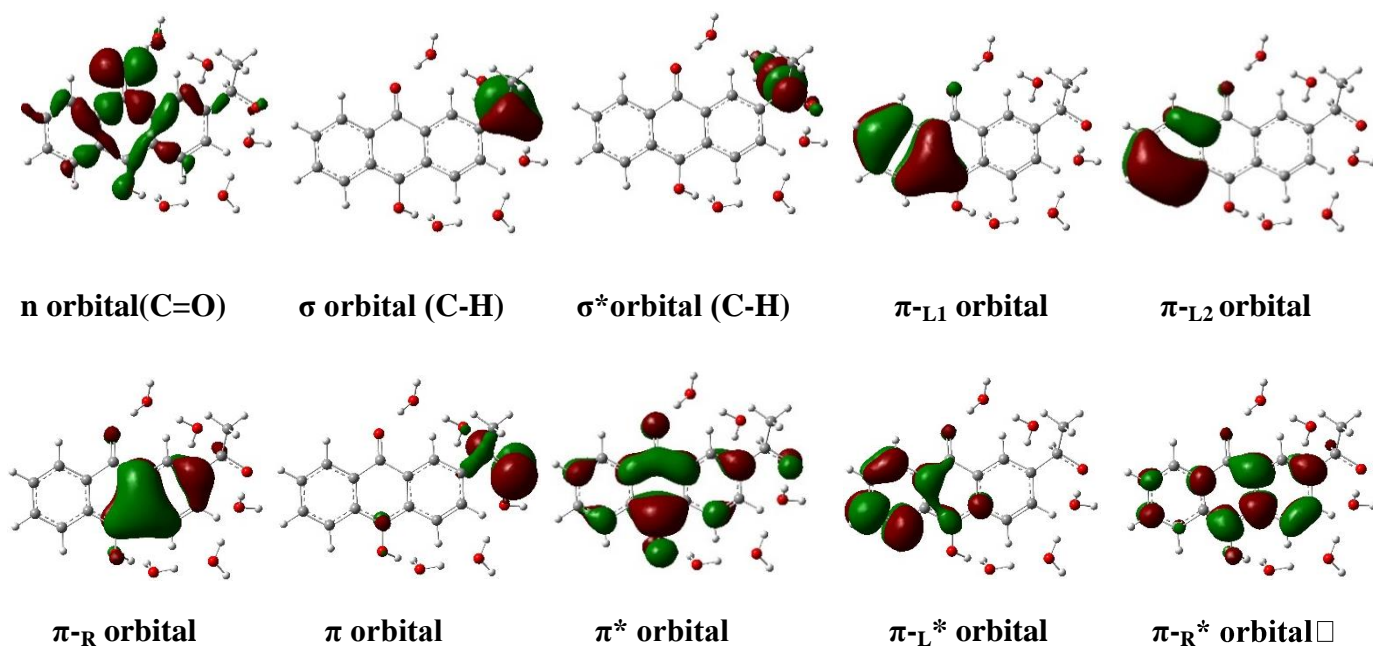
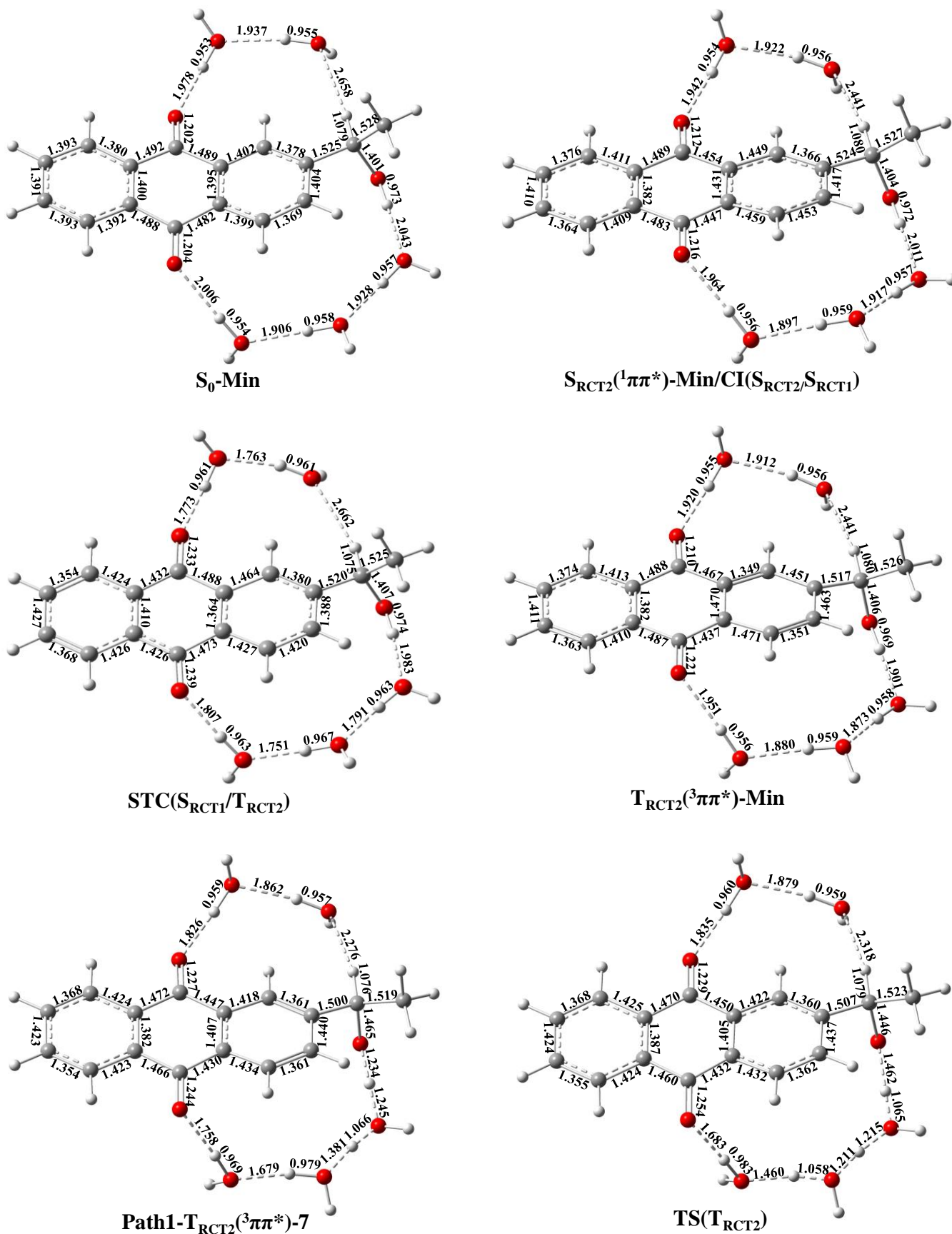


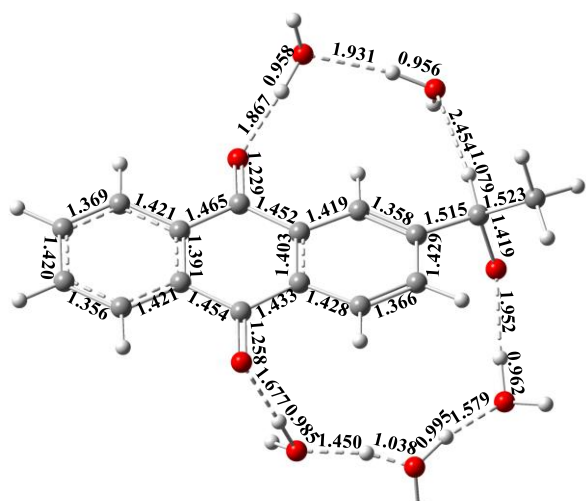
Figure S1-3. Molecular orbitals of 2-HEAQ·5H₂O used in defining the active space for the second step of ESIPT at the CASSCF(12e/10o) level of theory.



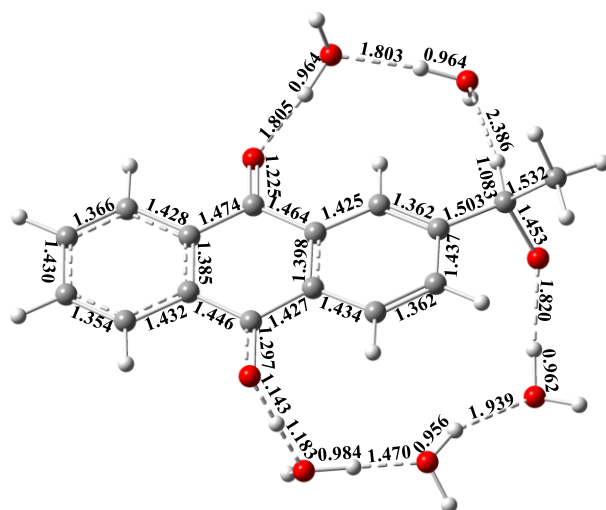
Section 2.Figures

Figure S2-1. Key structural parameters of the critical points for 2-HEAQ·5H₂O are shown along the ESIPT pathways of Figures 1 and 3 of the main article. The results were obtained from the CASSCF(12e/10o)/6-31G* calculations.

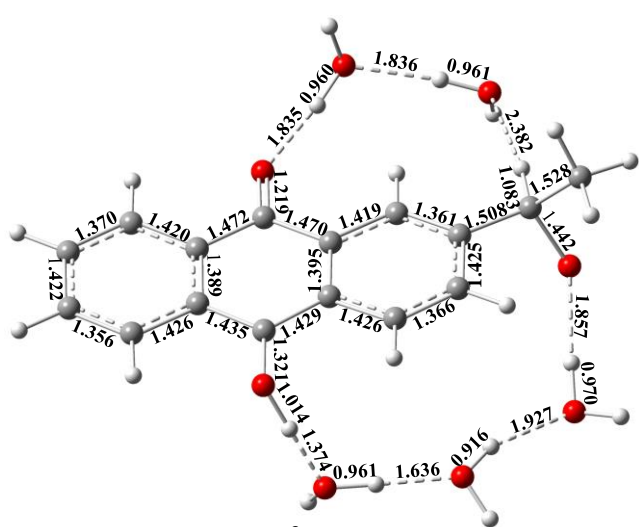




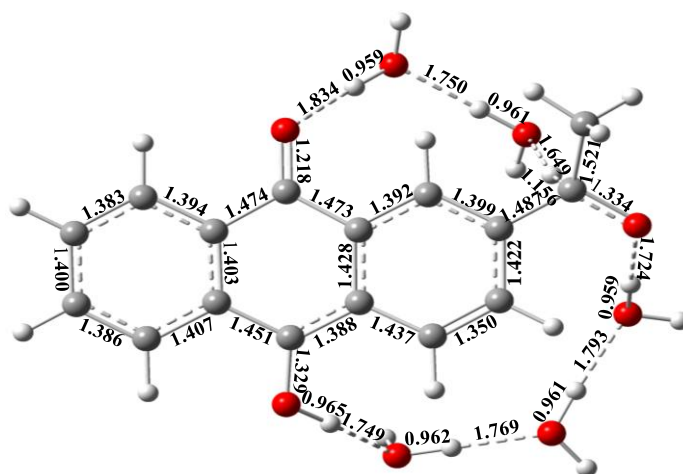
Path1- $T_{RCT2}(^3\pi\pi^*)-20$



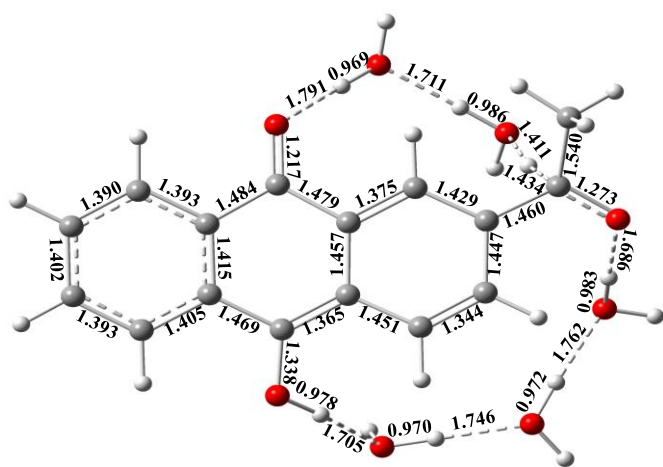
Path1- $T_{RCT2}(^3\pi\pi^*)-29$



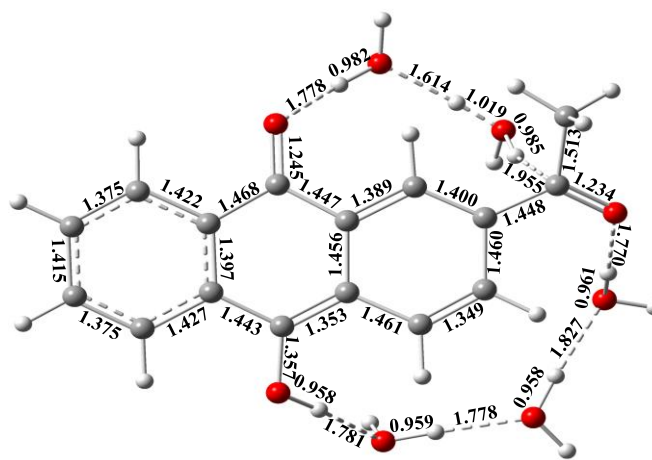
$T_{RCT2}(^3\pi\pi^*)-INT$



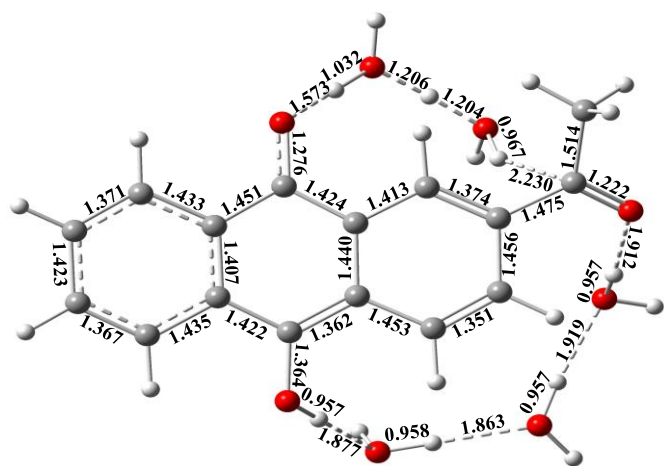
STC(T_{RCT2}/S_0)



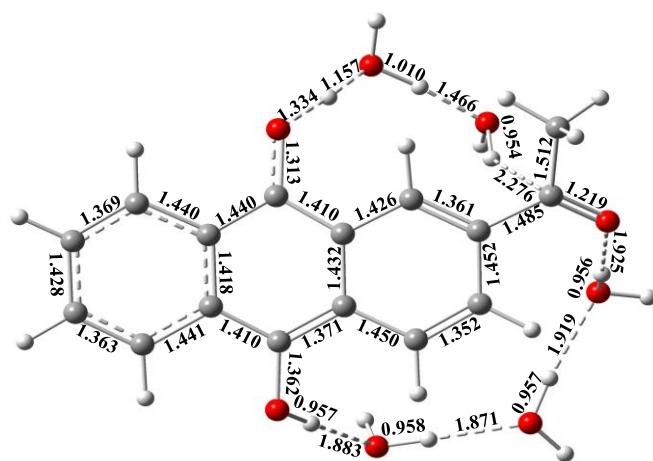
Local-Min(S_0)



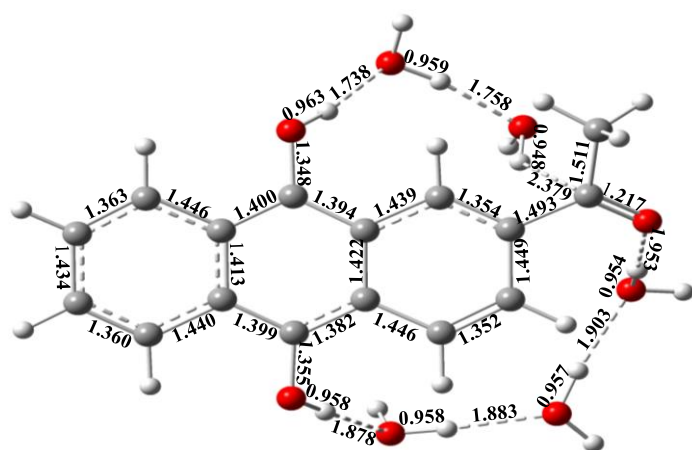
Path2- S_0-14



Path2-S₀-26



Path2-S₀-32



2-acetyl-9,10-dihydroanthracene

Figure S2-2. The schematic MEP for the deprotonation of 1'-substituted hydroxyl (O13-H14) in the $S_{\text{RCT1}}(1\pi\pi^*)$ state along the reaction coordinate of O13-H14 distance obtained at the CASPT2/CASSCF(12e/10o)/6-31G* level of theory.

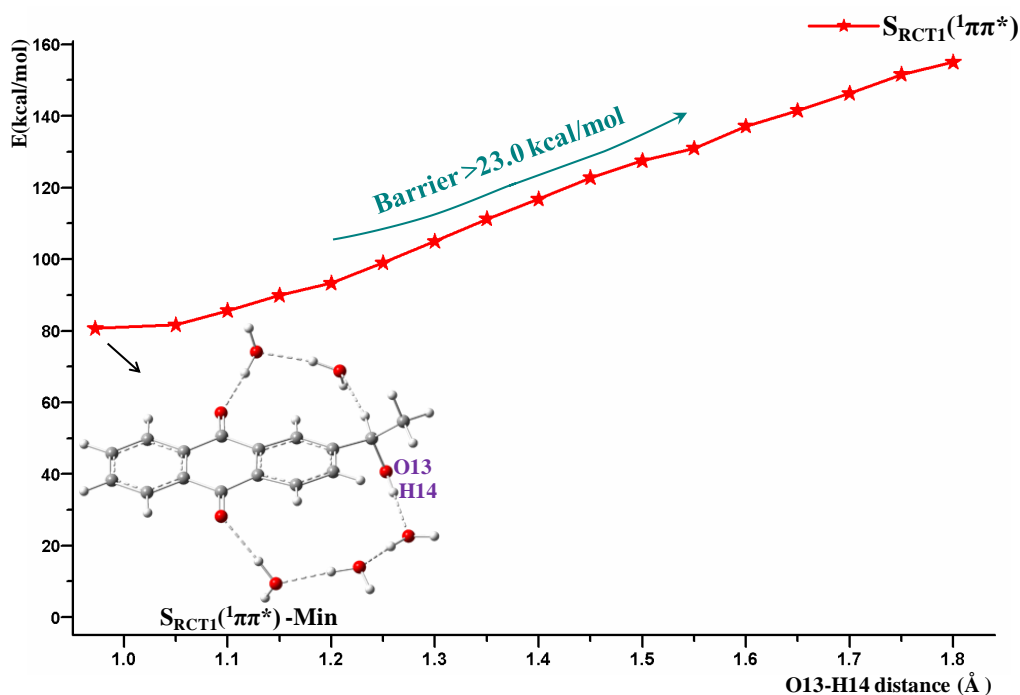
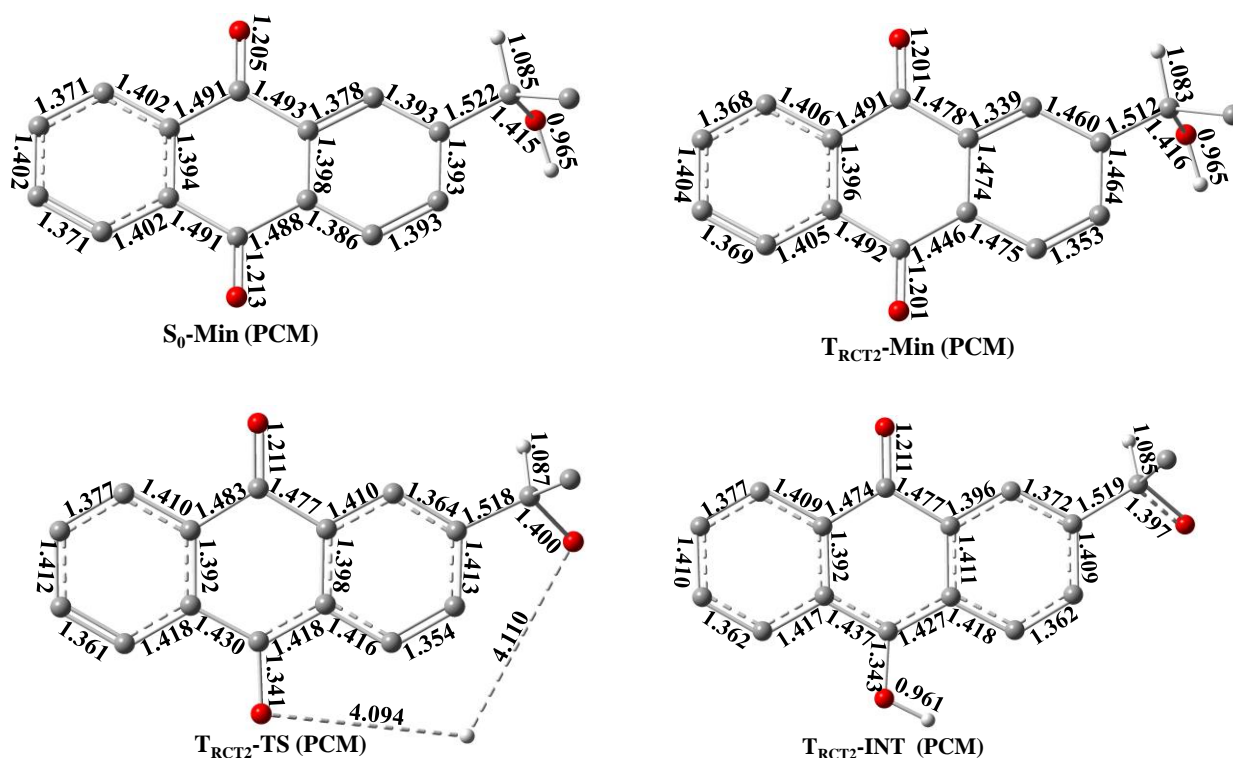


Figure S2-3. Key structural parameters (bond length in Å) of the critical points for 2-HEAQ are shown along the ESPT pathway. The results were obtained from the CASSCF(12e/10o)/6-31G**/PCM calculations.



Section 3. Tables

Table S3-1. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of 2-HEAQ·5H₂O along the reaction pathway of the first step of ES IPT between 1'-substituted hydroxyl (O13-H14) and carbonyl C10=O12 in the $S_{RCT2}(^1\pi\pi^*)$, $S_{RCT1}(^1\pi\pi^*)$ and $T_{RCT2}(^3\pi\pi^*)$ states obtained at the CASPT2//CASSCF(12e/10o)/6-31G* level of theory. The corresponding energy profiles are plotted in Figure 1 of the main article.

2-HEAQ·5H ₂ O	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S ₀ (singlet-state excitation)			
Root1	-1217.683070	-1221.097031	0
Root2		-1220.991491	66.227
Root3		-1220.962974	84.122
Root4		-1220.956094	88.439
Root5		-1220.954190	89.634
Root6	-1217.445716	-1220.922274	109.662
S ₀ (triplet-state excitation)			
Root1		-1220.987073	68.999
Root2	-1217.506376	-1220.977728	74.864
Root3		-1220.962709	84.288
Root4		-1220.955021	89.113
Root5		-1220.946303	94.583
Path1-S _{RCT2} (¹ ππ*)-1			
Root1		-1221.096538	0.309
Root2		-1220.978045	74.665
Root3		-1220.973672	77.409
Root4		-1220.948207	93.389
Root5	-1217.440961	-1220.941287	97.731
Path1-S _{RCT2} (¹ ππ*)-2			
Root1		-1221.079921	10.737
Root2		-1220.964607	83.097
Root3	-1217.500573	-1220.960589	85.619
Root4		-1220.954328	89.548
Root5		-1220.935961	101.073
CI(S _{RCT2} /S _{RCT1})/S _{RCT2} -min			
Root1		-1221.088181	5.553
Root2[S _{RCT1} (¹ ππ*)]	-1217.509007	-1220.971760	78.609
Root3[S _{RCT2} (¹ ππ*)]	-1217.493722	-1220.968433	80.697
Root4		-1220.938228	99.650
Root5		-1220.932025	103.543

Path1-S _{RCT1} (¹ $\pi\pi^*$)-1			
Root1		-1221.091702	3.344
Root2	-1217.509034	-1220.972715	78.009
Root3		-1220.970510	79.393
Root4		-1220.940013	98.530
Root5		-1220.933189	102.812
Path1-S _{RCT1} (¹ $\pi\pi^*$)-2			
Root1		-1221.082716	8.983
Root2	-1217.495617	-1220.974177	77.092
Root3		-1220.956483	88.195
Root4		-1220.933014	102.922
Root5		-1220.929683	105.013
STC(S _{RCT1} /T _{RCT2})-S _{RCT1} (¹ $\pi\pi^*$)			
Root1		-1221.083902	8.238
Root2	-1217.510261	-1220.975076	76.528
Root3		-1220.968171	80.861
Root4		-1220.939447	98.885
Root5		-1220.932016	103.548
STC(S _{RCT1} /T _{RCT2})-T _{RCT2} (³ $\pi\pi^*$)			
Root1	-1217.533741	-1220.982598	71.808
Root2		-1220.976296	75.762
Root3		-1220.973007	77.826
Root4		-1220.949625	92.499
Root5		-1220.943343	96.441
T _{RCT2} (³ $\pi\pi^*$)-Min			
Root1	-1217.563939	-1220.985951	69.704
Root2		-1220.959216	86.480
Root3		-1220.955582	88.761
Root4		-1220.935497	101.364
Root5		-1220.914275	114.681
Path1-T _{RCT2} (³ $\pi\pi^*$)-2			
Root1	-1217.544452	-1220.982809	71.675
Root2		-1220.954467	89.460
Root3		-1220.946417	94.512
Root4		-1220.931763	103.707
Root5		-1220.913772	114.997
Path1-T _{RCT2} (³ $\pi\pi^*$)-3			
Root1	-1217.538498	-1220.981093	72.752
Root2		-1220.952710	90.563
Root3		-1220.944892	95.469
Root4		-1220.929995	104.816
Root5		-1220.911948	116.141

Path1- $T_{RCT2}(^3\pi\pi^*)-4$			
Root1	-1217.532351	-1220.977330	75.114
Root2		-1220.948791	93.022
Root3		-1220.941315	97.713
Root4		-1220.925972	107.341
Root5		-1220.908179	118.506
Path1- $T_{RCT2}(^3\pi\pi^*)-5$			
Root1	-1217.508572	-1220.977156	75.223
Root2		-1220.940975	97.927
Root3		-1220.933259	102.768
Root4		-1220.904323	120.926
Root5		-1220.896004	126.146
Path1- $T_{RCT2}(^3\pi\pi^*)-6$			
Root1	-1217.502980	-1220.977529	74.989
Root2		-1220.941756	97.436
Root3		-1220.934328	102.098
Root4		-1220.945025	95.385
Root5		-1220.886008	132.419
Path1- $T_{RCT2}(^3\pi\pi^*)-7$			
Root1	-1217.504582	-1220.981706	72.367
Root2		-1220.941129	97.830
Root3		-1220.931000	104.186
Root4		-1220.913379	115.243
Root5		-1220.877412	137.813
Path1- $T_{RCT2}(^3\pi\pi^*)-8$			
Root1	-1217.504568	-1220.981585	72.443
Root2		-1220.941608	97.530
Root3		-1220.931386	103.944
Root4		-1220.909141	117.903
Root5		-1220.885266	132.885
Path1- $T_{RCT2}(^3\pi\pi^*)-9$			
Root1	-1217.504454	-1220.979036	74.043
Root2		-1220.947012	94.139
Root3		-1220.921265	110.295
Root4		-1220.904879	120.577
Root5		-1220.898437	124.619
Path1- $T_{RCT2}(^3\pi\pi^*)-10$			
Root1	-1217.50427	-1220.976770	75.465
Root2		-1220.949602	92.513
Root3		-1220.914871	114.307
Root4		-1220.897598	125.146
Root5		-1220.890857	129.376

Path1-T _{RCT2} (³ ππ*)-11			
Root1	-1217.511242	-1220.971748	78.616
Root2		-1220.948266	93.351
Root3		-1220.902514	122.061
Root4		-1220.878360	137.218
Root5		-1220.909722	117.538
Path1-T _{RCT2} (³ ππ*)-12			
Root1	-1217.512247	-1220.972049	78.427
Root2		-1220.949983	92.274
Root3		-1220.902279	122.209
Root4		-1220.879082	136.765
Root5		-1220.904216	120.993
TS(T _{RCT2})			
Root1	-1217.512687	-1220.971405	78.831
Root2		-1220.951942	91.045
Root3		-1220.901230	122.867
Root4		-1220.880747	135.720
Root5		-1220.903345	121.540
Path1-T _{RCT2} (³ ππ*)-14			
Root1	-1217.513755	-1220.972503	78.143
Root2		-1220.952504	90.692
Root3		-1220.901982	122.395
Root4		-1220.880940	135.599
Root5		-1220.899124	124.189
Path1-T _{RCT2} (³ ππ*)-15			
Root1	-1217.517538	-1220.97207	78.414
Root2		-1220.968766	80.488
Root3		-1220.971627	78.692
Root4		-1220.883810	133.798
Root5		-1220.894509	127.085
Path1-T _{RCT2} (³ ππ*)-16			
Root1	-1217.514637	-1220.972409	78.201
Root2		-1220.957534	87.536
Root3		-1220.90117	122.905
Root4		-1220.885735	132.590
Root5		-1220.877158	137.972
Path1-T _{RCT2} (³ ππ*)-17			
Root1	-1217.52301	-1220.971627	78.692
Root2		-1220.959355	86.393
Root3		-1220.899645	123.862
Root4		-1220.887321	131.595
Root5		-1220.879541	136.477
Path1-T _{RCT2} (³ ππ*)-18			

Root1	-1217.524647	-1220.970865	79.170
Root2		-1220.959831	86.094
Root3		-1220.898765	124.414
Root4		-1220.887764	131.317
Root5		-1220.878562	137.091
Path1- $T_{RCT2}(^3\pi\pi^*)-19$			
Root1	-1217.526035	-1220.971168	78.980
Root2		-1220.961449	85.079
Root3		-1220.898861	124.354
Root4		-1220.889212	130.408
Root5		-1220.878679	137.018
Path1- $T_{RCT2}(^3\pi\pi^*)-20$			
Root1	-1217.527288	-1220.969695	79.904
Root2		-1220.961855	84.824
Root3		-1220.896912	125.577
Root4		-1220.889347	130.323
Root5		-1220.876806	138.193
Path1- $T_{RCT2}(^3\pi\pi^*)-21$			
Root1	-1217.52805	-1220.971055	79.051
Root2		-1220.963683	83.677
Root3		-1220.897622	125.131
Root4		-1220.890564	129.560
Root5		-1220.877844	137.542
Path1- $T_{RCT2}(^3\pi\pi^*)-22$			
Root1	-1217.529265	-1220.972132	78.375
Root2		-1220.965476	82.552
Root3		-1220.897433	125.250
Root4		-1220.891265	129.120
Root5		-1220.878722	136.991
Path1- $T_{RCT2}(^3\pi\pi^*)-23$			
Root1	-1217.531973	-1220.975056	76.540
Root2		-1220.969009	80.335
Root3		-1220.897219	125.384
Root4		-1220.891885	128.731
Root5		-1220.883215	134.172
Path1- $T_{RCT2}(^3\pi\pi^*)-24$			
Root1	-1217.540294	-1220.97488	76.651
Root2		-1220.893496	127.720
Root3		-1220.870746	141.996
Root4		-1220.859874	148.818
Root5		-1220.822615	172.199
Path1- $T_{RCT2}(^3\pi\pi^*)-25$			
Root1	-1217.542469	-1220.982447	71.903

Root2		-1220.976314	75.751
Root3		-1220.897612	125.138
Root4		-1220.891692	128.852
Root5		-1220.878201	137.318
Path1-T _{RCT2} (³ ππ*)-26			
Root1	-1217.552717	-1220.986507	69.355
Root2		-1220.903799	121.255
Root3		-1220.887026	131.780
Root4		-1220.869802	142.589
Root5		-1220.834658	164.642
Path1-T _{RCT2} (³ ππ*)-27			
Root1	-1217.554862	-1220.988372	68.185
Root2		-1220.905528	120.170
Root3		-1220.889094	130.482
Root4		-1220.871813	141.326
Root5		-1220.836665	163.382
Path1-T _{RCT2} (³ ππ*)-28			
Root1	-1217.561595	-1220.992009	65.902
Root2		-1220.90683	119.353
Root3		-1220.893504	127.715
Root4		-1220.875947	138.732
Root5		-1220.840966	160.683
Path1-T _{RCT2} (³ ππ*)-29			
Root1	-1217.562891	-1220.99274	65.443
Root2		-1220.907115	119.174
Root3		-1220.894342	127.189
Root4		-1220.876827	138.180
Root5		-1220.841837	160.137
Path1-T _{RCT2} (³ ππ*)-30			
Root1	-1217.567448	-1220.995852	63.491
Root2		-1220.909441	117.714
Root3		-1220.897812	125.012
Root4		-1220.880611	135.806
Root5		-1220.845503	157.836
Path1-T _{RCT2} (³ ππ*)-31			
Root1	-1217.567118	-1220.997873	62.222
Root2		-1220.908304	118.428
Root3		-1220.896863	125.608
Root4		-1220.883753	133.834
Root5		-1220.845204	158.024
Path1-T _{RCT2} (³ ππ*)-32			
Root1	-1217.567354	-1220.997835	62.246
Root2		-1220.90821	118.487

Root3		-1220.896877	125.598
Root4		-1220.88375	133.836
Root5		-1220.845126	158.073
Path1- $T_{\text{RCT}2}(^3\pi\pi^*)$ -33			
Root1	-1217.573126	-1221.001146	60.169
Root2		-1220.910589	116.994
Root3		-1220.900525	123.309
Root4		-1220.888258	131.007
Root5		-1220.848954	155.670
Path1- $T_{\text{RCT}2}(^3\pi\pi^*)$ -34			
Root1	-1217.579007	-1221.003056	58.970
Root2		-1220.911854	116.200
Root3		-1220.903366	121.527
Root4		-1220.892619	128.271
Root5		-1220.851561	154.035
$T_{\text{RCT}2}(^3\pi\pi^*)$ -INT			
Root1	-1217.579944	-1221.003767	58.524
Root2		-1220.912619	115.720
Root3		-1220.904158	121.030
Root4		-1220.894171	127.297
Root5		-1220.852410	153.502

Table S3-2. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of 2-HEAQ-5H₂O along the reaction pathway of the second step of ESIPT between methylene C1'-H15 and carbonyl C9=O11 in the $T_{\text{RCT}2}(^3\pi\pi^*)$ and ground states obtained by the CASPT2//CASSCF(12e/10o)/6-31G* level of theory. The corresponding energy profiles are plotted in Figure 3 of the main article.

2-HEAQ-5H ₂ O	CASSCF		CASPT2	
	A.E.	A.E.	A.E.	R.E.
$T_{\text{RCT}2}(^3\pi\pi^*)$ -INT				
Root1	-1217.579944	-1221.003767		58.524
Root2		-1220.912619		115.720
Root3		-1220.904158		121.030
Root4		-1220.894171		127.297
Root5		-1220.85241		153.502
Path2- $T_{\text{RCT}2}(^3\pi\pi^*)$ -2				
Root1	-1217.583600	-1221.004853		57.843
Root2		-1220.911332		116.528
Root3		-1220.893692		127.597
Root4		-1220.886947		131.830
Root5		-1220.865340		145.388

Path2- $T_{RCT2}(^3\pi\pi^*)-3$			
Root1	-1217.581720	-1221.004144	58.288
Root2		-1220.910985	116.746
Root3		-1220.893470	127.737
Root4		-1220.886197	132.300
Root5		-1220.865111	145.532
Path2- $T_{RCT2}(^3\pi\pi^*)-4$			
Root1	-1217.579738	-1221.003239	58.855
Root2		-1220.910114	117.292
Root3		-1220.892558	128.309
Root4		-1220.885569	132.695
Root5		-1220.864182	146.115
Path2- $T_{RCT2}(^3\pi\pi^*)-5$			
Root1	-1217.577438	-1221.002210	59.501
Root2		-1220.909130	117.910
Root3		-1220.891616	128.900
Root4		-1220.884875	133.130
Root5		-1220.863227	146.715
Path2- $T_{RCT2}(^3\pi\pi^*)-6$			
Root1	-1217.574616	-1221.000977	60.275
Root2		-1220.908580	118.255
Root3		-1220.891246	129.132
Root4		-1220.883708	133.862
Root5		-1220.862832	146.962
Path2- $T_{RCT2}(^3\pi\pi^*)-7$			
Root1	-1217.571684	-1220.999428	61.247
Root2		-1220.906712	119.427
Root3		-1220.889667	130.123
Root4		-1220.882526	134.604
Root5		-1220.861093	148.053
Path2- $T_{RCT2}(^3\pi\pi^*)-8$			
Root1	-1217.568083	-1220.998059	62.106
Root2		-1220.905440	120.225
Root3		-1220.889021	130.528
Root4		-1220.881504	135.245
Root5		-1220.860190	148.620
Path2- $T_{RCT2}(^3\pi\pi^*)-9$			
Root1	-1217.552867	-1220.998551	61.797
Root2		-1220.905982	119.885
Root3		-1220.914068	114.811
Root4		-1220.876062	138.660
Root5		-1220.858480	149.693

STC(T_{RCT2}/S_0)- $T_{RCT2}(3\pi\pi^*)$			
Root1	-1217.545912	-1220.995758	63.550
Root2		-1220.906907	119.305
Root3		-1220.911019	116.724
Root4		-1220.875714	138.879
Root5		-1220.857435	150.349
STC(T_{RCT2}/S_0)- S_0			
Root1	-1217.565129	-1220.999397	61.266
Root2		-1220.915091	114.169
Root3		-1220.897070	125.477
Root4		-1220.870789	141.969
Root5		-1220.876217	138.563
Path2- S_0 -1			
Root1	-1217.543555	-1221.009543	54.900
Root2		-1220.936695	100.612
Root3		-1220.920119	111.014
Root4		-1220.902289	122.203
Root5		-1220.875706	138.884
Path2- S_0 -2			
Root1	-1217.549903	-1221.011868	53.441
Root2		-1220.933226	102.789
Root3		-1220.921206	110.332
Root4		-1220.897934	124.935
Root5		-1220.877870	137.526
Path2- S_0 -3			
Root1	-1217.536055	-1221.011563	53.632
Root2		-1220.928850	105.535
Root3		-1220.919734	111.255
Root4		-1220.903872	121.209
Root5		-1220.880070	136.145
Path2- S_0 -4			
Root1	-1217.533831	-1221.010879	54.061
Root2		-1220.929533	105.106
Root3		-1220.923330	108.999
Root4		-1220.900671	123.218
Root5		-1220.880984	135.572
Path2- S_0 -5			
Root1	-1217.531804	-1221.010406	54.358
Root2		-1220.929750	104.970
Root3		-1220.924864	108.036
Root4		-1220.897850	124.988
Root5		-1220.882378	134.697
Local-Min(S_0)			

Root1	-1217.530281	-1221.015654	51.065
Root2		-1220.934812	101.794
Root3		-1220.929489	105.134
Root4		-1220.902239	122.234
Root5		-1220.890340	129.701
Path2-S ₀ -7			
Root1	-1217.528358	-1221.015565	51.121
Root2		-1220.936580	100.684
Root3		-1220.924050	108.547
Root4		-1220.894488	127.097
Root5		-1220.884958	133.078
Path2-S ₀ -8			
Root1	-1217.536912	-1221.014248	51.947
Root2		-1220.940940	97.949
Root3		-1220.920671	110.668
Root4		-1220.897742	125.056
Root5		-1220.874655	139.543
Path2-S ₀ -9			
Root1	-1217.540511	-1221.015497	51.163
Root2		-1220.948554	93.171
Root3		-1220.920147	110.996
Root4		-1220.890645	129.509
Root5		-1220.875079	139.277
Path2-S ₀ -10			
Root1	-1217.545117	-1221.018183	49.478
Root2		-1220.953993	89.757
Root3		-1220.919815	111.205
Root4		-1220.892733	128.199
Root5		-1220.876704	138.257
Path2-S ₀ -11			
Root1	-1217.545467	-1221.020043	48.311
Root2		-1220.960194	85.866
Root3		-1220.920389	110.844
Root4		-1220.893167	127.926
Root5		-1220.893830	127.510
Path2-S ₀ -12			
Root1	-1217.550337	-1221.020242	48.186
Root2		-1220.959626	86.223
Root3		-1220.916558	113.249
Root4		-1220.896594	125.776
Root5		-1220.877179	137.959
Path2-S ₀ -13			
Root1	-1217.552226	-1221.021159	47.610

Root2		-1220.960954	85.389
Root3		-1220.916005	113.595
Root4		-1220.896884	125.594
Root5		-1220.876381	138.460
Path2-S ₀ -14			
Root1	-1217.553804	-1221.022205	46.954
Root2		-1220.962179	84.621
Root3		-1220.915855	113.690
Root4		-1220.896928	125.566
Root5		-1220.876136	138.614
Path2-S ₀ -15			
Root1	-1217.555250	-1221.023247	46.300
Root2		-1220.963217	83.970
Root3		-1220.915932	113.641
Root4		-1220.897383	125.281
Root5		-1220.876098	138.637
Path2-S ₀ -16			
Root1	-1217.556427	-1221.024239	45.678
Root2		-1220.964230	83.334
Root3		-1220.915858	113.688
Root4		-1220.897521	125.195
Root5		-1220.876232	138.553
Path2-S ₀ -17			
Root1	-1217.557621	-1221.025246	45.046
Root2		-1220.965073	82.805
Root3		-1220.916006	113.595
Root4		-1220.898205	124.765
Root5		-1220.876478	138.399
Path2-S ₀ -18			
Root1	-1217.558546	-1221.026115	44.500
Root2		-1220.965853	82.316
Root3		-1220.915788	113.732
Root4		-1220.898608	124.512
Root5		-1220.876714	138.251
Path2-S ₀ -19			
Root1	-1217.559098	-1221.028080	43.268
Root2		-1220.968594	80.595
Root3		-1220.919790	111.220
Root4		-1220.897192	125.401
Root5		-1220.904971	120.520
Path2-S ₀ -20			
Root1	-1217.560201	-1221.029016	42.680
Root2		-1220.969316	80.142

Root3		-1220.919853	111.181
Root4		-1220.897801	125.019
Root5		-1220.906170	119.767
Path2-S ₀ -21			
Root1	-1217.566838	-1221.029234	42.543
Root2		-1220.965273	82.679
Root3		-1220.924481	108.277
Root4		-1220.904894	120.568
Root5		-1220.898140	124.806
Path2-S ₀ -22			
Root1	-1217.567885	-1221.030368	41.832
Root2		-1220.965954	82.252
Root3		-1220.925878	107.400
Root4		-1220.905184	120.386
Root5		-1220.898656	124.482
Path2-S ₀ -23			
Root1	-1217.569040	-1221.031668	41.016
Root2		-1220.966727	81.767
Root3		-1220.927352	106.475
Root4		-1220.905659	120.088
Root5		-1220.899364	124.038
Path2-S ₀ -24			
Root1	-1217.570239	-1221.033118	40.106
Root2		-1220.967543	81.255
Root3		-1220.929028	105.424
Root4		-1220.906043	119.847
Root5		-1220.900136	123.554
Path2-S ₀ -25			
Root1	-1217.572529	-1221.034479	39.252
Root2		-1220.978635	74.295
Root3		-1220.926170	107.217
Root4		-1220.907990	118.625
Root5		-1220.880799	135.688
Path2-S ₀ -26			
Root1	-1217.574542	-1221.036430	38.027
Root2		-1220.979823	73.549
Root3		-1220.927350	106.477
Root4		-1220.909981	117.375
Root5		-1220.881959	134.960
Path2-S ₀ -27			
Root1	-1217.576936	-1221.038591	36.672
Root2		-1220.980926	72.857
Root3		-1220.928835	105.545

Root4		-1220.911602	116.358
Root5		-1220.883643	133.903
Path2-S ₀ -28			
Root1	-1217.579587	-1221.040978	35.173
Root2		-1220.981800	72.309
Root3		-1220.930715	104.365
Root4		-1220.912308	115.916
Root5		-1220.886523	132.096
Path2-S ₀ -29			
Root1	-1217.582564	-1221.043396	33.656
Root2		-1220.982456	71.897
Root3		-1220.932822	103.043
Root4		-1220.913211	115.349
Root5		-1220.890120	129.839
Path2-S ₀ -30			
Root1	-1217.585010	-1221.044796	32.778
Root2		-1220.979177	73.955
Root3		-1220.941219	97.773
Root4		-1220.898568	124.537
Root5		-1220.905994	119.878
Path2-S ₀ -31			
Root1	-1217.589433	-1221.047620	31.006
Root2		-1220.979394	73.818
Root3		-1220.943385	96.414
Root4		-1220.896995	125.525
Root5		-1220.908368	118.388
Path2-S ₀ -32			
Root1	-1217.594601	-1221.050995	28.888
Root2		-1220.979720	73.614
Root3		-1220.945622	95.010
Root4		-1220.896773	125.664
Root5		-1220.911170	116.629
Path2-S ₀ -33			
Root1	-1217.609304	-1221.055001	26.374
Root2		-1220.972519	78.133
Root3		-1220.948912	92.946
Root4		-1220.915719	113.775
Root5		-1220.911579	116.373
Path2-S ₀ -34			
Root1	-1217.615766	-1221.059618	23.477
Root2		-1220.973974	77.219
Root3		-1220.952945	90.416
Root4		-1220.917775	112.485

Root5		-1220.914389	114.609
Path2-S ₀ -35			
Root1	-1217.622970	-1221.064353	20.506
Root2		-1220.975681	76.149
Root3		-1220.956966	87.892
Root4		-1220.920249	110.933
Root5		-1220.917335	112.761
Path2-S ₀ -36			
Root1	-1217.629910	-1221.068844	17.688
Root2		-1220.978268	74.525
Root3		-1220.962035	84.711
Root4		-1220.924063	108.539
Root5		-1220.918990	111.722
Path2-S ₀ -37			
Root1	-1217.636794	-1221.072052	15.674
Root2		-1220.978370	74.461
Root3		-1220.963310	83.911
Root4		-1220.924399	108.328
Root5		-1220.922205	109.705
Path2-S ₀ -38			
Root1	-1217.661992	-1221.086622	6.532
Root2		-1220.986356	69.449
Root3		-1220.975472	76.279
Root4		-1220.936202	100.922
Root5		-1220.931775	103.700

Table S3-3. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of 2-HEAQ·5H₂O along the reaction coordinate of the deprotonation of 1'-substituted hydroxyl (O13-H14 distance) in the S_{RCT2}(¹ππ*) state obtained by the CASPT2//CASSCF(12e/10o)/6-31G* level of theory. The corresponding energy profiles are partially plotted by dotted line in Figure 1 of the main article.

2-HEAQ·5H ₂ O	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
CI(S _{RCT2} /S _{RCT1})/S _{RCT} -min			
Root1		-1221.088181	5.553
Root2		-1220.971760	78.609
Root3	-1217.493722	-1220.968433	80.697
Root4		-1220.938228	99.650
Root5		-1220.932025	103.543
S _{RCT} (¹ ππ*)-1.05			
Root1		-1221.085702	7.109

Root2		-1220.966876	81.673
Root3	-1217.492296	-1220.966425	81.956
Root4		-1220.934774	101.818
Root5		-1220.928316	105.871
$S_{\text{RCT}}(^1\pi\pi^*)-1.1$			
Root1		-1221.079707	10.871
Root2		-1220.960589	85.619
Root3	-1217.485004	-1220.960369	85.757
Root4		-1220.928901	105.503
Root5		-1220.922297	109.647
$S_{\text{RCT}}(^1\pi\pi^*)-1.15$			
Root1		-1221.072476	15.408
Root2		-1220.953735	89.920
Root3	-1217.477821	-1220.953587	90.012
Root4		-1220.922054	109.800
Root5		-1220.915321	114.025
$S_{\text{RCT}}(^1\pi\pi^*)-1.2$			
Root1		-1221.064176	20.617
Root2		-1220.948374	93.284
Root3	-1217.470837	-1220.945230	95.257
Root4		-1220.914747	114.385
Root5		-1220.908233	118.473

Table S3-4. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of the S_0 , $T_{\text{RCT}2}$ minimum, transition state ($T_{\text{RCT}2}$ -TS) and intermediate ($T_{\text{RCT}2}$ -INT) for 2-HEAQ·5H₂O along the reaction pathway of the first step of ESIPT in the $T_{\text{RCT}2}(^3\pi\pi^*)$ state obtained at the CASPT2//CASSCF(12e/10o)/6-31G** level of theory.

2-HEAQ·5H ₂ O	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0 -Min			
Root1		-1221.308888	0.000
Root2		-1221.167839	88.510
Root3		-1221.174812	84.134
Root4		-1221.165812	89.782
Root5	-1217.533870	-1221.133908	109.802
$T_{\text{RCT}2}$ -Min			
Root1	-1217.650470	-1221.202560	66.722
Root2		-1221.176045	83.361
Root3		-1221.166467	89.371
Root4		-1221.153553	97.474
Root5		-1221.135386	108.874

$T_{\text{RCT2-TS}}$			
Root1	-1217.604675	-1221.186522	76.786
Root2		-1221.166475	89.366
Root3		-1221.116762	120.562
Root4		-1221.095719	133.766
Root5		-1221.118657	119.372
$T_{\text{RCT2-INT}}$			
Root1	-1217.680590	-1221.223155	53.798
Root2		-1221.135244	108.963
Root3		-1221.126941	114.174
Root4		-1221.111348	123.959
Root5		-1221.075199	146.642

Table S3-5. The absolute energies (A.E.) in Hartree and relative energies (R.E.) in kcal/mol for the optimized structures of the S_0 , T_{RCT2} minimum, transition state ($T_{\text{RCT2-TS}}$) and intermediate ($T_{\text{RCT2-INT}}$) for 2-HEAQ along the reaction pathway of the first step of ESIPT in the $T_{\text{RCT2}}(^3\pi\pi^*)$ state obtained at the CASPT2//CASSCF(12e/10o)/6-31G** and the CASPT2//CASSCF(12e/10o)/6-31G**/PCM levels of theory.

2-HEAQ	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0 -Min (gas phase)			
Root1		-840.130750	0.000
Root2		-839.988733	89.117
Root3		-839.979812	94.715
Root4		-839.968968	101.520
Root5	-837.344975	-839.951810	112.287
$T_{\text{RCT2-Min}}$ (gas phase)			
Root1	-837.466872	-840.016335	71.797
Root2		-839.990390	88.077
Root3		-839.972242	99.465
Root4		-839.972927	99.036
Root5		-839.932086	124.664
$T_{\text{RCT2-TS}}$ (gas phase)			
Root1	-837.421970	-839.935312	122.639
Root2		-839.855148	172.943
Root3		-839.848672	177.007
Root4		-839.839827	182.557
Root5		-839.819611	195.243
$T_{\text{RCT2-INT}}$ (gas phase)			
Root1	-837.507282	-840.031756	62.120
Root2		-839.933578	123.728

Root3		-839.918436	133.229
Root4		-839.888918	151.752
Root5		-839.897483	146.377
S ₀ -Min (PCM)			
Root1		-840.126098	0.000
Root2		-839.984013	89.160
Root3		-839.976199	94.063
Root4		-839.967837	99.311
Root5	-837.3714436	-839.947825	111.868
T _{RCT2} -Min (PCM)			
Root1	-823.049987	-840.011173	72.117
Root2		-839.985968	87.933
Root3		-839.970276	97.780
Root4		-839.964873	101.170
Root5		-839.927678	124.511
T _{RCT2} -TS (PCM)			
Root1	-837.476679	-839.931671	122.005
Root2		-839.852499	171.686
Root3		-839.852084	171.947
Root4		-839.845469	176.097
Root5		-839.833735	183.461
T _{RCT2} -INT (PCM)			
Root1	-837.517261	-840.030418	60.040
Root2		-839.944204	114.140
Root3		-839.923082	127.395
Root4		-839.915053	132.433
Root5		-839.873969	158.214

Section 4. Cartesian Coordinates

S4-1. Cartesian coordinates of the critical points for 2-HEAQ·5H₂O along the reaction pathway of the first step of ES IPT between 1'-substituted hydroxyl (O13-H14) and carbonyl C10=O12 in the $S_{RCT2}(^1\pi\pi^*)$, $S_{RCT1}(^1\pi\pi^*)$ and $T_{RCT2}(^3\pi\pi^*)$ states obtained by the CASSCF(12e/10o)/6-31G* level of theory.

S₀

C	0.683402095	1.270527079	0.084227174
H	0.624713460	2.322118274	-0.122266004
C	-0.493982949	0.508752829	0.091610392
C	-1.800765101	1.173245425	-0.166236161
O	-1.886656733	2.335740190	-0.458138380
C	-3.034523018	0.346858782	-0.017240805
C	-4.266641523	0.959527022	-0.115016111
H	-4.311131994	2.016391156	-0.292212790
C	-5.435710554	0.212952320	0.015930449
H	-6.390639793	0.700217919	-0.053244670
C	-5.362182751	-1.159336323	0.232669658
H	-6.261308397	-1.739360648	0.331097420
C	-4.120326416	-1.785337377	0.316835448
H	-4.046368376	-2.843475108	0.474071423
C	-2.954661667	-1.034463473	0.199465528
C	-1.635029644	-1.718013818	0.277693206
O	-1.563885271	-2.919956440	0.308177022
C	-0.427929695	-0.861772241	0.345946420
C	0.811632919	-1.447017936	0.625874654
H	0.867856827	-2.496171502	0.841127804
C	1.948311121	-0.684047559	0.633318003
H	2.887746357	-1.154483710	0.846466038
C	1.905883076	0.689346216	0.344740629
C	3.193257259	1.504462190	0.271990255
C	4.004835223	1.448255825	1.565918381
H	4.872266416	2.090320922	1.466502862
H	3.417179755	1.790862490	2.411086569
H	4.356020561	0.442104560	1.774209224
O	1.958418894	4.994706247	-0.193925040
H	1.018920246	5.113269145	-0.317908724
H	2.353697180	5.199301671	-1.031051894
O	-0.883796058	5.077880496	-0.680050588
H	-1.227475573	4.188893738	-0.669442892
H	-1.473232261	5.591322427	-0.142902303
O	3.253910174	-4.094313359	-0.323930027
H	2.343017118	-4.218453489	-0.592390302
H	3.573679947	-4.963263392	-0.118909493
O	4.892436679	-1.724617394	-0.452893377
H	4.347739921	-2.511984165	-0.452475536
H	5.788557953	-2.033217040	-0.468592710
O	0.512196585	-4.551203842	-1.003475436

H	0.194673325	-4.550028878	-1.897714437
H	-0.160044794	-4.108696143	-0.490796510
H	2.919670981	2.532473305	0.089669966
O	3.959116647	1.117081525	-0.835289883
H	4.277123429	0.205685358	-0.714480072

S_{RCT2}-Min/CI(S_{RCT2}/S_{RCT1})

C	0.786395350	1.221689596	0.110896707
H	0.768748093	2.255065034	-0.185481714
C	-0.489633457	0.541071905	0.196766143
C	-1.719193491	1.267466058	-0.076286983
O	-1.736505059	2.461955171	-0.280297034
C	-2.983711874	0.481343148	-0.075133359
C	-4.193312437	1.157362905	-0.338800086
H	-4.162323463	2.212569762	-0.525067114
C	-5.380967802	0.463388937	-0.357608459
H	-6.302618037	0.977805354	-0.558453128
C	-5.390330165	-0.925329709	-0.116456396
H	-6.320740664	-1.463123112	-0.131411207
C	-4.222627248	-1.584469208	0.134709741
H	-4.207136727	-2.640382114	0.320899863
C	-3.002695975	-0.880617052	0.159610199
C	-1.752937807	-1.630078164	0.435698286
O	-1.751608048	-2.836819461	0.585183115
C	-0.531184355	-0.856638597	0.500226996
C	0.733430825	-1.488719220	0.859419074
H	0.752438337	-2.502370555	1.204054881
C	1.977545894	-0.743592795	0.772601736
H	2.882849441	-1.261108756	1.014388558
C	1.984020939	0.610670958	0.354956895
C	3.302245139	1.349394449	0.158297986
C	4.276110748	1.184185752	1.322200740
H	5.155287295	1.788281629	1.130963453
H	3.831893689	1.510763601	2.257399975
H	4.601687198	0.155129097	1.438064659
O	2.239833974	4.659177787	-0.337278060
H	1.326874132	4.918194361	-0.223354987
H	2.434755932	4.817762271	-1.250441881
O	-0.583250559	5.111047056	-0.129102153
H	-0.946518591	4.234966375	-0.231714263
H	-0.905338986	5.425299944	0.704590410
O	2.964460913	-4.097100996	-0.144627214
H	2.033779941	-4.187909754	-0.355946609
H	3.332756298	-4.964618493	-0.243661409
O	4.659562494	-1.921719441	-0.943520320
H	4.051661937	-2.623325075	-0.709840918
H	5.500958638	-2.167775654	-0.585050773
O	0.208564259	-4.516135848	-0.754941377
H	-0.084242423	-4.404502949	-1.649381973
H	-0.420485269	-4.038973447	-0.215756277
H	3.077188637	2.399580874	0.049583243

O	3.886610865	0.956719927	-1.056791345
H	4.138248030	0.018904266	-1.009982998

STC(S_{RCT1}/T_{RCT2})

C	0.726367811	1.326292846	0.062270203
H	0.646020432	2.374465683	-0.169165848
C	-0.494626941	0.522304040	0.140025807
C	-1.827468660	1.158932254	-0.040860637
O	-1.902392327	2.382041395	-0.178039330
C	-2.973411311	0.301054131	-0.031285218
C	-4.266860306	0.870411208	-0.204553123
H	-4.339931799	1.932756231	-0.331030787
C	-5.372473449	0.089276287	-0.213957399
H	-6.342355914	0.533381806	-0.346024661
C	-5.258485405	-1.323695644	-0.051617941
H	-6.143983504	-1.933382031	-0.060945605
C	-4.029393450	-1.899438279	0.115618859
H	-3.920497720	-2.959184429	0.240862152
C	-2.852603262	-1.094526054	0.133696536
C	-1.578469036	-1.709459667	0.309680432
O	-1.401412462	-2.932172946	0.401684547
C	-0.405272102	-0.820800401	0.361752799
C	0.884438220	-1.368953338	0.628774054
H	0.960530734	-2.411221964	0.864790779
C	2.052890860	-0.564506355	0.576916953
H	3.008401141	-1.009448566	0.757976314
C	1.980851019	0.781191151	0.244573724
C	3.256488405	1.582347292	0.042452212
C	4.117290235	1.654358610	1.299373060
H	4.994860528	2.253159313	1.089088372
H	3.573457518	2.114836973	2.117067694
H	4.448018634	0.669850210	1.612659110
O	1.553928558	4.817190161	-0.452940363
H	0.638769434	5.041553610	-0.262119113
H	1.777234245	5.269084000	-1.252511202
O	-1.113417952	4.995114491	-0.070004705
H	-1.375598116	4.074563924	-0.151085358
H	-1.688028470	5.404935404	0.557961655
O	3.180110395	-3.943863695	-0.177013792
H	2.263419726	-4.139910425	-0.413801042
H	3.534022737	-4.695270486	0.275096575
O	4.758360177	-1.713464909	-0.483012048
H	4.163263292	-2.468386982	-0.426737444
H	5.652978720	-2.009554540	-0.412844605
O	0.574867196	-4.548449729	-0.629636787
H	0.228227941	-4.808295994	-1.470373285
H	-0.123115197	-4.078182454	-0.160787699
H	2.979380521	2.578372801	-0.251650447
O	3.976914942	1.076854746	-1.055543932
H	4.293681226	0.171153163	-0.887536177

T_{RCT2}(³ππ*)-Min

C	0.694431059	1.271828876	0.197660481
H	0.704266438	2.304790026	-0.097217734
C	-0.481656854	0.615619353	0.270353932
C	-1.740090542	1.297054708	-0.052347341
O	-1.807799501	2.483590742	-0.281098508
C	-2.968658427	0.457994580	-0.093161348
C	-4.196117156	1.082486171	-0.410297263
H	-4.199970915	2.136696592	-0.605659639
C	-5.352289941	0.342215934	-0.466755792
H	-6.286491519	0.816091539	-0.707787694
C	-5.312535712	-1.044978231	-0.210332348
H	-6.219085767	-1.621555378	-0.254425633
C	-4.130834479	-1.653380214	0.093065294
H	-4.081177703	-2.706056646	0.292504711
C	-2.939400762	-0.901108510	0.156236184
C	-1.676695849	-1.610383933	0.494020937
O	-1.665723332	-2.819160181	0.667767728
C	-0.485555924	-0.814608281	0.610969933
C	0.780117921	-1.432189861	1.036916623
H	0.755866691	-2.442780571	1.388892298
C	1.938551034	-0.740030353	0.970134248
H	2.856541436	-1.215486962	1.252151039
C	1.967856124	0.643682384	0.497345159
C	3.261731668	1.340620696	0.123017248
C	4.366373617	1.187553594	1.164801671
H	5.229597455	1.760766243	0.846534169
H	4.045980500	1.559685154	2.133049958
H	4.677637199	0.154815180	1.278453233
O	2.178604128	4.642891384	-0.361830776
H	1.267746337	4.897734558	-0.222542055
H	2.346657799	4.799483938	-1.281046334
O	-0.628593557	5.095015753	-0.078167217
H	-1.005280459	4.225647167	-0.196225838
H	-0.923308469	5.390781924	0.772504606
O	3.036162531	-4.064300913	-0.248791002
H	2.093925608	-4.147042263	-0.405133879
H	3.402548125	-4.914672427	-0.450312503
O	4.566416741	-1.830656249	-1.065316777
H	4.003016377	-2.564930699	-0.818634908
H	5.425242317	-2.032420898	-0.721155548
O	0.267413912	-4.481158946	-0.698786786
H	-0.063781869	-4.383363466	-1.581503751
H	-0.347252619	-4.008978474	-0.139569821
H	3.047602512	2.392874886	0.012167458
O	3.671313467	0.894662464	-1.146021430
H	3.976010652	-0.023413343	-1.086849751

Path1-T_{RCT2}(³ππ*)-4

C	0.763560605	1.201340985	0.225141308
H	0.844702544	2.215740740	-0.121102074
C	-0.458352276	0.626276723	0.317233298
C	-1.670949862	1.357773892	-0.052961034
O	-1.687309715	2.536854967	-0.333193491
C	-2.940817792	0.573703329	-0.090983760
C	-4.136903063	1.256237647	-0.421361490
H	-4.087211996	2.308123917	-0.626576153
C	-5.326732426	0.573046609	-0.476130943
H	-6.236849084	1.089285390	-0.725029876
C	-5.357151281	-0.815376165	-0.206737200
H	-6.292775975	-1.344999982	-0.250239043
C	-4.208805249	-1.478382732	0.106079724
H	-4.209302882	-2.531462090	0.313216810
C	-2.980089862	-0.781377591	0.167951226
C	-1.753334663	-1.546587287	0.517915622
O	-1.784578304	-2.759951856	0.666917076
C	-0.542483977	-0.793344955	0.691671299
C	0.672130689	-1.460402379	1.186424632
H	0.573399147	-2.453817103	1.578480038
C	1.867379790	-0.837235181	1.118166974
H	2.753211498	-1.338503347	1.457364844
C	1.987795856	0.520599743	0.570613320
C	3.324861836	1.090939804	0.138015306
C	4.440511196	0.890581206	1.162688476
H	5.345485410	1.350046433	0.779635153
H	4.196352846	1.357954495	2.112879092
H	4.656754632	-0.158272702	1.348684262
O	2.487087672	4.356183034	-0.443101035
H	1.586608089	4.638204551	-0.280606106
H	2.625122346	4.460616624	-1.375075289
O	-0.253954858	4.942971826	-0.080311963
H	-0.723075662	4.120472485	-0.223768873
H	-0.472236434	5.219917972	0.799870483
O	2.770462803	-3.883716208	-0.416778564
H	1.815609957	-3.908574420	-0.557288663
H	3.103116365	-4.713053524	-0.736089760
O	4.366105044	-1.812618682	-1.066910437
H	3.709650866	-2.574101901	-0.839455990
H	5.175350960	-1.993090666	-0.603765354
O	0.101992520	-4.171974470	-0.822756696
H	-0.221408103	-3.971861945	-1.691898153
H	-0.512758803	-3.762022543	-0.210620982
H	3.201957007	2.158350171	0.000150667
O	3.640767181	0.549023317	-1.109317426
H	3.960001786	-0.489889943	-1.027505258

Path1-T_{RCT2}(³ππ*)-7

C	0.911193443	1.107571348	0.243439478
H	1.036810306	2.097103159	-0.147396930
C	-0.402777942	0.579885082	0.313153743
C	-1.524453634	1.395341778	-0.100855618
O	-1.414147467	2.567270276	-0.446657323
C	-2.841885814	0.738582524	-0.094631066
C	-3.987026482	1.499354090	-0.466054528
H	-3.849990953	2.528041848	-0.731712205
C	-5.225665562	0.919871680	-0.478876978
H	-6.091432710	1.492581944	-0.755900595
C	-5.368720630	-0.450755136	-0.125218421
H	-6.344735201	-0.901154945	-0.136005960
C	-4.284413465	-1.183440347	0.221724155
H	-4.370367704	-2.217540747	0.489325319
C	-2.990302226	-0.592826614	0.245988486
C	-1.840704801	-1.420375529	0.623905046
O	-1.957189768	-2.643460788	0.821014988
C	-0.576880689	-0.757060467	0.714483485
C	0.562450496	-1.485905870	1.191671091
H	0.407879813	-2.470040883	1.585765263
C	1.807078746	-0.935463761	1.166779286
H	2.636224278	-1.496931210	1.554518035
C	1.999119107	0.390204762	0.637167815
C	3.371266728	0.925838921	0.354487965
C	4.495827994	0.578020261	1.314220202
H	5.439110624	0.970874773	0.954115550
H	4.281005357	1.045042478	2.266863760
H	4.600022396	-0.486605676	1.475944654
O	2.916268757	4.130908956	-0.451833822
H	2.017247264	4.446371681	-0.357750030
H	3.119167009	4.223276501	-1.370404199
O	0.196238630	4.829881864	-0.290838523
H	-0.333799190	4.039067360	-0.404286650
H	-0.065200758	5.195103200	0.540950824
O	2.329605322	-3.863847766	-0.839150856
H	1.353194614	-3.796087916	-0.825272272
H	2.536793561	-4.664991635	-1.300697183
O	4.026655397	-2.131985391	-1.119489674
H	3.225080703	-2.827113673	-1.016022879
H	4.767040192	-2.451189214	-0.619257118
O	-0.315002972	-3.985107442	-0.868470350
H	-0.754347603	-3.750445130	-1.673040753
H	-0.849824339	-3.588740109	-0.164624100
H	3.361393286	1.983251547	0.155847649
O	3.645933157	0.307564128	-0.944924804
H	3.827208941	-0.912720368	-0.966462160

Path1-T_{RCT2}(³ππ*)-10

C	0.896829302	1.143391610	0.275403866
H	1.017067465	2.124225816	-0.133019998
C	-0.408433437	0.593671028	0.333966650
C	-1.545821742	1.386138830	-0.085272771
O	-1.450772904	2.559296818	-0.437972262
C	-2.849694714	0.713384125	-0.075901688
C	-4.007967079	1.455209410	-0.435761105
H	-3.892428100	2.488463686	-0.689766870
C	-5.236853893	0.853008404	-0.457490280
H	-6.110292693	1.415404930	-0.728417754
C	-5.354736486	-0.522368717	-0.124062287
H	-6.320045590	-0.993179224	-0.142439451
C	-4.257221713	-1.240180462	0.213975177
H	-4.327928699	-2.278587386	0.466027870
C	-2.975728891	-0.628316813	0.251014513
C	-1.813938910	-1.430113761	0.615357982
O	-1.892634250	-2.670644988	0.751161829
C	-0.563781134	-0.743159854	0.734123645
C	0.576641797	-1.445345022	1.234470613
H	0.436572394	-2.426479076	1.639258490
C	1.812685861	-0.869862038	1.217268966
H	2.646626686	-1.412660325	1.621077436
C	1.990946128	0.439150116	0.661727196
C	3.372367443	0.962893314	0.338389981
C	4.477993577	0.691689969	1.343263137
H	5.427213925	1.067826787	0.980223398
H	4.240429559	1.216153952	2.258269710
H	4.591697612	-0.358751056	1.576483108
O	2.837602257	4.094248799	-0.608275992
H	1.942709553	4.407225238	-0.465430239
H	2.954817933	4.094449024	-1.545467776
O	0.161483549	4.789477408	-0.287646237
H	-0.376787173	4.001863813	-0.401660781
H	-0.031344250	5.104523808	0.581738510
O	2.318819668	-3.861318273	-0.773882594
H	1.289199865	-3.726208695	-0.819788853
H	2.509081501	-4.655544610	-1.254968093
O	4.046809853	-2.214504677	-1.134660794
H	3.173902336	-2.927576529	-0.979087334
H	4.785822026	-2.493869518	-0.608455214
O	-0.243159980	-3.830656854	-0.954052191
H	-0.608203119	-3.455608294	-1.742383552
H	-0.803775669	-3.486362446	-0.225602655
H	3.343409816	2.013159327	0.104099160
O	3.666871267	0.291293817	-0.898717523
H	3.872382199	-1.131146369	-0.981164545

TS(T_{RCT2})

C	0.930724074	1.117541010	0.267728768
H	1.060176413	2.105145452	-0.130417589
C	-0.387606666	0.589805415	0.332726253
C	-1.511928183	1.409728175	-0.076033695
O	-1.394207830	2.583883351	-0.419977524
C	-2.828648191	0.756569677	-0.067483284
C	-3.974859459	1.520444751	-0.431371367
H	-3.834945396	2.552610796	-0.687174875
C	-5.213669087	0.940938650	-0.452969568
H	-6.080407090	1.516472498	-0.726075626
C	-5.358524654	-0.434603212	-0.114958393
H	-6.336267254	-0.883936999	-0.133837154
C	-4.274601106	-1.171974431	0.227041435
H	-4.360498617	-2.210133059	0.484242369
C	-2.978747096	-0.581832227	0.262693873
C	-1.832649565	-1.408781578	0.628837317
O	-1.943073336	-2.647664323	0.785898220
C	-0.567324817	-0.745381097	0.730082815
C	0.565702486	-1.471005975	1.219631954
H	0.404777871	-2.451029545	1.626001647
C	1.812639663	-0.924270466	1.189802725
H	2.642277515	-1.485181257	1.581312364
C	2.015619758	0.390444749	0.645987258
C	3.403132771	0.897608177	0.349904630
C	4.488325044	0.611988440	1.379424983
H	5.447022088	0.979793616	1.028789196
H	4.246240502	1.131699512	2.299210106
H	4.586349774	-0.444429439	1.601661097
O	2.959014187	4.107556999	-0.614856644
H	2.069028073	4.437573929	-0.479781309
H	3.091554868	4.135507882	-1.552517041
O	0.241365000	4.845254479	-0.321345851
H	-0.297436022	4.055209071	-0.409746152
H	0.017874788	5.206547642	0.525535176
O	2.158049413	-3.901237457	-0.841728954
H	1.111301814	-3.748194861	-0.872449001
H	2.351767868	-4.677176344	-1.355967185
O	3.947128348	-2.294194267	-1.107176507
H	2.989430491	-3.029869095	-0.969283024
H	4.690228146	-2.596576429	-0.596029957
O	-0.343315401	-3.823913093	-0.969502579
H	-0.739211335	-3.460564240	-1.752293809
H	-0.883286715	-3.476546790	-0.225086857
H	3.386214667	1.950775971	0.117926674
O	3.733131519	0.211732997	-0.879476406
H	3.847562501	-1.242368134	-0.974963344

Path1-T_{RCT2}(³ $\pi\pi^*$)-17

C	0.931638497	1.140581954	0.235444553
H	1.038830477	2.146071195	-0.129059692
C	-0.379612878	0.593139533	0.306211748
C	-1.520048064	1.407691303	-0.073014591
O	-1.417507256	2.587538796	-0.410641485
C	-2.829184952	0.741757741	-0.055912408
C	-3.986183185	1.494829355	-0.407554729
H	-3.853926376	2.528952477	-0.665929414
C	-5.221027980	0.905696625	-0.411992457
H	-6.097908411	1.473345367	-0.675137103
C	-5.352205749	-0.469639496	-0.066521837
H	-6.329069438	-0.924528159	-0.070465686
C	-4.257228883	-1.198327733	0.264667185
H	-4.329572647	-2.237225855	0.528635654
C	-2.963954618	-0.600013984	0.277431230
C	-1.807494383	-1.418147423	0.628403587
O	-1.914950978	-2.654004591	0.828329673
C	-0.540532848	-0.749059905	0.692389657
C	0.612979997	-1.475496732	1.127521933
H	0.466261425	-2.469598692	1.510737534
C	1.853406484	-0.911540710	1.089564356
H	2.700287111	-1.469133571	1.452070415
C	2.033114273	0.427876767	0.598296519
C	3.415546486	0.979271509	0.345006523
C	4.454531806	0.777607229	1.442928301
H	5.414504834	1.171463912	1.120703627
H	4.153195197	1.314573798	2.336890124
H	4.585222489	-0.269364028	1.698108403
O	2.919771826	4.234353509	-0.705348351
H	2.028196756	4.553838558	-0.554728292
H	3.028081285	4.262427071	-1.648553636
O	0.157316014	4.926027433	-0.356566894
H	-0.356588926	4.117035849	-0.426459083
H	-0.084993112	5.294847116	0.484679701
O	2.125843791	-4.057650753	-0.866444215
H	1.137140291	-3.830963830	-0.894556756
H	2.298346208	-4.777128491	-1.469726715
O	3.981507576	-2.518076387	-0.952507300
H	2.883014481	-3.312420307	-0.879467933
H	4.705295913	-2.777954466	-0.389358986
O	-0.383655810	-3.805951277	-1.023586664
H	-0.780275373	-3.369978123	-1.770861114
H	-0.899964656	-3.485508772	-0.252391185
H	3.362340037	2.026653252	0.083021573
O	3.826491504	0.251789175	-0.820652184
H	3.910584971	-1.554967677	-0.886029499

Path1-T_{RCT2}(³ππ*)-20

C	0.970820262	1.113885115	0.208039361
H	1.099146565	2.108406089	-0.170513108
C	-0.344977422	0.587916231	0.279971901
C	-1.470760431	1.416389570	-0.114932699
O	-1.339793290	2.591164539	-0.449719117
C	-2.793918135	0.790256619	-0.059439121
C	-3.935434796	1.562022165	-0.407187095
H	-3.789590646	2.586293976	-0.686954981
C	-5.184548717	1.001249600	-0.388346474
H	-6.046221499	1.587320970	-0.651591632
C	-5.340039541	-0.361994529	-0.021393990
H	-6.322047996	-0.800167664	-0.006433877
C	-4.258426300	-1.109921255	0.308611784
H	-4.358229886	-2.139779579	0.589276370
C	-2.954817536	-0.543169669	0.300947088
C	-1.814969054	-1.376763682	0.649199904
O	-1.944880725	-2.611546240	0.854032690
C	-0.531420045	-0.740320998	0.691581710
C	0.605395881	-1.478313796	1.141509734
H	0.446040528	-2.457243541	1.551066698
C	1.856730955	-0.933035726	1.092744791
H	2.693427518	-1.499656626	1.458905586
C	2.055986092	0.384827082	0.576078906
C	3.451344549	0.929501118	0.349256493
C	4.419328728	0.776420348	1.515449820
H	5.395477684	1.170650583	1.254560431
H	4.043614421	1.339538910	2.360418625
H	4.540056025	-0.257410024	1.816682805
O	3.006995016	4.267200175	-0.706062280
H	2.114379838	4.582340161	-0.570129737
H	3.156015568	4.350187583	-1.636664293
O	0.223034436	4.940837014	-0.412379381
H	-0.280136438	4.128324528	-0.484598980
H	-0.079821948	5.349797992	0.385232794
O	1.879220025	-4.228535274	-0.869921862
H	0.897185529	-3.893743789	-0.898643893
H	2.023753673	-4.860516834	-1.570179697
O	3.931093637	-2.700658847	-0.994944691
H	2.600924081	-3.544260443	-0.883450336
H	4.684058934	-2.986574521	-0.494204554
O	-0.537158967	-3.762764154	-1.063543293
H	-0.886138588	-3.240613579	-1.774975372
H	-1.026691908	-3.458338452	-0.264465433
H	3.381055353	1.970567824	0.073633935
O	3.959508916	0.203352573	-0.758314109
H	3.907823893	-1.741211027	-0.922707673

Path1-T_{RCT2}(³ππ*)-23

C	1.055721831	1.064853784	0.233628367
H	1.233532673	2.060832239	-0.118914069
C	-0.283879787	0.601046732	0.285830735
C	-1.370210139	1.494664971	-0.090136865
O	-1.176259920	2.650112763	-0.451109561
C	-2.724280865	0.937353950	-0.038386270
C	-3.825822010	1.774166885	-0.365811327
H	-3.628785306	2.794424060	-0.627579547
C	-5.101637522	1.278868145	-0.348584185
H	-5.933571305	1.912387289	-0.595997169
C	-5.324714144	-0.082334652	-0.005402522
H	-6.327783590	-0.469203586	0.007342370
C	-4.282757542	-0.891205513	0.303066497
H	-4.435172449	-1.919783314	0.563204976
C	-2.950334061	-0.391787922	0.297110094
C	-1.852852822	-1.285602534	0.614408347
O	-2.047231288	-2.527462896	0.777481497
C	-0.538085763	-0.721879510	0.667306291
C	0.561867629	-1.527523671	1.095011670
H	0.357724910	-2.507372946	1.481314332
C	1.839852418	-1.045357085	1.056774872
H	2.648821956	-1.671067318	1.386717173
C	2.104657577	0.273534743	0.577557549
C	3.520509233	0.768017860	0.365082718
C	4.456276058	0.632776173	1.562584172
H	5.448902413	0.986145373	1.307148293
H	4.079155585	1.243653945	2.372725330
H	4.534688644	-0.390635451	1.907724597
O	3.227381169	4.090188026	-0.748964675
H	2.342798251	4.427769042	-0.604482860
H	3.374225839	4.170111835	-1.679838193
O	0.531743526	4.841155070	-0.434531952
H	-0.024288929	4.064354778	-0.524267739
H	0.237172936	5.270466253	0.355173184
O	1.404970967	-4.279643228	-0.739146262
H	0.320642680	-3.915336485	-0.849364511
H	1.569286906	-5.002841225	-1.336533056
O	3.719746891	-2.839483990	-1.159662836
H	2.130109907	-3.623811712	-0.835027152
H	4.518361361	-3.206695815	-0.806931825
O	-0.847403576	-3.781236043	-1.015878610
H	-1.064654332	-3.213176284	-1.746693833
H	-1.333490879	-3.389834616	-0.213777687
H	3.485957123	1.802581195	0.060706339
O	4.058537887	-0.005247959	-0.693905015
H	3.788619839	-1.887575305	-1.037150540

Path1-T_{RCT2}(³ππ*)-26

C	1.114966642	1.035238485	0.241949589
H	1.324960262	2.043064652	-0.072461812
C	-0.249664542	0.621269024	0.272487070
C	-1.303136251	1.565921598	-0.094395690
O	-1.074312092	2.716054566	-0.451203207
C	-2.685084150	1.055975079	-0.034628945
C	-3.760426767	1.951748339	-0.326593851
H	-3.510599468	2.969793702	-0.566721570
C	-5.051098878	1.508737588	-0.298731641
H	-5.872048205	2.173148856	-0.516313700
C	-5.328859825	0.140692021	0.019761287
H	-6.354953243	-0.191401845	0.039001166
C	-4.318571740	-0.717177188	0.291995171
H	-4.497171379	-1.749719303	0.533249030
C	-2.957595585	-0.266578833	0.267855937
C	-1.887908206	-1.208526577	0.542916871
O	-2.137682386	-2.458534130	0.715059002
C	-0.557080951	-0.699570296	0.612372496
C	0.517010708	-1.571332049	0.995216529
H	0.268444121	-2.567572484	1.320931677
C	1.808269464	-1.141230116	0.990199199
H	2.596631623	-1.812575405	1.285545023
C	2.135523703	0.199891247	0.577701279
C	3.560495739	0.647149178	0.415488490
C	4.496173234	0.469476932	1.617246383
H	5.500578054	0.774104113	1.334327493
H	4.169895698	1.098911484	2.441246883
H	4.524475412	-0.561928526	1.954156821
O	3.439541176	3.902699732	-0.780357459
H	2.555252078	4.254503165	-0.629671940
H	3.564979606	3.948647891	-1.722529515
O	0.820418023	4.718519973	-0.440459660
H	0.191854947	3.995869494	-0.549966607
H	0.561564315	5.144597444	0.370752945
O	1.169245448	-4.205274859	-0.762400829
H	-0.201105345	-4.015975351	-0.807780143
H	1.424259171	-5.010438099	-1.198968916
O	3.632863389	-2.848737818	-1.221758733
H	1.894185687	-3.530857590	-0.858565893
H	4.415109598	-3.264504228	-0.872619597
O	-1.210073970	-3.914761338	-0.842929155
H	-1.396921890	-3.485315755	-1.678807885
H	-1.655020531	-3.280213130	-0.048663013
H	3.600271611	1.679545674	0.095426095
O	4.101654815	-0.190777898	-0.630852000
H	3.764047006	-1.915297171	-1.077391316

Path1-T_{RCT2}(³ππ*)-29

C	1.114027845	1.039019166	0.241077625
H	1.327623547	2.047459247	-0.066454784
C	-0.248683068	0.623975522	0.262647276
C	-1.303441517	1.568573797	-0.110704257
O	-1.072930394	2.719249246	-0.460980296
C	-2.686860556	1.065357783	-0.046169102
C	-3.758935323	1.963707094	-0.331849870
H	-3.507295507	2.981005095	-0.572521374
C	-5.051955462	1.524313894	-0.298953593
H	-5.871229568	2.191539527	-0.512510980
C	-5.332095955	0.158466272	0.018849243
H	-6.358824492	-0.170479390	0.042878534
C	-4.323228007	-0.704281091	0.286569992
H	-4.505563601	-1.735840333	0.528359721
C	-2.962319915	-0.258300216	0.256426499
C	-1.894345006	-1.195596506	0.526968500
O	-2.158068781	-2.451700653	0.715565663
C	-0.558787568	-0.696933136	0.598391135
C	0.511807496	-1.572548548	0.976275381
H	0.264267099	-2.570757273	1.292816427
C	1.804336047	-1.142136179	0.975301737
H	2.593856845	-1.814918761	1.262610529
C	2.131702270	0.199157778	0.576944269
C	3.561721869	0.639781660	0.437369751
C	4.466520729	0.457878130	1.660610003
H	5.480049098	0.753152276	1.402533873
H	4.123720167	1.092601987	2.473380304
H	4.477805624	-0.573284564	2.002579206
O	3.465688909	3.881997482	-0.773582244
H	2.578882547	4.229820216	-0.625003936
H	3.593896412	3.930071690	-1.715066533
O	0.848122426	4.698827800	-0.436937495
H	0.209785521	3.986043117	-0.554594511
H	0.590549020	5.123057765	0.375548937
O	1.193483909	-4.175162075	-0.723083817
H	-0.269598703	-4.042564147	-0.769902969
H	1.506900618	-4.996144344	-1.089130092
O	3.636050391	-2.838160311	-1.308261364
H	1.878994215	-3.521951638	-0.854357462
H	4.435034016	-3.269955664	-1.023923363
O	-1.249477101	-3.960424943	-0.801094957
H	-1.441096485	-3.593365462	-1.664170207
H	-1.715207353	-3.230886878	0.005726489
H	3.609335248	1.671063466	0.111182284
O	4.137312704	-0.200286902	-0.598664344
H	3.779876068	-1.902995652	-1.132196764

Path1-T_{RCT2}(³ππ*)-32

C	1.097498877	1.052211136	0.234844229
H	1.304519557	2.060162015	-0.075613097
C	-0.259657848	0.624745157	0.257138825
C	-1.325268925	1.557154761	-0.121071357
O	-1.104519344	2.709127726	-0.469378031
C	-2.704582628	1.044494166	-0.050589784
C	-3.783474728	1.931212854	-0.335986612
H	-3.542848651	2.949504798	-0.581241781
C	-5.073637241	1.480529975	-0.298241898
H	-5.897804903	2.140633930	-0.511926607
C	-5.340523209	0.115316837	0.024117516
H	-6.363361552	-0.223478059	0.052307474
C	-4.323595410	-0.738849367	0.292293542
H	-4.498540990	-1.770198151	0.538096653
C	-2.968488915	-0.281768768	0.257899901
C	-1.891298739	-1.202983599	0.528895866
O	-2.144899893	-2.466161506	0.727331184
C	-0.558307483	-0.696778929	0.597691637
C	0.516593253	-1.561356042	0.980281534
H	0.279389683	-2.560052108	1.299010166
C	1.805650571	-1.118145950	0.979150264
H	2.600708240	-1.781808331	1.270284911
C	2.120358848	0.221110045	0.577307999
C	3.550592039	0.667368744	0.446859206
C	4.436332590	0.488156324	1.682316415
H	5.452785463	0.787319473	1.443382758
H	4.075019493	1.120997606	2.487559100
H	4.446287716	-0.542670533	2.025369854
O	3.442364591	3.900599020	-0.780275357
H	2.552155592	4.240604579	-0.635971811
H	3.574420504	3.946498696	-1.720495712
O	0.811347063	4.703156624	-0.450976406
H	0.176237066	3.987690335	-0.565168541
H	0.553790897	5.128976734	0.359762199
O	1.270047194	-4.161746056	-0.759617880
H	-0.238841152	-4.045682420	-0.791454671
H	1.606952245	-4.998952164	-1.063311614
O	3.705195056	-2.824093531	-1.293703233
H	1.945406510	-3.520006530	-0.879172504
H	4.500491961	-3.245583967	-0.987646252
O	-1.210912753	-3.958905341	-0.812642959
H	-1.423666810	-3.662089013	-1.695773260
H	-1.704138970	-3.202954130	0.025873149
H	3.595057596	1.697632418	0.117013109
O	4.154031731	-0.166800762	-0.574388682
H	3.835605021	-1.882458590	-1.119116318

T_{RCT2}(³ππ*)-INT

C	1.056484497	1.078441691	0.224537286
H	1.246105178	2.088208711	-0.083267875
C	-0.285913451	0.620023542	0.244952251
C	-1.376287782	1.528214327	-0.137868313
O	-1.179845371	2.684748742	-0.469648376
C	-2.745991457	0.995537465	-0.059438385
C	-3.838203276	1.859453361	-0.336655629
H	-3.622655883	2.881667894	-0.582050777
C	-5.122027214	1.384312851	-0.293813796
H	-5.955645775	2.031219808	-0.502185180
C	-5.359291961	0.018479527	0.025025304
H	-6.372425671	-0.343289220	0.058061881
C	-4.325160938	-0.818575375	0.287725981
H	-4.485237490	-1.851035135	0.532396922
C	-2.983535927	-0.337209520	0.250037734
C	-1.887568336	-1.224460453	0.517791001
O	-2.134112773	-2.503258715	0.736527189
C	-0.557870642	-0.705436041	0.584988616
C	0.527850780	-1.547964206	0.966704179
H	0.317930203	-2.552503527	1.276734074
C	1.808702913	-1.072434010	0.966150220
H	2.616645080	-1.719352440	1.254094210
C	2.092408388	0.266802167	0.570783900
C	3.522440079	0.732239234	0.457851855
C	4.368100381	0.566214317	1.719775586
H	5.386743613	0.882437623	1.524195295
H	3.960209578	1.190437346	2.506548547
H	4.383197961	-0.462759457	2.066363734
O	3.382948003	3.953051943	-0.793394703
H	2.488641776	4.274855952	-0.652246996
H	3.518961310	4.000337507	-1.730462199
O	0.718323671	4.724201855	-0.461690460
H	0.093536639	4.002473446	-0.566435026
H	0.466155703	5.151530777	0.347003196
O	1.470643557	-4.141269971	-0.764571297
H	-0.162305123	-4.055343154	-0.811304358
H	1.870268331	-4.959056967	-1.037934956
O	3.867476970	-2.779643103	-1.263447777
H	2.128180088	-3.514559973	-0.879322785
H	4.665737389	-3.178724316	-0.943451712
O	-1.120149653	-3.983159990	-0.840411525
H	-1.340152284	-3.752150239	-1.735302303
H	-1.703707421	-3.136546116	0.071691642
H	3.558045675	1.761435584	0.123258238
O	4.196144615	-0.076163571	-0.527386965
H	3.965522624	-1.829174786	-1.095478970

S4-2. Cartesian coordinates of the critical points for 2-HEAQ·5H₂O along the reaction pathway of the second step of ES IPT between methylene C1'-H15 and carbonyl C9=O11 in the $T_{RCT_2}(^3\pi\pi^*)$ and ground states obtained by the CASSCF(12e/10o)/6-31G* level of theory.

Path2- $T_{RCT_2}(^3\pi\pi^*)$ -4

C	0.785247850	-1.244753919	-0.693070132
H	0.849779264	-2.306212327	-0.578128298
C	-0.458804120	-0.638020733	-0.481283796
C	-1.610987047	-1.484879113	-0.132720794
O	-1.489025831	-2.672670350	0.103263450
C	-2.920229818	-0.827950094	-0.088155690
C	-4.077963534	-1.610103078	0.072603918
H	-3.970669428	-2.675011277	0.144525897
C	-5.319199429	-1.008589167	0.130084441
H	-6.206362071	-1.604573318	0.240807855
C	-5.417194642	0.394922749	0.050813281
H	-6.381393585	0.866310513	0.100386858
C	-4.287418154	1.171126747	-0.087530980
H	-4.352028426	2.238663402	-0.144753721
C	-3.013392589	0.564548647	-0.173495664
C	-1.841291733	1.362727324	-0.334536634
O	-1.997822231	2.682581316	-0.309822677
C	-0.576350728	0.749681958	-0.575504315
C	0.574254673	1.504534783	-0.924123958
H	0.504375413	2.563019601	-1.069072412
C	1.780452193	0.900204326	-1.089391268
H	2.643280841	1.500499955	-1.306152053
C	1.913849437	-0.499110455	-0.965260208
C	3.258943665	-1.166731957	-0.790045175
C	3.538537963	-2.476577566	-1.504203608
H	4.442406677	-2.892312940	-1.073854084
H	2.736200905	-3.184234691	-1.344239961
H	3.683973884	-2.341304627	-2.568413648
O	2.832711632	-2.109017749	1.884183650
H	2.038780206	-2.638328647	1.793227452
H	2.591981620	-1.347350333	2.390569123
O	0.609669887	-3.689063336	1.656629442
H	-0.145506034	-3.356864513	1.170832011
H	0.777393754	-4.559101067	1.323630481
O	2.613965464	3.760553320	0.443981884
H	0.878108456	3.914197368	0.840644347
H	3.175207293	4.509204938	0.584843505
O	4.201674093	1.592469092	1.097246629
H	3.119749215	2.984615232	0.695466564
H	5.109791916	1.810563791	1.251865294
O	-0.053724185	3.989350819	1.061856022
H	-0.132671356	3.699997514	1.960171947
H	-1.241191905	3.152342718	0.060547010

H	3.233203844	-1.388417599	0.269208991
O	4.340026850	-0.311914680	-0.887510459
H	4.215060129	0.969806163	0.374186753

Path2-T_{RCT2}(³ππ*)-7

C	0.784088687	-1.250118596	-0.682561841
H	0.842224502	-2.315148337	-0.578040238
C	-0.458329171	-0.643144290	-0.475716915
C	-1.613964585	-1.489755259	-0.127968518
O	-1.498570754	-2.677424230	0.118611834
C	-2.919525272	-0.827179051	-0.089851799
C	-4.081268150	-1.604181346	0.071344140
H	-3.977287133	-2.668732393	0.146098075
C	-5.320222594	-0.999720569	0.126988254
H	-6.209365469	-1.592546299	0.239083150
C	-5.412708753	0.403427851	0.044976849
H	-6.377013479	0.874695310	0.095078237
C	-4.279586775	1.175179822	-0.093809944
H	-4.343382972	2.242531709	-0.151939831
C	-3.005973069	0.565677329	-0.177135459
C	-1.830649523	1.363066765	-0.335877929
O	-1.989561589	2.682015552	-0.302387801
C	-0.568522414	0.749390387	-0.570630444
C	0.585401723	1.506611920	-0.913276523
H	0.518695936	2.561763800	-1.087057993
C	1.790757496	0.901482802	-1.069028834
H	2.656612536	1.493390135	-1.301607781
C	1.910746781	-0.497694055	-0.958022857
C	3.248009721	-1.165067154	-0.785413821
C	3.535910831	-2.477860213	-1.488199483
H	4.439367819	-2.894495077	-1.056300539
H	2.729666481	-3.180505235	-1.329375843
H	3.685701314	-2.353098416	-2.553387411
O	2.813860302	-2.087935766	1.817499082
H	2.030990907	-2.638547641	1.765199976
H	2.601075918	-1.349664663	2.367753435
O	0.612412295	-3.675043510	1.656309893
H	-0.144529272	-3.342696014	1.172373494
H	0.774519898	-4.547626996	1.327655636
O	2.615072550	3.748234153	0.444007156
H	0.888245111	3.905453306	0.828624568
H	3.175249076	4.498730018	0.577794361
O	4.192402289	1.577414338	1.077049865
H	3.125112861	2.970970847	0.684493592
H	5.097508760	1.803832170	1.234736440
O	-0.043785080	3.988501770	1.047264869
H	-0.127526520	3.698862021	1.945015554
H	-1.229981153	3.157753217	0.055668548
H	3.136526992	-1.373528382	0.271086782
O	4.336454131	-0.325010944	-0.842345922

H	4.216325080	0.941897942	0.364086849
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STC(T_{RCT2}/S_0)

C	0.779091624	-1.262397953	-0.668912603
H	0.830880482	-2.329688662	-0.575489715
C	-0.460097362	-0.657417783	-0.475958909
C	-1.617836622	-1.499201925	-0.128420411
O	-1.510704164	-2.684077385	0.131251584
C	-2.929422511	-0.828563887	-0.089926482
C	-4.083595059	-1.594238661	0.068372977
H	-3.984577561	-2.659020191	0.145601972
C	-5.324091091	-0.986106759	0.122577005
H	-6.212838036	-1.579649006	0.235278287
C	-5.413475690	0.408209810	0.039087104
H	-6.376612786	0.883547668	0.089107869
C	-4.271284106	1.181287157	-0.100894387
H	-4.339033690	2.249001869	-0.158555091
C	-3.006477746	0.569737664	-0.178644375
C	-1.805091950	1.366735075	-0.342716298
O	-1.983138906	2.682513624	-0.297459640
C	-0.576272950	0.762444100	-0.567708216
C	0.602680805	1.510469151	-0.907946867
H	0.530436585	2.561936725	-1.101869151
C	1.802352484	0.905771424	-1.043919368
H	2.667134754	1.488341356	-1.303585385
C	1.926792764	-0.506110884	-0.931087094
C	3.264414342	-1.143664427	-0.808957806
C	3.533563771	-2.483730979	-1.475801289
H	4.436804071	-2.901844968	-1.046395727
H	2.720062406	-3.181550911	-1.319877996
H	3.684014789	-2.365307831	-2.540653893
O	2.798379205	-2.072986641	1.772702651
H	2.024679426	-2.642327883	1.750811149
H	2.604165360	-1.352785936	2.354505249
O	0.608857865	-3.666279176	1.657435950
H	-0.149139405	-3.334851507	1.173337883
H	0.766443658	-4.540889834	1.331710431
O	2.617474332	3.738532127	0.445260935
H	0.896682927	3.899985921	0.821474134
H	3.177303893	4.489820282	0.574325996
O	4.186284323	1.564020915	1.066268534
H	3.130170086	2.960048078	0.679912499
H	5.089747333	1.795089156	1.227428587
O	-0.036195898	3.986724269	1.037689565
H	-0.123224205	3.698779083	1.935651212
H	-1.222944852	3.164003970	0.051515149
H	3.035762621	-1.368085842	0.301484138
O	4.327701254	-0.337481795	-0.817944712
H	4.217313848	0.918394286	0.357785563

Path2-S₀-3

C	0.765187196	-1.270732484	-0.663654200
H	0.828532866	-2.333871089	-0.570887217
C	-0.451624809	-0.669014814	-0.475642990
C	-1.619797435	-1.505646547	-0.125379074
O	-1.512500372	-2.682271007	0.139127079
C	-2.937121585	-0.830855600	-0.091488431
C	-4.083186312	-1.591127919	0.064519375
H	-3.988525503	-2.657619523	0.143614317
C	-5.328321387	-0.980814293	0.117413116
H	-6.216726801	-1.575717532	0.229857788
C	-5.417097591	0.408200036	0.033589205
H	-6.378679646	0.887883005	0.083312506
C	-4.268797063	1.183604694	-0.106609620
H	-4.338951975	2.251743277	-0.163433626
C	-3.012480245	0.570988692	-0.180602160
C	-1.788719397	1.369638162	-0.345351272
O	-1.979650871	2.683521966	-0.291848198
C	-0.587601762	0.775184857	-0.565640096
C	0.612802018	1.509795064	-0.909542214
H	0.531641209	2.560907724	-1.104805666
C	1.806488412	0.913143043	-1.034244193
H	2.672649813	1.484558781	-1.301462601
C	1.958898138	-0.518548920	-0.904500764
C	3.295940680	-1.104713510	-0.852379027
C	3.531614536	-2.489490079	-1.462354239
H	4.436686218	-2.906238430	-1.040755693
H	2.715233955	-3.184856279	-1.314911942
H	3.684518238	-2.369269215	-2.530330455
O	2.789857070	-2.069555599	1.752948195
H	2.015890533	-2.647719569	1.740472936
H	2.600316686	-1.354267987	2.347040225
O	0.605249278	-3.659566806	1.658104688
H	-0.151291947	-3.328474698	1.171919396
H	0.762186904	-4.535113054	1.332958453
O	2.615713262	3.729894727	0.448817233
H	0.901600581	3.893610187	0.818986339
H	3.173482249	4.482839904	0.577163291
O	4.177890592	1.558931410	1.067851954
H	3.132867752	2.950907393	0.683311463
H	5.081857940	1.791630792	1.226701677
O	-0.033081405	3.983353124	1.032812604
H	-0.123930311	3.695894819	1.930584631
H	-1.216187179	3.166695096	0.053852541
H	2.974271410	-1.407398790	0.387069218
O	4.315409789	-0.342632257	-0.812871781
H	4.214358218	0.902808407	0.351407737

Local-Min(S₀)

C	0.774721943	-1.265421794	-0.664313957
H	0.838031153	-2.332662088	-0.568082948
C	-0.449335381	-0.668578586	-0.473005943
C	-1.609424852	-1.517391171	-0.122992916
O	-1.498458193	-2.699450328	0.146476105
C	-2.929350733	-0.839371565	-0.099280914
C	-4.083853234	-1.602874680	0.057285098
H	-3.985216712	-2.675110625	0.135257104
C	-5.330991086	-0.991483750	0.109993102
H	-6.225162257	-1.587557354	0.221202111
C	-5.424491520	0.404693658	0.029662096
H	-6.390025683	0.886996819	0.081714100
C	-4.277236011	1.183070002	-0.108690915
H	-4.344130239	2.256765846	-0.161971919
C	-3.014759804	0.570602345	-0.188072921
C	-1.798174069	1.378812487	-0.341538933
O	-1.980111356	2.702099601	-0.272087928
C	-0.593104978	0.777952644	-0.565345948
C	0.608557493	1.515537780	-0.909623977
H	0.520568173	2.572382234	-1.098373993
C	1.806769183	0.920244554	-1.040000985
H	2.683752423	1.490511708	-1.294857008
C	1.965018528	-0.511595060	-0.903983975
C	3.305341525	-1.088058090	-0.859548972
C	3.539196852	-2.482475607	-1.468733021
H	4.447066845	-2.904076492	-1.047018987
H	2.715140719	-3.178777794	-1.321112010
H	3.690442785	-2.366278417	-2.544554104
O	2.791972985	-2.077083240	1.740450229
H	1.999495214	-2.663277131	1.716364224
H	2.592184618	-1.353110269	2.333194271
O	0.606225922	-3.654004195	1.652302222
H	-0.150313469	-3.315530504	1.151153179
H	0.770684691	-4.529610706	1.315937197
O	2.605468184	3.719451641	0.459740129
H	0.905542232	3.883792399	0.821477156
H	3.156359512	4.481399457	0.592005141
O	4.163869549	1.559840256	1.071088175
H	3.132272862	2.938518750	0.697362146
H	5.070525959	1.799844094	1.229476185
O	-0.036649774	3.973775958	1.033633173
H	-0.134511915	3.684146967	1.934200240
H	-1.198048883	3.176271463	0.073057099
H	2.970564698	-1.462623712	0.483140131
O	4.322808693	-0.325305999	-0.806995966
H	4.200466104	0.901416809	0.342740120

Path2-S₀-8

C	0.761430725	-1.267775262	-0.655677017
H	0.826501948	-2.333595493	-0.561743388
C	-0.444351752	-0.678135734	-0.471323792
C	-1.610825780	-1.512272122	-0.120495546
O	-1.506058295	-2.695199066	0.156984434
C	-2.929754326	-0.834057424	-0.094802724
C	-4.093379028	-1.596215858	0.063804314
H	-3.993203589	-2.663972603	0.144895650
C	-5.327074592	-0.987034634	0.113024991
H	-6.220896982	-1.577652569	0.225458595
C	-5.419788669	0.408693962	0.026875082
H	-6.383701485	0.889093546	0.076173890
C	-4.275399830	1.183602810	-0.112958291
H	-4.341814961	2.253947353	-0.170965528
C	-3.010471436	0.569968327	-0.185459646
C	-1.788867794	1.370384159	-0.345597501
O	-1.977357253	2.698240809	-0.290155935
C	-0.598299318	0.777587433	-0.564907964
C	0.609202285	1.517066102	-0.911668560
H	0.525184346	2.566301051	-1.108267523
C	1.813327118	0.913742421	-1.033137096
H	2.681806246	1.481707272	-1.298840760
C	1.977868550	-0.525996632	-0.885101634
C	3.296957632	-1.083260199	-0.900516953
C	3.534332956	-2.491495152	-1.449935481
H	4.440733588	-2.911724262	-1.030828222
H	2.713674385	-3.185944019	-1.305446009
H	3.687737969	-2.383192546	-2.522007608
O	2.779915507	-2.038317848	1.700228112
H	2.005627918	-2.660522441	1.720067756
H	2.595357787	-1.347250684	2.339316619
O	0.608828299	-3.646177198	1.664746349
H	-0.154097882	-3.314196369	1.171460213
H	0.759429361	-4.525506148	1.340466531
O	2.613152647	3.720824888	0.450935438
H	0.902111084	3.887137116	0.812248638
H	3.164042642	4.478493830	0.577503975
O	4.169871880	1.551662610	1.072697821
H	3.132100376	2.944711532	0.686578138
H	5.071906222	1.795348633	1.227235088
O	-0.030608328	3.982832895	1.026990469
H	-0.129723884	3.692946354	1.922481472
H	-1.208975774	3.169104043	0.056308455
H	2.927000112	-1.536033344	0.659411109
O	4.320431570	-0.350167244	-0.800292523
H	4.204351741	0.902387685	0.348686521

Path2-S₀-11

C	0.777993873	-1.266201547	-0.654113600
H	0.819831055	-2.335506267	-0.560651738
C	-0.456314335	-0.680564933	-0.467433770
C	-1.606696002	-1.504946224	-0.119033330
O	-1.502233058	-2.703538312	0.166973099
C	-2.918488105	-0.831084443	-0.091442779
C	-4.092904742	-1.601639226	0.069052033
H	-3.994555245	-2.665745891	0.151335373
C	-5.327403423	-0.994292856	0.116055654
H	-6.219331888	-1.582547993	0.228701039
C	-5.415647116	0.408976910	0.025276822
H	-6.381707810	0.882134040	0.072086251
C	-4.277926895	1.176253379	-0.113832998
H	-4.343199225	2.245404702	-0.176366890
C	-2.999667981	0.560065314	-0.182962773
C	-1.795242485	1.359539206	-0.346445856
O	-1.985664712	2.698523977	-0.310458344
C	-0.600548062	0.770482598	-0.564570698
C	0.609386656	1.515166615	-0.910654984
H	0.524653966	2.563037228	-1.113826196
C	1.811386561	0.912794813	-1.022252063
H	2.676330749	1.482607916	-1.300570106
C	1.969653052	-0.532227522	-0.865398576
C	3.297056593	-1.072672780	-0.953606978
C	3.535231468	-2.493992657	-1.439298235
H	4.441152543	-2.908395277	-1.014601864
H	2.714074597	-3.185023541	-1.292726779
H	3.689957921	-2.394553188	-2.508817590
O	2.774365771	-2.009763883	1.674370003
H	2.001095250	-2.656235761	1.706694632
H	2.607380610	-1.332989124	2.336386570
O	0.630637012	-3.632982338	1.669406368
H	-0.154697869	-3.309485422	1.187768065
H	0.758200828	-4.523030948	1.361542798
O	2.612404735	3.728962825	0.445513247
H	0.893732107	3.891174601	0.808404721
H	3.165466050	4.484915798	0.570629772
O	4.172817423	1.547698464	1.081887487
H	3.125706217	2.953072421	0.681437874
H	5.073198193	1.800415706	1.230191686
O	-0.035183534	3.994801704	1.026631724
H	-0.133867191	3.697720390	1.919437274
H	-1.224808085	3.162102292	0.047610993
H	2.879706790	-1.562698824	0.764806342
O	4.310043429	-0.370606395	-0.795646850
H	4.204969624	0.914918904	0.355086742

Path2-S₀-14

C	0.786490253	-1.261076375	-0.651547450
H	0.820566225	-2.331547000	-0.572020624
C	-0.461125995	-0.679880495	-0.461354755
C	-1.594439992	-1.508284390	-0.112285847
O	-1.479100011	-2.714043666	0.176905503
C	-2.902164554	-0.841392170	-0.085126753
C	-4.085812021	-1.612085455	0.075869588
H	-3.988732475	-2.676903615	0.156566406
C	-5.320824903	-1.009674266	0.120153947
H	-6.215427988	-1.597412402	0.232523302
C	-5.412677214	0.399064729	0.026855577
H	-6.379591471	0.871964560	0.069692715
C	-4.278260197	1.163298856	-0.111287914
H	-4.345026649	2.231537771	-0.179330042
C	-2.991832146	0.549569623	-0.179798739
C	-1.806676354	1.354148451	-0.351447866
O	-2.000154807	2.697748944	-0.344907126
C	-0.607757192	0.765270880	-0.564735182
C	0.598163981	1.514694023	-0.909210309
H	0.515983343	2.561952664	-1.117243941
C	1.802873988	0.916909288	-1.014475644
H	2.662761035	1.490412762	-1.301923636
C	1.960755555	-0.526411035	-0.857757490
C	3.294778665	-1.070044875	-1.002638690
C	3.536855666	-2.494758028	-1.450351356
H	4.441906912	-2.890304464	-1.003261516
H	2.713049623	-3.175482237	-1.285135985
H	3.696813751	-2.419534275	-2.518297255
O	2.760193600	-2.012274278	1.702704995
H	1.972229679	-2.657994228	1.694442956
H	2.613418718	-1.315755043	2.347085179
O	0.666961553	-3.606183146	1.655074111
H	-0.145734150	-3.292403236	1.201738873
H	0.765099204	-4.513111399	1.386079308
O	2.608462068	3.746881893	0.436693320
H	0.876947303	3.900325812	0.808135597
H	3.164591425	4.500171507	0.565956449
O	4.178216671	1.546987440	1.104123350
H	3.113880370	2.969456728	0.678429030
H	5.077184199	1.814313017	1.235271698
O	-0.047977177	4.014938529	1.034634826
H	-0.144111645	3.701684034	1.922166045
H	-1.254164860	3.157664649	0.043014275
H	2.821611663	-1.561151102	0.829491635
O	4.301412670	-0.382403181	-0.812194471
H	4.202543966	0.942802618	0.357176771

Path2-S₀-17

C	0.789336078	-1.259415007	-0.652084523
H	0.819972382	-2.330568096	-0.588858230
C	-0.461550493	-0.678291084	-0.451687481
C	-1.584901789	-1.510701746	-0.101653265
O	-1.457521718	-2.719503331	0.190072570
C	-2.892173714	-0.848825793	-0.077071488
C	-4.079000922	-1.618363519	0.081805312
H	-3.984573163	-2.683660044	0.159877596
C	-5.313747845	-1.015949752	0.121529002
H	-6.208802954	-1.603343214	0.230924374
C	-5.407435343	0.394063683	0.026438903
H	-6.373219384	0.869535208	0.063941074
C	-4.274435986	1.156606790	-0.111604497
H	-4.339526968	2.224468428	-0.184244305
C	-2.986647887	0.543286305	-0.179223238
C	-1.811833293	1.351613734	-0.361834032
O	-2.006072136	2.697363449	-0.385300704
C	-0.610039216	0.762728077	-0.564214715
C	0.592603127	1.513838529	-0.907297042
H	0.508815390	2.560675235	-1.116481983
C	1.798502550	0.917817943	-1.010178588
H	2.654832722	1.495021049	-1.299022771
C	1.956358151	-0.525910158	-0.859861149
C	3.293209242	-1.074743673	-1.027884054
C	3.531811390	-2.503701573	-1.462588945
H	4.433025555	-2.883742957	-0.995413897
H	2.705570665	-3.176899093	-1.280812194
H	3.700591330	-2.461996225	-2.531841145
O	2.725297710	-2.016263910	1.727645076
H	1.923877214	-2.667136670	1.711199920
H	2.602443111	-1.325889910	2.383181767
O	0.687743735	-3.578031890	1.643965077
H	-0.136790638	-3.266111879	1.202924907
H	0.768576719	-4.497364994	1.413810053
O	2.613892935	3.761368734	0.429231877
H	0.863470207	3.913451286	0.811864503
H	3.174792915	4.510152076	0.566671288
O	4.188138586	1.538269626	1.130723699
H	3.108772433	2.981936368	0.682835119
H	5.086298801	1.815667214	1.248886142
O	-0.058199830	4.033180988	1.047459061
H	-0.148477087	3.705623139	1.930582800
H	-1.282580678	3.160895657	0.037443154
H	2.760278210	-1.552356658	0.864209430
O	4.296534106	-0.387978285	-0.840313707
H	4.203821913	0.960084447	0.364917535

Path2-S₀-20

C	0.793107085	-1.259166188	-0.654785296
H	0.820248274	-2.331008298	-0.606150578
C	-0.460681482	-0.676309707	-0.443267471
C	-1.576986964	-1.509301273	-0.090839806
O	-1.440671392	-2.721032976	0.205268635
C	-2.882848166	-0.851762642	-0.070565960
C	-4.073073983	-1.620766269	0.085778050
H	-3.980752752	-2.686534678	0.161770195
C	-5.306955644	-1.017859198	0.119606152
H	-6.202894320	-1.604584817	0.224493979
C	-5.401249261	0.393723381	0.023005090
H	-6.366482851	0.870576168	0.056377775
C	-4.269277143	1.154855081	-0.115113185
H	-4.331662855	2.222465403	-0.191046388
C	-2.979993964	0.541289868	-0.181293532
C	-1.812787092	1.350874061	-0.372535934
O	-2.005986160	2.698093576	-0.422456162
C	-0.608336233	0.760573532	-0.564676412
C	0.592000854	1.512651743	-0.905909476
H	0.506086733	2.559926730	-1.111417895
C	1.798447818	0.917095891	-1.009375312
H	2.654158857	1.496754750	-1.294066597
C	1.953563708	-0.527117647	-0.865397407
C	3.293551043	-1.081572520	-1.050147694
C	3.525402529	-2.516385438	-1.471065915
H	4.422058436	-2.890168465	-0.990954462
H	2.695897078	-3.182320477	-1.278071882
H	3.699663958	-2.501610137	-2.540506062
O	2.682539395	-2.020956405	1.746820063
H	1.868171625	-2.682632572	1.730576322
H	2.585480360	-1.348641340	2.424094624
O	0.689250239	-3.552564023	1.643420469
H	-0.134711049	-3.238911941	1.190208842
H	0.768970834	-4.477830210	1.438022447
O	2.624137563	3.771338286	0.427459361
H	0.853187547	3.928520190	0.818592108
H	3.189849601	4.515390814	0.572520729
O	4.198521573	1.526893342	1.154753924
H	3.108626126	2.990105795	0.693419622
H	5.096716809	1.806848289	1.268614981
O	-0.066472358	4.045434082	1.062097390
H	-0.148826653	3.708750349	1.942663303
H	-1.305619770	3.166469857	0.031598344
H	2.692856325	-1.539607407	0.894586692
O	4.293365773	-0.393907267	-0.868963823
H	4.208201675	0.966717006	0.376979773

Path2-S₀-23

C	0.800226884	-1.259127860	-0.661112112
H	0.823800868	-2.331442260	-0.630394818
C	-0.457044712	-0.672481994	-0.433991296
C	-1.564172853	-1.502649192	-0.073744159
O	-1.414448172	-2.719656199	0.234127836
C	-2.866964858	-0.852575585	-0.061990811
C	-4.062813634	-1.620388706	0.090854912
H	-3.972956077	-2.686573567	0.166557812
C	-5.295048044	-1.017393702	0.113279689
H	-6.192547476	-1.603255487	0.210371164
C	-5.390569882	0.396584081	0.013174867
H	-6.355722720	0.873782167	0.041688630
C	-4.260252486	1.155956923	-0.125225992
H	-4.319868467	2.223291062	-0.206257294
C	-2.968040538	0.542406357	-0.187922671
C	-1.810286698	1.351242336	-0.390465822
O	-1.999390908	2.699600704	-0.473951347
C	-0.601499628	0.758418839	-0.568966108
C	0.596957086	1.510732719	-0.906093085
H	0.510106038	2.560005858	-1.099993302
C	1.803246201	0.914210240	-1.013278518
H	2.661048274	1.495665143	-1.287203068
C	1.951595656	-0.530500494	-0.881721699
C	3.293986794	-1.096064558	-1.078425090
C	3.513866121	-2.539222294	-1.480034511
H	4.403452342	-2.911280415	-0.986372723
H	2.677908120	-3.192548077	-1.273525984
H	3.692428120	-2.555764999	-2.549171509
O	2.607024701	-2.029045504	1.772689332
H	1.747017213	-2.724219432	1.749014825
H	2.555554852	-1.393913068	2.487417561
O	0.669697129	-3.508748967	1.652259295
H	-0.151958810	-3.193063104	1.161312912
H	0.764687716	-4.438758725	1.472452364
O	2.641724880	3.782336801	0.436214990
H	0.840484149	3.953078370	0.831263564
H	3.216842001	4.518766341	0.585070940
O	4.213006006	1.507673042	1.185495211
H	3.113067919	2.997997670	0.714818904
H	5.112850661	1.780264181	1.305593554
O	-0.077719617	4.057190136	1.084160266
H	-0.145555760	3.713048856	1.963281070
H	-1.333106056	3.174478594	0.021571151
H	2.583512403	-1.512328553	0.946593877
O	4.291408384	-0.407621330	-0.909458017
H	4.219423175	0.964057388	0.397584255

Path2-S₀-26

C	0.805424061	-1.258562318	-0.665423145
H	0.827200790	-2.330867452	-0.640062415
C	-0.457216249	-0.670102014	-0.430929975
C	-1.556854908	-1.497770326	-0.064622659
O	-1.394190431	-2.721856936	0.254899051
C	-2.857601701	-0.855213793	-0.058339245
C	-4.058043783	-1.622174526	0.093144366
H	-3.969461681	-2.688270697	0.169157747
C	-5.289337052	-1.019598355	0.109962693
H	-6.187548338	-1.605048212	0.203803681
C	-5.386508870	0.396425595	0.007829457
H	-6.352305664	0.872466315	0.034636997
C	-4.257812963	1.155114240	-0.130741199
H	-4.316921987	2.222284736	-0.213934241
C	-2.962260203	0.541986503	-0.191953183
C	-1.811407744	1.350488317	-0.398293993
O	-1.997248597	2.698918796	-0.492089683
C	-0.598586381	0.756339955	-0.572579758
C	0.598059966	1.509918272	-0.907503453
H	0.511388277	2.560405513	-1.094574384
C	1.804555841	0.913181117	-1.018405246
H	2.663765536	1.495267164	-1.285980933
C	1.947629277	-0.530884867	-0.895649147
C	3.293552683	-1.102222424	-1.088706719
C	3.508730276	-2.547804030	-1.483358819
H	4.395614068	-2.920038499	-0.985415876
H	2.670351834	-3.196463401	-1.272431974
H	3.687917927	-2.573870730	-2.552263672
O	2.582047058	-2.029403243	1.784188708
H	1.641792529	-2.780542958	1.743946001
H	2.546211392	-1.410058694	2.510076772
O	0.663482398	-3.480233431	1.656131650
H	-0.170493602	-3.159607232	1.140235845
H	0.771235708	-4.412582618	1.485967541
O	2.646190003	3.785909282	0.443173579
H	0.834199609	3.962268951	0.836926374
H	3.225533494	4.519468384	0.590657131
O	4.216562019	1.502203074	1.194584778
H	3.113942744	3.000352646	0.724249329
H	5.117632868	1.767518535	1.321534008
O	-0.083939326	4.059279968	1.092273490
H	-0.145850292	3.714046392	1.971517306
H	-1.343357384	3.176041429	0.017501676
H	2.548077996	-1.500284114	0.974963085
O	4.288798032	-0.413285911	-0.922314151
H	4.223531283	0.960533729	0.406130780

Path2-S₀-29

C	0.809342783	-1.257589431	-0.668999288
H	0.830365751	-2.329591743	-0.647087904
C	-0.459746527	-0.667928317	-0.429087516
C	-1.550400808	-1.493190424	-0.056331923
O	-1.368368454	-2.727264202	0.278098513
C	-2.849700455	-0.860082827	-0.055671237
C	-4.055873527	-1.625085382	0.094251979
H	-3.968957063	-2.691143653	0.169578925
C	-5.286121999	-1.022604929	0.107200431
H	-6.185101793	-1.607513559	0.198938974
C	-5.385346268	0.395722927	0.004323116
H	-6.351848137	0.870493220	0.030492209
C	-4.258175015	1.153524031	-0.134153862
H	-4.317061007	2.220771464	-0.218130472
C	-2.959038979	0.540642260	-0.195288379
C	-1.815332609	1.349304802	-0.402622665
O	-1.997830475	2.697314521	-0.500578229
C	-0.598181301	0.754002400	-0.575900732
C	0.596135348	1.509347819	-0.909002999
H	0.509796930	2.560715908	-1.090698949
C	1.803102641	0.912980395	-1.023839764
H	2.663444992	1.495573044	-1.285891301
C	1.941634783	-0.529925484	-0.909088477
C	3.291995579	-1.105556008	-1.095674221
C	3.505088267	-2.551689879	-1.486998436
H	4.390315459	-2.923832462	-0.986487550
H	2.665492606	-3.197695352	-1.273584231
H	3.684258439	-2.581949589	-2.555788998
O	2.592885064	-2.019175364	1.792308467
H	1.533745208	-2.855041658	1.731427196
H	2.546985652	-1.409491332	2.520835830
O	0.652089143	-3.464383858	1.657929821
H	-0.203367613	-3.123295946	1.108281445
H	0.783185329	-4.394176230	1.491228700
O	2.646211080	3.787348220	0.447864697
H	0.829147686	3.966553683	0.840864025
H	3.227727791	4.519475369	0.594567343
O	4.216380554	1.501633674	1.197805044
H	3.112695335	3.001261847	0.729953363
H	5.118568284	1.760149000	1.330285727
O	-0.089300916	4.058812837	1.096798945
H	-0.147972603	3.713645736	1.976395643
H	-1.349882028	3.175719208	0.015860358
H	2.536779776	-1.488496680	0.995224065
O	4.284349238	-0.415704474	-0.928524411
H	4.224067531	0.957987169	0.411416625

Path2-S₀-32

C	0.812674673	-1.256268250	-0.673629017
H	0.833432598	-2.327519406	-0.654456428
C	-0.461728929	-0.664327145	-0.427918769
C	-1.542059975	-1.486037651	-0.046739576
O	-1.333960916	-2.733302813	0.307174462
C	-2.840920034	-0.865178158	-0.053279789
C	-4.054506186	-1.626677216	0.093271629
H	-3.970878786	-2.692779218	0.166676357
C	-5.283240317	-1.022993345	0.102283920
H	-6.183370325	-1.606981403	0.191450516
C	-5.384507892	0.397712550	-0.000121791
H	-6.351520788	0.871585918	0.025839524
C	-4.258302086	1.153858804	-0.137886107
H	-4.316620362	2.221384622	-0.221493261
C	-2.955906731	0.540140447	-0.199207005
C	-1.819326315	1.349305225	-0.406244133
O	-1.998185924	2.696260527	-0.505024307
C	-0.597516607	0.752950422	-0.579517844
C	0.594234014	1.510081217	-0.910508153
H	0.508399190	2.562467082	-1.085957426
C	1.801470912	0.913996728	-1.029570404
H	2.663129528	1.496874514	-1.285513278
C	1.935588325	-0.527813395	-0.922213247
C	3.290007069	-1.108087206	-1.103145415
C	3.500922732	-2.554103378	-1.492519697
H	4.384554443	-2.926592677	-0.989879502
H	2.660255561	-3.197742798	-1.277519796
H	3.680252683	-2.586402097	-2.561221753
O	2.614907172	-2.008613652	1.798539857
H	1.460519290	-2.909395792	1.722038914
H	2.549771776	-1.405158317	2.528442636
O	0.621057173	-3.467771232	1.659945044
H	-0.280210261	-3.079798841	1.047464893
H	0.787445523	-4.387781874	1.487246081
O	2.646401579	3.787487627	0.454372668
H	0.825989678	3.969521754	0.846637698
H	3.229787036	4.518317048	0.601023327
O	4.215459648	1.501204575	1.200435293
H	3.112020338	3.000839367	0.736741929
H	5.118937671	1.751903789	1.338875184
O	-0.093095433	4.057160761	1.102120854
H	-0.149492572	3.712594975	1.982256995
H	-1.353750589	3.175861604	0.015818964
H	2.531665347	-1.476331392	1.011043163
O	4.279217537	-0.417245598	-0.932659799
H	4.223980454	0.954333687	0.416925070

Path2-S₀-35

C	0.815571040	-1.254698223	-0.678445223
H	0.836585473	-2.325073951	-0.660586798
C	-0.462673698	-0.660945972	-0.427188856
C	-1.533486658	-1.477748085	-0.038130990
O	-1.303267159	-2.742365587	0.332140721
C	-2.833368357	-0.871340025	-0.050847195
C	-4.053441904	-1.629738924	0.091509772
H	-3.972838092	-2.695837794	0.162324639
C	-5.281044236	-1.024899235	0.097452934
H	-6.181911277	-1.608547222	0.184195127
C	-5.384917211	0.397594565	-0.003601542
H	-6.352463729	0.870375832	0.022692879
C	-4.259576192	1.152575920	-0.140514070
H	-4.317769031	2.220443766	-0.222927977
C	-2.954518811	0.538325977	-0.202361024
C	-1.823857311	1.348928863	-0.408280952
O	-2.000752634	2.694085318	-0.505593810
C	-0.597706777	0.752557952	-0.582509336
C	0.591283994	1.512168112	-0.911700099
H	0.505120878	2.565307864	-1.081669751
C	1.798935349	0.916939287	-1.034155836
H	2.661237328	1.500510686	-1.285279350
C	1.930454379	-0.523974408	-0.932284628
C	3.288301715	-1.107336171	-1.110324080
C	3.497899198	-2.552658914	-1.499418740
H	4.380572332	-2.925305586	-0.995535671
H	2.656937445	-3.195101574	-1.283440284
H	3.677449330	-2.585220593	-2.568053649
O	2.633605676	-1.999571013	1.800179889
H	1.429883918	-2.940818337	1.718607295
H	2.551199882	-1.402317381	2.531970984
O	0.610099441	-3.479458689	1.667225407
H	-0.387347700	-3.029646374	0.968508208
H	0.790937432	-4.389726971	1.479931888
O	2.643778209	3.788624972	0.460677132
H	0.821492999	3.971829310	0.852761829
H	3.228087848	4.518772595	0.607837055
O	4.212979833	1.502951712	1.201863780
H	3.109464555	3.001719098	0.742767665
H	5.117324691	1.747800639	1.345104230
O	-0.098437504	4.054789740	1.107368128
H	-0.152985392	3.711134081	1.988127042
H	-1.357916934	3.175593640	0.017058134
H	2.528348273	-1.467173028	1.019369999
O	4.274360293	-0.414903761	-0.936310254
H	4.222533340	0.953555511	0.420627784

Path2-S₀-38

C	0.856438600	-1.246563398	-0.708974348
H	0.910631917	-2.315765644	-0.680926038
C	-0.424448721	-0.653313548	-0.428381600
C	-1.521662631	-1.434153563	-0.068095335
O	-1.395432648	-2.751012433	0.190793469
C	-2.798368754	-0.861080760	-0.025329995
C	-3.993263291	-1.659224718	0.133564592
H	-3.898190015	-2.725985387	0.197800315
C	-5.222202790	-1.069490456	0.143839590
H	-6.112209479	-1.668070238	0.224394554
C	-5.346555353	0.355583604	0.046079868
H	-6.320591701	0.810826823	0.083729098
C	-4.239456497	1.132076647	-0.098885489
H	-4.308182741	2.197554198	-0.179867358
C	-2.929819685	0.538044804	-0.173499862
C	-1.804730549	1.340304184	-0.393026101
O	-1.987647470	2.679169462	-0.489292115
C	-0.567046162	0.754237354	-0.576143794
C	0.603760141	1.527222644	-0.926000458
H	0.505612136	2.583503026	-1.063797705
C	1.810081462	0.939263391	-1.094062638
H	2.669116745	1.532097456	-1.336648744
C	1.947358253	-0.500826788	-1.005691254
C	3.309672062	-1.081415238	-1.197615953
C	3.521321985	-2.525379409	-1.590837052
H	4.408572365	-2.894075058	-1.093072711
H	2.685653476	-3.168139834	-1.357596406
H	3.687151678	-2.565278426	-2.661985923
O	2.817270934	-1.931316843	1.785776049
H	1.484675263	-3.077791328	1.748019131
H	2.663180832	-1.379890220	2.542058652
O	0.668627096	-3.578889802	1.703605925
H	-0.643978861	-2.932690921	0.765706626
H	0.898273025	-4.456859540	1.436006800
O	2.654728585	3.810910499	0.471645547
H	0.825648517	3.988376545	0.880577692
H	3.243668149	4.540459983	0.603498479
O	4.253365175	1.543541480	1.151661676
H	3.132500233	3.025531979	0.738867279
H	5.163251137	1.745432354	1.324408118
O	-0.096571007	4.025647526	1.137895077
H	-0.127156094	3.701298353	2.027319851
H	-1.348374021	3.161490214	0.037041793
H	2.575910402	-1.392445495	1.044065760
O	4.287741561	-0.379199983	-1.023205100
H	4.262709942	0.968821443	0.389900541

S4-3. Cartesian coordinates of the S_0 and T_{RCT2} minima as well as transition state (T_{RCT2} -TS) and intermediate (T_{RCT2} -INT) along the reaction pathway of the first step of ES IPT in the T_{RCT2} state obtained by the CASSCF(12e/10o)/6-31G** level of theory.

S₀-Min

C	0.691514488	1.272153325	0.099180076
H	0.645099399	2.324346612	-0.107845739
C	-0.493504583	0.523823655	0.107065928
C	-1.791601111	1.203687071	-0.150090012
O	-1.854219020	2.367743089	-0.439202486
C	-3.038358087	0.391138903	-0.017989105
C	-4.263006573	1.018311444	-0.125489304
H	-4.292659300	2.076426198	-0.300284767
C	-5.440378426	0.284729515	-0.008588672
H	-6.389473857	0.782876464	-0.086519756
C	-5.385529840	-1.089223206	0.205602854
H	-6.293096339	-1.658317496	0.294006080
C	-4.152512485	-1.730482197	0.301487950
H	-4.091434730	-2.789984814	0.458255904
C	-2.976812593	-0.992075524	0.197049682
C	-1.664312778	-1.689546812	0.290782534
O	-1.609372226	-2.892242020	0.312398782
C	-0.444979192	-0.848413230	0.358406352
C	0.787831606	-1.447357012	0.637341523
H	0.832096822	-2.496697489	0.851180097
C	1.933707295	-0.698400434	0.641408933
H	2.868267978	-1.180904562	0.851689620
C	1.907224027	0.676110636	0.352507266
C	3.204173688	1.475400136	0.273127914
C	4.017295600	1.414341347	1.564664675
H	4.892620965	2.045408855	1.461314199
H	3.435210946	1.767439539	2.409824153
H	4.355754046	0.404599981	1.776041156
O	2.085172704	4.843070829	-0.272490839
H	1.150182420	5.007518226	-0.346842961
H	2.455824129	5.103981481	-1.101549760
O	-0.765489345	5.075249437	-0.634666538
H	-1.140035700	4.201889617	-0.634263040
H	-1.304710003	5.592759725	-0.056200229
O	3.192102758	-4.126084240	-0.324103544
H	2.281795343	-4.236505159	-0.591573798
H	3.503577968	-4.995751615	-0.124537123
O	4.863483513	-1.779205631	-0.453245941
H	4.308775050	-2.556318932	-0.455160989
H	5.754190325	-2.093538123	-0.470663699
O	0.444729264	-4.551057758	-1.001000447
H	0.131206396	-4.547273278	-1.892945714
H	-0.219865511	-4.101221503	-0.489090271
H	2.942098756	2.506834916	0.087653405

O	3.963533933	1.074364867	-0.834706380
H	4.270535712	0.162536974	-0.715159197

T_{RCT2}-Min

C	0.688947359	1.277114621	0.196591172
H	0.694849596	2.309468826	-0.101152897
C	-0.484335100	0.616208914	0.270727563
C	-1.745756083	1.291903077	-0.052809342
O	-1.819211944	2.479125825	-0.274910824
C	-2.970653965	0.447437307	-0.092820060
C	-4.200869913	1.066600244	-0.409459251
H	-4.209177790	2.121017711	-0.604101630
C	-5.353396715	0.320971038	-0.466248232
H	-6.289928737	0.790590043	-0.706891321
C	-5.307043699	-1.066195910	-0.211140547
H	-6.210979248	-1.646964644	-0.255617112
C	-4.122748011	-1.669365389	0.091526669
H	-4.067809887	-2.721979319	0.290170213
C	-2.934972051	-0.911448131	0.155520414
C	-1.668840826	-1.615401978	0.493225461
O	-1.651243116	-2.824544951	0.661681406
C	-0.481737272	-0.813899920	0.612311090
C	0.785752796	-1.424681439	1.043019465
H	0.764746714	-2.434313164	1.398598673
C	1.940989832	-0.727067410	0.976726621
H	2.860817464	-1.197359360	1.261916989
C	1.964782197	0.654841579	0.497560343
C	3.254225823	1.354244168	0.114517974
C	4.364211880	1.211851186	1.151896091
H	5.227199943	1.778044796	0.820844085
H	4.050775571	1.597783355	2.117099905
H	4.673035410	0.179576236	1.277422888
O	2.149906402	4.647432270	-0.388741081
H	1.242855892	4.901808630	-0.235563909
H	2.300160624	4.790728965	-1.311495235
O	-0.652210975	5.093778986	-0.057393204
H	-1.025255795	4.225195419	-0.180325982
H	-0.933889379	5.377380722	0.799966783
O	3.055197121	-4.066401662	-0.250740059
H	2.114328841	-4.146683031	-0.407850129
H	3.419433611	-4.912242217	-0.466867118
O	4.586199180	-1.819280806	-1.035643316
H	4.023721850	-2.557519095	-0.803346786
H	5.430647598	-2.006888042	-0.654231395
O	0.286622161	-4.478692218	-0.707024906
H	-0.042201381	-4.379592057	-1.588657963
H	-0.328211473	-4.009776087	-0.147697207
H	3.033877707	2.405070543	-0.002133139
O	3.660311999	0.902361845	-1.152482991
H	3.975098440	-0.012254305	-1.084920498

T_{RCT2}-TS

C	0.930724074	1.117541010	0.267728768
H	1.060176413	2.105145452	-0.130417589
C	-0.387606666	0.589805415	0.332726253
C	-1.511928183	1.409728175	-0.076033695
O	-1.394207830	2.583883351	-0.419977524
C	-2.828648191	0.756569677	-0.067483284
C	-3.974859459	1.520444751	-0.431371367
H	-3.834945396	2.552610796	-0.687174875
C	-5.213669087	0.940938650	-0.452969568
H	-6.080407090	1.516472498	-0.726075626
C	-5.358524654	-0.434603212	-0.114958393
H	-6.336267254	-0.883936999	-0.133837154
C	-4.274601106	-1.171974431	0.227041435
H	-4.360498617	-2.210133059	0.484242369
C	-2.978747096	-0.581832227	0.262693873
C	-1.832649565	-1.408781578	0.628837317
O	-1.943073336	-2.647664323	0.785898220
C	-0.567324817	-0.745381097	0.730082815
C	0.565702486	-1.471005975	1.219631954
H	0.404777872	-2.451029545	1.626001647
C	1.812639663	-0.924270466	1.189802725
H	2.642277515	-1.485181257	1.581312364
C	2.015619758	0.390444749	0.645987258
C	3.403132771	0.897608177	0.349904630
C	4.488325044	0.611988440	1.379424983
H	5.447022088	0.979793616	1.028789196
H	4.246240502	1.131699512	2.299210106
H	4.586349774	-0.444429438	1.601661097
O	2.959014187	4.107556999	-0.614856644
H	2.069028073	4.437573929	-0.479781309
H	3.091554868	4.135507882	-1.552517041
O	0.241364999	4.845254479	-0.321345851
H	-0.297436022	4.055209071	-0.409746152
H	0.017874788	5.206547642	0.525535176
O	2.158049413	-3.901237457	-0.841728954
H	1.111301814	-3.748194861	-0.872449001
H	2.351767868	-4.677176344	-1.355967185
O	3.947128348	-2.294194267	-1.107176507
H	2.989430491	-3.029869095	-0.969283024
H	4.690228146	-2.596576429	-0.596029957
O	-0.343315400	-3.823913093	-0.969502579
H	-0.739211335	-3.460564240	-1.752293809
H	-0.883286715	-3.476546790	-0.225086857
H	3.386214667	1.950775971	0.117926674
O	3.733131519	0.211732997	-0.879476406
H	3.847562501	-1.242368134	-0.974963344

T_{RCT2}-INT

C	1.018802997	1.096753023	0.220216528
H	1.191286337	2.110280376	-0.084708215
C	-0.312549336	0.614906339	0.243699307
C	-1.421467549	1.508979269	-0.122142236
O	-1.244003091	2.662939945	-0.467604205
C	-2.781349551	0.948914991	-0.060122871
C	-3.884847398	1.789853752	-0.351492761
H	-3.689933124	2.815155939	-0.599651810
C	-5.160495410	1.291869194	-0.315292018
H	-6.001301019	1.925586800	-0.532985801
C	-5.373427344	-0.073992524	0.009402837
H	-6.377742367	-0.458829399	0.037641942
C	-4.326668337	-0.890678908	0.283293045
H	-4.474292083	-1.923451761	0.531838206
C	-2.995758186	-0.385648257	0.255880119
C	-1.883299807	-1.250681948	0.537561761
O	-2.104573882	-2.532876221	0.764834975
C	-0.561642961	-0.712220718	0.591065560
C	0.533003507	-1.530261973	0.986817672
H	0.343383480	-2.536446326	1.302956357
C	1.806723610	-1.033694944	0.977568648
H	2.620341901	-1.672021367	1.268574224
C	2.069663202	0.303821399	0.567246244
C	3.491529058	0.812495017	0.467621983
C	4.304482787	0.721725217	1.760099993
H	5.313691329	1.078778544	1.590157170
H	3.843928445	1.345271016	2.517064256
H	4.354268407	-0.293249867	2.136223778
O	3.291470461	4.021942713	-0.818266230
H	2.398061188	4.331135180	-0.686608137
H	3.438728381	4.064395524	-1.748489241
O	0.603048821	4.758533419	-0.509920919
H	0.000808954	4.022436155	-0.594995384
H	0.345189406	5.205746833	0.279514598
O	1.648269622	-4.223919964	-0.793058401
H	-0.033024127	-4.122767061	-0.838907450
H	2.043513559	-5.037471870	-1.062103184
O	4.037466001	-2.726915231	-1.235567095
H	2.319350534	-3.552467252	-0.892795591
H	4.846551482	-3.091410011	-0.915609538
O	-0.999697401	-4.045556973	-0.871410580
H	-1.234315104	-3.841258026	-1.763440689
H	-1.648266573	-3.158347277	0.101368479
H	3.502581739	1.837439709	0.121392906
O	4.227258692	0.019282226	-0.494785890
H	4.087079792	-1.788778733	-1.068752990

S4-4. Cartesian coordinates of the S_0 and T_{RCT2} minima as well as transition state (T_{RCT2} -TS) and intermediate (T_{RCT2} -INT) along the reaction pathway of the first step of ESIPT in the T_{RCT2} state for the isolated 2-HEAQ (without water molecules). The results were obtained by the CASSCF(12e/10o)/6-31G** and CASSCF(12e/10o)/6-31G**/PCM levels of theory.

S_0 -Min (gas phase)

C	1.604452639	-0.908534624	-0.071918893
H	1.732488885	-1.974528436	-0.092918322
C	0.318629609	-0.403564400	-0.046767023
C	-0.831819443	-1.357594501	-0.064778971
O	-0.657252246	-2.539915262	-0.109945462
C	-2.208754965	-0.780061463	-0.029228331
C	-3.309043146	-1.649676667	-0.036700908
H	-3.130499451	-2.707350828	-0.068671282
C	-4.580897359	-1.142836556	-0.004759154
H	-5.425403028	-1.808650646	-0.010634646
C	-4.789743209	0.243392957	0.036135005
H	-5.792756657	0.630487598	0.061090197
C	-3.723611922	1.102780526	0.044706464
H	-3.864258217	2.166297471	0.075615026
C	-2.416329255	0.596065200	0.013752514
C	-1.271028215	1.552653939	0.023153714
O	-1.451155658	2.734857969	0.053892047
C	0.107551918	0.978343427	-0.002941312
C	1.204586683	1.836104833	0.014985599
H	1.039166457	2.895598109	0.053120260
C	2.495366978	1.315093185	-0.018103274
H	3.325787044	1.998061863	-0.006266775
C	2.713768425	-0.065034282	-0.068677970
C	4.113860595	-0.666347607	-0.034707767
C	5.101641756	-0.003386084	-0.988026905
H	6.044469870	-0.536688730	-0.952680421
H	4.730664781	-0.017482092	-2.007552779
H	5.296239328	1.029953248	-0.715830612
H	4.026974924	-1.708406822	-0.314667507
O	4.620666865	-0.701474477	1.279696323
H	4.747267871	0.200576069	1.593516863

T_{RCT2} -Min (gas phase)

C	1.554951976	-0.939299153	-0.137893582
H	1.692075782	-2.005612900	-0.153519979
C	0.308356293	-0.458560168	-0.116223506
C	-0.844268100	-1.392154162	-0.120139433
O	-0.698954551	-2.579626369	-0.211619626
C	-2.203802707	-0.781862264	-0.036405087
C	-3.319220828	-1.636649810	-0.026971512
H	-3.152228850	-2.695348226	-0.080403775

C	-4.582844890	-1.117946921	0.048433041
H	-5.435448770	-1.773419760	0.055484626
C	-4.772644269	0.271608002	0.116413086
H	-5.769552076	0.670877311	0.175360183
C	-3.696806263	1.116289728	0.107996746
H	-3.822018173	2.180785730	0.159493518
C	-2.393242490	0.598781314	0.032161435
C	-1.249788485	1.560317193	0.023669328
O	-1.429295208	2.753145362	0.074623332
C	0.082452849	0.998346735	-0.072946941
C	1.259373615	1.886757832	-0.109171067
H	1.080074049	2.943595375	-0.109010990
C	2.509776824	1.370907600	-0.139938563
H	3.354257384	2.034037285	-0.172225103
C	2.737148185	-0.076418839	-0.151924517
C	4.109728239	-0.684045326	0.030747980
C	5.196958183	-0.044633533	-0.826622568
H	6.128417808	-0.578584883	-0.680028088
H	4.936888981	-0.081016220	-1.879551576
H	5.365518684	0.993894158	-0.557971418
H	4.045546178	-1.731943006	-0.234867949
O	4.475315353	-0.697628809	1.394308575
H	4.623175531	0.206984287	1.691633289

T_{RCT2}-TS (gas phase)

C	-1.629980446	-1.004815503	-0.126599117
H	-1.752496547	-2.066856562	-0.237674837
C	-0.318683665	-0.497375875	-0.029511303
C	0.848275104	-1.407129788	-0.075458914
O	0.712395023	-2.599207218	-0.161977110
C	2.197359895	-0.780324734	-0.025624693
C	3.333758089	-1.609698215	-0.066351100
H	3.184276486	-2.670490876	-0.126448335
C	4.598566047	-1.065849384	-0.032101470
H	5.465405706	-1.700157044	-0.063879985
C	4.754153869	0.334837873	0.043157813
H	5.741991360	0.759889904	0.069603258
C	3.666740317	1.151478750	0.083595296
H	3.790791508	2.217195586	0.142343570
C	2.361082203	0.599444415	0.051500751
C	1.189765434	1.420596989	0.093663205
O	1.296909285	2.758869636	0.102847421
C	-0.125077278	0.882956900	0.079074620
C	-1.246977109	1.746614927	0.124814325
H	-1.096688140	2.800518886	0.245643942
C	-2.493096067	1.230660108	0.028769883
H	-3.349633655	1.874882195	0.041781355
C	-2.703673686	-0.159702417	-0.114026336
C	-4.141009880	-0.622122708	-0.263747695
C	-4.800023509	-0.980237749	1.070678311
H	-5.819256583	-1.309306812	0.906294675
H	-4.244473722	-1.771537927	1.560135685

H	-4.813579490	-0.119302960	1.730315215
H	-4.188439307	-1.488663260	-0.918976952
O	-4.912639481	0.359688086	-0.887699084
H	-2.638292081	3.883023255	-0.825508830

T_{RCT2}-INT (gas phase)

C	-1.672607044	-0.895463792	-0.179474366
H	-1.800270950	-1.959129224	-0.242712867
C	-0.367678254	-0.406429257	-0.109440113
C	0.754619531	-1.374299552	-0.120218149
O	0.553904781	-2.557548491	-0.193667842
C	2.123201202	-0.821205873	-0.042313979
C	3.217117908	-1.703730181	-0.046751692
H	3.021474010	-2.755931480	-0.109983848
C	4.503343126	-1.218043480	0.029189415
H	5.339766168	-1.891622474	0.025962170
C	4.713230200	0.172448505	0.111233323
H	5.715208589	0.557299331	0.171107881
C	3.662508301	1.037681601	0.116600871
H	3.829030660	2.094144275	0.179407968
C	2.335582284	0.549848992	0.039530290
C	1.214898829	1.450553586	0.042640739
O	1.524042982	2.759498267	0.122464834
C	-0.130695541	0.980343172	-0.028994831
C	-1.260527735	1.838272824	-0.026534034
H	-1.149534236	2.905662727	0.029471000
C	-2.523079901	1.334803604	-0.091009457
H	-3.355712594	2.013522205	-0.085641288
C	-2.754789182	-0.052994325	-0.170745406
C	-4.169293939	-0.607024599	-0.178675917
C	-4.693219680	-0.901794223	1.224080038
H	-5.707083337	-1.282083024	1.167515107
H	-4.070335433	-1.638535226	1.715780002
H	-4.696570992	0.002326664	1.822813477
H	-4.181575317	-1.514231697	-0.776140588
O	-5.003191916	0.280285917	-0.855646946
H	0.741896062	3.312890402	0.102520235

S₀-Min (PCM)

C	1.602340116	-0.907090383	-0.063621970
H	1.738936766	-1.972117462	-0.093555792
C	0.318986224	-0.404370331	-0.047518550
C	-0.833000054	-1.354113716	-0.075718382
O	-0.660860467	-2.541983906	-0.115826042
C	-2.207608164	-0.779253092	-0.033198478
C	-3.308948116	-1.646812622	-0.040596550
H	-3.140094086	-2.705683068	-0.076562909
C	-4.581776222	-1.139470904	-0.002716248
H	-5.425926437	-1.804627671	-0.009008587

C	-4.788788795	0.246782560	0.043967633
H	-5.790353557	0.635396897	0.073848775
C	-3.719887736	1.104898124	0.052031694
H	-3.867774590	2.166854171	0.087719296
C	-2.413112244	0.598226440	0.013450098
C	-1.264548672	1.548383653	0.021622685
O	-1.442374390	2.735658498	0.061101843
C	0.109110444	0.977256963	-0.009709897
C	1.202893083	1.828009336	0.000874097
H	1.043969233	2.889130156	0.025789432
C	2.496035128	1.310246128	-0.022155476
H	3.325016615	1.994279638	-0.020182596
C	2.711820725	-0.065199597	-0.050711630
C	4.109692425	-0.668261620	-0.036206351
C	5.093908825	0.003473374	-0.985473620
H	6.037180030	-0.530143479	-0.962258534
H	4.715188844	-0.006966491	-2.001779254
H	5.286456344	1.034066807	-0.704915352
H	4.020939917	-1.708166660	-0.321922595
O	4.616190343	-0.706543456	1.284170702
H	4.790115310	0.194702237	1.581341749

T_{RCT2}-Min (PCM)

C	1.554791704	-0.935121282	-0.152741112
H	1.699169355	-1.999497214	-0.183919579
C	0.305522793	-0.454256291	-0.144281569
C	-0.842288892	-1.385105590	-0.181677150
O	-0.694048485	-2.581172836	-0.193030257
C	-2.199801704	-0.780921054	-0.060445724
C	-3.314627844	-1.637163572	-0.024757430
H	-3.154667352	-2.696308100	-0.081902811
C	-4.578598047	-1.123243519	0.079912486
H	-5.428458074	-1.780758840	0.107083232
C	-4.770329368	0.265676028	0.151531366
H	-5.766263451	0.661907275	0.232978193
C	-3.695251725	1.112455924	0.118158082
H	-3.829748230	2.175167085	0.172269354
C	-2.390725426	0.600505924	0.012130967
C	-1.249870782	1.562034580	-0.018470730
O	-1.433267699	2.758273195	0.066983189
C	0.081005421	1.001896720	-0.090484595
C	1.261073587	1.887179216	-0.092957502
H	1.091550253	2.945011453	-0.078996042
C	2.511772177	1.371406059	-0.109845007
H	3.357723653	2.032634336	-0.113172100
C	2.734694014	-0.075008351	-0.135009503
C	4.105225941	-0.689684779	0.034545275
C	5.185022574	-0.039040028	-0.820754315
H	6.115227377	-0.580682266	-0.694020735
H	4.910242097	-0.061917269	-1.869709027

H	5.358532169	0.994086101	-0.536676469
H	4.033837020	-1.733337934	-0.244299087
O	4.476670544	-0.707438956	1.401158213
H	4.632333731	0.196744264	1.700354649

T_{RCT2}-TS (PCM)

C	-1.625972050	-1.002122129	-0.091958700
H	-1.753966898	-2.060359340	-0.225279437
C	-0.314794929	-0.493771610	0.016299908
C	0.848422866	-1.401128685	-0.045131322
O	0.705740418	-2.602123318	-0.098627961
C	2.196127960	-0.783913752	-0.016647446
C	3.334526671	-1.613343092	-0.070072333
H	3.194188357	-2.675673468	-0.118474501
C	4.599842799	-1.068892354	-0.064339129
H	5.466158196	-1.702867230	-0.105871208
C	4.756193858	0.333375570	-0.004778298
H	5.743587359	0.758625313	-0.000221998
C	3.668256039	1.150112674	0.048371879
H	3.795425280	2.216060691	0.096506225
C	2.362159232	0.596846853	0.045732686
C	1.193181564	1.418462431	0.108365908
O	1.309664150	2.754503289	0.086464818
C	-0.121230356	0.886000579	0.132274728
C	-1.249144122	1.738849791	0.197701192
H	-1.115516505	2.796850666	0.310456194
C	-2.496090723	1.219438492	0.111917940
H	-3.347607991	1.871711662	0.140522262
C	-2.703921765	-0.166892465	-0.066755488
C	-4.131616725	-0.641028693	-0.268301397
C	-4.901049044	-0.844021853	1.036002993
H	-5.829610413	-1.371602362	0.850866745
H	-4.296802208	-1.422849919	1.722503680
H	-5.127820863	0.109705244	1.500200176
H	-4.142709005	-1.569310476	-0.833137862
O	-4.843638176	0.281270883	-1.045094094
H	-2.448804148	3.612671880	-1.292111102

T_{RCT2}-INT (PCM)

C	-1.671555770	-0.902943131	-0.171630613
H	-1.810479329	-1.964760459	-0.228207851
C	-0.365480652	-0.412950426	-0.107129234
C	0.756696266	-1.373071956	-0.116415231
O	0.560291718	-2.566108282	-0.189650164
C	2.121004915	-0.821335336	-0.040503585
C	3.221121256	-1.701015904	-0.042107742
H	3.038053906	-2.755271500	-0.102248386
C	4.506600005	-1.213494540	0.033509309
H	5.344309049	-1.884642441	0.032869521
C	4.713221760	0.178586071	0.112449938

H	5.713681118	0.565620728	0.172388812
C	3.659217983	1.041151136	0.114436710
H	3.828811533	2.097004854	0.174893262
C	2.331467047	0.552235454	0.037636671
C	1.211793728	1.452314477	0.037336721
O	1.520372836	2.756899424	0.113663082
C	-0.131486258	0.976496313	-0.033320479
C	-1.259739234	1.835116203	-0.033724039
H	-1.147823665	2.900620314	0.019911561
C	-2.522701709	1.329424343	-0.093781851
H	-3.352496795	2.011014556	-0.081547636
C	-2.753680137	-0.059077177	-0.165902068
C	-4.166633918	-0.617365071	-0.163636381
C	-4.708687658	-0.841400594	1.243625401
H	-5.719261451	-1.230368098	1.190424429
H	-4.090489376	-1.552491154	1.776139515
H	-4.721160075	0.091043864	1.797583179
H	-4.174738792	-1.549487268	-0.718774747
O	-4.992989014	0.236023791	-0.898267114
H	0.743243835	3.321178000	0.095540746