Electronic supplementary information

Theoretical Investigations of the Chiral Transition of Serine and the Role of Water, Hydroxyl Radical and Hydroxide Ion

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Table S1. The high level Energy (E) at gas phase, Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the each reaction pathway of **S_1^{A}** chiral transition **R_1^{A}**.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total} (Kcal mol^{-1})	Ima (cm^{-1})
S_1^{A}	0.08153	-398.29013	-398.20860	0.00	
S_TS1^{A}	0.08001	-398.28279	-398.20278	3.66	530.32
S_2^{A}	0.08066	-398.28512	-398.20446	2.60	
TS2^{A}	0.07552	-398.18642	-398.11090	61.37	1706.62
3^{A}	0.08121	-398.24070	-398.15949	30.85	
Pathway A1					
TS3^{A1}	0.08055	-398.23732	-398.15677	32.55	307.79
4^{A1}	0.08098	-398.23898	-398.15800	31.78	
TS4^{A1}	0.08042	-398.23107	-398.15065	36.40	151.89
5^{A1}	0.08098	-398.23898	-398.15800	31.78	
TS5^{A1}	0.07537	-398.18472	-398.10935	62.34	1703.54
R_6^{A1}	0.08059	-398.28769	-398.20710	0.94	
R_TS6^{A1}	0.08039	-398.28645	-398.20606	1.60	230.00
R_1^{A1}	0.08153	-398.29013	-398.20860	0.00	
Pathway A2					
TS3^{A2}	0.07528	-398.18511	-398.10983	62.04	1703.50
R_4^{A2}	0.08067	-398.28577	-398.2051	2.20	
R_TS4^{A2}	0.07933	-398.27905	-398.19972	5.58	589.15
R_5^{A2}	0.08036	-398.28411	-398.20375	3.05	
R_TS5^{A2}	0.08016	-398.28359	-398.20343	3.25	237.77
R_6^{A2}	0.08036	-398.28534	-398.20498	2.27	
R_TS6^{A2}	0.08040	-398.28483	-398.20443	2.62	218.04
R_1^{A2}	0.08128	-398.29074	-398.20946	-0.53	

Table S2. The geometric parameters of S_1^{A} and R_1^{A1}.

Structures	C1-N5	C1-C8	C1-C3	C3-O13	C8-O9	C8-O10
S_1^{A}	1.46	1.52	1.55	1.41	1.21	1.35
R_1^{A1}	1.46	1.52	1.55	1.41	1.21	1.35

Structures	∠C3-C1-C8	∠C1-N5-H6	∠C1-C8-O9	∠O9-C8-O10
S_1^{A}	111.9	111.9	125.0	122.9
R_1^{A1}	111.9	111.9	125.0	122.9

Structures	∠H12-C1-N5-H7	∠C3-C1-C8-O9	∠C8-O9-O10-H11
S_1^{A}	-24.6	117.8	178.3
R_1^{A1}	24.6	-117.8	-178.3

Table S3. The high level Energy (E) at gas phase, Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the each reaction channel of **S_1^{B}** chiral transition **R_1^{B}.**

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total}(Kcal mol^{-1})	Ima (cm^{-1})
S_1^{B}	0.08194	-398.29141	-398.20947	0.00	
S_TS1^{B}	0.07982	-398.26809	-398.18827	13.32	539.83
S_2^{B}	0.08104	-398.28413	-398.20309	4.01	
TS2^{B}	0.07517	-398.18239	-398.10722	64.22	1685.36
3^{B}	0.08104	-398.23303	-398.15199	36.10	
Pathway **B1**					
TS3^{B1}	0.08035	-398.22981	-398.14946	37.69	282.33
4^{B1}	0.08069	-398.23106	-398.15037	37.12	
TS4^{B1}	0.07794	-398.22365	-398.14571	40.05	163.34
5^{B1}	0.08069	-398.23106	-398.15037	37.12	
TS5^{B1}	0.07515	-398.18026	-398.10511	65.55	1685.20
R_6^{B1}	0.08055	-398.28619	-398.20564	2.41	
R_TS6^{B1}	0.08041	-398.28554	-398.20513	2.73	201.95
R_7^{B1}	0.08154	-398.28887	-398.20733	1.34	
R_TS7^{B1}	0.08028	-398.28166	-398.20138	5.08	581.04
R_8^{B1}	0.08156	-398.28670	-398.20514	2.72	
R_TS8^{B1}	0.08017	-398.27019	-398.19002	12.22	605.12
R_1^{B1}	0.08194	-398.29141	-398.20947	0.00	
Pathway **B2**					
TS3^{B2}	0.07496	-398.18095	-398.10599	65.00	1684.38
R_4^{B2}	0.08035	-398.28382	-398.20347	3.77	
R_TS4^{B2}	0.07885	-398.26599	-398.18714	14.03	576.12
R_1^{B2}	0.08189	-398.28873	-398.20684	1.65	
Pathway **B3**					
TS3^{B3}	0.07733	-398.17279	-398.09546	71.61	1657.50
R_1^{B3}	0.08088	-398.28817	-398.20729	1.37	

Table S4. The high level Energy (E), Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the water-mediated proton transfer reactions for pathway **A1** at gas phase and solvent phase, respectively.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total}(Kcal mol^{-1})	Ima (cm^{-1})
gas phase					
S_2^{A1}·2H$_2$O	0.12130	-550.95585	-550.83455	0.00	
TS′2^{A1}	0.12143	-550.90649	-550.78506	31.09	769.77
3^{A1}·2H$_2$O	0.12481	-550.91979	-550.79498	24.85	
5^{A1}·2H$_2$O	0.12458	-550.91913	-550.79455	0.00	
TS′5^{A1}	0.12144	-550.90704	-550.7856	5.62	797.20
R_6^{A1}·2H$_2$O	0.12159	-550.95459	-550.833	-24.15	
solvent phase					
S_2^{A1}·2H$_2$O	0.12130	-550.98499	-550.86369	0.00	
TS′2^{A1}	0.12143	-550.94312	-550.82169	26.38	769.77
3^{A1}·2H$_2$O	0.12481	-550.95417	-550.82936	21.56	
5^{A1}·2H$_2$O	0.12458	-550.95257	-550.82799	0.00	
TS′5^{A1}	0.12144	-550.94187	-550.82043	4.75	797.20
R_6^{A1}·2H$_2$O	0.12159	-550.98294	-550.86135	-20.95	

Table S5. The high level Energy (E), Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the hydroxyl radical -mediated proton transfer reactions for pathway A1 at gas phase and solvent phase, respectively.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total}(Kcal mol^{-1})	Ima (cm^{-1})
gas phase					
S_2^{A1}·(H_2O·OH·)	0.10713	-550.25183	-550.14470	0.00	
TS″2^{A1}	0.10685	-550.20172	-550.09487	31.30	988.25
3^{A1}·(H_2O·OH·)	0.10978	-550.21352	-550.10374	25.73	
5^{A1}·(H_2O·OH·)	0.10978	-550.21352	-550.10374	0.00	
TS″5^{A1}	0.10702	-550.20234	-550.09532	5.29	1001.40
R_6^{A1}·(H_2O·OH·)	0.10755	-550. 25247	-550.14492	-25.87	
solvent phase					
S_2^{A1}·(H_2O·OH·)	0.10713	-550.21700	-550.10987	0.00	
TS″2^{A1}	0.10685	-550.19663	-550.08978	12.62	988.25
3^{A1}·(H_2O·OH·)	0.10978	-550.24913	-550.13935	-18.52	
5^{A1}·(H_2O·OH·)	0.10978	-550.24913	-550.13935	0.00	
TS″5^{A1}	0.10702	-550.19555	-550.08853	31.92	1001.40
R_6^{A1}·(H_2O·OH·)	0.10755	-550.21596	-550.10841	19.43	

Fig. S1 Intrinsic reaction coordinate for the proton transfer process from C1 to O19, from O19 to O16, from O16 to N5 atoms of 3^{A1}•(H_2O•OH•).

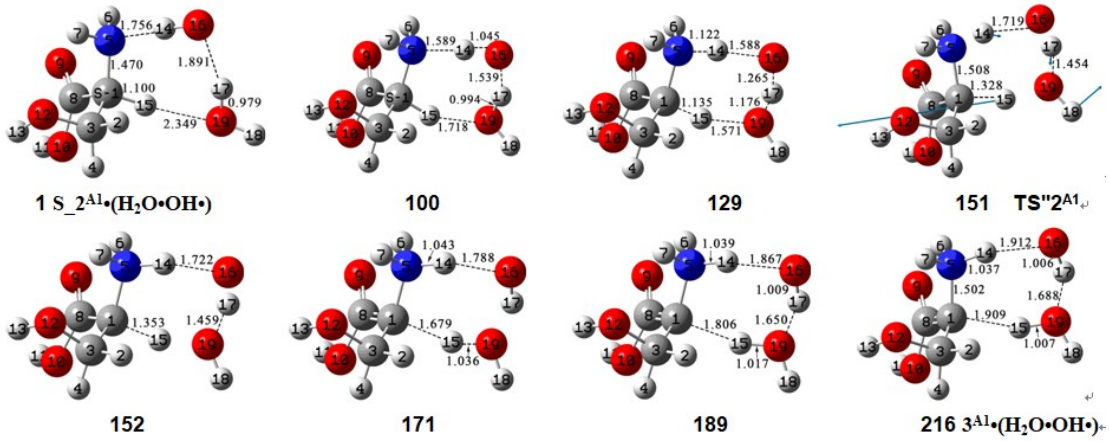


Fig.S2 The geomitries of some states for this S_2^{A1}•(H_2O•OH•)→$TS"2^{A1}$→3^{A1}•(H_2O•OH•) process.

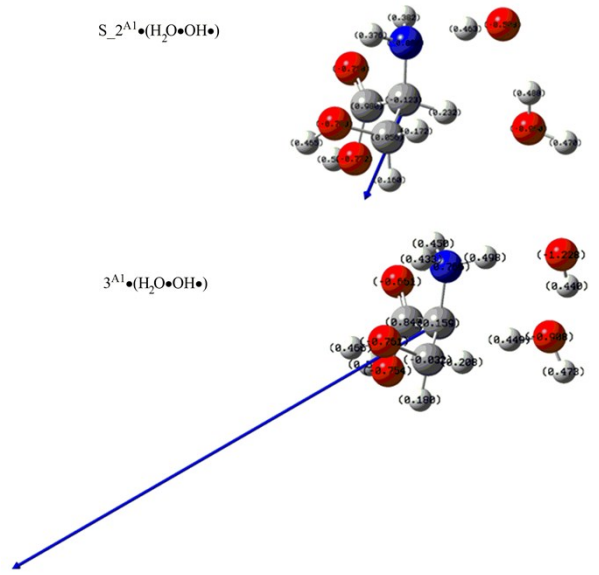


Fig.S3 *the NBO charge and the dipole moment of S_2^{A1}•(H_2O•OH•) and 3^{A1}•(H_2O•OH•)*

As shown in calculated free-energy profile in Fig.9, this step is very endothermic from S_2^{A1}•(H_2O•OH•) to 3^{A1}•(H_2O•OH•), by 25.7 kcal mol^{-1}. One reason is the NBO charges of oxygen atom OH• and α-carbon change from -0.508 and -0.123 to -1.228 and 0.159 a.u, respectively. The electronegativity on carboxyl oxygen and hydroxyl oxygen is also reduced, which make the dipole moment of the system to increase from 3.0920 cm to 12.9459 cm, resulting in the degree of charge separation is significantly increased. Another reason is carbon center undergoes a hybridization change from sp^3 to sp^2 in the transition state from S_2^{A1}•(H_2O•OH•) to 3^{A1}•(H_2O•OH•). However, when considered the solvation of the water environment, the 3^{A1}•(H_2O•OH•) is stable than the S_2^{A1}•(H_2O•OH•), by 18.5 kcal mol^{-1}. The reason may be caused by the dipole moment of 3^{A1}•(H_2O•OH•) is the bigger than that of S_2^{A1}•(H_2O•OH•), and the strong polar water solvent reduces the energy of the 3^{A1}•(H_2O•OH•) significantly more than that of the S_2^{A1}•(H_2O•OH•).

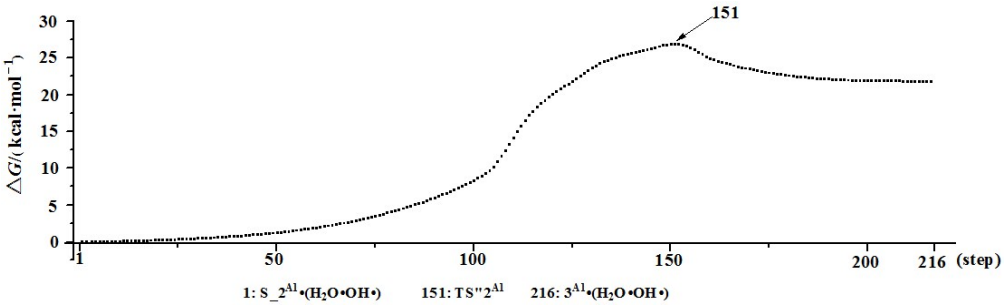


Table S6. The high level Energy (E), Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the hydroxide ion mediated proton transfer reactions for pathway **A1** at gas phase and solvent phase, respectively.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total} (kcal/mol)	Ima (cm^{-1})
gas phase					
S_2^{A1}·(H_2O·OH^-)	0.10500	-550.37091	-550.26591	0.0	
TS‴2^{A1}	0.10580	-550.36943	-550.26363	1.4	216.93
3''^{A1}·2H_2O	0.10774	-550.38647	-550.27873	-8.1	
5'^{A1}·2H_2O	0.10774	-550.38647	-550.27873	0.0	
TS‴5^{A1}	0.10580	-550.36943	-550.26363	9.5	216.92
R_6^{A1}·(H_2O·OH^-)	0.10500	-550.37091	-550.26591	8.1	
solvent phase					
S_2^{A1}·(H_2O·OH^-)	0.10500	-550.48423	-550.37923	0.0	
TS‴2^{A1}	0.10580	-550.47628	-550.37048	5.5	216.93
3''^{A1}·2H_2O	0.10774	-550.48534	-550.3776	1.0	
5'^{A1}·2H_2O	0.10774	-550.48534	-550.3776	0.0	
TS‴5^{A1}	0.10580	-550.47628	-550.37048	4.5	216.92
R_6^{A1}·(H_2O·OH^-)	0.10500	-550.48423	-550.37923	-1.0	

Table S7. The high level Energy (E), Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the water-mediated proton transfer reactions for pathway B1 at gas phase and solvent phase, respectively.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total}(Kcal mol^{-1})	Ima (cm^{-1})
gas phase					
S_2^{B1}·2H$_2$O	0.12210	-550.95614	-550.83404	0.00	
TS′2^{B1}	0.12103	-550.90333	-550.78230	32.50	858.23
3^{B1}-2H$_2$O	0.12437	-550.91467	-550.79033	27.46	
5^{B1}·2H$_2$O	0.12429	-550.91334	-550.78911	0.00	
TS′5^{B1}	0.12093	-550.90246	-550.78153	4.76	862.47
R_6^{B1}·2H$_2$O	0.12110	-550.95418	-550.83308	-27.62	
solvent phase					
S_2^{B1}·2H$_2$O	0.12210	-550.98377	-550.86167	0.00	
TS′2^{B1}	0.12103	-550.94053	-550.81950	26.49	858.23
3^{B1}·2H$_2$O	0.12437	-550.95161	-550.82724	21.63	
5^{B1}·2H$_2$O	0.12429	-550.94971	-550.82542	0.00	
TS′5^{B1}	0.12093	-550.93848	-550.81755	4.94	862.47
R_6^{B1}·2H$_2$O	0.12110	-550.98322	-550.86211	-23.05	

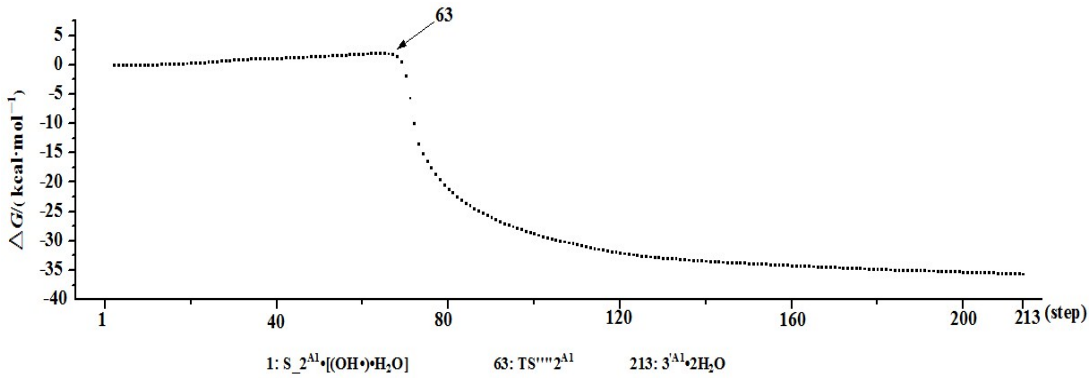


Fig. S4 Intrinsic reaction coordinate for the proton transfer process from C1 to O19 of $3'^{A1}$•2H_2O.

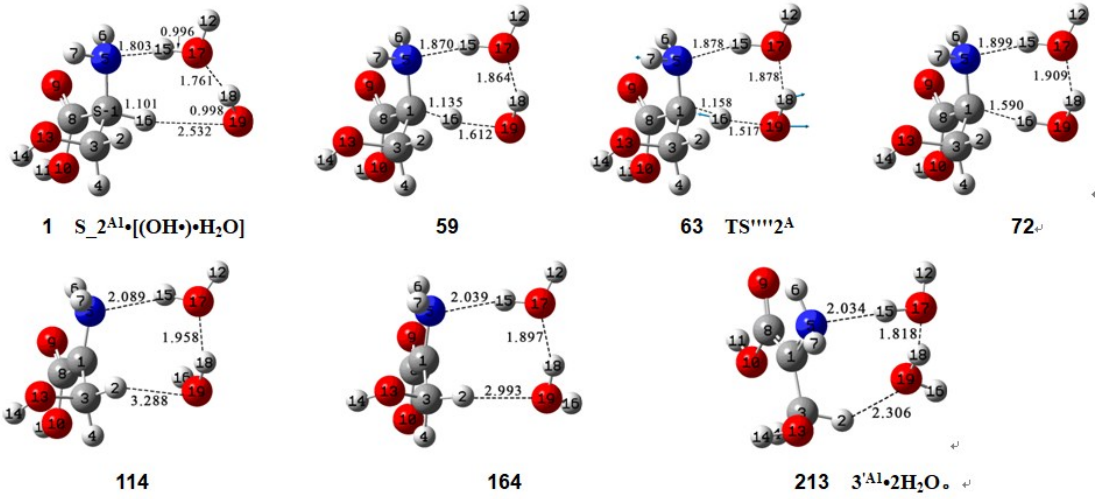
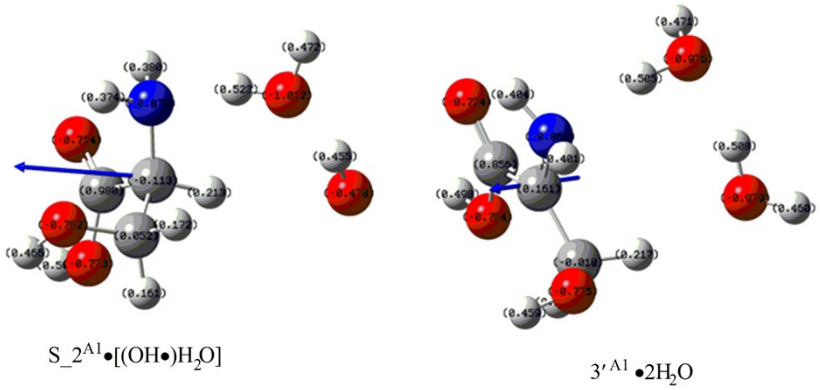


Fig.S5 The geomitries of some states for this S_2^{A1}•[(OH•)•H_2O]→TS""2^{A1}→$3'^{A1}$•2H_2O process



S_2^{A1}•[(OH•)H_2O] 3′^{A1} •2H_2O

Fig.S6 *the NBO charge and the dipole moment of S_2^{A1}•[(OH•)•H_2O] and 3'^{A1}•2H_2O*

However, from S_2^{A1}•[(OH•)•H_2O) to 3'^{A1}•2H_2O, 3'^{A1}•2H_2O is more stable than S_2^{A1}•(H_2O•OH•) in gas phase, by 37.6 kcal mol $^{-1}$ (Fig.9), one reason is the NBO charges of oxygen atom of water meleculer andα-carbon change from -1.012 and -0.113 to -0.976 and 0.161 a.u. and the electrical properties of methylene carbon changes from positively to negatively charged, resulting in the dipole moment of the system decrease from 2.6600 cm to 1.7762 cm, and the charge separation is reduced. Another reason is the skeleton atoms 1C, 3C, 8C, 5N, 9O, 10O and 13O form a super-conjugated large π bond in 3'^{A1} , and there are Intermolecular hydrogen bonds in 3'^{A1}•2H_2O. When considered the water solvation, the stability is hardly changed, the reason may be the dipole moment of 3'^{A1}•2$H_2O$and S_2^{A1}•[(OH•)•H_2O] are small, and the difference of both dipole moments is samll.

Table S8. The high level Energy (E), Thermal correction to Gibbs Free Energy (Gtc), total energies (G_{total}, including the ZPE correction) and relative total energies (ΔG_{total}), transition state imaginary frequency (Ima) at 298.15 K of all stationary points in the hydroxyl radical catalysed serine damage reactions for pathway **A1** at gas phase and solvent phase, respectively.

Structures	Gtc(Hartree)	E(Hartree)	G_{total}(Hartree)	ΔG_{total}(Kcal mol^{-1})	Ima (cm^{-1})
gas phase					
S_2^{A1}·[(OH·)·H_2O)]	0.10764	-550.25103	-550.14399	0.00	
TS′′′′2^{A1}	0.10779	-550.19134	-550.08355	37.96	791.41
3′^{A1}·2H_2O	0.10784	-550.31109	-550.20325	-37.22	
solvent phase					
S_2^{A1}·[(OH·)·H_2O)]	0.10764	-550.28018	-550.17254	0.00	
TS′′′′2^{A1}	0.10779	-550.24184	-550.13405	24.18	791.41
3′^{A1}·2H_2O	0.10784	-550.34326	-550.23542	-39.50	

Cartesian coordinates of stationary points optimized at the B3LYP/6-31+G(d, p) level

S_1[A]

C	-0.26295500	0.32611400	0.68393400
H	-2.19291700	-0.56351700	1.04295200
C	-1.31584600	-0.77103700	0.40963300
H	-0.92764900	-1.75838500	0.66836500
N	-0.77130800	1.60073600	0.17665800
H	-0.02457900	2.14957000	-0.24120000
H	-1.22399400	2.14617600	0.90145100
C	1.06847700	0.01725200	0.00969300
O	1.67331500	0.77903700	-0.71549200
O	1.53425600	-1.20584800	0.34145700
H	2.37969900	-1.33036500	-0.12221000
H	-0.05509000	0.33723100	1.76640000
O	-1.66766400	-0.79278000	-0.95914000
H	-1.81363300	0.13688600	-1.20652700

S_TS1[A]

C	0.27048100	0.32629100	-0.71168100
H	2.19933200	-0.59825700	-0.99331000
C	1.29108400	-0.79798600	-0.40255700
H	0.89202100	-1.76958600	-0.70365500
N	0.73419200	1.62833100	-0.31721500
H	0.28722200	2.09012900	0.45806100
H	1.60716000	1.98578500	-0.66372500
C	-1.04709800	0.05412800	0.00233200
O	-1.52738800	0.74761700	0.87293200
O	-1.63675800	-1.07571700	-0.44835900
H	-2.44829800	-1.20539200	0.07098800
H	0.05729500	0.27694900	-1.79205700
O	1.58836000	-0.88292000	0.97908100
H	1.78541900	0.01561800	1.28640200

S_2[A]

C	0.26788100	0.36543500	-0.70758400

H	2.21537800	-0.52423200	-0.97754300
C	1.28744700	-0.76841100	-0.43649000
H	0.90440200	-1.71447400	-0.82713800
N	0.70973800	1.69770600	-0.32663800
H	0.44786800	1.93604200	0.62445500
H	1.69632400	1.85919700	-0.49311700
C	-1.03629800	0.06520600	0.01725200
O	-1.45138900	0.66697300	0.98368100
O	-1.68439700	-0.98723300	-0.53158700
H	-2.47609900	-1.15325900	0.00793600
H	0.05419200	0.33960100	-1.78565400
O	1.53938300	-0.98496000	0.94266200
H	1.84680500	-0.15843600	1.34040900

TS2^{A}

C	0.17499100	0.30145500	-0.52430000
H	2.16925100	-0.12403000	-1.20143800
C	1.40793900	-0.53721400	-0.53229100
H	1.14961800	-1.53652300	-0.89768000
N	0.44342400	1.78811400	-0.10821300
H	-0.36248600	2.12502600	0.41975800
H	1.34216400	1.90153300	0.35536400
C	-1.10356600	-0.12056700	-0.02552600
O	-1.94527900	0.62921100	0.47763900
O	-1.35075200	-1.45619400	-0.18641800
H	-2.26145500	-1.59883400	0.11851400
H	0.23261900	1.43932100	-1.22601900
O	2.07505200	-0.60719700	0.74928000
H	1.51796600	-1.11189800	1.35769000

3^{A}

C	0.17182500	0.22360500	-0.43616700
H	2.08178500	-0.21061100	-1.33743300
C	1.41170900	-0.56496600	-0.54440700
H	1.15844400	-1.60703500	-0.76227000
N	0.35438000	1.66385900	-0.11500200
H	-0.59793500	1.92241900	0.23820900
H	1.06169800	1.80433900	0.61632800
C	-1.11014100	-0.15252900	-0.02612400
O	-1.98057500	0.66808200	0.37333200

O	-1.41096900	-1.48765800	-0.09116100
H	-2.33811800	-1.55593100	0.18443300
H	0.59696300	2.25060000	-0.91737000
O	2.25586000	-0.47325200	0.65037600
H	1.80161400	-0.94482800	1.36292800

TS3^{A1}

C	-0.15961800	0.19679000	0.46685800
H	-2.01341000	-0.41922800	1.39045200
C	-1.37535800	-0.63421500	0.52042400
H	-1.07475300	-1.68406000	0.56786000
N	-0.39581700	1.62780000	0.14059500
H	0.55068500	1.92133200	-0.20018600
H	-1.08987700	1.72831600	-0.61038000
C	1.12183600	-0.13867700	0.01999800
O	1.96518000	0.71156500	-0.37436300
O	1.45928200	-1.46591100	0.05645900
H	2.37926500	-1.50446000	-0.24714300
H	-0.67974400	2.20930500	0.93262200
O	-2.20955100	-0.36943000	-0.66173600
H	-2.54188700	-1.19899100	-1.02395700

4^{A1}

C	-0.16313100	0.17858400	0.45557100
H	-2.01001100	-0.46753700	1.37035900
C	-1.36665000	-0.66543700	0.49687000
H	-1.05662800	-1.71484000	0.52683600
N	-0.41060900	1.61400400	0.15992400
H	0.52772600	1.91655200	-0.19627000
H	-1.12724000	1.72000000	-0.56808400
C	1.12777500	-0.13519900	0.01743100
O	1.95984900	0.73357200	-0.35971500
O	1.48547200	-1.45518100	0.04400500
H	2.40262800	-1.47872200	-0.26954600
H	-0.67412700	2.18237900	0.96865400
O	-2.16450600	-0.39007900	-0.70246000
H	-3.02256800	-0.83004000	-0.62528600

TS4^{A1}

C	0.16254200	0.06806000	-0.00004100
H	1.26488900	-1.57623900	-0.88751000
C	1.28638500	-0.92333200	-0.00000400
H	1.26484900	-1.57622100	0.88751600
N	0.49286300	1.50312300	-0.00000700
H	-0.47314000	1.91557800	0.00001200
H	1.01691400	1.81430400	0.82346900
C	-1.20933700	-0.08964700	-0.00000500
O	-2.02913700	0.87780500	0.00002100
O	-1.67520300	-1.38325100	-0.00000100
H	-2.64162300	-1.30533000	0.00001700
H	1.01689800	1.81434800	-0.82347700
O	2.50476000	-0.14395800	0.00001600
H	3.26027400	-0.74355700	0.00003600

5^{A1}

C	0.16313100	0.17858300	0.45557000
H	1.05662700	-1.71484100	0.52683400
C	1.36665000	-0.66543700	0.49687000
H	2.01001000	-0.46753900	1.37036000
N	0.41060900	1.61400400	0.15992400
H	-0.52772600	1.91655200	-0.19626900
H	0.67412700	2.18237800	0.96865500
C	-1.12777500	-0.13519900	0.01743000
O	-1.95984900	0.73357200	-0.35971500
O	-1.48547300	-1.45518100	0.04400500
H	-2.40262900	-1.47872200	-0.26954600
H	1.12724000	1.72000100	-0.56808300
O	2.16450700	-0.39007900	-0.70245900
H	3.02257000	-0.83003800	-0.62528300

TS5^{A1}

C	0.16593100	0.26035600	0.53600000
H	1.06654900	-1.62754900	0.74012100
C	1.37545900	-0.60174000	0.51267000
H	2.10978700	-0.28554600	1.26823100
N	0.47498600	1.75134300	0.16140400
H	-0.33097400	2.11276800	-0.35108600

H	0.26413700	1.38098900	1.26681900
C	-1.11690100	-0.11712600	0.00833100
O	-1.92889000	0.67265500	-0.48216000
O	-1.41184500	-1.44174800	0.14712400
H	-2.31287900	-1.55255100	-0.19664200
H	1.36499200	1.84023200	-0.32396600
O	1.98807500	-0.52016100	-0.79807200
H	2.78783100	-1.06266000	-0.81045300

R_6^{A1}

C	0.25322500	0.41261500	0.66567400
H	0.99784400	-1.61077800	0.86893600
C	1.33866700	-0.64821900	0.47053300
H	2.23354600	-0.31942200	1.01332700
N	0.74303100	1.71073800	0.23976200
H	-0.00113700	2.40173700	0.27528000
H	0.03719500	0.44690000	1.74308800
C	-1.06302400	-0.00711500	-0.00879300
O	-1.70069000	0.67229200	-0.78252200
O	-1.48212900	-1.22979900	0.40621500
H	-2.32360900	-1.41364600	-0.04516900
H	1.04285200	1.65246900	-0.73075200
O	1.59487800	-0.73628200	-0.93347500
H	2.34240700	-1.32579100	-1.08926800

R_TS6^{A1}

C	-0.24421300	0.37720800	-0.67782900
H	-0.93262300	-1.67878800	-0.79224300
C	-1.30955300	-0.70703300	-0.45753800
H	-2.18817200	-0.43558800	-1.05141800
N	-0.77038000	1.67346700	-0.29016700
H	-0.08500000	2.40395200	-0.46095500
H	-0.02360600	0.38649600	-1.75427200
C	1.07317600	0.01103700	0.02190500
O	1.65197400	0.70041900	0.83253800
O	1.55830500	-1.18342900	-0.40199100
H	2.38835600	-1.34523600	0.07812900
H	-0.94485200	1.67252100	0.71240800
O	-1.63046800	-0.78589400	0.93466000
H	-2.57638600	-0.65366200	1.05863200

R_1^{A1}

C	-0.26295600	0.32611700	-0.68393400
H	-0.92764600	-1.75838300	-0.66837200
C	-1.31584200	-0.77103800	-0.40963300
H	-2.19291600	-0.56351500	-1.04294800
N	-0.77130900	1.60073900	-0.17666300
H	-1.22400100	2.14617800	-0.90145100
H	-0.05508500	0.33723100	-1.76639900
C	1.06847600	0.01725400	-0.00969200
O	1.67330800	0.77903400	0.71550200
O	1.53426000	-1.20584200	-0.34146500
H	2.37970100	-1.33036100	0.12220500
H	-0.02458700	2.14957500	0.24120600
O	-1.66766100	-0.79278800	0.95914100
H	-1.81363000	0.13687400	1.20653500

TS3^{A2}

C	0.19046900	0.15897500	0.17970700
H	1.40074800	-0.50554600	-1.47986800
C	1.27341000	-0.69027400	-0.40212300
H	1.00990900	-1.74529000	-0.26852700
N	0.43260200	1.69349800	-0.00875100
H	-0.39384400	2.16369100	-0.38006700
H	0.43080000	1.14347000	1.05287400
C	-1.21260900	-0.11929000	0.05159700
O	-2.09129700	0.74121400	-0.04972100
O	-1.52013400	-1.45004100	0.08316300
H	-2.48869200	-1.50165800	0.03799100
H	1.32854400	1.89938400	-0.44068700
O	2.56551400	-0.38998900	0.15060200
H	2.54403100	-0.61448100	1.09209600

R_4^{A2}

C	-0.22180400	0.17778100	-0.43897700
H	-1.02891200	-0.30365300	1.52580400
C	-1.14036200	-0.65633600	0.49578000
H	-0.86906000	-1.71943000	0.45379000
N	-0.52839700	1.59847100	-0.45939900

H	-0.07894100	2.06840700	0.32284400
H	-0.32429100	-0.23250400	-1.45334000
C	1.22000500	-0.02719000	-0.01024800
O	1.85679600	0.73725500	0.68259200
O	1.71679000	-1.20948200	-0.44794600
H	2.62086200	-1.29130600	-0.09829800
H	-1.53356900	1.73424000	-0.39430400
O	-2.51240100	-0.45913500	0.16690600
H	-2.72382500	-0.95968400	-0.63244200

R_TS4^{A2}

C	-0.22009300	0.23679100	-0.37854700
H	-1.08454400	-0.46733300	1.48109700
C	-1.18421300	-0.67837500	0.41294000
H	-0.95058000	-1.73324500	0.22735200
N	-0.49757200	1.61604100	-0.14192500
H	0.25668700	2.26106400	0.01578100
H	-0.31852400	-0.05252900	-1.44610900
C	1.23041800	-0.06145100	-0.03230900
O	2.04262200	0.74938600	0.35718500
O	1.54035300	-1.36632900	-0.23587100
H	2.48066700	-1.47558700	-0.01388800
H	-1.44930500	1.93574500	-0.15117000
O	-2.54057700	-0.38228400	0.08432600
H	-2.74724900	-0.76837900	-0.77722200

R_5^{A2}

C	0.21457700	0.27308600	0.32135700
H	1.15435800	-0.54312000	-1.44189200
C	1.21156300	-0.68193500	-0.35914200
H	0.97651900	-1.72315100	-0.11666700
N	0.47140000	1.63291100	-0.11559300
H	-0.22794200	2.28128600	0.23100900
H	0.32151200	0.12296500	1.41667500
C	-1.24116000	-0.07668000	0.04331100
O	-2.12429300	0.72885600	-0.15165400
O	-1.47254300	-1.41272300	0.10223200
H	-2.42688500	-1.54258600	-0.03319400
H	1.39884700	1.92874700	0.16942200
O	2.55232000	-0.35253300	0.00980200

H	2.75004800	-0.75015400	0.86758900

R_TS5^{A2}

C	0.21271800	0.27544200	0.32521600
H	1.11924100	-0.61386000	-1.42059700
C	1.20860400	-0.69068700	-0.33094000
H	0.99768200	-1.71862900	-0.02384700
N	0.47041100	1.62863000	-0.13779200
H	-0.25501700	2.26998700	0.16698400
H	0.32166900	0.14968100	1.42131600
C	-1.24102300	-0.07891300	0.04622700
O	-2.12937500	0.72538800	-0.13090000
O	-1.46664100	-1.41683400	0.08148500
H	-2.42120200	-1.54780200	-0.05132000
H	1.37580000	1.94593900	0.19252000
O	2.53394600	-0.29453500	0.04526200
H	2.98371800	-1.03292700	0.46969200

R_6^{A2}

C	-0.21588400	0.27414500	-0.31908500
H	-1.14896500	-0.62563400	1.40146200
C	-1.20692700	-0.70866200	0.30843500
H	-0.97222800	-1.73423100	0.00335800
N	-0.47920600	1.62037600	0.16520600
H	0.25524300	2.26199200	-0.11727200
H	-0.32416400	0.16669900	-1.41668500
C	1.23890000	-0.07691100	-0.04420300
O	2.12179400	0.73519500	0.12761100
O	1.47461000	-1.41183300	-0.07533000
H	2.43115100	-1.53391200	0.05189700
H	-1.37524800	1.94569100	-0.18176900
O	-2.50013900	-0.32022500	-0.16627800
H	-3.17800100	-0.77977100	0.34366200

R_TS6^{A2}

C	1.19724200	-0.72726000	-0.30523000
H	0.96397500	-1.75281600	-0.00286500
N	0.50677400	1.61301500	-0.10771300

H	-0.26315000	2.24150500	0.10100400
H	0.31086900	0.12585900	1.43505700
C	-1.23964200	-0.06595800	0.03835400
O	-2.09958700	0.75623300	-0.19461400
O	-1.50251600	-1.39376600	0.11001100
H	-2.45621100	-1.50420700	-0.04575000
H	1.35482300	1.95104600	0.33383600
O	2.51237600	-0.38556600	0.14675500
H	3.10596200	-0.32216000	-0.60924900

R_1^{A2}

C	0.23312700	0.16491600	0.41773200
H	0.98469800	-0.52616100	-1.50324700
C	1.14463100	-0.75383800	-0.43626200
H	0.89745000	-1.80417900	-0.26567000
N	0.70907700	1.53767100	0.28025800
H	0.28999800	1.97385800	-0.53898200
H	0.34465200	-0.14778500	1.46126800
C	-1.22572100	-0.01396200	0.01269000
O	-1.87792700	0.79100100	-0.61929200
O	-1.72023200	-1.21000700	0.40974700
H	-2.63659800	-1.27077300	0.08850200
H	0.45106300	2.10343900	1.08274600
O	2.49540800	-0.56504900	-0.07223700
H	2.61498800	0.39765000	0.00286900

S_1^{B}

C	-0.17461300	0.45075300	0.63748100
H	-2.30295400	0.24676100	0.94157200
C	-1.48481300	-0.33693100	0.50833300
H	-1.40188500	-1.28523200	1.04922800
N	-0.17434300	1.75378200	-0.04386500
H	-0.53284700	2.49601500	0.54809600
H	-0.75421100	1.70557400	-0.88067600
C	1.01339800	-0.38609400	0.10917500
O	1.96606900	0.33917600	-0.48822700
O	1.08069600	-1.58998100	0.23900500
H	1.61009200	1.26044800	-0.51743400
H	0.03003200	0.61621000	1.70380000
O	-1.82533500	-0.54625800	-0.86083200
H	-1.32310500	-1.30611500	-1.18703300

S_TS1^{B}

C	0.14179000	0.74873600	-0.37493000
H	2.07760600	0.46275900	-1.29276900
C	1.26616400	-0.16770700	-0.91627800
H	0.88981800	-0.77531400	-1.75238300
N	0.51027000	1.44323400	0.86515800
H	0.80794400	2.39502200	0.68127700
H	1.26874200	0.94860700	1.32941100
C	-1.12500300	-0.05736900	-0.10775600
O	-0.95961500	-0.99028300	0.91858900
O	-2.14897700	0.01788000	-0.73190000
H	-1.24004600	-0.61517400	1.76626400
H	-0.11769600	1.47495300	-1.15057600
O	1.84548000	-0.97801500	0.09751800
H	1.14892700	-1.53210600	0.48280000

S_2^{B}

C	0.16024700	0.75758600	-0.33653900
H	2.09959900	0.49319800	-1.24864600
C	1.28673800	-0.14811500	-0.89389300
H	0.91669000	-0.73005100	-1.75197100
N	0.51005700	1.47478100	0.89065400
H	1.07937100	2.28808100	0.67600700
H	1.05113500	0.86949700	1.50399000
C	-1.11821400	-0.03890100	-0.09205100

O	-0.93044800	-1.03209000	0.82663900
O	-2.18212300	0.13581600	-0.63998500
H	-1.78692600	-1.47609500	0.95277000
H	-0.10726200	1.48689200	-1.10623500
O	1.86542800	-0.99007000	0.09387200
H	1.18151400	-1.58766300	0.43019100

TS2^{B}

C	0.16856000	0.27488600	-0.52937300
H	2.20113700	0.03298300	-1.18950300
C	1.46846700	-0.45399700	-0.53824800
H	1.29143300	-1.46378100	-0.92158300
N	0.34201800	1.77465200	-0.07484300
H	1.22984100	1.92062800	0.40132600
H	-0.47099800	2.10148000	0.43909700
C	-1.03974100	-0.36158800	-0.08677900
O	-1.98529900	0.53677900	0.37846900
O	-1.28806600	-1.56167600	-0.13338700
H	-2.77128400	0.01097400	0.59707800
H	0.16487400	1.45031400	-1.19600900
O	2.11826800	-0.49255200	0.75421000
H	1.61793400	-1.09137000	1.32556400

3^{B}

C	-0.16472600	0.18169000	0.47626600
H	-2.11719200	-0.19351900	1.32515900
C	-1.44169100	-0.55328700	0.53890600
H	-1.23432400	-1.61076800	0.72348700
N	-0.35637800	1.62032600	0.12046300
H	-1.08565200	1.70686300	-0.60245000
H	0.53747000	1.96881600	-0.24803100
C	1.06289200	-0.36375700	0.07373100
O	1.98976500	0.63928800	-0.31757700
O	1.42112800	-1.54335900	0.04935600
H	2.80243100	0.16010100	-0.53856100
H	-0.62983200	2.20515800	0.91611600
O	-2.24650900	-0.37852100	-0.67879700
H	-1.83217800	-0.90607500	-1.37623600

TS3^{B1}

C	-0.15414900	0.15067900	0.48831600
H	-2.04532600	-0.42368500	1.38005600
C	-1.40774700	-0.62706200	0.50648400
H	-1.14303300	-1.68743800	0.50357000
N	-0.38535900	1.58696800	0.14981000
H	0.51448000	1.97172600	-0.16329900
H	-1.07281500	1.66228000	-0.61383200
C	1.08042800	-0.35662500	0.05728100
O	1.98349300	0.67599700	-0.31029000
O	1.46550500	-1.52659200	0.00450600
H	2.80766900	0.22101700	-0.53899200
H	-0.72452300	2.14518600	0.93895200
O	-2.21378700	-0.26757700	-0.67256100
H	-2.63182000	-1.05444700	-1.04086400

4^{B1}

C	-0.15734600	0.12659000	0.46067500
H	-2.03002500	-0.48756100	1.36442800
C	-1.39902300	-0.66442700	0.47722200
H	-1.12742500	-1.72374900	0.44163800
N	-0.40143000	1.57022100	0.16995400
H	0.47445100	1.95606800	-0.20450900
H	-1.14904100	1.65215600	-0.53363000
C	1.09416700	-0.35378700	0.04920000
O	1.98215600	0.70325000	-0.28884700
O	1.50407300	-1.51370100	-0.01191300
H	2.81154800	0.26572200	-0.53234500
H	-0.67271200	2.12096400	0.99078100
O	-2.19322900	-0.28135900	-0.69837500
H	-3.06757300	-0.69093100	-0.64555000

TS4^{B1}

C	0.15737500	0.03721300	-0.02253400
H	1.34589800	-1.55414400	-0.89143400
C	1.32713600	-0.90111800	-0.00490800
H	1.32001000	-1.55256800	0.88332500
N	0.46975800	1.48178800	-0.00315500
H	-0.44095800	1.96016600	-0.00734700

H	1.00115000	1.77430600	0.82529800
C	-1.17871300	-0.31747000	-0.00299900
O	-2.04170900	0.82129600	0.00746900
O	-1.68278600	-1.44895900	0.00336900
H	-2.93734100	0.45266900	0.01317600
H	1.01834600	1.78945800	-0.81389200
O	2.50919100	-0.06337900	0.01115300
H	3.29223300	-0.62580600	0.01968300

5^{B1}

C	0.15734600	0.12659000	0.46067600
H	1.12742500	-1.72375000	0.44163800
C	1.39902300	-0.66442800	0.47722200
H	2.03002500	-0.48756200	1.36442800
N	0.40143000	1.57022100	0.16995400
H	-0.47445000	1.95606800	-0.20451000
H	0.67271100	2.12096400	0.99078100
C	-1.09416700	-0.35378700	0.04920000
O	-1.98215600	0.70325100	-0.28884700
O	-1.50407300	-1.51370000	-0.01191300
H	-2.81154800	0.26572300	-0.53234400
H	1.14904300	1.65215600	-0.53362800
O	2.19322900	-0.28135900	-0.69837500
H	3.06757200	-0.69093100	-0.64555100

TS^{5B1}

C	0.16060200	0.20556700	0.53509700
H	1.15759500	-1.63038700	0.65508700
C	1.42193700	-0.57925600	0.49946000
H	2.12287900	-0.26950000	1.28830900
N	0.41305200	1.71711100	0.16635500
H	-0.38680400	2.10388000	-0.32620100
H	0.22081800	1.34274600	1.26553400
C	-1.07606100	-0.34841900	0.05659200
O	-1.95989700	0.62094100	-0.38949700
O	-1.40175400	-1.52841300	0.07729400
H	-2.77300100	0.14980700	-0.63144800
H	1.30100000	1.82857600	-0.31946500
O	2.05638000	-0.38132500	-0.78974600
H	2.86945600	-0.90187000	-0.82760500

R_6^{B1}

C	0.24740800	0.37314900	0.69632700
H	1.14955300	-1.58524400	0.80274000
C	1.41216600	-0.58523800	0.43979100
H	2.29092100	-0.20934000	0.97821700
N	0.60527500	1.71376700	0.26589200
H	-0.17265900	2.35696500	0.37210100
H	0.08195500	0.38231100	1.78227800
C	-1.03841200	-0.24164300	0.11468500
O	-1.69734500	0.58208700	-0.73339100
O	-1.45420700	-1.34340000	0.40818600
H	-2.49024700	0.10358400	-1.03067200
H	0.86482100	1.70365200	-0.71686000
O	1.64338700	-0.59366600	-0.97212900
H	2.37708500	-1.18607000	-1.17518200

R_TS6^{B1}

C	-0.22928000	0.43455200	-0.66029000
H	-1.24547700	-1.45196600	-0.90361400
C	-1.45303000	-0.46629800	-0.47851700
H	-2.30127000	-0.00888000	-1.00026400
N	-0.50671000	1.75949900	-0.13041500
H	0.31307000	2.35599400	-0.17784100
H	-0.05202500	0.52198000	-1.74262000
C	1.01431200	-0.29216800	-0.11848000
O	1.84651700	0.51726900	0.57875000
O	1.26821600	-1.46204500	-0.32177700
H	2.60866100	-0.02402300	0.84746000
H	-0.78096700	1.69043100	0.84638600
O	-1.74477100	-0.55396000	0.92207900
H	-1.94672800	-1.46665800	1.15469900

R_7^{B1}

C	-0.13136100	0.65268500	-0.47274000
H	-1.33594200	-0.80393400	-1.53392000

C	-1.45912500	-0.07288500	-0.72305700
H	-2.20012500	0.66877900	-1.03088000
N	-0.32225400	1.68985600	0.54208600
H	0.54916700	2.14132000	0.80129700
H	0.18686200	1.13714000	-1.40453300
C	0.96202000	-0.34466900	-0.07832200
O	2.19853500	0.20035200	-0.16089100
O	0.78521400	-1.48555100	0.31107600
H	2.83552100	-0.46441600	0.15432700
H	-0.75991400	1.29455200	1.37063400
O	-1.96928900	-0.68966600	0.45200200
H	-1.36467400	-1.41430300	0.67569600

R_TS7^{B1}

C	0.13157900	0.66877800	0.43537100
H	1.20228700	-0.83176300	1.58284900
C	1.41215200	-0.10669600	0.78301200
H	2.15981400	0.60415500	1.14489700
N	0.35739000	1.58958100	-0.64760500
H	-0.08418400	2.49013000	-0.66976100
H	-0.20032400	1.21516700	1.32655700
C	-0.98661200	-0.30984200	0.04426900
O	-2.21866400	0.20128300	0.25719600
O	-0.81799500	-1.41214600	-0.44857200
H	-2.86587500	-0.44038400	-0.08436700
H	1.05885500	1.36395600	-1.33289000
O	1.98060100	-0.74441400	-0.35234900
H	1.33344700	-1.39954800	-0.66016200

R_8^{B1}

C	1.38353200	-0.11399400	0.81570700
H	2.14689900	0.58562800	1.17093900
N	0.34126300	1.57773200	-0.74964500
H	0.76022100	2.45374100	-0.45361100
H	-0.21245600	1.28698700	1.24388700
C	-0.99759200	-0.26738300	0.01646000
O	-2.21561200	0.20167500	0.34396800
O	-0.83821000	-1.34172100	-0.53804800
H	-2.87417700	-0.43572600	0.01620400
H	0.97254300	1.13413100	-1.41358500

O	1.96217000	-0.81690100	-0.27373000
H	1.29585300	-1.44893400	-0.59012300

R_TS8^{B1}

C	0.10888600	0.61552000	0.48150500
H	1.36967000	-0.83297100	1.50044000
C	1.46530700	-0.06431900	0.72060700
H	2.18327200	0.68568600	1.06734900
N	0.11904000	1.62826600	-0.58573100
H	0.39145700	2.53881700	-0.23009900
H	-0.23224900	1.08961100	1.40933200
C	-0.96851300	-0.39316100	0.07817500
O	-2.24841700	0.09597300	0.18593000
O	-0.74114600	-1.52268900	-0.29060200
H	-2.54752800	0.47087400	-0.65476000
H	0.79073600	1.35186100	-1.29938600
O	2.00633600	-0.60962500	-0.47657900
H	1.44309300	-1.35925300	-0.72447200

R_1^{B1}

C	0.17461300	0.45075200	0.63748100
H	1.40188400	-1.28523400	1.04922600
C	1.48481200	-0.33693300	0.50833300
H	2.30295400	0.24675900	0.94157300
N	0.17434400	1.75378200	-0.04386400
H	0.53284700	2.49601500	0.54809700
H	-0.03003200	0.61620900	1.70380100
C	-1.01339800	-0.38609300	0.10917500
O	-1.96606800	0.33917700	-0.48822700
O	-1.08069700	-1.58998000	0.23900500
H	-1.61009000	1.26044800	-0.51743400
H	0.75421300	1.70557300	-0.88067500
O	1.82533400	-0.54625800	-0.86083300
H	1.32310400	-1.30611500	-1.18703400

TS3^{B2}

C	0.19010100	0.11706300	0.15854300

H	1.45983200	-0.52182800	-1.46433400
C	1.33007500	-0.67975800	-0.38278300
H	1.12506600	-1.74241600	-0.21618500
N	0.37197800	1.66307000	-0.05663000
H	0.32254300	1.15422700	1.01477600
H	-0.40192500	2.13232400	-0.52174100
C	-1.16327300	-0.34719600	0.05603100
O	-2.08383400	0.68724500	0.01495300
O	-1.53171400	-1.51597100	0.04095900
H	-2.95795400	0.26492800	0.00851100
H	1.30654700	1.88096000	-0.38986800
O	2.59267700	-0.27751900	0.17613200
H	2.58359200	-0.50038100	1.11815800

R_4^{B2}

C	-0.22806800	0.12784500	-0.46433600
H	-1.01820200	-0.23894000	1.53423300
C	-1.16447300	-0.62480000	0.52032000
H	-0.93851600	-1.69923400	0.51636100
N	-0.44408800	1.56859400	-0.51982900
H	-0.39973000	-0.28754600	-1.46468900
H	-0.12344000	2.01647200	0.33496500
C	1.20972400	-0.22652200	-0.12526100
O	1.77966000	0.65561500	0.73150100
O	1.78202800	-1.22256200	-0.51425600
H	2.68047200	0.33922500	0.91603300
H	-1.44058500	1.75071100	-0.61250600
O	-2.53197500	-0.38030700	0.20379200
H	-2.79218600	-0.94195000	-0.53822500

R_TS4^{B2}

C	-0.21816600	0.11803800	-0.45433000
H	-1.04061200	-0.24004600	1.53090500
C	-1.19208300	-0.60879000	0.51105600
H	-1.00060200	-1.68930400	0.49903400
N	-0.36448700	1.57019600	-0.49005600
H	-0.40217100	-0.26873300	-1.46367500
H	-0.22392300	1.95847200	0.44048100
C	1.21202200	-0.28035800	-0.11031900
O	1.85383000	0.59475400	0.74885400

O	1.71629200	-1.31718300	-0.45831800
H	2.37095400	1.25014800	0.25817700
H	-1.31447700	1.80187600	-0.76996700
O	-2.54743300	-0.31436000	0.18455500
H	-2.82990500	-0.88281300	-0.54372900

R_1^{B2}

C	-0.19383700	0.11725200	-0.46759400
H	-0.98631500	-0.40722800	1.48219300
C	-1.16118100	-0.67394000	0.43497000
H	-0.97268700	-1.74539200	0.31424300
N	-0.39839400	1.55817700	-0.27310300
H	-0.34312400	-0.20519500	-1.50721000
H	-1.36289100	1.74457500	-0.00693400
C	1.24772700	-0.26990000	-0.08514700
O	1.89941500	0.67475400	0.60878300
O	1.72845600	-1.34723200	-0.35769700
H	1.27275800	1.43612100	0.66744900
H	-0.20845400	2.08466700	-1.12122600
O	-2.52143600	-0.33573000	0.17566000
H	-2.81826000	-0.78959900	-0.62413900

TS3^{B3}

C	-0.24008600	0.01399800	-0.10108100
H	-1.66884300	-0.65571600	1.48715200
C	-1.40003400	-0.81434500	0.42808100
H	-1.19036000	-1.88090200	0.27861400
N	-0.59608500	1.44730700	0.22916400
H	-1.62740300	1.39294000	0.00702300
H	-0.11453800	2.11615700	-0.37204600
C	1.18261800	-0.29560300	-0.03317700
O	1.96409700	0.84270200	-0.13212800
O	1.68068400	-1.40387500	0.02036100
H	2.88674400	0.54116500	-0.17944400
H	-0.43983600	1.71275200	1.20568600
O	-2.36757600	-0.27532100	-0.47682500
H	-1.14579400	-0.08989700	-1.08533100

R_1^{B3}

C	-0.23893200	0.10780800	-0.44958200
H	-0.98162200	-0.45006000	1.51897100
C	-1.17562100	-0.71925400	0.46722400
H	-0.98003000	-1.78670100	0.34163100
N	-0.63896100	1.51095800	-0.36075000
H	-2.59856700	0.47710700	-0.01766100
H	-0.31473700	2.04820200	-1.15845600
C	1.21307000	-0.22113200	-0.11695600
O	1.80349400	0.71364000	0.67232100
O	1.78604100	-1.22858400	-0.47302100
H	2.70266900	0.39824900	0.86720400
H	-0.26614500	1.94860000	0.47785200
O	-2.52374500	-0.48265900	0.12149800
H	-0.40626500	-0.23582400	-1.47479300

S_2^{A1}-2H_2O

C	0.21188100	-0.05623900	0.03363500
H	-0.71877100	1.50865200	-1.09577100
C	0.28491300	1.09307800	-0.98015900
H	0.62012300	0.71655100	-1.95076300
N	-0.39155400	0.41909800	1.28586100
H	-0.19212400	-0.24785700	2.02972000
H	0.06563300	1.29105300	1.55299500
C	1.56089900	-0.72924300	0.27967200
O	1.95263600	-1.12750400	1.35618600
O	2.28692600	-0.87917800	-0.85735200
H	3.08909900	-1.37779300	-0.62384100
H	-3.70127300	0.45775000	1.44160000
O	1.11304100	2.16391800	-0.51899300
H	2.03297800	1.96574100	-0.73774300
H	-2.18578300	0.56393800	1.01586600
H	-0.44000400	-0.82648700	-0.40637700
O	-3.11998600	0.52213500	0.67514000
H	-2.92693100	-0.82176400	-0.53982200
H	-3.07815400	-1.57859300	-1.89659300
O	-2.50387600	-1.48317800	-1.12863000

TS′2^{A1}

C	0.16358000	0.04240100	-0.10385700
H	-0.53100800	1.80404400	-1.11241300
C	0.42209200	1.35293000	-0.82289400
H	1.00179200	1.16360400	-1.73060600
N	-0.55597800	0.31548500	1.19121700
H	-0.28170900	-0.41968000	1.85413700
H	-0.25220600	1.21917500	1.57065600
C	1.32668000	-0.81032700	0.20709500
O	1.47458200	-1.43283800	1.25353100
O	2.21512500	-0.90289700	-0.81360000
H	2.88073000	-1.55999900	-0.54975800
H	-3.82342200	-0.28420700	0.87399900
O	1.06337800	2.33224800	0.01850200
H	2.01439400	2.16048300	0.03491900
H	-1.62147500	0.30106700	1.04591400
H	-0.69914700	-0.61773800	-0.79400200
O	-3.09221800	0.17048100	0.44070700
H	-2.74577900	-0.42799900	-0.36154800
H	-1.98718500	-1.11073000	-2.18690900
O	-1.85302300	-1.16029900	-1.23226300

3^{A1}-2H_2O

C	-0.27586200	0.11956800	0.04662600
H	0.35198000	1.82049600	1.21271500
C	-0.56495800	1.32511800	0.87682600
H	-1.13740800	1.03146700	1.76204300
N	0.43972200	0.47274500	-1.22420600
H	0.15720400	-0.25706000	-1.89933100
H	0.12045500	1.38659500	-1.56888900
C	-1.25272900	-0.87293400	-0.25609200
O	-1.29078100	-1.53374900	-1.31045200
O	-2.16428300	-1.11181900	0.73993400
H	-2.70500800	-1.85416400	0.42680700
H	3.91272300	-0.08965300	-1.00730300
O	-1.26116100	2.37476800	0.13999400
H	-2.17507200	2.08759300	0.00561000
H	1.47609200	0.47733600	-1.12293700
H	1.08797200	-0.84613100	1.04568400
O	3.16327000	0.29902500	-0.54187300
H	2.97530900	-0.27027500	0.24487000
H	1.98526900	-1.09501600	2.32679900
O	1.98216900	-1.16959000	1.36479900

5^{A1}-$2H_2O$

C	0.29390600	0.12725600	0.06136000
H	1.28323700	1.02134400	1.69914600
C	0.59388200	1.31697600	0.90240100
H	-0.31187800	1.74011600	1.36110700
N	-0.42918600	0.49580100	-1.20020000
H	-0.16449600	-0.23758200	-1.87885600
C	1.27149400	-0.86058400	-0.26251000
O	1.28886700	-1.51215000	-1.32331000
O	2.18117300	-1.12650400	0.72328200
H	2.74222000	-1.83763400	0.37589200
H	-0.09073000	1.40287200	-1.54321100
O	1.19479400	2.34463500	0.05594800
H	1.27339900	3.16909100	0.55447400
H	-3.91890900	0.68485800	-0.40235500
H	-1.46261900	0.51791100	-1.09230100
H	-1.04871600	-0.80607500	1.06843400
O	-3.15869000	0.12919700	-0.60724700
H	-2.94307400	-0.39639300	0.20344100
H	-1.87205700	-2.06027200	1.57096100
O	-1.93586500	-1.10651900	1.43597100

TS′5^{A1}

C	0.18323400	0.04840700	0.10653300
H	1.10341000	1.16606100	1.67162700
C	0.43823400	1.35251700	0.82335200
H	-0.50850700	1.75947000	1.19992100
N	-0.53607000	0.31024500	-1.19181200
H	-0.25921600	-0.43283600	-1.84559000
C	1.34930000	-0.80387400	-0.20103100
O	1.48534400	-1.43354700	-1.24570000
O	2.22801200	-0.91247200	0.82112700
H	2.90849100	-1.54697100	0.54138400
H	-0.22778000	1.20841300	-1.57923100
O	1.03440700	2.27414600	-0.11648400
H	1.11972600	3.14587600	0.29023800
H	-3.82729400	0.48492100	-0.37331300

H	-1.59615100	0.29135800	-1.05470200
H	-0.68645500	-0.58671000	0.82131300
O	-3.08967200	-0.10114300	-0.57518200
H	-2.73475900	-0.52608900	0.32278100
H	-1.87493500	-1.85582000	1.68960900
O	-1.84417300	-0.93469500	1.40193000

R_6^{A1}-2H$_2$O

C	0.25683400	0.02245200	-0.14046700
H	0.56644300	-1.69477700	1.12534300
C	0.14061900	-0.68974600	1.20578900
H	-0.92082300	-0.77257300	1.46346000
N	-0.32028200	1.36945700	-0.05252700
H	-0.01288300	1.91951600	-0.85300200
C	1.69316700	0.05273400	-0.66774100
O	2.24792200	1.03699300	-1.10979600
O	2.27521100	-1.16824000	-0.65113600
H	3.16432600	-1.06931800	-1.03219600
H	0.07139300	1.82943300	0.76883000
O	0.85100300	0.10201200	2.16677400
H	0.76107400	-0.29682700	3.04055100
H	-3.59011200	1.43236300	0.43344900
H	-2.12292400	1.27078600	-0.12883600
H	-0.32984500	-0.57572500	-0.85094900
O	-3.07972700	1.03959100	-0.28390100
H	-2.91643100	-0.74812000	-0.54333200
H	-3.09788200	-2.12141200	-1.25891100
O	-2.52867000	-1.64437900	-0.64471700

S_2^{B1}-2H$_2$O

C	0.22209300	-0.05500600	-0.05313400
H	-0.73192700	1.72047300	-0.78829000
C	0.27069200	1.28701400	-0.78833200
H	0.58227500	1.12777200	-1.82677700
N	-0.32903300	0.14391700	1.30363000
H	-0.21350500	-0.69816800	1.86253700
H	0.18332600	0.89808100	1.76017400
C	1.60415300	-0.70729000	-0.03625800
O	1.62008100	-1.84772900	0.69348500
O	2.59751900	-0.28404400	-0.59647700
H	2.52291400	-2.20788800	0.65832500

H	-3.64572200	0.45176900	1.50687700
O	1.12164000	2.22431100	-0.13101300
H	2.03465400	1.96045500	-0.31746900
H	-2.12549100	0.47117000	1.08956900
H	-0.45381300	-0.72786400	-0.59957400
O	-3.05594900	0.54038900	0.74944400
H	-2.95685200	-0.67224000	-0.61987900
H	-3.14097900	-1.24282700	-2.05975400
O	-2.57494900	-1.28748300	-1.28104000

TS′2^{B1}

C	-0.16758600	0.03812400	0.13515300
H	0.67527400	1.86074000	0.90158300
C	-0.31217200	1.42465600	0.72768000
H	-0.83525500	1.35100000	1.68483900
N	0.51731600	0.15927400	-1.20793100
H	0.31260200	-0.66490200	-1.77601600
H	0.16999200	0.99167100	-1.69800000
C	-1.43082300	-0.71524900	0.04435100
O	-1.46599200	-1.58282800	-1.02086700
O	-2.35031400	-0.65530900	0.84243400
H	-2.28527100	-2.09837800	-0.94093200
H	3.82298800	-0.22969700	-0.86709900
O	-0.98486000	2.33418200	-0.16766600
H	-1.93832700	2.20226700	-0.07607500
H	1.58178000	0.22267200	-1.06756400
H	0.71192200	-0.62227100	0.83380900
O	3.05725000	0.18504100	-0.45404600
H	2.73845300	-0.41253500	0.35613200
H	1.99041400	-1.12892800	2.18944900
O	1.85612700	-1.16505300	1.23418000

3^{B1}-2H$_2$O

C	-0.27553300	0.11367600	0.08264100
H	0.48122900	1.86264400	1.09713300
C	-0.47011700	1.38956900	0.83327900
H	-1.02369900	1.18147900	1.75316100
N	0.40295700	0.38363700	-1.23616000
H	0.16674100	-0.37118500	-1.88608500
H	0.05764400	1.27183400	-1.62466600
C	-1.36511300	-0.80431200	-0.01587700

O	-1.31422700	-1.59056800	-1.17317500
O	-2.26139600	-0.99492500	0.80460900
H	-2.04331500	-2.22490600	-1.09310700
H	3.90138800	-0.05805300	-1.00791600
O	-1.15250200	2.40907900	0.04155400
H	-2.09056300	2.17496200	0.00895600
H	1.44055700	0.42756200	-1.13905200
H	1.07833000	-0.86097200	1.04244200
O	3.11922500	0.28403200	-0.56043700
H	2.94819400	-0.29102100	0.22754100
H	1.99246500	-1.18059300	2.29879200
O	1.97576200	-1.20896900	1.33440600

5^{B1}-2H_2O

C	0.30773300	0.13096600	0.09241800
H	1.22972100	1.17682100	1.66934500
C	0.52674600	1.38897000	0.85821400
H	-0.40424800	1.79051800	1.28419500
N	-0.38842100	0.41797500	-1.21257600
H	-0.15526200	-0.32709400	-1.87490300
C	1.37805700	-0.80929000	-0.02410600
O	1.30012300	-1.57316500	-1.19744500
O	2.25950700	-1.05307300	0.79460900
H	2.02572800	-2.21367800	-1.14002400
H	-0.04813400	1.31280100	-1.58805200
O	1.07410000	2.39099200	-0.05464900
H	1.14037300	3.24156000	0.39912000
H	-3.87545400	0.60200100	-0.49461900
H	-1.42432900	0.45068400	-1.10863700
H	-1.03346200	-0.76537900	1.10670900
O	-3.11256600	0.03764300	-0.66323100
H	-2.90890200	-0.44847600	0.17601400
H	-1.84261900	-1.98314700	1.72093600
O	-1.92862400	-1.05568700	1.46806500

TS′5^{B1}

C	0.20427200	0.05842700	0.14366200
H	1.05873300	1.33757700	1.60670900
C	0.36978700	1.42591500	0.76174000
H	-0.59708600	1.80008300	1.11994100

N	-0.49596800	0.20248400	-1.18991200
H	-0.26684000	-0.59497500	-1.78631100
C	1.45214600	-0.72257200	0.03852500
O	1.48567600	-1.52628200	-1.07986300
O	2.34019000	-0.75933300	0.86816500
H	2.29161900	-2.06418500	-1.01515100
H	-0.17556400	1.06112000	-1.65130100
O	0.89605300	2.31226300	-0.25326600
H	0.97798700	3.20591500	0.10278800
H	-3.79672200	0.42694400	-0.43131100
H	-1.55790400	0.21682900	-1.05368600
H	-0.67768500	-0.56688800	0.87322900
O	-3.05968800	-0.16945100	-0.60340600
H	-2.71875400	-0.56098700	0.31333500
H	-1.84656000	-1.80877500	1.77728600
O	-1.83431600	-0.91228000	1.41965700

R_6^{B1}-2H_2O

C	-0.26375900	-0.12682700	-0.03018500
H	-0.58717400	0.92426100	-1.87530200
C	-0.12692500	1.11878900	-0.90176200
H	0.93777100	1.33811600	-1.03891900
N	0.29453600	0.13280000	1.30471200
H	0.07161700	-0.63334200	1.93522200
C	-1.71149000	-0.62916700	-0.05853100
O	-2.17144900	-1.00455000	1.16227300
O	-2.37877900	-0.73890500	-1.06400900
H	-3.07416600	-1.34200800	1.03219700
H	-0.14390900	0.96813500	1.68911700
O	-0.79059200	2.18849400	-0.21443400
H	-0.81859300	2.96732200	-0.78267400
H	3.52630300	0.86995600	1.20815200
H	2.11004700	0.17400000	1.23300600
H	0.33701400	-0.90937800	-0.51386300
O	3.07913500	0.02916200	1.05745600
H	2.92804100	-0.73405100	-0.58940300
H	3.11007200	-1.79927600	-1.71461200
O	2.53096800	-1.09046400	-1.41291600

S_2^{A1}-(H_2O·OH·)

C	0.18922000	-0.11966200	-0.02451800

H	-0.88441300	1.71605700	-0.29348300
C	0.15344200	1.38093600	-0.34649100
H	0.51802300	1.55573900	-1.36225900
N	-0.41536400	-0.36345300	1.29256700
H	-0.12676900	-1.27995500	1.63311000
H	-0.03340600	0.31550800	1.95203100
C	1.58907700	-0.72446700	-0.11542700
O	2.03945600	-1.54796000	0.65275200
O	2.28597500	-0.27112400	-1.18661000
H	3.13061800	-0.75362100	-1.20801500
O	0.88073300	2.14820800	0.61607400
H	1.81026400	2.18584500	0.35606400
H	-2.16909000	-0.32135400	1.22653500
H	-0.41644800	-0.61894000	-0.79489300
O	-3.17343100	-0.34102400	1.05854600
H	-3.00816400	-0.33480900	-0.82504600
H	-3.24806600	-0.47458600	-2.35990200
O	-2.56466300	-0.32141800	-1.69744800

TS″2^{A1}

C	0.13999500	0.05043500	-0.11531200
H	-0.53438600	1.82410300	-1.12227200
C	0.41047400	1.36616400	-0.81593900
H	1.00831300	1.18598300	-1.71364700
N	-0.58349700	0.31122200	1.18167400
H	-0.31483000	-0.43616700	1.83522100
H	-0.28027800	1.20949800	1.57597000
C	1.28531000	-0.82055500	0.19157900
O	1.41537400	-1.45986200	1.23129900
O	2.18100000	-0.91404000	-0.82328300
H	2.83726100	-1.58047500	-0.55951300
O	1.03417600	2.33885600	0.04810800
H	1.98563100	2.17116000	0.07894100
H	-1.63569700	0.30297400	1.04300500
H	-0.77419000	-0.61306700	-0.81390800
O	-3.25626900	0.12674100	0.49709500
H	-2.88013300	-0.47187700	-0.28913600
H	-2.04387400	-1.26946900	-2.11356500
O	-1.91153300	-1.10138100	-1.17256700

3^{A1}-(H_2O·OH·)

C	0.53635200	1.33656400	-0.87286200
H	1.11610700	1.05622500	-1.75741500
N	-0.46530500	0.46111400	1.21792600
H	-0.19207100	-0.28375300	1.88153600
H	-0.13118600	1.36501900	1.57629800
C	1.22068700	-0.87711500	0.23279600
O	1.26002800	-1.54172400	1.28319400
O	2.12690900	-1.10957500	-0.76724300
H	2.67463600	-1.84950500	-0.46007700
O	1.22342100	2.37276700	-0.11136000
H	2.14279700	2.09730800	0.00930100
H	-1.49785200	0.48629300	1.12324200
H	-1.13552000	-0.81563400	-1.00375400
O	-3.32211200	0.29441900	0.58310500
H	-3.07964300	-0.29652200	-0.19391900
H	-2.07500900	-1.35493800	-2.18624000
O	-2.05920300	-1.13195400	-1.24810000

5^{A1}-(H_2O·OH·)

C	-0.23963300	0.11726900	-0.06322700
H	0.37749600	1.83593400	-1.21146700
C	-0.53635100	1.33656400	-0.87286200
H	-1.11610600	1.05622600	-1.75741500
N	0.46530600	0.46111300	1.21792600
H	0.19207100	-0.28375400	1.88153600
H	0.13118600	1.36501800	1.57629800
C	-1.22068800	-0.87711500	0.23279600
O	-1.26002800	-1.54172400	1.28319400
O	-2.12690900	-1.10957400	-0.76724300
H	-2.67463600	-1.84950400	-0.46007700
O	-1.22342100	2.37276800	-0.11136000
H	-2.14279700	2.09730900	0.00930100
H	1.49785200	0.48629300	1.12324200
H	1.13552000	-0.81563500	-1.00375400
O	3.32211200	0.29442000	0.58310500
H	3.07964300	-0.29652200	-0.19391900
H	2.07500800	-1.35494100	-2.18623900
O	2.05920300	-1.13195500	-1.24810000

TS″5A1

C	0.15803600	0.06324400	0.11486800
H	1.14512500	1.18481400	1.63466400
C	0.46772700	1.37334800	0.79633400
H	-0.45577500	1.82242200	1.18300800
N	-0.56056200	0.31844600	-1.18637100
H	-0.27138400	-0.42753400	-1.83450300
C	1.27700600	-0.84657500	-0.18111000
O	1.37363800	-1.50469100	-1.21421400
O	2.16046500	-0.97473700	0.83483800
H	2.81040700	-1.64267200	0.56045800
H	-0.25991100	1.21935800	-1.57565600
O	1.07325900	2.25441100	-0.17661000
H	1.17369400	3.13835600	0.19958300
H	-1.61108900	0.29364700	-1.06042600
H	-0.77521100	-0.53310500	0.85905200
O	-3.23884000	-0.06635300	-0.59494800
H	-2.86302400	-0.42052400	0.32782200
H	-1.97843900	-1.63951900	1.85321700
O	-1.91940700	-0.80418700	1.37303700

R_6^{A1}-(H_2O·OH·)

C	0.21641200	-0.07480700	0.12836600
H	0.52914600	2.04192500	-0.13427700
C	0.09442400	1.20733400	-0.69359000
H	-0.96852600	1.40976900	-0.86542000
N	-0.37195800	-1.20385000	-0.60551000
H	-0.03213100	-2.07717900	-0.20449100
C	1.65664300	-0.36958400	0.55248600
O	2.20023300	-1.44879400	0.44555700
O	2.25280300	0.69747700	1.12947000
H	3.14423500	0.41971800	1.40120700
H	-0.01524300	-1.18208100	-1.56111300
O	0.79065400	0.98592600	-1.92556800
H	0.66973300	1.74725600	-2.50567200
H	-2.11409500	-1.19632700	-0.54368900
H	-0.35725100	0.09481300	1.04957500
O	-3.12225900	-1.12533000	-0.40245300
H	-3.00250200	0.30702200	0.81994400
H	-3.28180300	1.34112900	1.95304600
O	-2.59302300	1.00862600	1.36623000

S_2^{A1}-[(OH·)·H_2O)]

C	0.19038400	-0.06260300	0.01992100
H	-0.72807800	1.57453600	-1.01663200
C	0.27258400	1.14532600	-0.92409500
H	0.60877600	0.82620500	-1.91463800
N	-0.40580200	0.34311600	1.29934000
H	-0.20355900	-0.36283100	2.00564400
H	0.05338100	1.19944200	1.61018200
C	1.53444300	-0.76257800	0.22253000
O	1.92085400	-1.22693000	1.27375600
O	2.25550800	-0.85011000	-0.92237700
H	3.05460700	-1.36872700	-0.72410800
H	-3.73669300	0.57501400	1.29865300
O	1.10592000	2.17777500	-0.39322200
H	2.02359900	1.99985100	-0.63725800
H	-2.17660300	0.50118600	1.00188400
H	-0.46806300	-0.80304100	-0.46030600
O	-3.08583200	0.46922100	0.59565600
H	-3.04346400	-0.81383300	-0.60944000
O	-2.76242100	-1.52626600	-1.24875000

TS‴2^{A1}

C	0.13927800	0.04470200	-0.10958900
H	-0.55529200	1.82047700	-1.10132000
C	0.39446300	1.37523800	-0.79123000
H	1.00438700	1.21583900	-1.68416400
N	-0.58576900	0.27834000	1.19150000
H	-0.28543200	-0.46182400	1.83967900
H	-0.30479300	1.18573800	1.58144900
C	1.29381400	-0.81849600	0.18536700
O	1.41516900	-1.48615300	1.20991400
O	2.20569600	-0.86805300	-0.81527800
H	2.86227700	-1.54042200	-0.56814500
H	-3.93821500	-0.36894800	0.69009300
O	0.99189600	2.34404100	0.09505900
H	1.94661100	2.19623600	0.12654700
H	-1.63679500	0.23643900	1.05581500
H	-0.72964800	-0.58537600	-0.87743800
O	-3.12844100	0.04594900	0.37264300
H	-2.77700900	-0.47579200	-0.44526500
O	-1.79070100	-1.13321100	-1.44546700

$3'^{A1}$-$2H_2O$

C	0.64024800	0.25651800	0.33984100
H	-0.92006400	1.34608200	-0.64185600
C	0.08114800	1.52767300	-0.22979900
H	0.72316400	1.89149100	-1.03621000
N	0.07576100	-0.21945600	1.50569000
H	0.63207000	-0.91845200	1.98926500
H	-0.33458200	0.49661500	2.09719800
C	1.63180700	-0.58720600	-0.27331600
O	2.01751400	-1.65463700	0.21131400
O	2.12805600	-0.10370500	-1.44979400
H	2.78024000	-0.75272100	-1.75933500
H	-2.01146000	-2.66405000	0.23977500
O	-0.09976700	2.51710500	0.79998700
H	0.76028500	2.90362900	1.01351600
H	-1.50018600	-1.36339700	0.91825100
H	-3.70406500	0.51468300	-1.41750900
O	-2.29306400	-1.79000200	0.53778000
H	-2.77912000	-0.54978700	-0.76192300
O	-2.78971700	0.21251200	-1.37445700

S_2^{A1}·(H_2O·OH^-)

C	0.17410300	-0.25840900	-0.08892400
H	0.38883000	-2.34884100	0.24742100
C	0.97637900	-1.45477800	0.45061700
H	1.10641900	-1.35321700	1.53389100
N	-0.49971200	-0.53811800	-1.35473600
H	-1.47940900	-0.25907700	-1.28442700
H	-0.08235900	-0.00968200	-2.11266400
C	1.00629900	0.99107700	-0.13458100
O	0.99652300	1.85529600	-0.98140100
O	1.87062500	1.09512700	0.93622100
H	2.28917000	1.96267300	0.84285000
O	2.25715700	-1.67477700	-0.17141000
H	2.82535100	-0.95076100	0.11212300
H	-3.70220200	-1.00821500	-0.56279800
H	-0.62071000	-0.05650300	0.68828000
O	-3.54170200	-0.06055200	-0.56447100
H	-3.04041400	0.11054100	0.34471400
H	-2.52000600	-0.02268300	2.35969100
O	-2.15852500	0.28931200	1.52498500

TS′′′2^{A1}

C	0.10877700	0.04861900	0.13963600
H	-0.65025300	1.94772000	-0.43686600
C	0.27354000	1.38509000	-0.56383600
H	0.44233900	1.22739700	-1.63431400
N	-0.56326800	0.16953900	1.43731800
H	-0.93985700	-0.73591500	1.69957100
H	0.09090800	0.43667800	2.16856700
C	1.33030900	-0.77619800	0.17495300
O	1.66021200	-1.59088800	1.01786700
O	2.14858300	-0.59100300	-0.93338400
H	2.84274100	-1.25839200	-0.84146300
O	1.32454600	2.23521800	-0.03857600
H	2.15385600	1.78782500	-0.23869900
H	-2.82776100	0.59065300	0.84112800
H	-0.69626700	-0.57352700	-0.56839000
O	-3.54091700	0.26701400	0.27509100
H	-3.03529700	-0.32116400	-0.35523800
H	-1.79424300	-1.06601800	-2.15241400
O	-1.83230600	-1.21622700	-1.20195200

3′′^{A1}·2H$_2$O

C	0.27399500	0.20810300	0.22133300
H	-0.76716600	1.65652500	-0.94897500
C	0.25203900	1.30451000	-0.76831000
H	0.69672400	0.98235400	-1.71454800
N	-0.58955400	0.38221000	1.39064700
H	-0.45983900	-0.43446400	1.98386100
H	-0.27889500	1.17986600	1.94684000
C	1.31344400	-0.72214600	0.32416500
O	1.53850500	-1.52820600	1.25065800
O	2.17422900	-0.79096800	-0.79850400
H	2.72904500	-1.55202600	-0.58737100
O	0.95512500	2.53679400	-0.33800100
H	1.82091600	2.23635500	-0.03913700
H	-2.48368700	0.34976300	0.86990200
H	-0.93965500	-1.06749700	-0.84893900
O	-3.35576300	0.15518700	0.45939200
H	-3.10556600	-0.44872600	-0.25483300

H	-1.41162900	-1.28382700	-2.29292900
O	-1.65087600	-1.50238200	-1.38748600

$5'^{A1}\cdot 2H_2O$

C	-0.27399600	0.20810300	0.22133300
H	0.76716500	1.65652500	-0.94897500
C	-0.25204000	1.30451000	-0.76831000
H	-0.69672500	0.98235500	-1.71454800
N	0.58955300	0.38221000	1.39064700
H	0.45983800	-0.43446400	1.98386100
H	0.27889500	1.17986600	1.94684100
C	-1.31344400	-0.72214700	0.32416500
O	-1.53850400	-1.52820700	1.25065700
O	-2.17422900	-0.79096900	-0.79850400
H	-2.72904400	-1.55202800	-0.58737100
O	-0.95512600	2.53679500	-0.33800100
H	-1.82091600	2.23635600	-0.03913600
H	2.48368700	0.34976300	0.86990300
H	0.93965500	-1.06749800	-0.84894100
O	3.35576300	0.15518600	0.45939300
H	3.10556600	-0.44872700	-0.25483200
H	1.41163400	-1.28382000	-2.29293000
O	1.65087700	-1.50238100	-1.38748700

$TS''''5^{A1}$

C	-0.10877700	0.04861900	0.13963600
H	0.65025200	1.94772000	-0.43686800
C	-0.27354200	1.38509000	-0.56383700
H	-0.44234100	1.22739600	-1.63431500
N	0.56326800	0.16954000	1.43731700
H	0.93985900	-0.73591300	1.69957000
H	-0.09090800	0.43667900	2.16856700
C	-1.33030800	-0.77619900	0.17495300
O	-1.66021100	-1.59088900	1.01786800
O	-2.14858300	-0.59100400	-0.93338300
H	-2.84274100	-1.25839300	-0.84146300
O	-1.32454800	2.23521700	-0.03857600
H	-2.15385700	1.78782400	-0.23869900
H	2.82776000	0.59065300	0.84112900
H	0.69626600	-0.57352600	-0.56839000
O	3.54091600	0.26701500	0.27509300

H	3.03529600	-0.32116400	-0.35523800
H	1.79424600	-1.06601600	-2.15241500
O	1.83230800	-1.21622600	-1.20195300

R_6^{A1}·(H_2O·OH^-)

C	-0.17410300	0.25840700	0.08892500
H	-0.38882200	2.34884000	-0.24741500
C	-0.97637300	1.45478000	-0.45061400
H	-1.10641200	1.35322200	-1.53388900
N	0.49971200	0.53811000	1.35473900
H	1.47941000	0.25907100	1.28442800
H	0.08236100	0.00966900	2.11266400
C	-1.00630300	-0.99107700	0.13457900
O	-0.99653000	-1.85529700	0.98139700
O	-1.87062900	-1.09512000	-0.93622300
H	-2.28917800	-1.96266500	-0.84285400
O	-2.25715200	1.67478200	0.17141200
H	-2.82534700	0.95076800	-0.11212300
H	3.70220100	1.00821400	0.56279900
H	0.62071000	0.05650000	-0.68828000
O	3.54170400	0.06055000	0.56447000
H	3.04041500	-0.11054200	-0.34471400
H	2.52000400	0.02268500	-2.35969000
O	2.15852500	-0.28931300	-1.52498500