Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Protonation State Control of Electric Field Induced Molecular Switching Mechanism

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1.1 Electric Field Modification of the Ground State Potential Energy Surface of HO−AB−OH

Table S1: Relative energies in kcal mol^{-1} of optimized S_0 stationary points of HO-AB-OH under F_{NN} field computed using B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{NN} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_0 trans	-1.78	0.18	1.12	1.06	0.00	-2.05	-5.10	-9.15	-14.23
S_0 rot ts	32.99	42.71	45.13	45.93	45.22	43.00	39.27	34.01	27.19
S_0 rot inv ts	42.45	45.18	46.24	45.89	44.21	41.19	36.80	31.00	23.59
S_0 inv ts	32.36	38.32	42.66	45.47	46.78	46.60	44.90	41.60	36.65
S_0 cis	12.58	15.52	17.21	17.71	17.05	15.23	12.23	8.02	2.54

Table S2: Relative energies in kcal mol^{-1} of optimized S_0 stationary points of HO-AB-OH under F_{OC} field computed using B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{OC} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_0 trans	-13.48	-7.51	-3.34	-0.86	0.00	-0.75	-3.11	-7.17	-13.03
S_0 rot ts	38.68	42.66	45.03	45.88	45.22	43.02	39.24	33.82	26.70
S_0 rot inv ts	43.23	45.22	46.05	45.72	44.21	41.34	36.99	30.84	23.38
S_0 inv ts	40.91	44.23	46.31	47.16	46.79	45.17	42.26	38.01	32.34
S_0 cis	17.92	19.11	19.35	18.67	17.05	14.50	11.01	6.55	1.11

Table S3: HO-AB-OH molecules ΔG relative barrier heights from the S_0 cis structure in kcal mol^{-1} for the three transition states examined in all two electric fields.

Structure	Field Strength (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
F_{NN} S_0 rot ts	20.56	26.90	27.96	28.44	28.46	28.05	27.26	26.11	24.59
F_{NN} S_0 rot inv ts	28.60	28.14	27.70	27.02	26.05	23.38	22.39	20.78	18.39
F_{NN} S_0 inv ts	18.78	21.50	25.40	27.64	29.51	31.02	32.14	32.88	33.18
F_{OC} S_0 rot ts	20.20	23.24	25.80	27.49	28.46	28.78	28.43	27.36	25.45
F_{OC} S_0 rot inv ts	23.92	24.86	25.63	26.12	26.05	23.70	23.47	21.38	21.12
F_{OC} S_0 inv ts	22.85	24.95	26.78	28.31	29.51	30.35	30.84	30.93	30.56

1.2 Electric Field Modification of the Ground State Potential Energy Surface of HO−AB−O$^-$

Table S4: Relative energies in kcal mol^{-1} of optimized S_0 stationary points of HO-AB-O$^-$ under F_{NN} field computed using B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{NN} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_0 trans	3.27	4.42	4.25	2.77	0.00	-4.05	-9.35	-15.91	-23.70
S_0 rot ts	23.55	27.07	29.32	30.28	29.89	28.09	24.81	19.92	13.29
S_0 rot inv ts	46.24	48.03	47.85	45.78	41.89	36.22	28.79	19.61	8.55
S_0 inv ts	46.29	48.05	47.79	45.61	41.58	35.75	28.14	18.74	7.43
S_0 cis	24.34	25.08	24.10	21.40	17.02	10.95	3.24	-6.10	-17.14

Table S5: Relative energies in kcal mol^{-1} of optimized S_0 stationary points of HO-AB-O$^-$ under F_{OC} field computed using B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{OC} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_0 trans	10.09	11.17	9.82	6.08	0.00	-8.37	-18.95	-31.69	-46.54
S_0 rot ts	24.19	27.88	30.07	30.77	29.89	27.33	22.93	16.46	7.69
S_0 rot inv ts	49.27	50.66	49.75	46.79	41.89	35.11	26.47	15.96	3.49
S_0 inv ts	50.33	51.09	49.48	46.28	41.58	35.44	27.83	18.71	8.01
S_0 cis	24.55	24.44	23.13	20.65	17.02	12.24	6.32	-0.75	-9.02

Table S6: HO-AB-O$^-$ molecules ΔG relative barrier heights from the S_0 cis structure in kcal mol^{-1} for the three transition states examined in all two electric fields.

Structure	Field Strength (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
F_{NN} S_0 rot ts	-1.52	1.10	4.18	7.64	11.31	15.97	20.41	24.89	29.45
F_{NN} S_0 rot inv ts	20.52	21.61	22.45	23.13	23.71	24.14	24.38	24.51	24.46
F_{NN} S_0 inv ts	20.63	21.70	22.47	23.04	23.49	23.76	23.82	23.71	23.38
F_{OC} S_0 rot ts	-1.46	2.41	5.95	9.05	11.31	13.86	15.53	16.33	16.28
F_{OC} S_0 rot inv ts	22.96	24.66	25.24	24.90	23.71	21.68	18.90	15.38	11.19
F_{OC} S_0 inv ts	24.32	25.09	25.05	24.49	23.49	22.16	20.41	18.22	15.60

2 Photoisomerization Pathways of 4,4'-dihydroxyazobenzene

2.1 Electric Field Modification of Excited State Potential Energy Surfaces of HO−AB−OH

Table S7: Relative energies in kcal mol^{-1} of S_1 and S_2 transition energies from the relative S_0 stationary points of HO-AB-OH under F_{NN} field computed using TD-B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{NN} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_1 trans	59.72	61.91	63.02	63.06	62.03	59.94	56.79	52.57	47.25
S_1 rot ts	35.96	44.72	48.93	50.49	50.15	48.04	44.14	38.38	30.59
S_1 rot inv ts	51.74	55.86	59.58	62.25	63.62	63.67	62.43	59.95	57.23
S_1 inv ts	58.68	63.94	67.48	69.49	70.10	69.40	67.47	64.21	59.61
S_1 cis	70.84	73.83	75.33	75.65	74.85	72.98	70.03	65.94	60.62
S_2 trans	59.14	75.78	78.21	79.17	78.51	76.19	72.26	66.88	60.16
S_2 rot ts	86.52	98.67	109.91	115.03	114.12	111.48	107.14	101.11	85.34
S_2 rot inv ts	63.23	80.77	95.41	102.54	108.14	112.01	105.27	89.59	75.63
S_2 inv ts	64.56	89.25	105.23	112.73	113.68	109.33	103.77	90.06	72.92
S_2 cis	71.79	89.15	102.19	105.61	106.53	103.16	97.48	89.64	78.21

Table S8: Relative energies in kcal mol^{-1} of S_1 and S_2 transition energies from the relative S_0 stationary points of HO-AB-OH under F_{OC} field computed using TD-B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{OC} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_1 trans	39.97	53.52	58.29	61.09	62.03	61.14	58.40	53.71	39.39
S_1 rot ts	40.79	46.34	49.45	50.67	50.13	47.80	43.62	37.43	28.77
S_1 rot inv ts	53.08	57.44	60.68	62.75	63.62	63.52	62.77	60.46	55.72
S_1 inv ts	64.10	67.42	69.52	70.40	70.10	68.60	65.90	61.95	56.68
S_1 cis	75.79	76.97	77.19	76.47	74.85	72.33	68.92	64.61	59.35
S_2 trans	46.70	63.38	71.80	76.64	78.51	76.99	72.47	62.90	46.99
S_2 rot ts	86.62	99.37	111.05	114.84	114.13	111.77	107.77	102.11	94.72
S_2 rot inv ts	67.29	84.45	95.83	102.66	108.13	112.36	114.05	110.42	97.61
S_2 inv ts	77.46	94.47	107.22	113.53	113.68	109.53	104.15	97.53	89.10
S_2 cis	86.42	98.60	106.55	108.36	106.53	102.35	96.71	90.22	82.98

2.2 Electric Field Modification of Excited State Potential Energy Surfaces of HO−AB−O$^-$

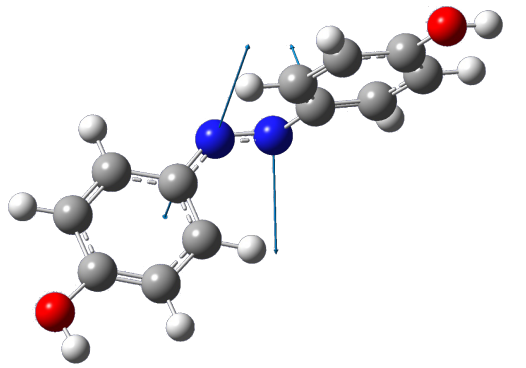
Table S9: Relative energies in kcal mol^{-1} of S_1 and S_2 transition energies from the relative S_0 stationary points of deprotonated HO-AB-O$^-$ under F_{NN} field computed using TD-B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{NN} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_1 trans	34.11	48.23	57.62	62.39	64.49	60.75	55.74	49.39	31.66
S_1 rot ts	47.86	47.33	45.71	43.21	39.87	35.62	30.10	22.39	16.83
S_1 rot inv ts	61.65	77.85	80.69	77.85	73.10	66.44	57.92	47.70	36.38
S_1 inv ts	61.36	77.52	81.25	78.41	73.61	66.86	58.19	47.79	36.20
S_1 cis	51.09	62.88	71.45	77.63	75.24	69.73	61.76	51.52	39.23
S_2 trans	45.79	54.32	64.22	66.91	64.96	63.00	58.43	49.47	41.80
S_2 rot ts	49.91	64.15	74.38	81.09	85.44	87.36	75.80	59.50	41.15
S_2 rot inv ts	72.41	81.65	88.31	93.91	96.62	95.79	92.65	79.25	57.81
S_2 inv ts	71.33	82.07	87.76	93.57	96.45	95.62	92.52	79.19	57.28
S_2 cis	58.16	70.88	78.81	78.82	83.34	85.04	81.18	62.54	40.70

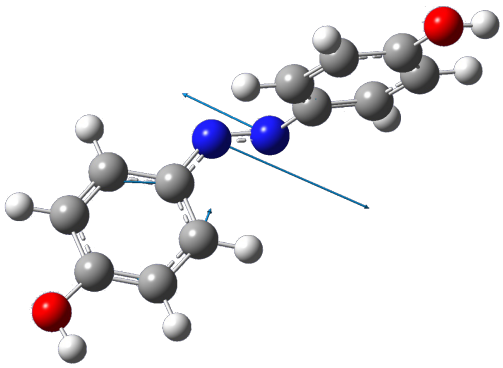
Table S10: Relative energies in kcal mol^{-1} of S_1 and S_2 transition energies from the relative S_0 stationary points of deprotonated HO-AB-O$^-$ under F_{OC} field computed using TD-B3LYP. Energies are shown relative to the zero-field S_0 trans.

Structure	F_{OC} field (10^{-3} a.u.)								
	-10.0	-7.5	-5.0	-2.5	0.0	2.5	5.0	7.5	10.0
S_1 trans	16.82	31.86	44.86	55.88	64.51	56.16	45.40	32.27	16.86
S_1 rot ts	45.00	50.53	47.94	44.35	39.88	34.40	27.25	18.75	13.00
S_1 rot inv ts	57.61	69.50	80.75	78.33	73.11	65.78	56.38	45.06	32.32
S_1 inv ts	59.82	65.05	76.98	78.06	73.62	67.41	59.43	49.73	38.29
S_1 cis	43.09	54.41	65.02	74.66	75.26	71.46	65.88	58.50	47.11
S_2 trans	40.31	57.46	70.44	70.11	64.98	59.10	49.58	37.83	19.66
S_2 rot ts	52.97	58.29	69.36	78.47	85.44	87.92	73.45	55.37	34.74
S_2 rot inv ts	66.26	82.41	81.50	89.99	96.62	96.20	92.01	71.19	46.55
S_2 inv ts	77.68	81.81	80.76	87.77	96.48	96.33	90.99	70.79	47.97
S_2 cis	68.63	76.49	77.87	77.52	83.34	85.35	82.51	66.08	49.51

2.3 S_0/S_1 Branching Space Normal Modes



(a) Gradient Difference X_1



(b) Derivative Coupling X_2

Figure S1: Gradient difference (a) and derivative coupling (b) vectors that define the branching space of the anti and syn protonated derivatives of AB around the S_0/S_1 CI computed using CAS(10,8)/6-31+G(d)

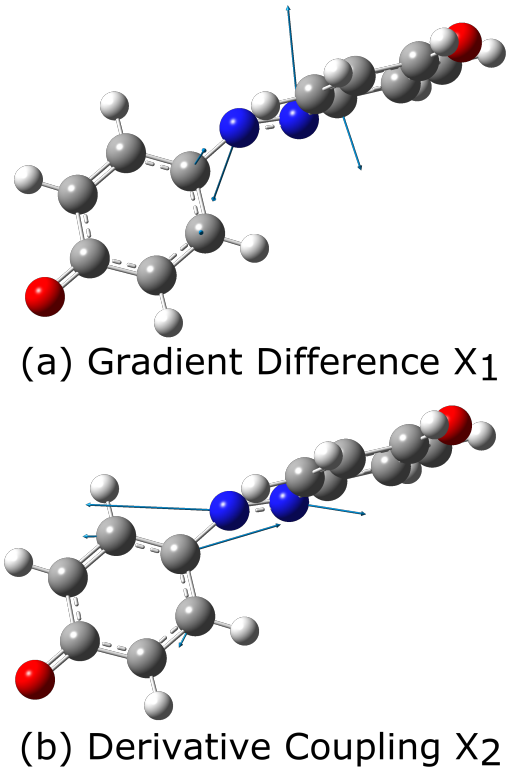


Figure S2: Gradient difference (a) and derivative coupling (b) vectors that define the branching space of the anti and syn deprotonated derivatives of AB around the S_0/S_1 CI computed using CAS(10,8)/6-31+G(d).

2.4 Potential Energy Surfaces of Deprotonated Molecule Under Applied Field

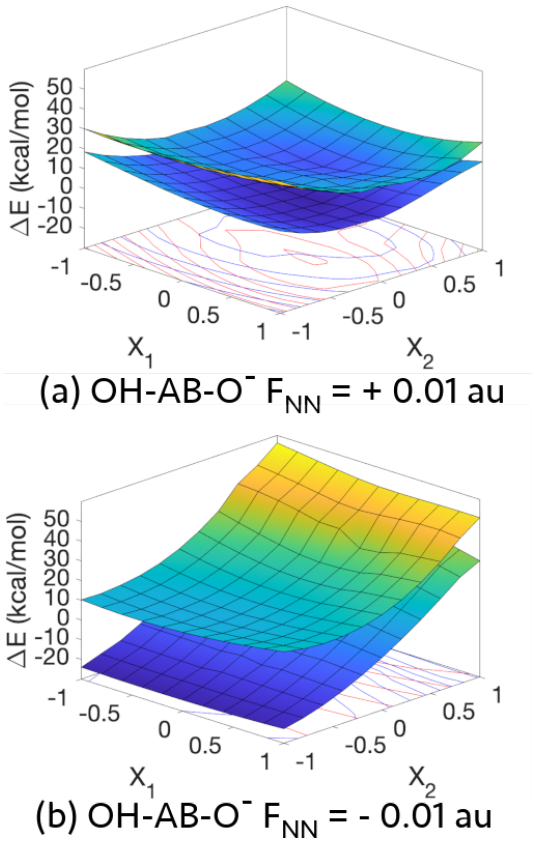


Figure S3: S_0 and S_1 potential energy surfaces of HO−AB−O$^-$ under F_{NN} field in the S_0/S_1 branching space. The difference between potential energy surfaces are shown in fig. **??**.

3 Cartesian coordinates and energies of protonated OH−AB−O structures in field free conditions

3.1 Field Free OH−AB−OH Trans Structure S_0 State

E_h = -723.3779

Cartesian Coordinates:

N	-0.00128	0.00192	-0.62662
N	0.00021	-0.00016	0.62917
C	-1.63098	1.89578	-0.53855
C	-2.41183	2.80297	-1.23120
C	-2.41157	2.80258	-2.63255
C	-1.62373	1.88723	-3.33267
H	-0.22229	0.25891	-3.15788
H	-1.62424	1.88798	0.54417
H	-3.03234	3.52400	-0.71059
H	-1.62170	1.88476	-4.41983
C	-0.84061	0.97742	-2.63111
C	-0.83271	0.96824	-1.23266
C	0.83167	-0.96659	1.23674
C	0.83966	-0.97584	2.63818
C	1.62763	-1.89171	0.54396
C	1.61912	-1.88170	3.34265
H	0.22039	-0.25602	3.16217
C	2.40834	-2.79906	1.24276
H	1.62296	-1.88635	-0.53884
C	2.40720	-2.79771	2.64428
H	1.63032	-1.89469	4.42646
H	3.02392	-3.51464	0.70212
O	3.15800	-3.67052	3.37796
H	3.66018	-4.25460	2.79682
O	-3.20427	3.72357	-3.25436
H	-3.13162	3.63913	-4.21287

3.2 Field Free OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3058

Cartesian Coordinates:

N	-1.28728	-1.24392	-0.54024
N	-1.28728	-1.24392	0.76630
C	1.15263	-1.26580	-0.62002
C	2.29877	-1.23145	-1.39471
C	2.21155	-1.30819	-2.78695
C	0.95370	-1.40757	-3.40982
H	-1.17134	-1.49208	-3.12017
H	1.21557	-1.19841	0.45836
H	3.27802	-1.13704	-0.93806
H	0.88895	-1.46442	-4.49399
C	-0.19616	-1.42354	-2.65148
C	-0.13279	-1.34011	-1.23199
C	-1.29239	-0.00756	1.34283
C	-1.29261	0.04453	2.76556
C	-1.15967	1.21197	0.62686
C	-1.16027	1.23862	3.43475
H	-1.38562	-0.88937	3.30851
C	-1.02470	2.41053	1.30960
H	-1.14064	1.19170	-0.45433
C	-1.02815	2.43479	2.70796
H	-1.14680	1.28086	4.51796
H	-0.89582	3.33608	0.75287
O	-0.87577	3.58229	3.42606
H	-0.80380	4.34360	2.83696
O	3.37642	-1.25489	-3.49642
H	3.19879	-1.31257	-4.44316

3.3 Field Free OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3074

Cartesian Coordinates:

N	0.98742	-0.75489	-1.29485
N	0.98742	-0.75489	-0.07228
C	-0.84900	0.96675	-1.32185
C	-1.70375	1.76260	-2.06295
C	-1.65223	1.72376	-3.46387
C	-0.74243	0.88597	-4.11454
H	0.82839	-0.57107	-3.84266
H	-0.87867	0.99026	-0.23775
H	-2.41907	2.42253	-1.58523
H	-0.70390	0.85844	-5.20046
C	0.11322	0.08885	-3.36327
C	0.06416	0.12458	-1.97068
C	0.91462	-0.84606	1.26123
C	1.63007	0.04990	2.09602
C	0.13967	-1.85914	1.87526
C	1.56902	-0.07683	3.47598
H	2.23699	0.82723	1.64663
C	0.07882	-1.94578	3.26332
H	-0.40862	-2.56213	1.25947
C	0.79122	-1.06649	4.07463
H	2.12842	0.60600	4.10653
H	-0.53367	-2.72718	3.70829
O	0.76774	-1.11847	5.45464
H	0.22728	-1.86160	5.74597
O	-2.51953	2.53118	-4.13442
H	-2.40703	2.43576	-5.08823

3.4 Field Free OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3033

Cartesian Coordinates:

N	0.96424	-0.91484	-1.28492
N	0.96437	-0.91475	-0.03953
C	-0.47814	1.15997	-1.41711
C	-1.26535	2.00272	-2.18651
C	-1.49703	1.69882	-3.53255
C	-0.91811	0.56302	-4.10442
H	0.36327	-1.13982	-3.75701
H	-0.27945	1.40393	-0.37992
H	-1.70414	2.90355	-1.77120
H	-1.09056	0.33124	-5.15286
C	-0.11191	-0.26294	-3.32941
C	0.09635	0.01111	-1.97642
C	0.87055	-0.84421	1.30279
C	1.81204	-1.54989	2.10133
C	-0.20004	-0.20725	1.98361
C	1.72801	-1.56847	3.48005
H	2.61295	-2.07128	1.59015
C	-0.31781	-0.26954	3.36405
H	-0.95668	0.31024	1.40633
C	0.65572	-0.93320	4.11829
H	2.45912	-2.09492	4.08340
H	-1.15890	0.20865	3.86119
O	0.60919	-1.00467	5.47713
H	-0.16964	-0.54580	5.81538
O	-2.29025	2.55913	-4.23880
H	-2.37570	2.26312	-5.15314

3.5 Field Free OH−AB−OH Cis Structure S_0 State

E_h = -723.3507

Cartesian Coordinates:

N	0.50021	-2.26792	-0.35763
N	0.48368	-2.12615	0.88121
C	1.05689	0.02044	-1.20722
C	0.99868	0.94203	-2.24162
C	0.23050	0.67203	-3.37782
C	-0.44775	-0.54381	-3.48659
H	-0.83621	-2.44826	-2.55834
H	1.65727	0.23880	-0.33244
H	1.54485	1.87711	-2.18778
H	-1.02743	-0.77016	-4.37813
C	-0.35143	-1.48245	-2.46487
C	0.36373	-1.19628	-1.29893
C	0.11487	-0.91722	1.55456
C	0.83430	-0.60312	2.71474
C	-1.02094	-0.16423	1.23505
C	0.48373	0.48823	3.49597
H	1.67870	-1.22623	2.98927
C	-1.40135	0.90416	2.03878
H	-1.61915	-0.41978	0.36890
C	-0.63985	1.24652	3.15972
H	1.05101	0.75095	4.38161
H	-2.29490	1.47256	1.79201
O	-0.95586	2.29750	3.97413
H	-1.75058	2.74299	3.65661
O	0.19872	1.62850	-4.35372
H	-0.33795	1.33202	-5.09870

4 Cartesian coordinates and energies of protonated OH−AB−O structures in F_{NN} conditions

4.1 F_{NN} -0.0025 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3762

Cartesian Coordinates:

N	0.00150	-0.00132	-0.63066
N	0.00338	-0.00390	0.62536
C	-1.62836	1.89274	-0.53993
C	-2.41136	2.80247	-1.22830
C	-2.41368	2.80505	-2.62828
C	-1.62746	1.89152	-3.33150
H	-0.22429	0.26115	-3.16326
H	-1.61943	1.88244	0.54280
H	-3.02996	3.52134	-0.70242
H	-1.62825	1.89234	-4.41940
C	-0.84197	0.97894	-2.63426
C	-0.83119	0.96643	-1.23682
C	0.83377	-0.96904	1.23134
C	0.83929	-0.97546	2.63405
C	1.63097	-1.89557	0.54076
C	1.61671	-1.87893	3.34160
H	0.21962	-0.25525	3.15654
C	2.41006	-2.80100	1.24284
H	1.62802	-1.89218	-0.54206
C	2.40631	-2.79665	2.64589
H	1.62636	-1.89013	4.42513
H	3.02729	-3.51845	0.70658
O	3.15254	-3.66407	3.38291
H	3.65940	-4.25378	2.81161
O	-3.20829	3.72828	-3.25288
H	-3.13056	3.63791	-4.20995

4.2 F_{NN} -0.0025 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3047

Cartesian Coordinates:

N	-1.28836	-1.23016	-0.54525
N	-1.28807	-1.23316	0.76130
C	1.15148	-1.24146	-0.62737
C	2.30043	-1.21838	-1.40218
C	2.21675	-1.31433	-2.79091
C	0.96040	-1.42194	-3.41194
H	-1.16653	-1.50687	-3.12617
H	1.21731	-1.16182	0.44995
H	3.27755	-1.12217	-0.94112
H	0.89660	-1.49614	-4.49593
C	-0.19270	-1.42796	-2.65578
C	-0.13397	-1.32588	-1.23757
C	-1.29187	0.00132	1.34042
C	-1.29169	0.04312	2.76421
C	-1.16312	1.22444	0.62889
C	-1.16013	1.23185	3.44058
H	-1.38299	-0.89431	3.30095
C	-1.02905	2.41755	1.31682
H	-1.14745	1.20637	-0.45251
C	-1.03152	2.43234	2.71846
H	-1.14550	1.26984	4.52361
H	-0.90126	3.34798	0.76822
O	-0.88323	3.56978	3.44065
H	-0.81217	4.34083	2.86393
O	3.38575	-1.27256	-3.50843
H	3.19662	-1.36416	-4.44961

4.3 F_{NN} -0.0025 au OH−AB−OH Rotation Inversion TS Structure

S_0 State

E_h = -723.3047

Cartesian Coordinates:

N	0.98068	-0.76500	-1.29450
N	0.98199	-0.76292	-0.07336
C	-0.86293	0.95614	-1.32598
C	-1.71750	1.75499	-2.06670
C	-1.65389	1.72813	-3.46568
C	-0.73581	0.90023	-4.11611
H	0.83924	-0.55580	-3.84260
H	-0.89966	0.96982	-0.24183
H	-2.43946	2.40631	-1.58706
H	-0.68890	0.88356	-5.20264
C	0.11736	0.09869	-3.36505
C	0.05788	0.12376	-1.97424
C	0.90968	-0.85176	1.26690
C	1.63275	0.04199	2.09362
C	0.13904	-1.86416	1.88106
C	1.57652	-0.08176	3.47356
H	2.24025	0.81698	1.64082
C	0.07847	-1.94682	3.27034
H	-0.41081	-2.56868	1.26821
C	0.79548	-1.06707	4.07789
H	2.14016	0.59869	4.10245
H	-0.53490	-2.72487	3.71872
O	0.78021	-1.10797	5.45136
H	0.23021	-1.83546	5.76444
O	-2.52035	2.53776	-4.14379
H	-2.38917	2.44447	-5.09493

4.4 F_{NN} -0.0025 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3054

Cartesian Coordinates:

N	0.97838	-0.90249	-1.28268
N	0.96859	-0.91227	-0.03756
C	-0.47020	1.17109	-1.42158
C	-1.25713	2.01446	-2.19349
C	-1.49329	1.70442	-3.53543
C	-0.92085	0.56370	-4.10263
H	0.35655	-1.14330	-3.74915
H	-0.27131	1.41683	-0.38476
H	-1.69316	2.91684	-1.77852
H	-1.09958	0.32646	-5.14961
C	-0.11487	-0.26190	-3.32583
C	0.09960	0.01840	-1.97591
C	0.86303	-0.85379	1.30443
C	1.81032	-1.55268	2.10292
C	-0.20802	-0.21549	1.98499
C	1.72657	-1.57119	3.48005
H	2.61545	-2.06808	1.59228
C	-0.32437	-0.27366	3.36412
H	-0.96553	0.30066	1.40725
C	0.65218	-0.93675	4.11968
H	2.46009	-2.09091	4.08590
H	-1.16413	0.20468	3.86226
O	0.61306	-1.00964	5.47100
H	-0.15887	-0.55181	5.82740
O	-2.28590	2.56448	-4.25252
H	-2.39452	2.23587	-5.15270

4.5 F_{NN} -0.0025 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3496

Cartesian Coordinates:

N	0.52793	-2.25981	-0.35359
N	0.50698	-2.11993	0.88487
C	1.10046	0.01115	-1.22644
C	1.04356	0.92880	-2.26607
C	0.24601	0.67038	-3.38259
C	-0.46753	-0.52593	-3.46683
H	-0.89196	-2.41188	-2.51391
H	1.71937	0.22078	-0.36230
H	1.60967	1.85270	-2.22487
H	-1.07541	-0.74109	-4.34300
C	-0.37601	-1.46046	-2.43993
C	0.37589	-1.18794	-1.29497
C	0.11853	-0.92006	1.55783
C	0.83291	-0.59811	2.72017
C	-1.01778	-0.17234	1.22724
C	0.47473	0.49487	3.49341
H	1.67548	-1.21890	3.00469
C	-1.40790	0.89636	2.02550
H	-1.61307	-0.43677	0.36164
C	-0.65274	1.24641	3.14958
H	1.03244	0.76148	4.38366
H	-2.30532	1.45724	1.77613
O	-0.97246	2.29539	3.95756
H	-1.80057	2.70516	3.67936
O	0.21710	1.61867	-4.37449
H	-0.38657	1.34204	-5.07389

4.6 F_{NN} -0.0050 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3761

Cartesian Coordinates:

N	0.00412	-0.00440	-0.63493
N	0.00646	-0.00751	0.62198
C	-1.62564	1.88957	-0.54117
C	-2.41084	2.80187	-1.22532
C	-2.41550	2.80718	-2.62399
C	-1.63097	1.89561	-3.33056
H	-0.22617	0.26329	-3.16902
H	-1.61447	1.87666	0.54155
H	-3.02748	3.51848	-0.69410
H	-1.63474	1.89988	-4.41919
C	-0.84313	0.98026	-2.63764
C	-0.82934	0.96425	-1.24077
C	0.83550	-0.97109	1.22612
C	0.83894	-0.97508	2.63044
C	1.63402	-1.89912	0.53773
C	1.61426	-1.87607	3.34081
H	0.21884	-0.25438	3.15147
C	2.41140	-2.80255	1.24284
H	1.63288	-1.89784	-0.54523
C	2.40555	-2.79574	2.64764
H	1.62252	-1.88566	4.42427
H	3.03016	-3.52177	0.71055
O	3.14720	-3.65781	3.38729
H	3.65857	-4.25278	2.82554
O	-3.21223	3.73291	-3.25143
H	-3.12949	3.63670	-4.20716

4.7 F_{NN} -0.0050 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3059

Cartesian Coordinates:

N	-1.28506	-1.20793	-0.55374
N	-1.28397	-1.21695	0.75400
C	1.15540	-1.20799	-0.64076
C	2.30604	-1.20410	-1.41676
C	2.22403	-1.32428	-2.80171
C	0.96804	-1.43580	-3.41924
H	-1.16058	-1.51497	-3.13429
H	1.22601	-1.11420	0.43510
H	3.28202	-1.11013	-0.95256
H	0.90369	-1.52954	-4.50264
C	-0.18728	-1.42605	-2.66385
C	-0.13165	-1.30145	-1.24691
C	-1.28631	0.01344	1.33811
C	-1.28522	0.04134	2.76354
C	-1.16741	1.24368	0.63498
C	-1.16048	1.22321	3.45087
H	-1.37067	-0.90155	3.29138
C	-1.04063	2.42941	1.33168
H	-1.15593	1.23154	-0.44673
C	-1.04232	2.43087	2.73726
H	-1.14531	1.25365	4.53398
H	-0.91999	3.36719	0.79417
O	-0.90571	3.55723	3.46639
H	-0.84043	4.34001	2.90457
O	3.39662	-1.30083	-3.52868
H	3.20039	-1.48170	-4.45492

4.8 F_{NN} -0.0050 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3042

Cartesian Coordinates:

N	0.9662	-0.77731	-1.29243
N	0.96890	-0.77086	-0.07230
C	-0.88369	0.94444	-1.33268
C	-1.73664	1.74550	-2.07552
C	-1.65532	1.73287	-3.47223
C	-0.72502	0.91714	-4.11971
H	0.85445	-0.53659	-3.84021
H	-0.93137	0.94745	-0.24873
H	-2.46808	2.38643	-1.59610
H	-0.66514	0.91335	-5.20663
C	0.12352	0.11137	-3.36655
C	0.04884	0.12392	-1.97749
C	0.89676	-0.85441	1.27460
C	1.63222	0.03497	2.09201
C	0.13436	-1.86846	1.89154
C	1.58794	-0.08872	3.47182
H	2.23921	0.80762	1.63433
C	0.07804	-1.94758	3.28186
H	-0.41855	-2.57447	1.28291
C	0.80474	-1.06945	4.08406
H	2.16047	0.58691	4.09751
H	-0.53575	-2.72168	3.73539
O	0.80362	-1.10162	5.45080
H	0.24774	-1.81461	5.78715
O	-2.51952	2.54405	-4.16055
H	-2.36133	2.45898	-5.10796

4.9 F_{NN} -0.0050 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3099

Cartesian Coordinates:

N	0.98887	-0.89106	-1.28011
N	0.97110	-0.90902	-0.03456
C	-0.46294	1.18315	-1.42669
C	-1.24744	2.02757	-2.20274
C	-1.48624	1.71165	-3.54113
C	-0.92054	0.56524	-4.10258
H	0.34919	-1.14780	-3.74023
H	-0.26571	1.43082	-0.38991
H	-1.68095	2.93172	-1.78878
H	-1.10357	0.32311	-5.14867
C	-0.11788	-0.26104	-3.32226
C	0.10149	0.02518	-1.97458
C	0.85620	-0.86059	1.30584
C	1.80898	-1.55432	2.10467
C	-0.21558	-0.22160	1.98800
C	1.72577	-1.57425	3.47993
H	2.61780	-2.06399	1.59404
C	-0.33034	-0.27742	3.36564
H	-0.97442	0.29363	1.41070
C	0.64919	-0.94108	4.12207
H	2.46123	-2.08880	4.08757
H	-1.16886	0.20037	3.86546
O	0.61714	-1.01752	5.46581
H	-0.14823	-0.56251	5.84120
O	-2.27535	2.57240	-4.27125
H	-2.42681	2.20011	-5.14757

4.10 F_{NN} -0.0050 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3504

Cartesian Coordinates:

N	0.55211	-2.24937	-0.34995
N	0.52699	-2.11163	0.88882
C	1.14145	0.00349	-1.24796
C	1.08808	0.91376	-2.29589
C	0.26544	0.66395	-3.39423
C	-0.48135	-0.51247	-3.45220
H	-0.94387	-2.37469	-2.46845
H	1.77674	0.20697	-0.39409
H	1.67300	1.82651	-2.26859
H	-1.11276	-0.71908	-4.31449
C	-0.39799	-1.43845	-2.41622
C	0.38649	-1.17758	-1.29073
C	0.12140	-0.92118	1.56125
C	0.83114	-0.59260	2.72611
C	-1.01603	-0.17814	1.22158
C	0.46558	0.50075	3.49315
H	1.67208	-1.21123	3.01939
C	-1.41595	0.88894	2.01651
H	-1.60926	-0.45095	0.35700
C	-0.66653	1.24538	3.14399
H	1.01445	0.77034	4.38783
H	-2.31814	1.44170	1.76675
O	-0.99034	2.29071	3.94766
H	-1.84535	2.66867	3.70789
O	0.24204	1.59985	-4.40647
H	-0.44567	1.36457	-5.03989

4.11 F_{NN} -0.0075 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3776

Cartesian Coordinates:

N	0.00689	-0.00767	-0.63998
N	0.00973	-0.01134	0.61843
C	-1.62257	1.88598	-0.54253
C	-2.40997	2.80088	-1.22188
C	-2.41751	2.80955	-2.61954
C	-1.63476	1.90002	-3.32979
H	-0.22825	0.26566	-3.17597
H	-1.60899	1.87026	0.54024
H	-3.02453	3.51508	-0.68494
H	-1.64182	1.90813	-4.41936
C	-0.84436	0.98166	-2.64169
C	-0.82697	0.96144	-1.24518
C	0.83716	-0.97306	1.22048
C	0.83846	-0.97455	2.62669
C	1.63725	-1.90291	0.53442
C	1.61161	-1.87299	3.34021
H	0.21792	-0.25334	3.14626
C	2.41282	-2.80420	1.24283
H	1.63802	-1.90384	-0.54868
C	2.40458	-2.79460	2.64961
H	1.61843	-1.88088	4.42365
H	3.03316	-3.52523	0.71471
O	3.14157	-3.65120	3.39221
H	3.65774	-4.25173	2.84077
O	-3.21638	3.73781	-3.24943
H	-3.12880	3.63597	-4.20385

4.12 F_{NN} -0.0075 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3098

Cartesian Coordinates:

N	-1.27796	-1.17222	-0.56945
N	-1.27363	-1.19294	0.74008
C	1.16283	-1.14490	-0.66792
C	2.31307	-1.16844	-1.44764
C	2.23072	-1.32796	-2.82672
C	0.97363	-1.44741	-3.43726
H	-1.15592	-1.52338	-3.14740
H	1.24126	-1.02881	0.40522
H	3.28917	-1.07529	-0.98297
H	0.90781	-1.56674	-4.51897
C	-0.18211	-1.41674	-2.68061
C	-0.12706	-1.25816	-1.26571
C	-1.27593	0.03048	1.33432
C	-1.27131	0.03579	2.76189
C	-1.17561	1.27277	0.64704
C	-1.15877	1.20671	3.46766
H	-1.34529	-0.91615	3.27488
C	-1.06179	2.44701	1.35956
H	-1.17164	1.27374	-0.43501
C	-1.06005	2.42617	2.76964
H	-1.14193	1.22321	4.55099
H	-0.95658	3.39588	0.83883
O	-0.94208	3.53719	3.51224
H	-0.88965	4.33625	2.97175
O	3.40526	-1.32806	-3.56920
H	3.23685	-1.76388	-4.41197

4.13 F_{NN} -0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3058

Cartesian Coordinates:

N	0.93749	-0.79276	-1.28702
N	0.94164	-0.77800	-0.06686
C	-0.91509	0.93107	-1.34343
C	-1.76528	1.73164	-2.09279
C	-1.65748	1.73662	-3.48617
C	-0.70760	0.93773	-4.12583
H	0.87806	-0.50962	-3.83352
H	-0.98008	0.92273	-0.26027
H	-2.51138	2.35855	-1.61719
H	-0.62763	0.94938	-5.21255
C	0.13404	0.12938	-3.36689
C	0.03680	0.12670	-1.97962
C	0.86883	-0.85095	1.28521
C	1.62621	0.02931	2.09123
C	0.12331	-1.87213	1.90981
C	1.60727	-0.09996	3.47009
H	2.23032	0.79976	1.62584
C	0.07756	-1.94809	3.30054
H	-0.43508	-2.57958	1.30760
C	0.82320	-1.07525	4.09417
H	2.19740	0.56576	4.08977
H	-0.53604	-2.71670	3.76263
O	0.84699	-1.10301	5.45317
H	0.28419	-1.79805	5.81606
O	-2.51890	2.54618	-4.18962
H	-2.31218	2.48854	-5.12946

4.14 F_{NN} -0.0075 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3168

Cartesian Coordinates:

N	0.99790	-0.87954	-1.27765
N	0.97324	-0.90432	-0.03074
C	-0.45235	1.19794	-1.43342
C	-1.23268	2.04344	-2.21527
C	-1.47453	1.72047	-3.54989
C	-0.91689	0.56694	-4.10410
H	0.34123	-1.15406	-3.73004
H	-0.25727	1.44859	-0.39681
H	-1.66318	2.95009	-1.80338
H	-1.10317	0.31995	-5.14957
C	-0.11993	-0.26053	-3.31873
C	0.10476	0.03235	-1.97291
C	0.85052	-0.86419	1.30688
C	1.80809	-1.55450	2.10685
C	-0.22290	-0.22552	1.99180
C	1.72460	-1.57787	3.47989
H	2.62055	-2.05838	1.59612
C	-0.33698	-0.28119	3.36763
H	-0.98293	0.28946	1.41527
C	0.64501	-0.94695	4.12497
H	2.46121	-2.08871	4.08909
H	-1.17465	0.19521	3.86937
O	0.61892	-1.02923	5.46092
H	-0.14034	-0.57896	5.85596
O	-2.25814	2.58220	-4.29570
H	-2.48801	2.15124	-5.12663

4.15 F_{NN} -0.0075 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3531

Cartesian Coordinates:

N	0.57605	-2.23714	-0.34609
N	0.54650	-2.10112	0.89345
C	1.18375	-0.00540	-1.27306
C	1.13482	0.89422	-2.33207
C	0.28764	0.65185	-3.41156
C	-0.49247	-0.50300	-3.44015
H	-0.99526	-2.33552	-2.41935
H	1.83599	0.19277	-0.43059
H	1.73908	1.79480	-2.32133
H	-1.14548	-0.70229	-4.28873
C	-0.41898	-1.41641	-2.39191
C	0.39740	-1.16652	-1.28613
C	0.12419	-0.92051	1.56452
C	0.82926	-0.58517	2.73223
C	-1.01522	-0.18248	1.21681
C	0.45548	0.50730	3.49431
H	1.66931	-1.20099	3.03343
C	-1.42616	0.88106	2.01004
H	-1.60664	-0.46363	0.35346
C	-0.68272	1.24353	3.14139
H	0.99586	0.77991	4.39320
H	-2.33412	1.42447	1.76112
O	-1.01229	2.28352	3.94240
H	-1.88911	2.63238	3.73922
O	0.26927	1.57203	-4.44774
H	-0.51242	1.41058	-4.98810

4.16 F_{NN} -0.0100 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3807

Cartesian Coordinates:

N	0.00977	-0.01106	-0.64566
N	0.01311	-0.01531	0.61490
C	-1.61915	1.88198	-0.54398
C	-2.40882	2.79955	-1.21814
C	-2.41956	2.81196	-2.61497
C	-1.63869	1.90459	-3.32927
H	-0.23047	0.26819	-3.18407
H	-1.60302	1.86328	0.53886
H	-3.02114	3.51117	-0.67511
H	-1.64935	1.91690	-4.41990
C	-0.84558	0.98303	-2.64639
C	-0.82410	0.95806	-1.24993
C	0.83862	-0.97479	1.21462
C	0.83791	-0.97393	2.62307
C	1.64056	-1.90678	0.53104
C	1.60879	-1.86971	3.33986
H	0.21689	-0.25218	3.14116
C	2.41416	-2.80576	1.24281
H	1.64331	-1.91003	-0.55225
C	2.40353	-2.79336	2.65188
H	1.61419	-1.87593	4.42340
H	3.03610	-3.52863	0.71890
O	3.13578	-3.64441	3.39734
H	3.65685	-4.25060	2.85665
O	-3.22073	3.74294	-3.24698
H	-3.12851	3.63572	-4.20014

4.17 F_{NN} -0.0100 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3253

Cartesian Coordinates:

N	-1.33364	-1.14256	-0.59504
N	-1.29117	-1.17716	0.71622
C	1.10068	-1.18281	-0.76040
C	2.22722	-1.23240	-1.57487
C	2.10973	-1.37230	-2.95462
C	0.83714	-1.44879	-3.53266
H	-1.28378	-1.45946	-3.18568
H	1.21507	-1.08428	0.31128
H	3.21098	-1.16794	-1.11292
H	0.75433	-1.57498	-4.60954
C	-0.29560	-1.38158	-2.74285
C	-0.20726	-1.24272	-1.32472
C	-1.25264	0.03770	1.32136
C	-1.20597	0.02548	2.75034
C	-1.17999	1.29042	0.64566
C	-1.07210	1.18675	3.46718
H	-1.26503	-0.93217	3.25462
C	-1.05082	2.45427	1.36683
H	-1.21841	1.30174	-0.43589
C	-1.00405	2.41556	2.78037
H	-1.02296	1.19230	4.54983
H	-0.97415	3.41200	0.85742
O	-0.87486	3.51333	3.52954
H	-0.85752	4.32620	3.00696
O	3.21747	-1.42503	-3.80090
H	4.01064	-1.47746	-3.25427

4.18 F_{NN} -0.0100 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3102

Cartesian Coordinates:

N	0.88044	-0.81585	-1.27633
N	0.88715	-0.78565	-0.05282
C	-0.97168	0.90308	-1.36078
C	-1.81579	1.69947	-2.12526
C	-1.66274	1.73332	-3.51176
C	-0.67705	0.96311	-4.13393
H	0.92078	-0.46581	-3.81770
H	-1.06915	0.87950	-0.28035
H	-2.58689	2.30397	-1.66022
H	-0.56261	0.99755	-5.21851
C	0.15353	0.15534	-3.36338
C	0.01691	0.12652	-1.97789
C	0.81387	-0.83845	1.29823
C	1.61008	0.02640	2.08788
C	0.09951	-1.87456	1.94304
C	1.64165	-0.11595	3.46273
H	2.20661	0.79355	1.60724
C	0.07642	-1.94554	3.33207
H	-0.47088	-2.58287	1.35289
C	0.85867	-1.08269	4.10805
H	2.26497	0.53145	4.06897
H	-0.53566	-2.70413	3.81161
O	0.92577	-1.11003	5.45610
H	0.35986	-1.78450	5.85376
O	-2.51998	2.53594	-4.24087
H	-2.19722	2.58611	-5.14786

4.19 F_{NN} -0.0100 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3263

Cartesian Coordinates:

N	1.01257	-0.86411	-1.27575
N	0.97998	-0.89510	-0.02660
C	-0.42533	1.22178	-1.44569
C	-1.20096	2.06698	-2.23575
C	-1.45414	1.72996	-3.56316
C	-0.91179	0.56387	-4.10609
H	0.32854	-1.16787	-3.71570
H	-0.22746	1.48042	-0.41137
H	-1.62355	2.97996	-1.82933
H	-1.10579	0.30859	-5.14911
C	-0.12100	-0.26334	-3.31432
C	0.11623	0.04245	-1.97215
C	0.84855	-0.86253	1.30689
C	1.80979	-1.54978	2.11052
C	-0.23069	-0.22834	1.99352
C	1.72149	-1.58044	3.48071
H	2.62844	-2.04515	1.60122
C	-0.34878	-0.28826	3.36676
H	-0.99100	0.28622	1.41634
C	0.63470	-0.95631	4.12698
H	2.45804	-2.08799	4.09270
H	-1.18857	0.18315	3.86905
O	0.60929	-1.04913	5.45466
H	-0.14621	-0.60726	5.86833
O	-2.23300	2.59087	-4.32893
H	-2.61725	2.08528	-5.05382

4.20 F_{NN} -0.0100 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3578

Cartesian Coordinates:

N	0.60025	-2.22443	-0.34117
N	0.56596	-2.08878	0.89947
C	1.22779	-0.01786	-1.30254
C	1.18311	0.86682	-2.37608
C	0.31142	0.63010	-3.43551
C	-0.50141	-0.50169	-3.43095
H	-1.04432	-2.29788	-2.36588
H	1.89793	0.17628	-0.47307
H	1.80704	1.75409	-2.38566
H	-1.17383	-0.69541	-4.26601
C	-0.43823	-1.39754	-2.36698
C	0.40943	-1.15682	-1.28108
C	0.12758	-0.91774	1.56749
C	0.82773	-0.57443	2.73817
C	-1.01513	-0.18596	1.21218
C	0.44448	0.51653	3.49548
H	1.66780	-1.18619	3.04711
C	-1.43862	0.87275	2.00428
H	-1.60492	-0.47665	0.35064
C	-0.70145	1.24216	3.13964
H	0.97654	0.79310	4.39820
H	-2.35357	1.40489	1.75705
O	-1.03876	2.27552	3.93880
H	-1.93378	2.59653	3.77073
O	0.29456	1.53158	-4.49988
H	-0.58384	1.50925	-4.89569

4.21 F_{NN} +0.0025 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3811

Cartesian Coordinates:

N	-0.00399	0.00512	-0.62249
N	-0.00298	0.00356	0.63363
C	-1.63359	1.89883	-0.53721
C	-2.41221	2.80341	-1.23428
C	-2.40947	2.80012	-2.63714
C	-1.61996	1.88283	-3.33417
H	-0.22030	0.25662	-3.15290
H	-1.62916	1.89375	0.54554
H	-3.03450	3.52653	-0.71870
H	-1.61512	1.87708	-4.42072
C	-0.83924	0.97584	-2.62820
C	-0.83419	0.96999	-1.22851
C	0.82895	-0.96338	1.24242
C	0.84003	-0.97626	2.64294
C	1.62411	-1.88757	0.54732
C	1.62174	-1.88476	3.34396
H	0.22132	-0.25712	3.16901
C	2.40647	-2.79686	1.24236
H	1.61742	-1.87984	-0.53545
C	2.40823	-2.79890	2.64266
H	1.63480	-1.89993	4.42816
H	3.02040	-3.51051	0.69723
O	3.16364	-3.67707	3.37261
H	3.66094	-4.25571	2.78184
O	-3.20024	3.71884	-3.25613
H	-3.13268	3.64027	-4.21608

4.22 F_{NN} +0.0025 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3093

Cartesian Coordinates:

N	-1.28203	-1.25058	-0.53763
N	-1.28212	-1.24978	0.76998
C	1.15857	-1.28687	-0.61697
C	2.30107	-1.24908	-1.39263
C	2.20846	-1.30924	-2.78840
C	0.94809	-1.39436	-3.41179
H	-1.17497	-1.46886	-3.11544
H	1.22033	-1.23148	0.46224
H	3.28337	-1.16198	-0.94142
H	0.88126	-1.43610	-4.49580
C	-0.19771	-1.41319	-2.64983
C	-0.12823	-1.34668	-1.22879
C	-1.28775	-0.01330	1.34565
C	-1.28811	0.04653	2.76790
C	-1.15636	1.20562	0.62821
C	-1.16105	1.24516	3.43273
H	-1.37922	-0.88535	3.31518
C	-1.02679	2.40825	1.30845
H	-1.13479	1.18595	-0.45288
C	-1.03177	2.43922	2.70415
H	-1.14969	1.28930	4.51644
H	-0.90233	3.33099	0.74575
O	-0.88271	3.59664	3.42012
H	-0.81457	4.34944	2.82005
O	3.36900	-1.25331	-3.49070
H	3.20332	-1.29282	-4.44131

4.23 F_{NN} +0.0025 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3122

Cartesian Coordinates:

N	0.98879	-0.74602	-1.29338
N	0.98695	-0.74623	-0.06915
C	-0.83973	0.97768	-1.32018
C	-1.69313	1.77000	-2.06392
C	-1.64974	1.71974	-3.46673
C	-0.74570	0.87285	-4.11529
H	0.82040	-0.58486	-3.84088
H	-0.86504	1.01127	-0.23625
H	-2.40348	2.43802	-1.59009
H	-0.71222	0.83522	-5.20052
C	0.11039	0.08029	-3.36159
C	0.06809	0.12612	-1.96714
C	0.91281	-0.83744	1.25786
C	1.62317	0.05986	2.10008
C	0.13497	-1.85196	1.87328
C	1.56247	-0.07240	3.47998
H	2.22902	0.83943	1.65328
C	0.07633	-1.94289	3.26009
H	-0.41324	-2.55302	1.25540
C	0.78863	-1.06648	4.07435
H	2.12123	0.61063	4.11149
H	-0.53615	-2.72641	3.70268
O	0.76014	-1.13097	5.46090
H	0.25588	-1.90665	5.73082
O	-2.51646	2.52431	-4.13210
H	-2.41781	2.42917	-5.08808

4.24 F_{NN} +0.0025 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3036

Cartesian Coordinates:

N	0.94606	-0.92771	-1.28656
N	0.95815	-0.91631	-0.04031
C	-0.48802	1.14976	-1.41309
C	-1.27327	1.99218	-2.18170
C	-1.49834	1.69457	-3.53253
C	-0.91321	0.56278	-4.10775
H	0.36854	-1.13766	-3.76330
H	-0.29143	1.39211	-0.37520
H	-1.71519	2.89171	-1.76698
H	-1.07756	0.33668	-5.15808
C	-0.10987	-0.26445	-3.33260
C	0.09076	0.00323	-1.97576
C	0.87851	-0.83207	1.30093
C	1.81436	-1.54571	2.09981
C	-0.19193	-0.19728	1.98424
C	1.73063	-1.56593	3.47985
H	2.61070	-2.07306	1.58750
C	-0.31044	-0.26545	3.36583
H	-0.94856	0.32159	1.40858
C	0.66039	-0.93059	4.11804
H	2.45919	-2.10058	4.07962
H	-1.15291	0.21173	3.86291
O	0.60651	-1.00254	5.48463
H	-0.17966	-0.54449	5.80543
O	-2.28913	2.55610	-4.22994
H	-2.36219	2.28532	-5.15371

4.25 F_{NN} +0.0025 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3536

Cartesian Coordinates:

N	0.46968	-2.27292	-0.36239
N	0.45789	-2.12931	0.87750
C	1.01081	0.03156	-1.19106
C	0.95349	0.95389	-2.22299
C	0.21842	0.66992	-3.37986
C	-0.42336	-0.56468	-3.51049
H	-0.77848	-2.48270	-2.60077
H	1.59130	0.26061	-0.30585
H	1.47917	1.89987	-2.15821
H	-0.97146	-0.80408	-4.41780
C	-0.32535	-1.50356	-2.49043
C	0.34964	-1.20245	-1.30275
C	0.11024	-0.91191	1.55103
C	0.83567	-0.60704	2.70916
C	-1.02566	-0.15308	1.24509
C	0.49289	0.48082	3.50097
H	1.68230	-1.23257	2.97181
C	-1.39643	0.91260	2.05721
H	-1.62760	-0.39823	0.37859
C	-0.62803	1.24522	3.17537
H	1.07068	0.73844	4.38170
H	-2.28686	1.48824	1.81542
O	-0.94086	2.29625	3.99900
H	-1.69794	2.77818	3.64505
O	0.18643	1.63085	-4.34331
H	-0.29281	1.32431	-5.12324

4.26 F_{NN} +0.0050 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3860

Cartesian Coordinates:

N	-0.00671	0.00830	-0.61908
N	-0.00605	0.00715	0.63806
C	-1.63599	1.90163	-0.53582
C	-2.41227	2.80348	-1.23681
C	-2.40756	2.79788	-2.64167
C	-1.61633	1.87860	-3.33570
H	-0.21842	0.25445	-3.14851
H	-1.63379	1.89914	0.54704
H	-3.03639	3.52872	-0.72624
H	-1.60890	1.86983	-4.42186
C	-0.83796	0.97435	-2.62565
C	-0.83510	0.97105	-1.22442
C	0.82619	-0.96015	1.24774
C	0.84027	-0.97652	2.64753
C	1.62069	-1.88357	0.55028
C	1.62422	-1.88764	3.34540
H	0.22216	-0.25808	3.17578
C	2.40463	-2.79470	1.24184
H	1.61206	-1.87358	-0.53246
C	2.40896	-2.79975	2.64109
H	1.63902	-1.90486	4.43002
H	3.01688	-3.50639	0.69227
O	3.16912	-3.68345	3.36772
H	3.66180	-4.25680	2.76783
O	-3.19619	3.71410	-3.25764
H	-3.13393	3.64170	-4.21905

4.27 F_{NN} +0.0050 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3153

Cartesian Coordinates:

N	-1.27302	-1.24952	-0.53773
N	-1.27296	-1.25008	0.77218
C	1.16891	-1.30378	-0.61826
C	2.30672	-1.27137	-1.39578
C	2.20782	-1.31913	-2.79549
C	0.94415	-1.38462	-3.41758
H	-1.17698	-1.43888	-3.11235
H	1.23089	-1.25861	0.46156
H	3.29315	-1.19680	-0.95144
H	0.87419	-1.41511	-4.50133
C	-0.19711	-1.39837	-2.65088
C	-0.12087	-1.34518	-1.22819
C	-1.27808	-0.01529	1.34862
C	-1.27828	0.04922	2.77112
C	-1.15288	1.20604	0.63289
C	-1.16267	1.25141	3.43484
H	-1.36397	-0.88225	3.32061
C	-1.03463	2.41127	1.31348
H	-1.12892	1.18993	-0.44819
C	-1.04235	2.44551	2.70725
H	-1.15448	1.29486	4.51923
H	-0.91913	3.33309	0.74716
O	-0.90403	3.61210	3.42366
H	-0.84558	4.35866	2.81498
O	3.36402	-1.27130	-3.49164
H	3.20940	-1.29766	-4.44548

4.28 F_{NN} +0.0050 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3192

Cartesian Coordinates:

N	0.98343	-0.73837	-1.28934
N	0.97883	-0.73671	-0.06323
C	-0.83694	0.98851	-1.32135
C	-1.68594	1.77750	-2.07093
C	-1.64494	1.71672	-3.47569
C	-0.74419	0.86085	-4.11897
H	0.81554	-0.59804	-3.83612
H	-0.86212	1.03182	-0.23773
H	-2.39317	2.45351	-1.60381
H	-0.71141	0.81398	-5.20346
C	0.10888	0.07238	-3.35964
C	0.06810	0.12779	-1.96318
C	0.90216	-0.82551	1.25733
C	1.60943	0.07294	2.10630
C	0.12206	-1.84152	1.87613
C	1.55525	-0.06790	3.48603
H	2.21314	0.85495	1.66098
C	0.06954	-1.93776	3.26159
H	-0.42838	-2.53978	1.25719
C	0.78731	-1.06716	4.07756
H	2.11725	0.61315	4.11755
H	-0.54373	-2.72195	3.70327
O	0.75885	-1.14759	5.47126
H	0.33470	-1.97668	5.71880
O	-2.50804	2.51890	-4.13893
H	-2.41907	2.42523	-5.09672

4.29 F_{NN} +0.0050 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3063

Cartesian Coordinates:

N	0.92362	-0.94097	-1.28710
N	0.94995	-0.91664	-0.03973
C	-0.50017	1.14041	-1.40941
C	-1.28116	1.98287	-2.17911
C	-1.49778	1.69135	-3.53531
C	-0.90719	0.56222	-4.11239
H	0.37142	-1.13749	-3.76767
H	-0.30730	1.38150	-0.37061
H	-1.72617	2.88168	-1.76625
H	-1.06215	0.34168	-5.16479
C	-0.10955	-0.26692	-3.33517
C	0.08201	-0.00540	-1.97380
C	0.88707	-0.81694	1.29899
C	1.81791	-1.53936	2.09831
C	-0.18413	-0.18625	1.98696
C	1.73496	-1.56322	3.47931
H	2.60967	-2.07200	1.58423
C	-0.30231	-0.26222	3.36958
H	-0.94214	0.33357	1.41428
C	0.66653	-0.92901	4.11907
H	2.46107	-2.10752	4.07414
H	-1.14666	0.21244	3.86753
O	0.60489	-1.00362	5.49381
H	-0.18868	-0.54714	5.79727
O	-2.28295	2.55510	-4.22559
H	-2.34865	2.30583	-5.15666

4.30 F_{NN} +0.0050 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3584

Cartesian Coordinates:

N	0.43617	-2.27435	-0.36801
N	0.42990	-2.12925	0.87378
C	0.96175	0.04531	-1.17832
C	0.90781	0.96509	-2.21070
C	0.20981	0.66461	-3.38889
C	-0.39490	-0.58786	-3.53805
H	-0.72016	-2.51453	-2.64016
H	1.52076	0.28729	-0.28301
H	1.41266	1.92164	-2.13701
H	-0.90823	-0.84209	-4.46101
C	-0.29870	-1.52313	-2.51605
C	0.33287	-1.20567	-1.30648
C	0.10501	-0.90457	1.54750
C	0.83742	-0.60997	2.70360
C	-1.03168	-0.13938	1.25775
C	0.50245	0.47242	3.50842
H	1.68672	-1.23786	2.95257
C	-1.39293	0.92118	2.08093
H	-1.63839	-0.37323	0.39149
C	-0.61699	1.24227	3.19652
H	1.09155	0.72380	4.38399
H	-2.28121	1.50348	1.84667
O	-0.92701	2.29155	4.03197
H	-1.64291	2.80998	3.64554
O	0.18120	1.62617	-4.34363
H	-0.24922	1.31529	-5.15068

4.31 F_{NN} +0.0075 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3924

Cartesian Coordinates:

N	-0.00961	0.01170	-0.61546
N	-0.00932	0.01096	0.64329
C	-1.63853	1.90458	-0.53429
C	-2.41236	2.80356	-1.23952
C	-2.40537	2.79532	-2.64653
C	-1.61238	1.87401	-3.33754
H	-0.21633	0.25206	-3.14409
H	-1.63867	1.90480	0.54869
H	-3.03832	3.53092	-0.73406
H	-1.60232	1.86219	-4.42335
C	-0.83649	0.97266	-2.62312
C	-0.83592	0.97202	-1.21997
C	0.82286	-0.95625	1.25362
C	0.84054	-0.97680	2.65299
C	1.61680	-1.87904	0.55352
C	1.62691	-1.89076	3.34714
H	0.22317	-0.25919	3.18390
C	2.40238	-2.79209	1.24104
H	1.60608	-1.86661	-0.52926
C	2.40988	-2.80083	2.63941
H	1.64384	-1.91045	4.43237
H	3.01276	-3.50163	0.68649
O	3.17494	-3.69025	3.36193
H	3.66272	-4.25792	2.75253
O	-3.19189	3.70908	-3.25954
H	-3.13496	3.64287	-4.22248

4.32 F_{NN} +0.0075 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3236

Cartesian Coordinates:

N	-1.26025	-1.24186	-0.53979
N	-1.25979	-1.24579	0.77342
C	1.18326	-1.31831	-0.62312
C	2.31545	-1.29871	-1.40367
C	2.20889	-1.33648	-2.80763
C	0.94147	-1.37671	-3.42714
H	-1.17712	-1.40139	-3.11068
H	1.24684	-1.28298	0.45712
H	3.30656	-1.24249	-0.96722
H	0.86741	-1.39841	-4.51050
C	-0.19435	-1.37866	-2.65428
C	-0.11048	-1.33673	-1.22960
C	-1.26350	-0.01420	1.35221
C	-1.26323	0.05284	2.77558
C	-1.14878	1.21207	0.64078
C	-1.16518	1.25789	3.44057
H	-1.34051	-0.87946	3.32579
C	-1.04765	2.41848	1.32394
H	-1.12297	1.20190	-0.44037
C	-1.05934	2.45382	2.71643
H	-1.16150	1.29865	4.52596
H	-0.94528	3.34092	0.75574
O	-0.93896	3.62943	3.43486
H	-0.89523	4.37064	2.81857
O	3.36047	-1.30598	-3.49840
H	3.21706	-1.32430	-4.45530

4.33 F_{NN} +0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3284

Cartesian Coordinates:

N	0.96890	-0.73205	-1.28145
N	0.95981	-0.72575	-0.05304
C	-0.84215	1.00003	-1.32628
C	-1.68209	1.78613	-2.08610
C	-1.63612	1.71524	-3.49293
C	-0.73599	0.84978	-4.12645
H	0.81417	-0.61173	-3.82698
H	-0.87278	1.05313	-0.24315
H	-2.38823	2.47037	-1.62941
H	-0.69817	0.79405	-5.21009
C	0.10898	0.06466	-3.35705
C	0.06307	0.12940	-1.95831
C	0.87848	-0.80898	1.26122
C	1.58452	0.09036	2.11628
C	0.09576	-1.82620	1.88504
C	1.54424	-0.06380	3.49551
H	2.18445	0.87567	1.67169
C	0.05530	-1.93111	3.26871
H	-0.46016	-2.51961	1.26556
C	0.78542	-1.07025	4.08531
H	2.11403	0.61223	4.12635
H	-0.55867	-2.71482	3.71122
O	0.76611	-1.17461	5.48655
H	0.49617	-2.07253	5.70856
O	-2.49124	2.51582	-4.15829
H	-2.40721	2.42385	-5.11756

4.34 F_{NN} +0.0075 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3115

Cartesian Coordinates:

N	0.89937	-0.95259	-1.28726
N	0.94075	-0.91519	-0.03820
C	-0.51376	1.13250	-1.40645
C	-1.28867	1.97492	-2.17869
C	-1.49564	1.68870	-3.54044
C	-0.90152	0.56028	-4.11792
H	0.37037	-1.14042	-3.77022
H	-0.32636	1.37275	-0.36645
H	-1.73624	2.87363	-1.76841
H	-1.04729	0.34383	-5.17211
C	-0.11199	-0.27108	-3.33721
C	0.07102	-0.01459	-1.97084
C	0.89540	-0.80022	1.29659
C	1.82276	-1.53052	2.09700
C	-0.17558	-0.17268	1.99167
C	1.74120	-1.55914	3.47868
H	2.60959	-2.06832	1.58046
C	-0.29216	-0.25662	3.37524
H	-0.93580	0.34786	1.42274
C	0.67437	-0.92672	4.12169
H	2.46430	-2.11412	4.06816
H	-1.13709	0.21673	3.87526
O	0.60641	-1.00507	5.50410
H	-0.20502	-0.57003	5.79056
O	-2.27376	2.55485	-4.22530
H	-2.33256	2.32521	-5.16277

4.35 F_{NN} +0.0075 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3651

Cartesian Coordinates:

N	0.40041	-2.27201	-0.37460
N	0.40033	-2.12574	0.87004
C	0.91019	0.06180	-1.16953
C	0.86189	0.97583	-2.20505
C	0.20436	0.65650	-3.40459
C	-0.36315	-0.61294	-3.56840
H	-0.66219	-2.54361	-2.67557
H	1.44643	0.31895	-0.26480
H	1.34567	1.94265	-2.12478
H	-0.83933	-0.88354	-4.50613
C	-0.27196	-1.54096	-2.54119
C	0.31368	-1.20598	-1.31017
C	0.09923	-0.89519	1.54383
C	0.83960	-0.61182	2.69793
C	-1.03873	-0.12307	1.27276
C	0.51227	0.46288	3.51830
H	1.69200	-1.24186	2.93140
C	-1.39076	0.92982	2.10972
H	-1.65101	-0.34438	0.40712
C	-0.60695	1.23735	3.22315
H	1.11332	0.70685	4.38851
H	-2.27776	1.51820	1.88544
O	-0.91460	2.28296	4.07311
H	-1.58649	2.83747	3.65880
O	0.18254	1.61524	-4.35388
H	-0.20526	1.30284	-5.18267

4.36 F_{NN} +0.0100 au OH−AB−OH Trans Structure S_0 State

E_h = -723.4005

Cartesian Coordinates:

N	-0.01266	0.01525	-0.61183
N	-0.01270	0.01491	0.64923
C	-1.64117	1.90763	-0.53265
C	-2.41238	2.80357	-1.24223
C	-2.40308	2.79265	-2.65170
C	-1.60823	1.86918	-3.33963
H	-0.21412	0.24951	-3.13970
H	-1.64375	1.91068	0.55047
H	-3.04021	3.53309	-0.74199
H	-1.59553	1.85431	-4.42519
C	-0.83494	0.97087	-2.62068
C	-0.83655	0.97275	-1.21522
C	0.81903	-0.95177	1.25987
C	0.84081	-0.97708	2.65912
C	1.61255	-1.87410	0.55686
C	1.62979	-1.89410	3.34915
H	0.22433	-0.26050	3.19322
C	2.39984	-2.78915	1.23993
H	1.59957	-1.85905	-0.52598
C	2.41085	-2.80197	2.63761
H	1.64913	-1.91659	4.43510
H	3.00821	-3.49635	0.68001
O	3.18102	-3.69735	3.35556
H	3.66377	-4.25917	2.73657
O	-3.18736	3.70380	-3.26185
H	-3.13581	3.64386	-4.22637

4.37 F_{NN} +0.0100 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3345

Cartesian Coordinates:

N	-1.24354	-1.22741	-0.54371
N	-1.24246	-1.23666	0.77379
C	1.20162	-1.33041	-0.63152
C	2.32697	-1.33133	-1.41633
C	2.21153	-1.36161	-2.82489
C	0.94015	-1.37084	-3.44040
H	-1.17488	-1.35632	-3.11045
H	1.26824	-1.30442	0.44898
H	3.32300	-1.29960	-0.98879
H	0.86100	-1.38627	-4.52332
C	-0.18909	-1.35419	-2.65998
C	-0.09681	-1.32129	-1.23292
C	-1.24376	-0.00968	1.35646
C	-1.24271	0.05772	2.78137
C	-1.14338	1.22382	0.65190
C	-1.16872	1.26478	3.44999
H	-1.30903	-0.87648	3.33085
C	-1.06502	2.42978	1.33976
H	-1.11607	1.22191	-0.42935
C	-1.08251	2.46397	2.73164
H	-1.17131	1.30085	4.53666
H	-0.97932	3.35409	0.77135
O	-0.98743	3.64809	3.45362
H	-0.96620	4.38479	2.83079
O	3.35774	-1.35790	-3.51120
H	3.22528	-1.37125	-4.47106

4.38 F_{NN} +0.0100 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3403

Cartesian Coordinates:

N	0.91882	-0.73756	-1.25724
N	0.89443	-0.72047	-0.02644
C	-0.87612	1.00711	-1.34201
C	-1.68610	1.79685	-2.12686
C	-1.60306	1.72376	-3.53531
C	-0.69309	0.84829	-4.14351
H	0.83191	-0.62501	-3.79982
H	-0.93772	1.06421	-0.26030
H	-2.39990	2.48817	-1.69341
H	-0.62554	0.78971	-5.22543
C	0.12093	0.05838	-3.34926
C	0.03979	0.12594	-1.94849
C	0.79604	-0.79072	1.27958
C	1.50665	0.10814	2.13986
C	-0.00365	-1.80050	1.91006
C	1.49298	-0.07267	3.51569
H	2.09719	0.90048	1.69518
C	-0.01476	-1.92856	3.28938
H	-0.58192	-2.47423	1.28902
C	0.74958	-1.09256	4.10508
H	2.07653	0.59251	4.14701
H	-0.62575	-2.70852	3.73935
O	0.77394	-1.26527	5.51326
H	1.16007	-2.13063	5.69258
O	-2.43083	2.52984	-4.21674
H	-2.33385	2.44258	-5.17632

4.39 F_{NN} +0.0100 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3195

Cartesian Coordinates:

N	0.87232	-0.96279	-1.28595
N	0.93008	-0.91147	-0.03499
C	-0.52892	1.12708	-1.40453
C	-1.29543	1.96927	-2.18154
C	-1.49188	1.68680	-3.54917
C	-0.89589	0.55670	-4.12466
H	0.36536	-1.14666	-3.76975
H	-0.34805	1.36761	-0.36341
H	-1.74508	2.86904	-1.77591
H	-1.03189	0.34313	-5.18053
C	-0.11723	-0.27688	-3.33818
C	0.05684	-0.02377	-1.96643
C	0.90349	-0.78060	1.29453
C	1.82899	-1.51854	2.09581
C	-0.16756	-0.15732	1.99935
C	1.74931	-1.55469	3.47781
H	2.61122	-2.06016	1.57594
C	-0.28045	-0.25042	3.38381
H	-0.93131	0.36381	1.43586
C	0.68421	-0.92513	4.12592
H	2.46962	-2.12204	4.06000
H	-1.12558	0.22110	3.88734
O	0.60960	-1.01030	5.51672
H	-0.22417	-0.60766	5.78536
O	-2.25936	2.55609	-4.23063
H	-2.31613	2.34172	-5.17289

4.40 F_{NN} +0.0100 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3738

Cartesian Coordinates:

N	0.36471	-2.26622	-0.38190
N	0.37128	-2.11882	0.86640
C	0.85747	0.08030	-1.16478
C	0.81675	0.98600	-2.20556
C	0.20212	0.64616	-3.42576
C	-0.32931	-0.63913	-3.60008
H	-0.60665	-2.56958	-2.70650
H	1.36999	0.35423	-0.25147
H	1.27970	1.96259	-2.12115
H	-0.76729	-0.92686	-4.55099
C	-0.24611	-1.55694	-2.56515
C	0.29265	-1.20373	-1.31406
C	0.09296	-0.88409	1.53992
C	0.84217	-0.61206	2.69198
C	-1.04669	-0.10478	1.28938
C	0.52168	0.45256	3.53017
H	1.69835	-1.24355	2.90819
C	-1.39044	0.93762	2.14275
H	-1.66481	-0.31240	0.42446
C	-0.59889	1.23009	3.25454
H	1.13515	0.68852	4.39474
H	-2.27711	1.53118	1.93046
O	-0.90541	2.27021	4.12140
H	-1.52953	2.86079	3.68291
O	0.19059	1.59908	-4.37222
H	-0.15959	1.28707	-5.21891

5 Cartesian coordinates and energies of protonated OH−AB−O structures in F_{OC} conditions

5.1 F_{OC} -0.0025 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3792

Cartesian Coordinates:

O	0.40457	-0.47019	-5.86933
C	0.40615	-0.47206	-4.49682
C	1.13248	-1.31596	-2.36080
C	0.32825	-0.38154	-1.70230
C	-0.44182	0.51317	-2.46644
C	-0.40325	0.46834	-3.84990
C	1.17468	-1.36498	-3.75058
H	1.72325	-2.00238	-1.76427
H	-1.06435	1.23648	-1.95447
H	-0.99279	1.15332	-4.45000
H	1.80495	-2.09726	-4.25048
N	0.36288	-0.42178	-0.28965
N	-0.36267	0.42152	0.29429
C	-0.32906	0.38243	1.70218
C	-1.13706	1.32179	2.36009
C	0.43989	-0.51155	2.46601
C	-1.18513	1.37770	3.74364
H	-1.72615	2.00665	1.76004
C	0.39606	-0.46058	3.84907
H	1.06457	-1.23784	1.96161
C	-0.41671	0.48439	4.49497
H	-1.80601	2.09954	4.26110
H	0.99204	-1.15351	4.43775
O	-0.49941	0.58057	5.84666
H	0.06318	-0.07351	6.28000
H	0.99680	-1.15822	-6.19532

5.2 F_{OC} -0.0025 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3047

Cartesian Coordinates:

O	1.30080	-1.42534	-4.66810
C	1.27858	-1.41403	-3.29359
C	1.13151	-2.54068	-1.16238
C	1.18063	-1.29181	-0.48141
C	1.30017	-0.10773	-1.26524
C	1.33053	-0.17872	-2.64972
C	1.17958	-2.59541	-2.53900
H	1.05199	-3.44651	-0.57206
H	1.33496	0.85123	-0.76466
H	1.39128	0.72357	-3.24914
H	1.13609	-3.55918	-3.04237
N	1.03256	-1.27961	0.85954
N	1.15886	-0.17099	1.53531
C	-0.01018	0.48531	1.79049
C	0.08374	1.70033	2.52594
C	-1.27650	0.10511	1.27165
C	-1.01713	2.50023	2.72061
H	1.05264	1.98053	2.92336
C	-2.38018	0.91549	1.47147
H	-1.36102	-0.81365	0.70695
C	-2.26175	2.10878	2.19649
H	-0.95224	3.42852	3.27630
H	-3.34315	0.63201	1.05285
O	-3.30840	2.94891	2.40130
H	-4.12989	2.56057	2.07501
H	1.26827	-2.33569	-4.98501

5.3 F_{OC} -0.0025 au OH−AB−OH Rotation Inversion TS Structure

S_0 State

E_h = -723.3050

Cartesian Coordinates:

O	1.22553	-1.41680	-5.15678
C	1.21051	-1.40723	-3.78849
C	1.84114	-2.28989	-1.63847
C	1.10827	-1.28367	-1.01442
C	0.42346	-0.33401	-1.78151
C	0.47288	-0.39368	-3.16449
C	1.89448	-2.35661	-3.02658
H	2.36328	-3.01296	-1.02084
H	-0.14117	0.44715	-1.28341
H	-0.04768	0.33155	-3.78013
H	2.46672	-3.14191	-3.51477
N	1.11517	-1.31846	0.43566
N	0.48276	-0.46128	1.03134
C	-0.30176	0.40550	1.69194
C	0.16343	1.70207	2.02181
C	-1.59643	0.02578	2.11500
C	-0.64106	2.56962	2.74588
H	1.16298	2.00166	1.72901
C	-2.39326	0.92995	2.81183
H	-1.96356	-0.96965	1.89519
C	-1.92637	2.20062	3.14032
H	-0.27070	3.55218	3.01751
H	-3.39055	0.61893	3.11407
O	-2.67601	3.13062	3.82710
H	-3.43955	2.70871	4.23780
H	1.76622	-2.14964	-5.47531

5.4 F_{OC} -0.0025 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3027

Cartesian Coordinates:

O	1.23567	-1.41164	-5.14309
C	1.22204	-1.40103	-3.76916
C	1.63188	-2.41374	-1.62157
C	1.14545	-1.27411	-0.97936
C	0.72271	-0.18542	-1.75099
C	0.76453	-0.24180	-3.13777
C	1.65521	-2.48971	-3.00979
H	1.98451	-3.23775	-1.00975
H	0.38702	0.71855	-1.25559
H	0.45642	0.60153	-3.74691
H	2.01857	-3.38980	-3.50142
N	1.20413	-1.31124	0.46842
N	0.52365	-0.49307	1.11329
C	-0.26577	0.42113	1.71031
C	-0.14457	0.62613	3.11264
C	-1.30423	1.12248	1.04270
C	-0.96253	1.50657	3.79178
H	0.62241	0.06937	3.63804
C	-2.16089	1.96771	1.72995
H	-1.44654	0.96469	-0.01991
C	-1.98211	2.17711	3.10357
H	-0.85701	1.66879	4.85841
H	-2.96459	2.47774	1.20351
O	-2.77038	3.01159	3.82690
H	-3.45662	3.40669	3.27502
H	1.58331	-2.25513	-5.45627

5.5 F_{OC} -0.0025 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3481

Cartesian Coordinates:

O	1.03726	-1.74312	-4.21379
C	1.04609	-1.67857	-2.84206
C	0.84182	-2.66841	-0.65282
C	1.08352	-1.42840	-0.05654
C	1.35155	-0.32057	-0.87355
C	1.34235	-0.44671	-2.25583
C	0.79095	-2.78999	-2.03763
H	0.69229	-3.53537	-0.01840
H	1.58505	0.63785	-0.42560
H	1.56648	0.40095	-2.89398
H	0.58039	-3.75710	-2.48864
N	1.25774	-1.42349	1.36701
N	0.82462	-0.53746	2.12757
C	-0.08854	0.49186	1.73573
C	0.11291	1.75397	2.31014
C	-1.24740	0.26134	0.98593
C	-0.77598	2.79177	2.07398
H	0.97827	1.90573	2.94603
C	-2.16378	1.28696	0.78376
H	-1.44797	-0.72234	0.57897
C	-1.92198	2.55903	1.31007
H	-0.61893	3.77443	2.50361
H	-3.07317	1.09440	0.21930
O	-2.77764	3.60828	1.12412
H	-3.57924	3.31362	0.67551
H	0.85282	-2.64686	-4.49588

5.6 F_{OC} -0.0050 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3832

Cartesian Coordinates:

O	0.40635	-0.47225	-5.87865
C	0.40303	-0.46844	-4.49853
C	1.13131	-1.31457	-2.36312
C	0.32817	-0.38147	-1.70151
C	-0.44189	0.51318	-2.46589
C	-0.40495	0.47025	-3.85112
C	1.17131	-1.36102	-3.75370
H	1.72260	-2.00154	-1.76775
H	-1.06361	1.23551	-1.95112
H	-0.99623	1.15721	-4.44816
H	1.80188	-2.09360	-4.25442
N	0.36435	-0.42351	-0.28855
N	-0.36171	0.42042	0.29819
C	-0.32667	0.37967	1.70154
C	-1.13600	1.32062	2.36000
C	0.44307	-0.51528	2.46730
C	-1.18465	1.37722	3.74147
H	-1.72509	2.00552	1.76004
C	0.39904	-0.46407	3.84887
H	1.06835	-1.24230	1.96502
C	-0.41550	0.48300	4.49521
H	-1.80472	2.09814	4.26068
H	0.99404	-1.15592	4.43881
O	-0.50319	0.58496	5.83839
H	0.05353	-0.06236	6.29059
H	1.00251	-1.16479	-6.18660

5.7 F_{OC} -0.0050 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3061

Cartesian Coordinates:

O	1.35654	-1.44867	-4.69138
C	1.30308	-1.42219	-3.30827
C	1.11090	-2.53892	-1.17421
C	1.15491	-1.28859	-0.49430
C	1.28595	-0.10878	-1.28297
C	1.34461	-0.18696	-2.66863
C	1.18297	-2.59773	-2.55040
H	1.02161	-3.44334	-0.58310
H	1.31762	0.85322	-0.78794
H	1.42592	0.71488	-3.26718
H	1.14565	-3.56503	-3.04905
N	1.00954	-1.27375	0.84574
N	1.14128	-0.16576	1.51882
C	-0.02484	0.49552	1.77520
C	0.08379	1.71033	2.50899
C	-1.29938	0.11135	1.27921
C	-1.01134	2.51410	2.71710
H	1.05732	1.98273	2.90017
C	-2.39733	0.92162	1.49437
H	-1.39211	-0.81500	0.72797
C	-2.26409	2.11958	2.21502
H	-0.94000	3.43828	3.27842
H	-3.37001	0.63586	1.10094
O	-3.30435	2.95681	2.43505
H	-4.14122	2.54915	2.17790
H	1.37475	-2.36750	-4.98290

5.8 F_{OC} -0.0050 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3045

Cartesian Coordinates:

O	1.25152	-1.43177	-5.17156
C	1.22190	-1.41139	-3.79674
C	1.82881	-2.29460	-1.64026
C	1.10464	-1.27815	-1.02495
C	0.43590	-0.32414	-1.79832
C	0.49290	-0.38811	-3.18270
C	1.88871	-2.36632	-3.02846
H	2.33885	-3.02044	-1.01561
H	-0.12112	0.46479	-1.30343
H	-0.01475	0.34316	-3.80255
H	2.45492	-3.16042	-3.51064
N	1.10653	-1.30864	0.43204
N	0.47100	-0.45221	1.02208
C	-0.32008	0.41742	1.67923
C	0.14373	1.71383	2.00485
C	-1.60443	0.02609	2.11900
C	-0.65805	2.57619	2.73830
H	1.14337	2.01417	1.71296
C	-2.40144	0.92647	2.82024
H	-1.96170	-0.97625	1.91482
C	-1.93835	2.20067	3.14371
H	-0.28708	3.55611	3.01787
H	-3.39155	0.60894	3.13735
O	-2.68687	3.12844	3.82864
H	-3.38220	2.69779	4.33998
H	1.79356	-2.17308	-5.46661

5.9 F_{OC} -0.0050 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3041

Cartesian Coordinates:

O	1.26099	-1.42485	-5.15621
C	1.23014	-1.40274	-3.77555
C	1.61476	-2.41326	-1.62286
C	1.13422	-1.26778	-0.98661
C	0.72360	-0.17962	-1.76402
C	0.77651	-0.23973	-3.15249
C	1.64675	-2.49315	-3.01064
H	1.95890	-3.23638	-1.00483
H	0.38911	0.72705	-1.27219
H	0.48045	0.60612	-3.76483
H	2.00605	-3.39854	-3.49693
N	1.20452	-1.29872	0.46424
N	0.52072	-0.48566	1.11088
C	-0.27334	0.42208	1.71018
C	-0.14064	0.63121	3.11172
C	-1.31606	1.12194	1.04634
C	-0.95563	1.50949	3.79520
H	0.63074	0.07721	3.63335
C	-2.16819	1.96705	1.73727
H	-1.46379	0.96146	-0.01553
C	-1.98141	2.17725	3.11195
H	-0.84482	1.67301	4.86094
H	-2.97661	2.47611	1.21716
O	-2.76232	3.00819	3.83884
H	-3.46767	3.39176	3.30303
H	1.61534	-2.27386	-5.44546

5.10 F_{OC} -0.0050 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3470

Cartesian Coordinates:

O	1.07214	-1.76626	-4.22707
C	1.06482	-1.68343	-2.84980
C	0.80404	-2.65258	-0.65721
C	1.07886	-1.41700	-0.06617
C	1.38456	-0.32254	-0.88695
C	1.38679	-0.45685	-2.26985
C	0.76630	-2.78055	-2.04203
H	0.62257	-3.51091	-0.01941
H	1.63933	0.63115	-0.44016
H	1.64188	0.38153	-2.90906
H	0.53221	-3.74456	-2.48919
N	1.26483	-1.40702	1.35680
N	0.83320	-0.52230	2.11763
C	-0.08810	0.49934	1.73088
C	0.11319	1.76347	2.30186
C	-1.24999	0.26123	0.98830
C	-0.78016	2.79739	2.06701
H	0.97639	1.91690	2.94006
C	-2.17125	1.28320	0.78947
H	-1.45217	-0.72630	0.59143
C	-1.93033	2.55726	1.31159
H	-0.62908	3.77880	2.50134
H	-3.08636	1.08571	0.23591
O	-2.79103	3.60294	1.12493
H	-3.63274	3.28754	0.77484
H	0.87957	-2.67438	-4.48816

5.11 F_{OC} -0.0075 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3898

Cartesian Coordinates:

O	0.40841	-0.47465	-5.88867
C	0.40011	-0.46506	-4.49968
C	1.13053	-1.31355	-2.36514
C	0.32791	-0.38121	-1.69915
C	-0.44212	0.51325	-2.46514
C	-0.40656	0.47194	-3.85242
C	1.16851	-1.35763	-3.75624
H	1.72227	-2.00094	-1.77086
H	-1.06321	1.23471	-1.94822
H	-0.99963	1.16084	-4.44613
H	1.79928	-2.09033	-4.25785
N	0.36599	-0.42548	-0.28831
N	-0.36157	0.42033	0.30273
C	-0.32478	0.37751	1.69926
C	-1.13547	1.32019	2.36060
C	0.44577	-0.51853	2.46834
C	-1.18452	1.37724	3.73909
H	-1.72465	2.00531	1.76076
C	0.40182	-0.46743	3.84784
H	1.07165	-1.24635	1.96796
C	-0.41434	0.48166	4.49637
H	-1.80371	2.09726	4.26058
H	0.99613	-1.15857	4.43889
O	-0.50580	0.58801	5.83058
H	0.04500	-0.05260	6.30090
H	1.00831	-1.17136	-6.17911

5.12 F_{OC} -0.0075 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3099

Cartesian Coordinates:

O	1.42977	-1.48421	-4.72019
C	1.33245	-1.43671	-3.32948
C	1.07540	-2.53615	-1.19232
C	1.11728	-1.28229	-0.51560
C	1.26579	-0.10911	-1.31246
C	1.36351	-0.19954	-2.69759
C	1.17893	-2.60379	-2.56654
H	0.96989	-3.43698	-0.59832
H	1.29604	0.85739	-0.82603
H	1.47591	0.69939	-3.29649
H	1.14451	-3.57558	-3.05802
N	0.97867	-1.26426	0.82291
N	1.11839	-0.15603	1.49290
C	-0.04328	0.51063	1.75353
C	0.08354	1.72554	2.48500
C	-1.32971	0.11989	1.29264
C	-1.00517	2.53140	2.71576
H	1.06445	1.99210	2.86134
C	-2.42117	0.92727	1.53382
H	-1.43377	-0.81446	0.75674
C	-2.26940	2.13089	2.24830
H	-0.92393	3.45200	3.28137
H	-3.40615	0.63621	1.17701
O	-3.30275	2.96197	2.49444
H	-4.15126	2.53972	2.30709
H	1.56380	-2.40410	-4.97527

5.13 F_{OC} -0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3058

Cartesian Coordinates:

O	1.27853	-1.45090	-5.18810
C	1.23405	-1.41717	-3.80687
C	1.81729	-2.29727	-1.64274
C	1.10124	-1.27016	-1.03705
C	0.44784	-0.31370	-1.81849
C	0.51260	-0.38414	-3.20414
C	1.88446	-2.37580	-3.03064
H	2.31509	-3.02476	-1.00989
H	-0.10223	0.48320	-1.32807
H	0.01731	0.35163	-3.82941
H	2.44564	-3.17865	-3.50561
N	1.09484	-1.29846	0.42657
N	0.45619	-0.44227	1.01103
C	-0.34126	0.43041	1.66408
C	0.12275	1.72573	1.98849
C	-1.61370	0.02695	2.12490
C	-0.67357	2.58157	2.73552
H	1.12187	2.02707	1.69554
C	-2.40890	0.92243	2.83385
H	-1.96144	-0.98163	1.93552
C	-1.94825	2.19950	3.15394
H	-0.30060	3.55794	3.02415
H	-3.39073	0.59810	3.16802
O	-2.69262	3.12312	3.84232
H	-3.33213	2.69456	4.42439
H	1.82445	-2.19874	-5.45808

5.14 F_{OC} -0.0075 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3074

Cartesian Coordinates:

O	1.29191	-1.44013	-5.17047
C	1.23984	-1.40582	-3.78334
C	1.59386	-2.41339	-1.62462
C	1.11870	-1.26142	-0.99483
C	0.72176	-0.17410	-1.77989
C	0.78919	-0.23864	-3.16969
C	1.63701	-2.49810	-3.01158
H	1.92828	-3.23536	-0.99953
H	0.38790	0.73580	-1.29299
H	0.50787	0.60990	-3.78615
H	1.99223	-3.40948	-3.49124
N	1.20236	-1.28572	0.45774
N	0.51611	-0.47703	1.10716
C	-0.28108	0.42421	1.70932
C	-0.13516	0.63808	3.11023
C	-1.33039	1.12163	1.05117
C	-0.94664	1.51362	3.79930
H	0.64176	0.08740	3.62699
C	-2.17727	1.96606	1.74705
H	-1.48553	0.95787	-0.00963
C	-1.98041	2.17763	3.12268
H	-0.82912	1.67867	4.86407
H	-2.99175	2.47329	1.23467
O	-2.75340	3.00441	3.85419
H	-3.47800	3.37683	3.33630
H	1.66229	-2.29060	-5.43397

5.15 F_{OC} -0.0075 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3474

Cartesian Coordinates:

O	1.10978	-1.79455	-4.24185
C	1.08437	-1.69110	-2.85942
C	0.76769	-2.63626	-0.66372
C	1.07120	-1.40451	-0.07779
C	1.41181	-0.32426	-0.90313
C	1.42765	-0.46875	-2.28625
C	0.74474	-2.77274	-2.04809
H	0.55662	-3.48497	-0.02217
H	1.68534	0.62529	-0.45833
H	1.71305	0.35927	-2.92664
H	0.49041	-3.73415	-2.49094
N	1.26882	-1.39095	1.34421
N	0.83935	-0.50773	2.10630
C	-0.08898	0.50728	1.72573
C	0.11288	1.77278	2.29424
C	-1.25485	0.26239	0.99134
C	-0.78462	2.80354	2.06139
H	0.97438	1.92719	2.93437
C	-2.18058	1.28120	0.79709
H	-1.45939	-0.72880	0.60476
C	-1.93932	2.55704	1.31512
H	-0.63846	3.78354	2.50039
H	-3.10188	1.07974	0.25535
O	-2.80528	3.59974	1.12793
H	-3.68004	3.27185	0.88751
H	0.92479	-2.71029	-4.48041

5.16 F_{OC} -0.0100 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3993

Cartesian Coordinates:

O	0.41091	-0.47755	-5.89912
C	0.39739	-0.46191	-4.50125
C	1.12967	-1.31246	-2.36728
C	0.32730	-0.38055	-1.69534
C	-0.44280	0.51386	-2.46473
C	-0.40816	0.47364	-3.85374
C	1.16588	-1.35445	-3.75837
H	1.72194	-2.00038	-1.77412
H	-1.06367	1.23495	-1.94679
H	-1.00295	1.16444	-4.44454
H	1.79703	-2.08749	-4.26065
N	0.36781	-0.42767	-0.28928
N	-0.36213	0.42103	0.30777
C	-0.32302	0.37550	1.69617
C	-1.13523	1.32007	2.36182
C	0.44875	-0.52209	2.46947
C	-1.18459	1.37748	3.73715
H	-1.72453	2.00543	1.76225
C	0.40505	-0.47129	3.84670
H	1.07505	-1.25051	1.97062
C	-0.41302	0.48016	4.49753
H	-1.80288	2.09655	4.26103
H	0.99864	-1.16169	4.43892
O	-0.50821	0.59084	5.82291
H	0.03665	-0.04300	6.31112
H	1.01449	-1.17835	-6.17121

5.17 F_{OC} -0.0100 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3162

Cartesian Coordinates:

O	1.53102	-1.54193	-4.75427
C	1.36658	-1.46291	-3.35901
C	1.01519	-2.53280	-1.21963
C	1.06229	-1.27257	-0.54933
C	1.23757	-0.10987	-1.35877
C	1.38881	-0.22098	-2.73990
C	1.16156	-2.61688	-2.58904
H	0.88242	-3.42628	-0.61983
H	1.26975	0.86309	-0.88523
H	1.54780	0.67049	-3.34060
H	1.12537	-3.59398	-3.07044
N	0.93621	-1.24960	0.78705
N	1.08756	-0.13959	1.45234
C	-0.06733	0.53310	1.72105
C	0.08252	1.74918	2.44819
C	-1.36980	0.13147	1.31356
C	-0.99812	2.55439	2.71442
H	1.07422	2.01305	2.79716
C	-2.45305	0.93167	1.59595
H	-1.48927	-0.81199	0.79677
C	-2.27762	2.14266	2.30076
H	-0.90223	3.47233	3.28202
H	-3.45261	0.63010	1.29307
O	-3.30210	2.96274	2.58895
H	-4.15834	2.52840	2.47702
H	1.87334	-2.42209	-4.94768

5.18 F_{OC} -0.0100 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3090

Cartesian Coordinates:

O	1.30909	-1.47845	-5.20756
C	1.24819	-1.42702	-3.82018
C	1.81824	-2.28936	-1.64547
C	1.09491	-1.26031	-1.05124
C	0.44240	-0.31400	-1.84522
C	0.51654	-0.39490	-3.23176
C	1.89730	-2.37622	-3.03224
H	2.31175	-3.01102	-1.00229
H	-0.11316	0.48430	-1.36278
H	0.02108	0.33476	-3.86503
H	2.46810	-3.17944	-3.49684
N	1.06561	-1.29509	0.41579
N	0.42728	-0.43456	0.99433
C	-0.37194	0.44527	1.64011
C	0.10406	1.73312	1.97602
C	-1.63379	0.03600	2.12655
C	-0.67636	2.58194	2.74674
H	1.10468	2.02922	1.68236
C	-2.41965	0.92805	2.84830
H	-1.97922	-0.97507	1.94628
C	-1.94903	2.20151	3.17579
H	-0.29138	3.54786	3.05366
H	-3.39553	0.60304	3.19789
O	-2.67763	3.12043	3.87825
H	-3.28842	2.69925	4.49660
H	1.87559	-2.22079	-5.44885

5.19 F_{OC} -0.0100 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3127

Cartesian Coordinates:

O	1.32903	-1.45764	-5.18561
C	1.25095	-1.41041	-3.79244
C	1.56707	-2.41473	-1.62693
C	1.09853	-1.25483	-1.00435
C	0.71837	-0.16819	-1.79868
C	0.80411	-0.23804	-3.18953
C	1.62385	-2.50536	-3.01255
H	1.88940	-3.23559	-0.99376
H	0.38606	0.74607	-1.31828
H	0.54203	0.61378	-3.81098
H	1.97346	-3.42380	-3.48454
N	1.19793	-1.27153	0.44878
N	0.51038	-0.46648	1.10196
C	-0.28823	0.42835	1.70763
C	-0.12692	0.64822	3.10782
C	-1.34740	1.12113	1.05729
C	-0.93494	1.51974	3.80384
H	0.65735	0.10230	3.61848
C	-2.18885	1.96355	1.75958
H	-1.51207	0.95314	-0.00195
C	-1.97959	2.17759	3.13589
H	-0.80896	1.68687	4.86744
H	-3.01139	2.46713	1.25648
O	-2.74464	2.99903	3.87312
H	-3.48903	3.35981	3.37514
H	1.72580	-2.30448	-5.42092

5.20 F_{OC} -0.0100 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3493

Cartesian Coordinates:

O	1.15025	-1.82786	-4.25755
C	1.10442	-1.70136	-2.87068
C	0.73163	-2.61949	-0.67224
C	1.06084	-1.39118	-0.09134
C	1.43453	-0.32589	-0.92177
C	1.46586	-0.48235	-2.30462
C	0.72489	-2.76628	-2.05569
H	0.49236	-3.45779	-0.02685
H	1.72524	0.61987	-0.47952
H	1.78175	0.33404	-2.94622
H	0.45251	-3.72540	-2.49395
N	1.27051	-1.37476	1.32933
N	0.84368	-0.49316	2.09331
C	-0.09137	0.51562	1.71979
C	0.11163	1.78208	2.28637
C	-1.26174	0.26434	0.99414
C	-0.79002	2.81012	2.05588
H	0.97185	1.93707	2.92804
C	-2.19164	1.28030	0.80529
H	-1.46895	-0.73034	0.61787
C	-1.94940	2.55781	1.31930
H	-0.64787	3.78879	2.49903
H	-3.11910	1.07586	0.27549
O	-2.82134	3.59787	1.13063
H	-3.72177	3.26825	1.02432
H	0.99073	-2.75436	-4.47137

5.21 F_{OC} +0.0025 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3790

Cartesian Coordinates:

O	0.40148	-0.46662	-5.85125
C	0.41234	-0.47925	-4.49390
C	1.13536	-1.31937	-2.35658
C	0.32842	-0.38168	-1.70116
C	-0.44211	0.51365	-2.46740
C	-0.40024	0.46497	-3.84700
C	1.18178	-1.37331	-3.74398
H	1.72533	-2.00493	-1.75815
H	-1.06633	1.23901	-1.96129
H	-0.98636	1.14603	-4.45352
H	1.81153	-2.10509	-4.24257
N	0.36088	-0.41940	-0.29348
N	-0.36563	0.42494	0.28803
C	-0.33396	0.38809	1.70094
C	-1.13985	1.32491	2.36078
C	0.43393	-0.50456	2.46334
C	-1.18661	1.37930	3.74770
H	-1.72906	2.00985	1.76086
C	0.39059	-0.45416	3.84886
H	1.05739	-1.22934	1.95466
C	-0.41909	0.48712	4.49497
H	-1.80909	2.10293	4.26208
H	0.98855	-1.14931	4.43550
O	-0.49136	0.57121	5.86310
H	0.08206	-0.09534	6.25954
H	0.98538	-1.14507	-6.21306

5.22 F_{OC} +0.0025 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3093

Cartesian Coordinates:

O	1.23788	-1.40232	-4.63568
C	1.25046	-1.41047	-3.28038
C	1.14545	-2.54127	-1.15115
C	1.20881	-1.29087	-0.47216
C	1.32337	-0.10322	-1.25459
C	1.32245	-0.17012	-2.63377
C	1.16600	-2.59787	-2.52597
H	1.07014	-3.44516	-0.55727
H	1.36900	0.85261	-0.74889
H	1.36604	0.72793	-3.23987
H	1.10740	-3.55766	-3.03296
N	1.06185	-1.28357	0.86812
N	1.18183	-0.17158	1.54980
C	0.01012	0.47537	1.80752
C	0.08170	1.69117	2.54618
C	-1.24947	0.09735	1.26957
C	-1.03018	2.47970	2.73395
H	1.04723	1.99151	2.93818
C	-2.36424	0.90123	1.46300
H	-1.32568	-0.80665	0.68098
C	-2.26669	2.08727	2.19330
H	-0.97093	3.41711	3.27602
H	-3.31520	0.61468	1.01910
O	-3.32828	2.92548	2.39218
H	-4.10520	2.59787	1.92256
H	1.17791	-2.29732	-4.99320

5.23 F_{OC} +0.0025 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3120

Cartesian Coordinates:

O	1.16418	-1.38486	-5.12895
C	1.18203	-1.39500	-3.77449
C	1.86415	-2.27632	-1.63948
C	1.11814	-1.28893	-0.99405
C	0.40038	-0.34766	-1.74799
C	0.43091	-0.39942	-3.12786
C	1.90064	-2.33398	-3.02670
H	2.41059	-2.99408	-1.03701
H	-0.17654	0.41888	-1.24200
H	-0.11504	0.31425	-3.73417
H	2.48210	-3.10267	-3.52826
N	1.13834	-1.33724	0.44078
N	0.51079	-0.48176	1.05277
C	-0.26082	0.37415	1.72452
C	0.20376	1.67184	2.06707
C	-1.57165	0.00918	2.12464
C	-0.60915	2.54565	2.77480
H	1.19917	1.97638	1.76552
C	-2.36539	0.91188	2.82533
H	-1.95278	-0.97345	1.87308
C	-1.89839	2.18109	3.15667
H	-0.24646	3.53740	3.02415
H	-3.36808	0.60526	3.11631
O	-2.65227	3.10174	3.86906
H	-3.58286	2.85379	3.83073
H	1.70299	-2.09757	-5.49522

5.24 F_{OC} +0.0025 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3058

Cartesian Coordinates:

O	1.20008	-1.39048	-5.11995
C	1.21127	-1.40071	-3.76045
C	1.65868	-2.41558	-1.62027
C	1.15720	-1.28669	-0.96744
C	0.71366	-0.19772	-1.73217
C	0.74216	-0.24830	-3.11499
C	1.67216	-2.48581	-3.00815
H	2.02600	-3.24000	-1.01791
H	0.37286	0.70166	-1.23294
H	0.41524	0.58970	-3.72066
H	2.04571	-3.37601	-3.50777
N	1.19648	-1.33572	0.47115
N	0.52467	-0.50562	1.11532
C	-0.25147	0.42105	1.70936
C	-0.14980	0.61904	3.11391
C	-1.28598	1.12505	1.03826
C	-0.97212	1.50307	3.78735
H	0.61011	0.05732	3.64506
C	-2.14908	1.97029	1.72110
H	-1.42152	0.97250	-0.02537
C	-1.98224	2.17819	3.09271
H	-0.87403	1.66231	4.85582
H	-2.94492	2.48215	1.18446
O	-2.78295	3.02047	3.81125
H	-3.43634	3.43289	3.23288
H	1.54648	-2.21741	-5.47759

5.25 F_{OC} +0.0025 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3547

Cartesian Coordinates:

O	0.97995	-1.71260	-4.19139
C	1.01491	-1.67782	-2.83197
C	0.91862	-2.69701	-0.64899
C	1.08570	-1.44850	-0.04184
C	1.27644	-0.31861	-0.85433
C	1.25121	-0.43414	-2.23428
C	0.84835	-2.81217	-2.03271
H	0.83495	-3.57693	-0.02018
H	1.46390	0.64954	-0.40650
H	1.41484	0.42766	-2.87128
H	0.69179	-3.78570	-2.48988
N	1.23580	-1.45644	1.38086
N	0.80108	-0.56750	2.14299
C	-0.09278	0.47928	1.74309
C	0.11097	1.73607	2.32632
C	-1.24844	0.26590	0.98198
C	-0.76900	2.78304	2.09046
H	0.98196	1.88284	2.95639
C	-2.15451	1.29978	0.77708
H	-1.44810	-0.70961	0.55556
C	-1.90839	2.56711	1.31279
H	-0.59783	3.76747	2.51137
H	-3.05394	1.11931	0.19351
O	-2.75548	3.62450	1.13003
H	-3.46569	3.38686	0.52151
H	0.83316	-2.61053	-4.51358

5.26 F_{OC} +0.0050 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3828

Cartesian Coordinates:

O	0.39999	-0.46491	-5.84215
C	0.41541	-0.48282	-4.49267
C	1.13718	-1.32150	-2.35480
C	0.32860	-0.38187	-1.69932
C	-0.44242	0.51407	-2.46776
C	-0.39898	0.46355	-3.84521
C	1.18560	-1.37779	-3.74055
H	1.72683	-2.00672	-1.75561
H	-1.06746	1.24041	-1.96454
H	-0.98340	1.14266	-4.45509
H	1.81510	-2.10932	-4.23876
N	0.36043	-0.41886	-0.29613
N	-0.36754	0.42715	0.28574
C	-0.33639	0.39090	1.69895
C	-1.14150	1.32677	2.36123
C	0.43118	-0.50134	2.46202
C	-1.18760	1.38040	3.74949
H	-1.73083	2.01184	1.76151
C	0.38797	-0.45108	3.84856
H	1.05409	-1.22544	1.95137
C	-0.42036	0.48859	4.49522
H	-1.81095	2.10501	4.26236
H	0.98690	-1.14733	4.43450
O	-0.48721	0.56638	5.87159
H	0.09132	-0.10607	6.24950
H	0.97935	-1.13811	-6.22242

5.27 F_{OC} +0.0050 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3153

Cartesian Coordinates:

O	1.23181	-1.40054	-4.62628
C	1.24789	-1.41424	-3.28057
C	1.14408	-2.54093	-1.15046
C	1.21317	-1.28773	-0.47393
C	1.33210	-0.10020	-1.25914
C	1.32689	-0.16913	-2.63502
C	1.16106	-2.60279	-2.52348
H	1.06566	-3.44199	-0.55262
H	1.38280	0.85551	-0.75363
H	1.37057	0.72493	-3.24658
H	1.09706	-3.56202	-3.02983
N	1.06887	-1.28316	0.86480
N	1.18783	-0.16887	1.55021
C	0.01611	0.47429	1.81101
C	0.07964	1.69026	2.55178
C	-1.24447	0.09538	1.27398
C	-1.03767	2.47204	2.74403
H	1.04578	2.00237	2.93379
C	-2.36433	0.89354	1.47392
H	-1.31993	-0.80138	0.67449
C	-2.27360	2.07683	2.20599
H	-0.97831	3.41448	3.27824
H	-3.31288	0.60324	1.02706
O	-3.34438	2.91072	2.41125
H	-4.09040	2.62912	1.86770
H	1.16640	-2.28854	-5.00216

5.28 F_{OC} +0.0050 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3189

Cartesian Coordinates:

O	1.13221	-1.36660	-5.11538
C	1.16689	-1.38635	-3.76864
C	1.87523	-2.26695	-1.64189
C	1.12400	-1.28779	-0.98493
C	0.39066	-0.34988	-1.73202
C	0.41089	-0.39833	-3.11017
C	1.90196	-2.32122	-3.02807
H	2.43381	-2.98169	-1.04702
H	-0.19036	0.41069	-1.22200
H	-0.14593	0.31054	-3.71190
H	2.48647	-3.08232	-3.53671
N	1.15561	-1.34174	0.44179
N	0.52583	-0.49144	1.06359
C	-0.24272	0.35245	1.74188
C	0.21261	1.65492	2.08898
C	-1.55631	-0.02015	2.14244
C	-0.61036	2.52247	2.79419
H	1.20221	1.97001	1.77921
C	-2.35296	0.87388	2.84685
H	-1.93305	-1.00164	1.87959
C	-1.89636	2.14874	3.17536
H	-0.25944	3.52112	3.03406
H	-3.35338	0.56475	3.14094
O	-2.67285	3.05307	3.90374
H	-3.56647	3.06910	3.54215
H	1.67049	-2.06709	-5.50680

5.29 F_{OC} +0.0050 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3105

Cartesian Coordinates:

O	1.18980	-1.38185	-5.11004
C	1.20896	-1.40184	-3.75798
C	1.67062	-2.41636	-1.62036
C	1.15826	-1.29305	-0.96261
C	0.70444	-0.20490	-1.72622
C	0.73027	-0.25326	-3.10683
C	1.68300	-2.48461	-3.00745
H	2.04524	-3.23986	-1.02127
H	0.35822	0.69191	-1.22659
H	0.39465	0.58133	-3.71209
H	2.06397	-3.36958	-3.50974
N	1.18950	-1.34807	0.46971
N	0.52240	-0.51146	1.11514
C	-0.24565	0.42055	1.70845
C	-0.15246	0.61550	3.11471
C	-1.27985	1.12682	1.03761
C	-0.97567	1.50156	3.78662
H	0.60445	0.05110	3.64792
C	-2.14435	1.97244	1.71957
H	-1.41419	0.97690	-0.02632
C	-1.98176	2.17968	3.09036
H	-0.87980	1.65919	4.85613
H	-2.93673	2.48568	1.17895
O	-2.78740	3.02649	3.80741
H	-3.42244	3.45010	3.21680
H	1.53884	-2.19880	-5.48894

5.30 F_{OC} +0.0050 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3603

Cartesian Coordinates:

O	0.95763	-1.70445	-4.18208
C	1.00284	-1.68152	-2.82919
C	0.95575	-2.70943	-0.64876
C	1.08400	-1.45749	-0.03621
C	1.23746	-0.31936	-0.84801
C	1.20729	-0.43208	-2.22648
C	0.87919	-2.82417	-2.03152
H	0.90378	-3.59340	-0.02209
H	1.40193	0.65330	-0.40139
H	1.34273	0.43442	-2.86354
H	0.75105	-3.80033	-2.49104
N	1.22229	-1.47231	1.38493
N	0.78725	-0.58152	2.14869
C	-0.09607	0.47426	1.74568
C	0.10961	1.72812	2.33371
C	-1.25134	0.27024	0.98023
C	-0.76612	2.78008	2.09943
H	0.98401	1.87186	2.96024
C	-2.15192	1.30865	0.77514
H	-1.45150	-0.70096	0.54440
C	-1.90300	2.57322	1.31630
H	-0.58721	3.76508	2.51634
H	-3.04666	1.13510	0.18262
O	-2.74618	3.63510	1.13557
H	-3.41189	3.42858	0.46794
H	0.83456	-2.59921	-4.52390

5.31 F_{OC} +0.0075 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3893

Cartesian Coordinates:

O	0.39884	-0.46361	-5.83346
C	0.41826	-0.48614	-4.49247
C	1.13892	-1.32356	-2.35367
C	0.32882	-0.38209	-1.69600
C	-0.44296	0.51479	-2.46812
C	-0.39814	0.46266	-3.84267
C	1.18924	-1.38209	-3.73709
H	1.72839	-2.00859	-1.75377
H	-1.06881	1.24214	-1.96754
H	-0.98090	1.13989	-4.45621
H	1.81865	-2.11356	-4.23500
N	0.36068	-0.41911	-0.29960
N	-0.36970	0.42964	0.28444
C	-0.33841	0.39324	1.69550
C	-1.14296	1.32840	2.36135
C	0.42911	-0.49889	2.46082
C	-1.18864	1.38153	3.75106
H	-1.73245	2.01359	1.76197
C	0.38571	-0.44841	3.84825
H	1.05151	-1.22235	1.94861
C	-0.42168	0.49011	4.49500
H	-1.81295	2.10722	4.26191
H	0.98538	-1.14548	4.43380
O	-0.48361	0.56218	5.88079
H	0.09959	-0.11563	6.24127
H	0.97344	-1.13132	-6.23215

5.32 F_{OC} +0.0075 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3240

Cartesian Coordinates:

O	1.24362	-1.40535	-4.62176
C	1.25343	-1.42187	-3.28551
C	1.13805	-2.54044	-1.15309
C	1.21088	-1.28311	-0.47985
C	1.33810	-0.09688	-1.27004
C	1.33643	-0.17049	-2.64232
C	1.15846	-2.61031	-2.52380
H	1.05352	-3.43747	-0.54994
H	1.39290	0.85965	-0.76645
H	1.38561	0.71830	-3.26085
H	1.09136	-3.56998	-3.02806
N	1.07053	-1.28141	0.85658
N	1.18996	-0.16438	1.54628
C	0.01918	0.47566	1.81127
C	0.07680	1.69175	2.55452
C	-1.24529	0.09462	1.28198
C	-1.04579	2.46619	2.75633
H	1.04480	2.01673	2.92183
C	-2.36970	0.88554	1.49457
H	-1.32245	-0.79507	0.67227
C	-2.28336	2.06656	2.22810
H	-0.98460	3.41385	3.28215
H	-3.31822	0.59019	1.05079
O	-3.36474	2.89389	2.44548
H	-4.07332	2.67177	1.82920
H	1.17562	-2.28674	-5.01511

5.33 F_{OC} +0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3287

Cartesian Coordinates:

O	1.12323	-1.34724	-5.10638
C	1.16345	-1.37831	-3.76733
C	1.89547	-2.24938	-1.64475
C	1.12474	-1.28657	-0.97995
C	0.36806	-0.36197	-1.72513
C	0.38681	-0.40703	-3.10125
C	1.91957	-2.30178	-3.02935
H	2.47278	-2.95261	-1.05403
H	-0.22699	0.38713	-1.21451
H	-0.18364	0.29172	-3.70189
H	2.51828	-3.04887	-3.54150
N	1.17640	-1.33403	0.43823
N	0.52828	-0.49844	1.06706
C	-0.25232	0.32091	1.74946
C	0.17278	1.64065	2.08555
C	-1.55138	-0.08493	2.17986
C	-0.66157	2.48522	2.80339
H	1.14772	1.98069	1.75617
C	-2.36367	0.79449	2.88215
H	-1.90680	-1.07568	1.92154
C	-1.93690	2.08267	3.19845
H	-0.32412	3.49050	3.04027
H	-3.36018	0.47993	3.17873
O	-2.77076	2.94553	3.93112
H	-3.22301	3.54346	3.32293
H	1.67248	-2.02750	-5.51963

5.34 F_{OC} +0.0075 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3173

Cartesian Coordinates:

O	1.18436	-1.37489	-5.10144
C	1.20877	-1.40386	-3.75703
C	1.68160	-2.41698	-1.62100
C	1.15633	-1.29929	-0.95867
C	0.69246	-0.21256	-1.72279
C	0.71816	-0.25924	-3.10106
C	1.69540	-2.48393	-3.00683
H	2.06336	-3.23878	-1.02406
H	0.33889	0.68144	-1.22374
H	0.37426	0.57132	-3.70696
H	2.08525	-3.36353	-3.51090
N	1.18089	-1.36022	0.46648
N	0.51840	-0.51695	1.11429
C	-0.24096	0.41944	1.70743
C	-0.15528	0.61184	3.11579
C	-1.27582	1.12888	1.03812
C	-0.97852	1.50026	3.78703
H	0.59895	0.04473	3.65065
C	-2.14019	1.97554	1.71996
H	-1.41030	0.98171	-0.02603
C	-1.98077	2.18199	3.09013
H	-0.88380	1.65619	4.85766
H	-2.92907	2.49087	1.17598
O	-2.79015	3.03435	3.80624
H	-3.40763	3.46831	3.20454
H	1.53772	-2.18100	-5.50084

5.35 F_{OC} +0.0075 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3674

Cartesian Coordinates:

O	0.93953	-1.70129	-4.17432
C	0.99311	-1.68808	-2.82816
C	0.99215	-2.72053	-0.64948
C	1.08031	-1.46565	-0.03165
C	1.19720	-0.32117	-0.84432
C	1.16413	-0.43287	-2.22103
C	0.91177	-2.83685	-2.03099
H	0.97129	-3.60686	-0.02416
H	1.33844	0.65593	-0.39999
H	1.27247	0.43677	-2.85889
H	0.81335	-3.81537	-2.49208
N	1.20689	-1.48796	1.38698
N	0.77190	-0.59503	2.15320
C	-0.10006	0.46999	1.74794
C	0.10806	1.72074	2.34123
C	-1.25558	0.27617	0.97874
C	-0.76334	2.77807	2.10943
H	0.98611	1.86095	2.96406
C	-2.15038	1.31950	0.77427
H	-1.45700	-0.69050	0.53359
C	-1.89816	2.58095	1.32153
H	-0.57625	3.76328	2.52291
H	-3.04068	1.15345	0.17325
O	-2.73732	3.64771	1.14329
H	-3.36049	3.47278	0.42696
H	0.84203	-2.59232	-4.53529

5.36 F_{OC} +0.0100 au OH−AB−OH Trans Structure S_0 State

E_h = -723.3986

Cartesian Coordinates:

O	0.39729	-0.46185	-5.82488
C	0.42086	-0.48917	-4.49220
C	1.14130	-1.32633	-2.35321
C	0.32942	-0.38275	-1.69179
C	-0.44342	0.51539	-2.46839
C	-0.39764	0.46211	-3.84004
C	1.19320	-1.38671	-3.73393
H	1.73067	-2.01126	-1.75285
H	-1.06988	1.24348	-1.96996
H	-0.97888	1.13762	-4.45694
H	1.82237	-2.11794	-4.23203
N	0.36166	-0.42022	-0.30341
N	-0.37211	0.43243	0.28422
C	-0.34035	0.39549	1.69052
C	-1.14461	1.33027	2.36153
C	0.42722	-0.49666	2.45986
C	-1.18992	1.38297	3.75219
H	-1.73439	2.01578	1.76271
C	0.38336	-0.44567	3.84784
H	1.04946	-1.21991	1.94699
C	-0.42316	0.49181	4.49514
H	-1.81529	2.10986	4.26099
H	0.98377	-1.14357	4.43333
O	-0.48021	0.55821	5.89033
H	0.10755	-0.12482	6.23286
H	0.96705	-1.12398	-6.24188

5.37 F_{OC} +0.0100 au OH−AB−OH Rotation TS Structure S_0 State

E_h = -723.3353

Cartesian Coordinates:

O	1.27237	-1.41629	-4.62186
C	1.26648	-1.43311	-3.29508
C	1.12824	-2.53973	-1.15913
C	1.20223	-1.27699	-0.48997
C	1.34078	-0.09320	-1.28705
C	1.35009	-0.17397	-2.65542
C	1.15846	-2.62027	-2.52697
H	1.03542	-3.43164	-0.54953
H	1.39855	0.86508	-0.78705
H	1.40977	0.70834	-3.28217
H	1.09101	-3.58136	-3.02778
N	1.06727	-1.27832	0.84375
N	1.18845	-0.15819	1.53814
C	0.01927	0.47910	1.80862
C	0.07283	1.69530	2.55471
C	-1.25176	0.09400	1.29413
C	-1.05499	2.46168	2.77056
H	1.04351	2.03468	2.90267
C	-2.38018	0.87577	1.52532
H	-1.33286	-0.78922	0.67549
C	-2.29612	2.05549	2.25948
H	-0.99071	3.41490	3.28723
H	-3.33092	0.57378	1.09080
O	-3.38996	2.87367	2.49385
H	-4.04996	2.73314	1.80393
H	1.20451	-2.29142	-5.03212

5.38 F_{OC} +0.0100 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -723.3406

Cartesian Coordinates:

O	1.11978	-1.34351	-5.09880
C	1.16425	-1.38010	-3.76709
C	1.89538	-2.25124	-1.64442
C	1.12348	-1.28709	-0.97578
C	0.36627	-0.36118	-1.72395
C	0.38615	-0.40714	-3.09799
C	1.92136	-2.30498	-3.02706
H	2.47272	-2.95485	-1.05402
H	-0.22958	0.38903	-1.21603
H	-0.18301	0.29050	-3.70107
H	2.52013	-3.05172	-3.53909
N	1.17678	-1.33787	0.43445
N	0.52935	-0.49976	1.06826
C	-0.24596	0.31696	1.75158
C	0.18051	1.63842	2.09263
C	-1.54990	-0.08227	2.18417
C	-0.65211	2.48505	2.80943
H	1.15123	1.98085	1.75323
C	-2.35856	0.79851	2.88847
H	-1.91390	-1.06691	1.91436
C	-1.92751	2.08505	3.20824
H	-0.31765	3.49431	3.03451
H	-3.35988	0.48883	3.17577
O	-2.76487	2.96179	3.92785
H	-3.26003	3.50544	3.30187
H	1.66430	-2.01758	-5.53029

5.39 F_{OC} +0.0100 au OH−AB−OH Inversion TS Structure S_0 State

E_h = -723.3263

Cartesian Coordinates:

O	1.18360	-1.36948	-5.09423
C	1.21073	-1.40669	-3.75764
C	1.69205	-2.41734	-1.62230
C	1.15178	-1.30535	-0.95565
C	0.67783	-0.22073	-1.72195
C	0.70569	-0.26626	-3.09772
C	1.70967	-2.48366	-3.00637
H	2.08092	-3.23659	-1.02637
H	0.31474	0.67003	-1.22439
H	0.35361	0.55953	-3.70530
H	2.10986	-3.35768	-3.51133
N	1.17121	-1.37203	0.46150
N	0.51278	-0.52219	1.11293
C	-0.23775	0.41722	1.70643
C	-0.15864	0.60771	3.11738
C	-1.27418	1.13088	1.03991
C	-0.98091	1.49905	3.78871
H	0.59327	0.03790	3.65355
C	-2.13669	1.97943	1.72230
H	-1.41022	0.98649	-0.02432
C	-1.97939	2.18515	3.09208
H	-0.88621	1.65340	4.86054
H	-2.92201	2.49760	1.17553
O	-2.79124	3.04431	3.80765
H	-3.39069	3.48897	3.19552
H	1.54248	-2.16406	-5.51353

5.40 F_{OC} +0.0100 au OH−AB−OH Cis Structure S_0 State

E_h = -723.3761

Cartesian Coordinates:

O	0.92458	-1.70168	-4.16769
C	0.98511	-1.69654	-2.82841
C	1.02686	-2.73019	-0.65072
C	1.07538	-1.47305	-0.02781
C	1.15719	-0.32398	-0.84254
C	1.12255	-0.43590	-2.21738
C	0.94452	-2.84948	-2.03074
H	1.03561	-3.61740	-0.02617
H	1.27587	0.65725	-0.40128
H	1.20532	0.43549	-2.85666
H	0.87581	-3.82975	-2.49282
N	1.19137	-1.50275	1.38751
N	0.75658	-0.60745	2.15695
C	-0.10437	0.46624	1.75042
C	0.10629	1.71402	2.34889
C	-1.26045	0.28289	0.97774
C	-0.76098	2.77674	2.11998
H	0.98825	1.85076	2.96765
C	-2.14954	1.33109	0.77432
H	-1.46332	-0.67915	0.52338
C	-1.89403	2.58937	1.32789
H	-0.56555	3.76212	2.52999
H	-3.03544	1.17267	0.16504
O	-2.72943	3.66099	1.15220
H	-3.31143	3.51754	0.39497
H	0.85272	-2.58802	-4.54771

6 Cartesian coordinates and energies of deprotonated OH−AB−O$^-$ structures in field free conditions

6.1 Field Free OH−AB−O$^-$ Trans Structure S_0 State

E_h = -722.8491

Cartesian Coordinates:

N	0.03222	0.09777	-0.67632
N	0.03422	0.10218	0.60875
C	-0.75140	-2.27269	-0.52984
C	-1.13334	-3.43113	-1.19763
C	-1.14597	-3.47502	-2.59303
C	-0.77218	-2.34670	-3.31954
H	-0.09760	-0.30468	-3.20596
H	-0.74103	-2.23687	0.55236
H	-1.42533	-4.31211	-0.62567
H	-0.78431	-2.38776	-4.40416
C	-0.39068	-1.18940	-2.64965
C	-0.36936	-1.11963	-1.24450
C	0.41190	1.24852	1.24400
C	0.40642	1.22685	2.66708
C	0.81051	2.46245	0.60576
C	0.76620	2.31800	3.41311
H	0.10201	0.29945	3.14730
C	1.17210	3.55952	1.33654
H	0.81783	2.48826	-0.47883
C	1.17657	3.56881	2.79683
H	0.75654	2.28440	4.49940
H	1.47500	4.48200	0.84679
O	1.51021	4.57928	3.45929
O	-1.51986	-4.60912	-3.29669
H	-1.75061	-5.30443	-2.66989

6.2 Field Free OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8014

Cartesian Coordinates:

N	1.55106	-0.45182	-0.46892
N	1.52165	-0.47879	0.85010
C	0.40958	1.69293	-0.71938
C	-0.06188	2.69282	-1.57115
C	0.13092	2.62040	-2.94554
C	0.80938	1.51793	-3.47543
H	1.80707	-0.33808	-3.07494
H	0.23506	1.76697	0.34792
H	-0.59476	3.54255	-1.14166
H	0.95840	1.46054	-4.55035
C	1.28209	0.51246	-2.65077
C	1.09989	0.55132	-1.23221
C	0.49997	-1.08216	1.45595
C	0.56082	-1.18951	2.89094
C	-0.65889	-1.62973	0.79224
C	-0.44636	-1.74686	3.61091
H	1.44858	-0.78672	3.37127
C	-1.67327	-2.18604	1.50278
H	-0.68882	-1.56812	-0.28999
C	-1.64355	-2.28787	2.96546
H	-0.40551	-1.81145	4.69446
H	-2.55908	-2.57991	1.01185
O	-2.57544	-2.79711	3.61196
O	-0.33558	3.59766	-3.83356
H	-0.78026	4.28271	-3.32212

6.3 Field Free OH−AB−O$^-$ Rotation Inversion TS Structure S_0 State

E_h = -722.7823

Cartesian Coordinates:

N	0.22463	1.23072	-1.28034
N	0.25336	1.23035	-0.01258
C	-0.66908	-1.13011	-1.29826
C	-0.98934	-2.27220	-2.03016
C	-0.72688	-2.32595	-3.39859
C	-0.15574	-1.22464	-4.03659
H	0.57694	0.78812	-3.78404
H	-0.88315	-1.08402	-0.23726
H	-1.45155	-3.12471	-1.53193
H	0.04276	-1.27675	-5.10282
C	0.14543	-0.08434	-3.30147
C	-0.08846	-0.01702	-1.91928
C	0.32913	1.22312	1.30142
C	0.25852	0.02878	2.11494
C	0.51406	2.45329	2.04081
C	0.36555	0.05443	3.47618
H	0.14095	-0.92268	1.60298
C	0.59997	2.49779	3.40192
H	0.57580	3.36540	1.45157
C	0.53366	1.29514	4.22345
H	0.32276	-0.86208	4.06008
H	0.72958	3.44064	3.92817
O	0.61578	1.32380	5.47108
O	-1.02118	-3.44086	-4.16719
H	-1.40087	-4.12061	-3.59850

6.4 Field Free OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7828

Cartesian Coordinates:

N	0.39605	1.28823	-1.25376
N	0.39620	1.29212	0.01409
C	-0.71526	-0.97806	-1.34512
C	-1.10406	-2.07970	-2.10608
C	-0.75778	-2.15903	-3.45415
C	-0.03579	-1.12151	-4.04485
H	0.87679	0.80689	-3.73077
H	-0.99796	-0.91376	-0.30136
H	-1.68487	-2.87951	-1.64628
H	0.22656	-1.19296	-5.09605
C	0.33038	-0.01853	-3.28307
C	0.01636	0.07051	-1.91806
C	0.38167	1.18212	1.32850
C	0.57057	2.35525	2.15113
C	0.22071	-0.05632	2.06036
C	0.57134	2.31518	3.51546
H	0.70504	3.29576	1.62222
C	0.24810	-0.11656	3.42456
H	0.10525	-0.97195	1.48660
C	0.41136	1.07016	4.25601
H	0.70279	3.21957	4.10480
H	0.14105	-1.06444	3.94700
O	0.41621	1.02085	5.50586
O	-1.11292	-3.23671	-4.24932
H	-1.59454	-3.87610	-3.71185

6.5 Field Free OH−AB−O^- Cis Structure S_0 State

E_h = -722.8220

Cartesian Coordinates:

N	1.43738	-1.59385	-0.64643
N	1.44322	-1.59459	0.62977
C	0.94026	0.73865	-1.32159
C	0.43294	1.62274	-2.26757
C	-0.28160	1.14659	-3.36848
C	-0.46532	-0.22395	-3.52656
H	-0.05683	-2.17757	-2.72069
H	1.47959	1.12229	-0.46273
H	0.59218	2.69315	-2.14327
H	-1.01628	-0.58806	-4.38812
C	0.06347	-1.10682	-2.58850
C	0.75689	-0.64920	-1.45636
C	0.59485	-0.91434	1.47886
C	0.99761	-0.93016	2.84644
C	-0.66628	-0.30510	1.19269
C	0.27337	-0.32516	3.83937
H	1.93176	-1.43922	3.07136
C	-1.41960	0.27164	2.18084
H	-1.05892	-0.32648	0.18382
C	-0.99238	0.33434	3.57296
H	0.61753	-0.33712	4.87043
H	-2.39009	0.70493	1.95147
O	-1.67728	0.89236	4.46313
O	-0.81222	1.99162	-4.32983
H	-0.67372	2.90520	-4.05478

7 Cartesian coordinates and energies of deprotonated OH−AB−O$^-$ structures in F_{NN} conditions

7.1 F_{NN} -0.0025 au OH−AB−O$^-$ Trans Structure S_0 State

E_h = -722.8447

Cartesian Coordinates:

N	0.03288	0.09971	-0.67939
N	0.03503	0.10435	0.61138
C	-0.74998	-2.26849	-0.53069
C	-1.13186	-3.42668	-1.19839
C	-1.14519	-3.47255	-2.59360
C	-0.77162	-2.34490	-3.32048
H	-0.09639	-0.30106	-3.20748
H	-0.73967	-2.23296	0.55148
H	-1.42338	-4.30629	-0.62401
H	-0.78373	-2.38584	-4.40584
C	-0.38972	-1.18650	-2.65175
C	-0.36714	-1.11301	-1.24509
C	0.41050	1.24401	1.24561
C	0.40554	1.22418	2.67276
C	0.80933	2.45883	0.60391
C	0.76489	2.31398	3.41610
H	0.10142	0.29799	3.15468
C	1.17056	3.55477	1.33173
H	0.81538	2.48101	-0.48068
C	1.17556	3.56477	2.79451
H	0.75592	2.28298	4.50190
H	1.47387	4.47886	0.84517
O	1.50886	4.57573	3.44830
O	-1.52139	-4.61355	-3.29524
H	-1.74962	-5.30142	-2.65937

7.2 F_{NN} -0.0025 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8008

Cartesian Coordinates:

N	1.54258	-0.45172	-0.47305
N	1.51449	-0.47765	0.85136
C	0.39936	1.69354	-0.72418
C	-0.06891	2.69252	-1.57537
C	0.12351	2.62051	-2.95112
C	0.79695	1.51623	-3.48029
H	1.79033	-0.34500	-3.07897
H	0.23016	1.77292	0.34359
H	-0.59887	3.54360	-1.14446
H	0.94895	1.45839	-4.55563
C	1.26610	0.50690	-2.65559
C	1.08816	0.54568	-1.23438
C	0.50064	-1.08160	1.45937
C	0.55691	-1.17931	2.89885
C	-0.65336	-1.64349	0.79348
C	-0.44782	-1.73790	3.61805
H	1.43837	-0.76602	3.38112
C	-1.66312	-2.20376	1.50205
H	-0.67784	-1.58944	-0.28925
C	-1.63769	-2.29471	2.96858
H	-0.41224	-1.79419	4.70174
H	-2.54354	-2.61296	1.01390
O	-2.56638	-2.81100	3.60652
O	-0.34872	3.60557	-3.83750
H	-0.68694	4.33702	-3.30901

7.3 F_{NN} -0.0025 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7761

Cartesian Coordinates:

N	0.23829	1.23067	-1.28559
N	0.26321	1.23078	-0.01204
C	-0.65643	-1.12501	-1.29622
C	-0.98433	-2.26635	-2.02472
C	-0.73502	-2.32213	-3.39501
C	-0.16932	-1.22152	-4.03830
H	0.57108	0.79151	-3.79269
H	-0.85884	-1.07974	-0.23319
H	-1.44146	-3.11786	-1.51960
H	0.02399	-1.27488	-5.10618
C	0.13996	-0.08000	-3.30702
C	-0.08032	-0.00843	-1.92143
C	0.33439	1.22378	1.29615
C	0.25598	0.02433	2.11102
C	0.51932	2.45591	2.04166
C	0.35490	0.04618	3.46922
H	0.13875	-0.92603	1.59680
C	0.59890	2.49752	3.39993
H	0.58502	3.36911	1.45440
C	0.52475	1.28927	4.21903
H	0.30564	-0.86857	4.05459
H	0.72772	3.43619	3.93288
O	0.60182	1.31524	5.46061
O	-1.04043	-3.44378	-4.15954
H	-1.37494	-4.13057	-3.57114

7.4 F_{NN} -0.0025 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7764

Cartesian Coordinates:

N	0.41429	1.28558	-1.25854
N	0.41076	1.29037	0.01514
C	-0.69810	-0.97574	-1.34102
C	-1.09716	-2.07489	-2.09922
C	-0.76877	-2.15318	-3.45126
C	-0.05392	-1.11495	-4.04873
H	0.86858	0.81206	-3.74141
H	-0.96596	-0.91502	-0.29351
H	-1.67131	-2.87505	-1.63108
H	0.20048	-1.18613	-5.10268
C	0.32335	-0.01273	-3.29003
C	0.02763	0.07760	-1.91947
C	0.39149	1.18194	1.32333
C	0.57840	2.35704	2.15227
C	0.22245	-0.06121	2.05610
C	0.56800	2.31556	3.51317
H	0.71886	3.29799	1.62561
C	0.23686	-0.12367	3.41667
H	0.11217	-0.97647	1.48066
C	0.39588	1.06618	4.25069
H	0.69652	3.21585	4.10856
H	0.12341	-1.06948	3.94066
O	0.38771	1.01554	5.49403
O	-1.13859	-3.23577	-4.24308
H	-1.56977	-3.88993	-3.68099

7.5 F_{NN} -0.0025 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8150

Cartesian Coordinates:

N	1.42099	-1.63632	-0.65254
N	1.42973	-1.64594	0.62959
C	0.92439	0.70879	-1.28086
C	0.42636	1.61125	-2.21218
C	-0.26973	1.15834	-3.33501
C	-0.43857	-0.20786	-3.53136
H	-0.03517	-2.18008	-2.76214
H	1.44127	1.07573	-0.40144
H	0.57316	2.67947	-2.05593
H	-0.98317	-0.55517	-4.40460
C	0.08266	-1.11190	-2.60714
C	0.75542	-0.68051	-1.45091
C	0.59055	-0.95698	1.46853
C	1.00075	-0.92544	2.83741
C	-0.67656	-0.36212	1.16662
C	0.29164	-0.26888	3.80490
H	1.93225	-1.43131	3.07875
C	-1.41714	0.26285	2.13040
H	-1.08183	-0.44077	0.16540
C	-0.96808	0.39782	3.51345
H	0.64075	-0.23669	4.83318
H	-2.39314	0.68109	1.89701
O	-1.63292	1.01544	4.37183
O	-0.79557	2.03447	-4.28057
H	-0.76751	2.92662	-3.91617

7.6 F_{NN} -0.0050 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8423

Cartesian Coordinates:

N	0.03389	0.10257	-0.68490
N	0.03599	0.10744	0.61231
C	-0.74798	-2.26311	-0.53245
C	-1.12998	-3.42154	-1.19810
C	-1.14473	-3.47099	-2.59326
C	-0.77184	-2.34480	-3.32202
H	-0.09602	-0.29890	-3.21346
H	-0.73716	-2.22664	0.54965
H	-1.42067	-4.29917	-0.62012
H	-0.78452	-2.38698	-4.40816
C	-0.38910	-1.18399	-2.65617
C	-0.36446	-1.10496	-1.24798
C	0.40924	1.24024	1.24634
C	0.40431	1.22118	2.67770
C	0.80884	2.45676	0.60243
C	0.76303	2.30903	3.41964
H	0.10025	0.29574	3.16036
C	1.16946	3.55079	1.32866
H	0.81418	2.47631	-0.48213
C	1.17412	3.56030	2.79410
H	0.75444	2.27972	4.50503
H	1.47356	4.47679	0.84607
O	1.50743	4.57118	3.44028
O	-1.52340	-4.61934	-3.29167
H	-1.74882	-5.29969	-2.64663

7.7 F_{NN} -0.0050 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8024

Cartesian Coordinates:

N	1.53256	-0.45349	-0.47936
N	1.50679	-0.47872	0.85069
C	0.38736	1.69242	-0.72967
C	-0.07436	2.69271	-1.57918
C	0.12120	2.62341	-2.95629
C	0.79093	1.51824	-3.48551
H	1.77942	-0.34876	-3.08461
H	0.22026	1.77406	0.33827
H	-0.60109	3.54512	-1.14659
H	0.94875	1.46256	-4.56111
C	1.25425	0.50334	-2.66175
C	1.07633	0.53922	-1.23801
C	0.50008	-1.08140	1.46204
C	0.55401	-1.17128	2.90579
C	-0.65113	-1.65516	0.79577
C	-0.44776	-1.73079	3.62559
H	1.43068	-0.74960	3.38891
C	-1.65594	-2.21852	1.50425
H	-0.67251	-1.60743	-0.28731
C	-1.63239	-2.30067	2.97426
H	-0.41521	-1.78033	4.70939
H	-2.53257	-2.64063	1.02009
O	-2.55771	-2.82296	3.60540
O	-0.34960	3.62046	-3.83978
H	-0.62126	4.37234	-3.30145

7.8 F_{NN} -0.0050 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7728

Cartesian Coordinates:

N	0.26164	1.22688	-1.29161
N	0.28003	1.22852	-0.01134
C	-0.64042	-1.12091	-1.29404
C	-0.98044	-2.25967	-2.01957
C	-0.74702	-2.31737	-3.39237
C	-0.18382	-1.21874	-4.04088
H	0.57094	0.79173	-3.80282
H	-0.82999	-1.07675	-0.22885
H	-1.43417	-3.10906	-1.50733
H	0.00219	-1.27316	-5.11099
C	0.13850	-0.07766	-3.31336
C	-0.06579	-0.00161	-1.92342
C	0.34386	1.22262	1.29129
C	0.26337	0.01806	2.10842
C	0.51964	2.45849	2.04273
C	0.35100	0.03809	3.46400
H	0.15453	-0.93233	1.59230
C	0.58823	2.49883	3.39849
H	0.58561	3.37261	1.45685
C	0.51165	1.28527	4.21600
H	0.30046	-0.87481	4.05149
H	0.70878	3.43465	3.93763
O	0.57925	1.31016	5.45219
O	-1.06793	-3.44463	-4.15294
H	-1.36747	-4.13360	-3.54829

7.9 F_{NN} -0.0050 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7729

Cartesian Coordinates:

N	0.44488	1.27754	-1.26379
N	0.43455	1.28459	0.01651
C	-0.67570	-0.97490	-1.33600
C	-1.09131	-2.06852	-2.09191
C	-0.78530	-2.14511	-3.44906
C	-0.07470	-1.10827	-4.05365
H	0.86576	0.81321	-3.75406
H	-0.92572	-0.91844	-0.28416
H	-1.66048	-2.86743	-1.61500
H	0.16844	-1.17873	-5.11130
C	0.32013	-0.00938	-3.29795
C	0.04690	0.08193	-1.92054
C	0.40684	1.17919	1.31861
C	0.58084	2.35883	2.15304
C	0.23628	-0.06904	2.05361
C	0.55316	2.31804	3.51053
H	0.72363	3.30023	1.62777
C	0.23314	-0.13131	3.41077
H	0.14106	-0.98550	1.47725
C	0.37413	1.06429	4.24625
H	0.67002	3.21605	4.11104
H	0.11921	-1.07517	3.93749
O	0.34650	1.01443	5.48328
O	-1.17607	-3.23053	-4.23775
H	-1.56292	-3.89453	-3.65512

7.10 F_{NN} -0.0050 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8107

Cartesian Coordinates:

N	1.39816	-1.67500	-0.65852
N	1.41134	-1.69361	0.63012
C	0.89599	0.68248	-1.23828
C	0.41272	1.60157	-2.15883
C	-0.25414	1.17097	-3.30876
C	-0.40376	-0.19044	-3.54297
H	-0.00470	-2.17956	-2.80886
H	1.38410	1.03403	-0.33672
H	0.54360	2.66684	-1.97051
H	-0.93401	-0.52214	-4.43195
C	0.10518	-1.11410	-2.62936
C	0.74737	-0.70856	-1.44415
C	0.58415	-0.99661	1.46210
C	1.00297	-0.92560	2.83101
C	-0.68888	-0.41356	1.14949
C	0.31212	-0.22046	3.77393
H	1.92995	-1.43248	3.08597
C	-1.41364	0.25677	2.09013
H	-1.10795	-0.54543	0.15926
C	-0.93879	0.45860	3.45960
H	0.66699	-0.15013	4.79780
H	-2.39503	0.66233	1.85750
O	-1.57823	1.13602	4.28463
O	-0.77283	2.07658	-4.24074
H	-0.85214	2.93338	-3.80568

7.11 F_{NN} -0.0075 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8420

Cartesian Coordinates:

N	0.03497	0.10574	-0.69086
N	0.03689	0.11031	0.61314
C	-0.74585	-2.25711	-0.53455
C	-1.12798	-3.41585	-1.19751
C	-1.14430	-3.46959	-2.59294
C	-0.77215	-2.34522	-3.32406
H	-0.09564	-0.29709	-3.22139
H	-0.73441	-2.21917	0.54749
H	-1.41779	-4.29118	-0.61536
H	-0.78557	-2.38931	-4.41116
C	-0.38841	-1.18146	-2.66180
C	-0.36154	-1.09616	-1.25175
C	0.40796	1.23643	1.24704
C	0.40307	1.21792	2.68270
C	0.80835	2.45487	0.60100
C	0.76116	2.30382	3.42352
H	0.09911	0.29317	3.16606
C	1.16830	3.54685	1.32596
H	0.81299	2.47201	-0.48359
C	1.17261	3.55570	2.79430
H	0.75298	2.27608	4.50867
H	1.47317	4.47484	0.84751
O	1.50595	4.56648	3.43309
O	-1.52564	-4.62592	-3.28731
H	-1.74816	-5.29821	-2.63269

7.12 F_{NN} -0.0075 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8059

Cartesian Coordinates:

N	1.52041	-0.45623	-0.48727
N	1.49766	-0.48054	0.84845
C	0.37177	1.68969	-0.73666
C	-0.08137	2.69238	-1.58412
C	0.12131	2.62786	-2.96245
C	0.78927	1.52276	-3.49176
H	1.77279	-0.35011	-3.09135
H	0.20368	1.77156	0.33113
H	-0.60599	3.54545	-1.15002
H	0.95667	1.47163	-4.56730
C	1.24436	0.50097	-2.66939
C	1.06285	0.53221	-1.24319
C	0.49784	-1.08093	1.46456
C	0.55174	-1.16406	2.91235
C	-0.65182	-1.66560	0.79959
C	-0.44584	-1.72530	3.63419
H	1.42444	-0.73456	3.39525
C	-1.65062	-2.23248	1.50969
H	-0.67242	-1.62323	-0.28377
C	-1.62626	-2.30766	2.98289
H	-0.41427	-1.76917	4.71808
H	-2.52439	-2.66639	1.03062
O	-2.54722	-2.83656	3.60867
O	-0.34291	3.63941	-3.84244
H	-0.56057	4.40305	-3.29593

7.13 F_{NN} -0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -722.7725

Cartesian Coordinates:

N	0.29429	1.21995	-1.29807
N	0.30380	1.22402	-0.01074
C	-0.62359	-1.11650	-1.29169
C	-0.98116	-2.25051	-2.01436
C	-0.76479	-2.31088	-3.39004
C	-0.19856	-1.21690	-4.04365
H	0.57970	0.78723	-3.81411
H	-0.79992	-1.07299	-0.22436
H	-1.43526	-3.09574	-1.49505
H	-0.02028	-1.27304	-5.11624
C	0.14239	-0.07792	-3.32012
C	-0.04530	0.00357	-1.92546
C	0.35847	1.21983	1.28680
C	0.28519	0.00962	2.10619
C	0.51310	2.46109	2.04392
C	0.35812	0.02925	3.45950
H	0.19534	-0.94173	1.58797
C	0.56620	2.50121	3.39746
H	0.57347	3.37638	1.45919
C	0.49503	1.28214	4.21380
H	0.31379	-0.88213	4.04936
H	0.66904	3.43542	3.94245
O	0.54845	1.30702	5.44515
O	-1.10705	-3.44218	-4.14662
H	-1.37784	-4.13059	-3.52770

7.14 F_{NN} -0.0075 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.7725

Cartesian Coordinates:

N	0.48667	1.26429	-1.26914
N	0.46709	1.27496	0.01824
C	-0.64890	-0.97563	-1.33014
C	-1.08685	-2.06055	-2.08417
C	-0.80730	-2.13473	-3.44734
C	-0.09736	-1.10144	-4.05896
H	0.86919	0.80995	-3.76813
H	-0.87878	-0.92432	-0.27368
H	-1.65296	-2.85659	-1.59825
H	0.13178	-1.17048	-5.12111
C	0.32124	-0.00868	-3.30626
C	0.07368	0.08341	-1.92105
C	0.42810	1.17397	1.31454
C	0.57696	2.36074	2.15296
C	0.26434	-0.07977	2.05302
C	0.52593	2.32243	3.50691
H	0.71762	3.30269	1.62815
C	0.23865	-0.13953	3.40689
H	0.19530	-0.99876	1.47676
C	0.34577	1.06432	4.24199
H	0.62165	3.22006	4.11118
H	0.13097	-1.08158	3.93756
O	0.29068	1.01721	5.47266
O	-1.22513	-3.22037	-4.23306
H	-1.57510	-3.89013	-3.63371

7.15 F_{NN} -0.0075 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8091

Cartesian Coordinates:

N	1.37070	-1.70641	-0.66397
N	1.38925	-1.73228	0.63170
C	0.85861	0.66189	-1.20034
C	0.39494	1.59406	-2.11576
C	-0.23496	1.18255	-3.29439
C	-0.36372	-0.17444	-3.56086
H	0.03073	-2.17698	-2.85485
H	1.31425	1.00147	-0.27775
H	0.50864	2.65607	-1.89938
H	-0.87429	-0.49355	-4.46702
C	0.12909	-1.11405	-2.65317
C	0.73431	-0.73136	-1.43753
C	0.57686	-1.02818	1.46014
C	1.00382	-0.93144	2.82949
C	-0.70128	-0.45157	1.14245
C	0.33260	-0.18625	3.75221
H	1.92417	-1.44464	3.09433
C	-1.40867	0.25614	2.06434
H	-1.13368	-0.62595	0.16422
C	-0.90691	0.51063	3.41891
H	0.69260	-0.08889	4.77169
H	-2.39435	0.65393	1.83714
O	-1.51774	1.24166	4.21243
O	-0.74534	2.11351	-4.21688
H	-0.92909	2.92598	-3.73094

7.16 F_{NN} -0.0100 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8439

Cartesian Coordinates:

N	0.03630	0.10967	-0.69894
N	0.03807	0.11397	0.61244
C	-0.74338	-2.24990	-0.53742
C	-1.12578	-3.40942	-1.19623
C	-1.14417	-3.46907	-2.59224
C	-0.77293	-2.34717	-3.32690
H	-0.09565	-0.29664	-3.23309
H	-0.73103	-2.20947	0.54454
H	-1.41453	-4.28174	-0.60879
H	-0.78743	-2.39437	-4.41508
C	-0.38786	-1.17948	-2.66966
C	-0.35831	-1.08637	-1.25748
C	0.40694	1.23336	1.24705
C	0.40175	1.21426	2.68705
C	0.80829	2.45443	0.59992
C	0.75904	2.29771	3.42794
H	0.09779	0.28979	3.17031
C	1.16736	3.54367	1.32489
H	0.81255	2.47020	-0.48470
C	1.17097	3.55061	2.79623
H	0.75100	2.27067	4.51293
H	1.47306	4.47399	0.85125
O	1.50419	4.56099	3.42846
O	-1.52841	-4.63417	-3.28094
H	-1.74774	-5.29756	-2.61601

7.17 F_{NN} -0.0100 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8116

Cartesian Coordinates:

N	1.50536	-0.45969	-0.49680
N	1.48614	-0.48258	0.84447
C	0.35117	1.68516	-0.74581
C	-0.09118	2.69134	-1.59099
C	0.12316	2.63376	-2.97020
C	0.79170	1.52983	-3.49934
H	1.77007	-0.34897	-3.09921
H	0.17868	1.76531	0.32146
H	-0.61510	3.54435	-1.15570
H	0.97345	1.48591	-4.57419
C	1.23552	0.49961	-2.67875
C	1.04651	0.52456	-1.25030
C	0.49329	-1.08001	1.46699
C	0.54982	-1.15689	2.91855
C	-0.65591	-1.67535	0.80537
C	-0.44163	-1.72141	3.64427
H	1.41916	-0.71930	3.39981
C	-1.64698	-2.24681	1.51908
H	-0.67844	-1.63733	-0.27822
C	-1.61845	-2.31691	2.99527
H	-0.40864	-1.76047	4.72825
H	-2.51874	-2.69203	1.04651
O	-2.53316	-2.85412	3.61738
O	-0.32867	3.66253	-3.84603
H	-0.49603	4.43365	-3.29204

7.18 F_{NN} -0.0100 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7754

Cartesian Coordinates:

N	0.34436	1.20794	-1.30434
N	0.34065	1.21601	-0.01070
C	-0.60236	-1.11186	-1.28859
C	-0.98641	-2.23773	-2.00832
C	-0.78991	-2.30146	-3.38740
C	-0.21095	-1.21690	-4.04610
H	0.60682	0.77350	-3.82661
H	-0.76450	-1.06853	-0.21906
H	-1.44656	-3.07545	-1.48164
H	-0.04128	-1.27538	-5.12168
C	0.15834	-0.08353	-3.32687
C	-0.01278	0.00498	-1.92751
C	0.38166	1.21484	1.28251
C	0.32761	-0.00116	2.10410
C	0.49570	2.46355	2.04396
C	0.37710	0.02034	3.45571
H	0.27346	-0.95427	1.58396
C	0.52359	2.50491	3.39560
H	0.54350	3.37982	1.45966
C	0.46662	1.28069	4.21167
H	0.34799	-0.88944	4.04858
H	0.59392	3.43901	3.94545
O	0.49402	1.30721	5.43875
O	-1.16396	-3.43320	-4.13956
H	-1.41397	-4.11825	-3.50797

7.19 F_{NN} -0.0100 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.7753

Cartesian Coordinates:

N	0.54413	1.24458	-1.27341
N	0.51205	1.26054	0.02001
C	-0.61704	-0.97745	-1.32263
C	-1.08643	-2.04884	-2.07501
C	-0.83854	-2.11932	-3.44511
C	-0.12125	-1.09480	-4.06365
H	0.88609	0.79773	-3.78259
H	-0.82348	-0.93218	-0.26112
H	-1.65341	-2.83900	-1.57994
H	0.09137	-1.16205	-5.13108
C	0.33104	-0.01310	-3.31384
C	0.11073	0.08019	-1.92086
C	0.45802	1.16570	1.31106
C	0.56258	2.36255	2.15058
C	0.31504	-0.09408	2.05399
C	0.47980	2.32823	3.50039
H	0.69357	3.30540	1.62497
C	0.25902	-0.14904	3.40436
H	0.28905	-1.01650	1.47934
C	0.30815	1.06529	4.23629
H	0.53992	3.22750	4.10643
H	0.16765	-1.08944	3.94057
O	0.21386	1.02236	5.45959
O	-1.29395	-3.20031	-4.22785
H	-1.61472	-3.87247	-3.61463

7.20 F_{NN} -0.0100 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8103

Cartesian Coordinates:

N	1.33965	-1.72792	-0.66916
N	1.36388	-1.75747	0.63427
C	0.81359	0.64900	-1.17215
C	0.37418	1.58923	-2.08938
C	-0.21126	1.19142	-3.29692
C	-0.31886	-0.16246	-3.58684
H	0.07020	-2.17389	-2.89789
H	1.23358	0.98172	-0.23065
H	0.46991	2.64846	-1.85141
H	-0.80537	-0.47378	-4.51025
C	0.15413	-1.11280	-2.67882
C	0.71730	-0.74763	-1.43302
C	0.56937	-1.04747	1.46270
C	1.00353	-0.94257	2.83428
C	-0.71307	-0.47039	1.14672
C	0.35214	-0.17034	3.74539
H	1.91562	-1.46749	3.10336
C	-1.40250	0.26248	2.05808
H	-1.15787	-0.67191	0.17896
C	-0.87465	0.54903	3.40023
H	0.71626	-0.06053	4.76193
H	-2.39103	0.65861	1.84116
O	-1.45594	1.32190	4.16902
O	-0.71366	2.14195	-4.21534
H	-0.99857	2.90477	-3.69807

7.21 F_{NN} +0.0025 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8555

Cartesian Coordinates:

N	0.03134	0.09549	-0.67377
N	0.03369	0.09992	0.60610
C	-0.75317	-2.27643	-0.52893
C	-1.13512	-3.43515	-1.19729
C	-1.14682	-3.47788	-2.59339
C	-0.77230	-2.34876	-3.31943
H	-0.09818	-0.30879	-3.20493
H	-0.74326	-2.24065	0.55342
H	-1.42786	-4.31712	-0.62733
H	-0.78413	-2.39007	-4.40356
C	-0.39138	-1.19292	-2.64842
C	-0.37158	-1.12626	-1.24380
C	0.41357	1.25312	1.24229
C	0.40785	1.22943	2.66150
C	0.81147	2.46664	0.60761
C	0.76804	2.32190	3.41049
H	0.10335	0.30071	3.13992
C	1.17333	3.56464	1.34169
H	0.81969	2.49642	-0.47699
C	1.17811	3.57274	2.79971
H	0.75776	2.28561	4.49741
H	1.47527	4.48576	0.84883
O	1.51110	4.58311	3.47099
O	-1.51869	-4.60620	-3.29788
H	-1.75201	-5.30732	-2.67872

7.22 F_{NN} +0.0025 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8043

Cartesian Coordinates:

N	1.55536	-0.45259	-0.46787
N	1.52638	-0.48098	0.84639
C	0.41188	1.69007	-0.71627
C	-0.06107	2.69142	-1.56817
C	0.13934	2.62263	-2.94100
C	0.82619	1.52395	-3.47179
H	1.82719	-0.32772	-3.07202
H	0.22795	1.75604	0.34996
H	-0.60083	3.53765	-1.14104
H	0.97784	1.47075	-4.54587
C	1.29856	0.52009	-2.64790
C	1.10699	0.55631	-1.23194
C	0.49789	-1.08327	1.45221
C	0.56609	-1.20067	2.88269
C	-0.66701	-1.61699	0.79340
C	-0.44198	-1.75735	3.60552
H	1.46097	-0.80856	3.35945
C	-1.68448	-2.16958	1.50865
H	-0.70516	-1.54815	-0.28824
C	-1.64768	-2.28253	2.96712
H	-0.39332	-1.83064	4.68889
H	-2.57635	-2.54823	1.01671
O	-2.58164	-2.78460	3.62467
O	-0.31670	3.59587	-3.82908
H	-0.85531	4.23123	-3.34465

7.23 F_{NN} +0.0025 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7914

Cartesian Coordinates:

N	0.22304	1.22694	-1.27635
N	0.25102	1.22736	-0.01318
C	-0.67677	-1.13591	-1.29967
C	-0.99564	-2.27643	-2.03522
C	-0.72470	-2.32806	-3.40298
C	-0.14651	-1.22719	-4.03633
H	0.58519	0.78285	-3.77800
H	-0.89892	-1.08989	-0.24004
H	-1.46461	-3.12872	-1.54340
H	0.05398	-1.27747	-5.10169
C	0.15229	-0.08954	-3.29748
C	-0.09000	-0.02652	-1.91728
C	0.32796	1.22076	1.30667
C	0.26727	0.03165	2.11986
C	0.50669	2.45027	2.04011
C	0.37940	0.06270	3.48448
H	0.15406	-0.92161	1.61036
C	0.59426	2.49888	3.40441
H	0.56316	3.36110	1.44849
C	0.53847	1.30215	4.22894
H	0.34573	-0.85533	4.06749
H	0.71939	3.44680	3.92364
O	0.62210	1.33477	5.48330
O	-1.01430	-3.43459	-4.17580
H	-1.42992	-4.10936	-3.62673

7.24 F_{NN} +0.0025 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.7921

Cartesian Coordinates:

N	0.39230	1.28443	-1.24950
N	0.39220	1.28889	0.01370
C	-0.72458	-0.98372	-1.34782
C	-1.10998	-2.08425	-2.11276
C	-0.75362	-2.16216	-3.45924
C	-0.02487	-1.12534	-4.04394
H	0.88404	0.80130	-3.72322
H	-1.01669	-0.91858	-0.30639
H	-1.69724	-2.88331	-1.66043
H	0.23980	-1.19457	-5.09412
C	0.33693	-0.02460	-3.27821
C	0.01270	0.06077	-1.91610
C	0.37749	1.17898	1.33430
C	0.56133	2.35254	2.14963
C	0.22631	-0.05402	2.06753
C	0.56702	2.31676	3.51751
H	0.68918	3.29190	1.61717
C	0.26218	-0.10883	3.43571
H	0.11172	-0.97180	1.49713
C	0.42082	1.07715	4.26291
H	0.69553	3.22702	4.09941
H	0.16406	-1.05819	3.95816
O	0.43334	1.03190	5.51980
O	-1.10115	-3.23218	-4.25869
H	-1.62557	-3.85861	-3.74668

7.25 F_{NN} +0.0025 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8316

Cartesian Coordinates:

N	1.44657	-1.55129	-0.64078
N	1.45115	-1.54428	0.63005
C	0.94286	0.76965	-1.35586
C	0.43214	1.63556	-2.31873
C	-0.28905	1.13710	-3.40521
C	-0.48190	-0.23711	-3.52928
H	-0.06735	-2.17239	-2.68981
H	1.49692	1.16953	-0.51367
H	0.59949	2.70732	-2.22296
H	-1.03035	-0.61740	-4.38485
C	0.04934	-1.09935	-2.57578
C	0.75163	-0.61699	-1.46024
C	0.59626	-0.87266	1.49190
C	0.99440	-0.93743	2.85582
C	-0.65971	-0.24965	1.22541
C	0.25919	-0.38215	3.87288
H	1.92995	-1.45211	3.06241
C	-1.42191	0.28031	2.23720
H	-1.04248	-0.21625	0.21312
C	-1.01036	0.27389	3.63269
H	0.60049	-0.43907	4.90421
H	-2.38792	0.72790	2.01597
O	-1.70896	0.77757	4.55174
O	-0.82094	1.95234	-4.38297
H	-0.57893	2.86886	-4.20705

7.26 F_{NN} +0.0050 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8640

Cartesian Coordinates:

N	0.03063	0.09364	-0.67165
N	0.03294	0.09735	0.60362
C	-0.75457	-2.27953	-0.52842
C	-1.13656	-3.43857	-1.19637
C	-1.14766	-3.48072	-2.59330
C	-0.77270	-2.35116	-3.31954
H	-0.09906	-0.31299	-3.20614
H	-0.74478	-2.24314	0.55404
H	-1.42983	-4.32130	-0.62784
H	-0.78458	-2.39343	-4.40327
C	-0.39208	-1.19599	-2.64824
C	-0.37340	-1.13162	-1.24412
C	0.41505	1.25742	1.24063
C	0.40898	1.23169	2.65619
C	0.81250	2.47062	0.60941
C	0.76958	2.32549	3.40823
H	0.10436	0.30168	3.13285
C	1.17460	3.56947	1.34695
H	0.82176	2.50430	-0.47523
C	1.17930	3.57637	2.80291
H	0.75873	2.28664	4.49592
H	1.47581	4.48921	0.85109
O	1.51208	4.58661	3.48301
O	-1.51762	-4.60352	-3.29833
H	-1.75340	-5.31056	-2.68690

7.27 F_{NN} +0.0050 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8095

Cartesian Coordinates:

N	1.55541	-0.45164	-0.46907
N	1.52717	-0.48079	0.84109
C	0.40511	1.68652	-0.71663
C	-0.07242	2.68622	-1.56978
C	0.14300	2.62372	-2.94056
C	0.84274	1.53074	-3.47106
H	1.84750	-0.31590	-3.07003
H	0.20970	1.74368	0.34802
H	-0.62713	3.52458	-1.14689
H	1.00237	1.48451	-4.54377
C	1.31176	0.52775	-2.64750
C	1.10783	0.56110	-1.23394
C	0.49389	-1.08341	1.44918
C	0.57125	-1.20947	2.87529
C	-0.67590	-1.60827	0.79769
C	-0.43548	-1.76795	3.60278
H	1.47246	-0.82529	3.34742
C	-1.69404	-2.15977	1.52013
H	-0.72410	-1.53463	-0.28335
C	-1.64856	-2.28194	2.97413
H	-0.37731	-1.84894	4.68598
H	-2.59063	-2.52733	1.02835
O	-2.58243	-2.77919	3.64505
O	-0.30653	3.58913	-3.82995
H	-0.86453	4.22073	-3.36276

7.28 F_{NN} +0.0050 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8032

Cartesian Coordinates:

N	0.24296	1.21640	-1.27391
N	0.26328	1.21980	-0.01402
C	-0.67782	-1.14216	-1.30034
C	-1.00467	-2.27803	-2.03990
C	-0.73088	-2.32788	-3.40834
C	-0.14108	-1.23020	-4.03780
H	0.60322	0.77196	-3.77446
H	-0.90420	-1.09629	-0.24131
H	-1.48339	-3.12781	-1.55360
H	0.05718	-1.27873	-5.10326
C	0.16519	-0.09807	-3.29510
C	-0.08002	-0.03869	-1.91523
C	0.33358	1.21563	1.31170
C	0.29005	0.03193	2.12600
C	0.49151	2.44691	2.03952
C	0.40297	0.07097	3.49444
H	0.19289	-0.92468	1.61953
C	0.57201	2.50171	3.40752
H	0.53745	3.35634	1.44501
C	0.53632	1.31117	4.23580
H	0.38675	-0.84833	4.07724
H	0.68000	3.45637	3.91940
O	0.61627	1.34969	5.49774
O	-1.02457	-3.42391	-4.18527
H	-1.48237	-4.08850	-3.65779

7.29 F_{NN} +0.0050 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.8042

Cartesian Coordinates:

N	0.41205	1.27136	-1.24605
N	0.40462	1.27888	0.01365
C	-0.72442	-0.99121	-1.34856
C	-1.11700	-2.08610	-2.11823
C	-0.75926	-2.16135	-3.46573
C	-0.02113	-1.12791	-4.04604
H	0.89740	0.79052	-3.71949
H	-1.01955	-0.92655	-0.30763
H	-1.71226	-2.88227	-1.67186
H	0.23945	-1.19389	-5.09705
C	0.34727	-0.03361	-3.27579
C	0.02150	0.04719	-1.91376
C	0.38082	1.17190	1.34011
C	0.54393	2.34934	2.14743
C	0.24708	-0.05568	2.07690
C	0.54502	2.32080	3.51898
H	0.66002	3.28753	1.61036
C	0.28648	-0.10168	3.44949
H	0.14608	-0.97794	1.51118
C	0.42236	1.08675	4.27095
H	0.65718	3.23937	4.09225
H	0.20612	-1.05250	3.97341
O	0.43623	1.04845	5.53557
O	-1.10925	-3.22032	-4.26973
H	-1.67749	-3.82959	-3.78448

7.30 F_{NN} +0.0050 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8439

Cartesian Coordinates:

N	1.43793	-1.52086	-0.63764
N	1.44395	-1.50646	0.62858
C	0.92288	0.79464	-1.37608
C	0.42061	1.64613	-2.35765
C	-0.28683	1.13001	-3.44535
C	-0.47776	-0.24752	-3.54977
H	-0.05579	-2.16842	-2.68763
H	1.47533	1.20787	-0.53906
H	0.58910	2.71879	-2.28006
H	-1.00797	-0.64048	-4.41067
C	0.04680	-1.09342	-2.58022
C	0.73513	-0.59179	-1.46437
C	0.59051	-0.83667	1.50574
C	0.99257	-0.94317	2.86255
C	-0.66207	-0.20218	1.26433
C	0.25593	-0.42741	3.90268
H	1.92880	-1.46500	3.04802
C	-1.42439	0.28985	2.29945
H	-1.04276	-0.12432	0.25352
C	-1.01617	0.22744	3.69197
H	0.60149	-0.52264	4.93073
H	-2.38798	0.74913	2.09140
O	-1.71843	0.68846	4.63823
O	-0.80944	1.92082	-4.44029
H	-0.50092	2.82909	-4.34218

7.31 F_{NN} +0.0075 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8744

Cartesian Coordinates:

N	0.03008	0.09212	-0.67125
N	0.03237	0.09539	0.60021
C	-0.75563	-2.28180	-0.52830
C	-1.13774	-3.44139	-1.19499
C	-1.14870	-3.48408	-2.59294
C	-0.77346	-2.35447	-3.32019
H	-0.10032	-0.31803	-3.20984
H	-0.74573	-2.24427	0.55427
H	-1.43138	-4.32448	-0.62707
H	-0.78570	-2.39843	-4.40364
C	-0.39296	-1.19940	-2.64956
C	-0.37488	-1.13602	-1.24557
C	0.41662	1.26200	1.23834
C	0.40998	1.23373	2.65055
C	0.81389	2.47553	0.61134
C	0.77085	2.32844	3.40640
H	0.10512	0.30220	3.12490
C	1.17606	3.57470	1.35314
H	0.82444	2.51367	-0.47334
C	1.18034	3.57962	2.80726
H	0.75925	2.28660	4.49497
H	1.47669	4.49334	0.85486
O	1.51284	4.58949	3.49673
O	-1.51697	-4.60204	-3.29754
H	-1.75498	-5.31446	-2.69324

7.32 F_{NN} +0.0075 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8173

Cartesian Coordinates:

N	1.55118	-0.44862	-0.47262
N	1.52328	-0.47894	0.83518
C	0.39473	1.68626	-0.71965
C	-0.08475	2.68391	-1.57452
C	0.14927	2.62782	-2.94351
C	0.86050	1.53908	-3.47284
H	1.86379	-0.30505	-3.06880
H	0.18710	1.73427	0.34309
H	-0.65559	3.51438	-1.15834
H	1.03022	1.50009	-4.54387
C	1.32194	0.53560	-2.64895
C	1.10390	0.56668	-1.23743
C	0.48738	-1.08231	1.44684
C	0.57495	-1.21713	2.86909
C	-0.68697	-1.60314	0.80492
C	-0.42816	-1.78028	3.60250
H	1.48185	-0.83864	3.33598
C	-1.70293	-2.15668	1.53667
H	-0.74732	-1.52684	-0.27549
C	-1.64764	-2.28688	2.98597
H	-0.35823	-1.86903	4.68554
H	-2.60279	-2.51757	1.04563
O	-2.57960	-2.78210	3.67200
O	-0.29008	3.58579	-3.83410
H	-0.85492	4.22347	-3.38347

7.33 F_{NN} +0.0075 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8178

Cartesian Coordinates:

N	0.30952	1.19202	-1.27326
N	0.30633	1.20332	-0.01585
C	-0.67066	-1.14563	-1.29995
C	-1.02571	-2.27018	-2.04358
C	-0.75500	-2.32143	-3.41416
C	-0.13868	-1.23611	-4.04103
H	0.65155	0.74511	-3.77355
H	-0.89599	-1.09784	-0.24045
H	-1.52493	-3.11035	-1.56163
H	0.05319	-1.28511	-5.10739
C	0.19575	-0.11556	-3.29456
C	-0.04674	-0.05656	-1.91357
C	0.35217	1.20567	1.31567
C	0.34520	0.02778	2.13251
C	0.45416	2.44218	2.03814
C	0.45167	0.07891	3.50559
H	0.29038	-0.93399	1.62933
C	0.50961	2.50534	3.41069
H	0.47496	3.35043	1.44057
C	0.52059	1.32193	4.24374
H	0.47431	-0.84076	4.08878
H	0.57000	3.46880	3.91521
O	0.58774	1.36939	5.51451
O	-1.07241	-3.40175	-4.19472
H	-1.57438	-4.05000	-3.68743

7.34 F_{NN} +0.0075 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.8192

Cartesian Coordinates:

N	0.48102	1.23868	-1.24251
N	0.45018	1.25493	0.01428
C	-0.71000	-0.99933	-1.34662
C	-1.13040	-2.07932	-2.12225
C	-0.78300	-2.15182	-3.47432
C	-0.02557	-1.13011	-4.05211
H	0.93324	0.76457	-3.71941
H	-0.99825	-0.93601	-0.30337
H	-1.74026	-2.86638	-1.68002
H	0.22276	-1.19263	-5.10605
C	0.37085	-0.05100	-3.27603
C	0.05472	0.02549	-1.91074
C	0.39696	1.15754	1.34539
C	0.50642	2.34460	2.14215
C	0.29658	-0.06384	2.08984
C	0.48414	2.32784	3.51728
H	0.59916	3.28164	1.59868
C	0.33109	-0.09472	3.46764
H	0.23397	-0.99421	1.53171
C	0.40798	1.10060	4.27974
H	0.55164	3.25859	4.07909
H	0.28732	-1.04623	3.99587
O	0.41311	1.07460	5.55330
O	-1.15564	-3.19203	-4.28354
H	-1.76478	-3.77999	-3.82214

7.35 F_{NN} +0.0075 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8588

Cartesian Coordinates:

N	1.40229	-1.51117	-0.63895
N	1.41323	-1.48770	0.62349
C	0.87138	0.80780	-1.37955
C	0.39321	1.65125	-2.38102
C	-0.27194	1.12430	-3.49105
C	-0.44570	-0.25700	-3.59635
H	-0.01563	-2.16920	-2.72557
H	1.39917	1.23027	-0.53118
H	0.55251	2.72513	-2.30601
H	-0.93575	-0.65705	-4.47729
C	0.05928	-1.09288	-2.61022
C	0.70260	-0.57986	-1.47183
C	0.57396	-0.80772	1.51900
C	0.99311	-0.94418	2.86493
C	-0.67697	-0.16372	1.31049
C	0.26865	-0.45419	3.92946
H	1.92946	-1.47455	3.02470
C	-1.42676	0.30249	2.37112
H	-1.06739	-0.05428	0.30597
C	-1.00546	0.20069	3.75486
H	0.62945	-0.57790	4.95032
H	-2.39028	0.77065	2.18263
O	-1.69873	0.63250	4.72976
O	-0.76914	1.89785	-4.50456
H	-0.43402	2.80036	-4.44693

7.36 F_{NN} +0.0100 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8868

Cartesian Coordinates:

N	0.02965	0.09087	-0.67236
N	0.03195	0.09391	0.59597
C	-0.75637	-2.28336	-0.52855
C	-1.13872	-3.44373	-1.19320
C	-1.14992	-3.48797	-2.59239
C	-0.77456	-2.35859	-3.32137
H	-0.10192	-0.32385	-3.21576
H	-0.74617	-2.24424	0.55415
H	-1.43256	-4.32683	-0.62519
H	-0.78744	-2.40494	-4.40463
C	-0.39400	-1.20315	-2.65222
C	-0.37608	-1.13961	-1.24802
C	0.41831	1.26690	1.23557
C	0.41088	1.23563	2.64471
C	0.81562	2.48125	0.61340
C	0.77189	2.33091	3.40500
H	0.10567	0.30241	3.11635
C	1.17770	3.58031	1.36017
H	0.82767	2.52441	-0.47130
C	1.18129	3.58253	2.81264
H	0.75938	2.28575	4.49457
H	1.47785	4.49805	0.85987
O	1.51341	4.59193	3.51200
O	-1.51670	-4.60162	-3.29573
H	-1.75676	-5.31904	-2.69814

7.37 F_{NN} +0.0100 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8279

Cartesian Coordinates:

N	1.54083	-0.44408	-0.47975
N	1.51235	-0.47657	0.82676
C	0.37922	1.68911	-0.72646
C	-0.09647	2.68598	-1.58326
C	0.16092	2.63717	-2.95033
C	0.88176	1.55086	-3.47753
H	1.87631	-0.29444	-3.06885
H	0.15759	1.72812	0.33378
H	-0.68263	3.50960	-1.17557
H	1.06485	1.52019	-4.54638
C	1.32945	0.54456	-2.65301
C	1.09374	0.57284	-1.24331
C	0.47640	-1.08098	1.44489
C	0.57680	-1.22306	2.86361
C	-0.70195	-1.60393	0.81609
C	-0.41963	-1.79363	3.60557
H	1.48905	-0.84760	3.32362
C	-1.71218	-2.16253	1.56026
H	-0.77698	-1.52856	-0.26369
C	-1.64449	-2.29815	3.00493
H	-0.33461	-1.88973	4.68824
H	-2.61383	-2.52267	1.07158
O	-2.57163	-2.79487	3.70868
O	-0.26190	3.59042	-3.84144
H	-0.83189	4.23610	-3.40861

7.38 F_{NN} +0.0100 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8355

Cartesian Coordinates:

N	0.46637	1.13242	-1.26975
N	0.40966	1.16281	-0.01681
C	-0.65251	-1.14294	-1.29751
C	-1.07370	-2.23999	-2.04626
C	-0.81423	-2.29781	-3.42110
C	-0.13929	-1.24555	-4.04562
H	0.76460	0.68270	-3.77264
H	-0.86742	-1.09028	-0.23566
H	-1.61579	-3.05511	-1.56815
H	0.04118	-1.29875	-5.11367
C	0.26324	-0.15217	-3.29418
C	0.02949	-0.08829	-1.91073
C	0.39512	1.18191	1.31796
C	0.46867	0.01703	2.14406
C	0.36717	2.42621	2.02885
C	0.55445	0.09345	3.52310
H	0.51042	-0.95026	1.64977
C	0.36703	2.50093	3.40603
H	0.32781	3.32993	1.42550
C	0.48217	1.33644	4.25130
H	0.66079	-0.81805	4.11127
H	0.31765	3.47269	3.89719
O	0.52043	1.40195	5.53331
O	-1.19128	-3.34862	-4.20539
H	-1.74941	-3.96504	-3.71730

7.39 F_{NN} +0.0100 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.8372

Cartesian Coordinates:

N	0.63205	1.16431	-1.23237
N	0.55106	1.20052	0.01894
C	-0.68164	-1.00567	-1.34196
C	-1.16418	-2.05143	-2.12681
C	-0.83862	-2.12190	-3.48692
C	-0.03678	-1.13180	-4.06155
H	1.02148	0.70396	-3.71758
H	-0.95081	-0.94447	-0.29312
H	-1.80563	-2.81500	-1.68877
H	0.19216	-1.19165	-5.11991
C	0.42403	-0.08689	-3.27602
C	0.12682	-0.01353	-1.90506
C	0.43404	1.12652	1.35043
C	0.42428	2.33046	2.12518
C	0.40425	-0.08273	2.11313
C	0.35237	2.33223	3.50255
H	0.46300	3.26421	1.56966
C	0.42124	-0.08327	3.49762
H	0.42743	-1.02511	1.57188
C	0.37287	1.12161	4.28826
H	0.32102	3.27845	4.04273
H	0.45299	-1.02892	4.03864
O	0.35634	1.12047	5.57289
O	-1.26764	-3.12589	-4.30396
H	-1.91887	-3.68300	-3.86199

7.40 F_{NN} +0.0100 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8764

Cartesian Coordinates:

N	1.32889	-1.52879	-0.64635
N	1.34893	-1.49319	0.61330
C	0.78341	0.80495	-1.36875
C	0.34837	1.64860	-2.39019
C	-0.24073	1.12014	-3.54350
C	-0.38111	-0.26489	-3.67092
H	0.05349	-2.17407	-2.80337
H	1.25965	1.23125	-0.49230
H	0.48668	2.72401	-2.30094
H	-0.80529	-0.66409	-4.58565
C	0.08725	-1.09821	-2.66762
C	0.65005	-0.58470	-1.48514
C	0.54321	-0.78555	1.53061
C	0.99698	-0.93692	2.86108
C	-0.70796	-0.13479	1.36572
C	0.30138	-0.45805	3.95332
H	1.93344	-1.47598	2.98882
C	-1.42984	0.31793	2.45625
H	-1.12289	-0.00762	0.37262
C	-0.97600	0.19437	3.82514
H	0.69189	-0.59773	4.96239
H	-2.39621	0.79105	2.29547
O	-1.64615	0.60822	4.83303
O	-0.69157	1.88494	-4.57661
H	-0.36530	2.79106	-4.52020

8 Cartesian coordinates and energies of deprotonated OH−AB−O$^-$ structures in F_{OC} conditions

8.1 F_{OC} -0.0025 au OH−AB−O$^-$ Trans Structure S_0 State

E_h = -722.8394

Cartesian Coordinates:

O	-0.24308	-0.73366	-5.81885
C	-0.21743	-0.65662	-4.42569
C	-0.57273	-1.73403	-2.30164
C	-0.18950	-0.57307	-1.59827
C	0.18184	0.55271	-2.36626
C	0.16622	0.50585	-3.75606
H	-0.88640	-2.68384	-4.21542
H	-0.85982	-2.60416	-1.71963
H	0.47928	1.45414	-1.84529
H	0.45752	1.38910	-4.32686
N	-0.21053	-0.63686	-0.20603
N	0.15429	0.46357	0.37049
C	0.16540	0.49788	1.72408
C	0.57226	1.72408	2.33381
C	-0.19429	-0.58457	2.59203
C	0.62320	1.87940	3.68942
H	0.84361	2.54035	1.66799
C	-0.14889	-0.44576	3.94720
H	-0.50430	-1.51904	2.13706
C	0.26387	0.79873	4.59932
H	0.93429	2.81690	4.14173
H	-0.42148	-1.26584	4.60645
O	0.30269	0.91782	5.83928
C	-0.58820	-1.78046	-3.69152
H	0.03792	0.11928	-6.16906

8.2 F_{OC} -0.0025 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8000

Cartesian Coordinates:

N	0.82445	1.47200	-0.09610
N	0.34487	1.37355	1.13493
C	-1.21228	0.74906	-1.23606
C	-1.87455	0.51443	-2.43948
C	-1.25535	0.74357	-3.66357
C	0.05451	1.23115	-3.67576
H	1.74776	1.86266	-2.51608
H	-1.71294	0.54579	-0.29630
H	-2.89904	0.13883	-2.41075
H	0.54106	1.41098	-4.63161
C	0.73091	1.48187	-2.49353
C	0.13231	1.24479	-1.21276
C	0.51596	0.23829	1.80082
C	0.06423	0.20224	3.17188
C	1.10999	-0.96357	1.25835
C	0.13459	-0.92726	3.91857
H	-0.35311	1.12220	3.57168
C	1.18581	-2.09761	1.99532
H	1.48243	-0.91852	0.24092
C	0.69281	-2.17004	3.37807
H	-0.22163	-0.95819	4.94374
H	1.61549	-3.01119	1.59342
O	0.74850	-3.21799	4.03677
O	-1.89721	0.50554	-4.89506
H	-2.70082	0.00664	-4.71131

8.3 F_{OC} -0.0025 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7745

Cartesian Coordinates:

N	-0.98771	1.42247	-0.48080
N	-0.55163	0.94995	0.61822
C	-0.24527	-0.65133	-1.69953
C	-0.04139	-1.30630	-2.91211
C	-0.26419	-0.64162	-4.11661
C	-0.70900	0.68001	-4.10412
H	-1.28621	2.34666	-2.85927
H	-0.08222	-1.17058	-0.76298
H	0.28958	-2.34580	-2.91712
H	-0.88020	1.19062	-5.04772
C	-0.92618	1.32183	-2.88977
C	-0.68573	0.68085	-1.66284
C	-0.06371	0.49298	1.74474
C	0.88041	-0.60628	1.83266
C	-0.43140	1.08514	3.01848
C	1.39348	-1.04589	3.01514
H	1.20060	-1.06779	0.90194
C	0.05401	0.64203	4.21079
H	-1.13587	1.91275	2.98060
C	1.01063	-0.45926	4.29805
H	2.11069	-1.86231	3.05273
H	-0.24785	1.09794	5.15018
O	1.46741	-0.87018	5.38045
O	-0.06452	-1.25852	-5.35006
H	0.25328	-2.15445	-5.18887

8.4 F_{OC} -0.0025 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7753

Cartesian Coordinates:

O	-0.55345	-1.74431	-5.12551
C	-0.52106	-1.67896	-3.73419
C	-1.17238	-2.63086	-1.62107
C	-0.51152	-1.61056	-0.91671
C	0.16480	-0.63486	-1.66476
C	0.16542	-0.67261	-3.05805
H	-1.72602	-3.44480	-3.54595
H	-1.67507	-3.39935	-1.04043
H	0.71009	0.14102	-1.14169
H	0.70987	0.08751	-3.62050
N	-0.50108	-1.71613	0.51118
N	-0.17127	-0.67928	1.16939
C	0.16335	0.45054	1.75109
C	0.42492	0.48921	3.17572
C	0.27158	1.72948	1.07494
C	0.78339	1.62736	3.83422
H	0.33289	-0.45444	3.70752
C	0.59833	2.88182	1.72539
H	0.04603	1.75853	0.01207
C	0.90129	2.91321	3.15394
H	0.98752	1.61993	4.90168
H	0.65459	3.83203	1.19906
O	1.23252	3.96266	3.74031
C	-1.19390	-2.66352	-3.01085
H	-0.06254	-0.99003	-5.47133

8.5 F_{OC} -0.0025 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8162

Cartesian Coordinates:

O	-0.52239	-1.71229	-4.45592
C	-0.47701	-1.70428	-3.06409
C	-1.58047	-2.14179	-0.96781
C	-0.46401	-1.69342	-0.24213
C	0.66429	-1.27852	-0.97560
C	0.65839	-1.29037	-2.36505
H	-2.47622	-2.46064	-2.90925
H	-2.44497	-2.49390	-0.41372
H	1.54457	-0.93568	-0.44377
H	1.54574	-0.96636	-2.90866
N	-0.42961	-1.89834	1.15734
N	-0.00911	-1.04052	2.00568
C	0.20218	0.30390	1.80965
C	0.94055	0.95275	2.84407
C	-0.30496	1.13774	0.76505
C	1.25725	2.28412	2.79907
H	1.26793	0.33082	3.67328
C	-0.03142	2.47807	0.72848
H	-0.95320	0.71429	0.00757
C	0.81295	3.14260	1.71448
H	1.84169	2.74644	3.58981
H	-0.45335	3.10835	-0.05081
O	1.10350	4.35897	1.63384
C	-1.59752	-2.13376	-2.36131
H	0.27376	-1.27958	-4.78480

8.6 F_{OC} -0.0050 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8334

Cartesian Coordinates:

O	-0.23739	-0.71613	-5.82608
C	-0.21681	-0.65456	-4.42224
C	-0.57585	-1.74289	-2.30338
C	-0.19321	-0.58443	-1.58727
C	0.17991	0.54615	-2.35588
C	0.16565	0.50357	-3.74545
H	-0.88710	-2.68465	-4.21962
H	-0.86410	-2.61611	-1.72636
H	0.47665	1.44488	-1.82999
H	0.45848	1.39093	-4.31149
N	-0.21552	-0.65221	-0.20511
N	0.15258	0.45845	0.37403
C	0.16443	0.49490	1.71832
C	0.57329	1.72778	2.32646
C	-0.19560	-0.58922	2.59283
C	0.62562	1.88738	3.67724
H	0.84348	2.54099	1.65658
C	-0.14901	-0.44675	3.94402
H	-0.50566	-1.52441	2.14022
C	0.26570	0.80440	4.59097
H	0.93620	2.82386	4.13108
H	-0.41972	-1.26163	4.60970
O	0.30576	0.92748	5.82375
C	-0.58886	-1.78171	-3.69360
H	0.04684	0.14584	-6.15044

8.7 F_{OC} -0.0050 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8012

Cartesian Coordinates:

N	0.83026	1.47408	-0.10011
N	0.35409	1.37565	1.13815
C	-1.21632	0.76054	-1.23143
C	-1.88237	0.53131	-2.43113
C	-1.26275	0.74791	-3.65914
C	0.05042	1.22461	-3.67607
H	1.75115	1.85207	-2.52093
H	-1.71758	0.56680	-0.28997
H	-2.91212	0.16965	-2.39830
H	0.53878	1.39592	-4.63361
C	0.73180	1.47753	-2.49595
C	0.13625	1.24736	-1.20896
C	0.52624	0.24575	1.80349
C	0.06544	0.20273	3.17535
C	1.13214	-0.95337	1.26042
C	0.12149	-0.93201	3.91227
H	-0.34816	1.12151	3.58087
C	1.19737	-2.09072	1.98852
H	1.52451	-0.89796	0.25105
C	0.67270	-2.17577	3.36201
H	-0.24126	-0.96968	4.93456
H	1.64014	-3.00065	1.59258
O	0.70138	-3.23388	3.99898
O	-1.92093	0.50443	-4.89035
H	-2.67392	-0.06459	-4.69618

8.8 F_{OC} -0.0050 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7698

Cartesian Coordinates:

N	-0.95975	1.44521	-0.49007
N	-0.53256	0.96500	0.61661
C	-0.23844	-0.63764	-1.69231
C	-0.04931	-1.30362	-2.90045
C	-0.27526	-0.64968	-4.10975
C	-0.70888	0.67575	-4.10612
H	-1.26430	2.35969	-2.87229
H	-0.07327	-1.14983	-0.75243
H	0.27347	-2.34649	-2.89654
H	-0.88206	1.18181	-5.05284
C	-0.91255	1.33152	-2.89636
C	-0.66977	0.70186	-1.66087
C	-0.05659	0.50507	1.73966
C	0.90264	-0.58852	1.82287
C	-0.44658	1.07583	3.02257
C	1.40743	-1.03809	3.00100
H	1.23842	-1.03031	0.88778
C	0.02886	0.62065	4.21097
H	-1.16100	1.89482	2.98971
C	0.99998	-0.47285	4.29012
H	2.13455	-1.84536	3.03974
H	-0.28764	1.05521	5.15508
O	1.45030	-0.89427	5.36470
O	-0.08609	-1.28965	-5.34211
H	0.22537	-2.18315	-5.15650

8.9 F_{OC} -0.0050 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7702

Cartesian Coordinates:

O	-0.50459	-1.73374	-5.12676
C	-0.50016	-1.67661	-3.72650
C	-1.18557	-2.63072	-1.62499
C	-0.53782	-1.60918	-0.90611
C	0.14892	-0.63034	-1.64607
C	0.17256	-0.66982	-3.03866
H	-1.70842	-3.44477	-3.55735
H	-1.69573	-3.40047	-1.05254
H	0.68341	0.14604	-1.11303
H	0.72594	0.09222	-3.59187
N	-0.54022	-1.71529	0.51369
N	-0.20291	-0.67744	1.17414
C	0.13841	0.44557	1.75363
C	0.43753	0.48525	3.17482
C	0.22441	1.72792	1.07329
C	0.82025	1.62087	3.81999
H	0.35550	-0.45632	3.71132
C	0.57154	2.87762	1.71198
H	-0.04016	1.75545	0.01908
C	0.92835	2.90520	3.13097
H	1.05360	1.61544	4.88099
H	0.60885	3.83084	1.18926
O	1.29365	3.95077	3.69574
C	-1.18407	-2.66227	-3.01537
H	-0.00494	-0.97265	-5.44419

8.10 F_{OC} -0.0050 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8122

Cartesian Coordinates:

O	-0.47277	-1.66500	-4.44600
C	-0.45402	-1.68177	-3.04618
C	-1.57735	-2.16449	-0.97056
C	-0.48187	-1.69713	-0.22295
C	0.65003	-1.25424	-0.93870
C	0.66394	-1.25458	-2.32695
H	-2.44083	-2.47943	-2.92702
H	-2.44262	-2.53715	-0.43136
H	1.51440	-0.89758	-0.39053
H	1.55325	-0.90804	-2.85439
N	-0.46242	-1.90627	1.17235
N	-0.04658	-1.04653	2.02301
C	0.16825	0.29254	1.82639
C	0.94305	0.94522	2.83305
C	-0.36221	1.11785	0.78643
C	1.29308	2.26561	2.74537
H	1.27516	0.33520	3.66876
C	-0.05816	2.44851	0.71104
H	-1.05536	0.69311	0.06989
C	0.84978	3.10601	1.64508
H	1.90689	2.73152	3.51080
H	-0.50091	3.07839	-0.05721
O	1.18913	4.30377	1.50763
C	-1.57412	-2.14292	-2.36509
H	0.29084	-1.15399	-4.73747

8.11 F_{OC} -0.0075 au OH−AB−O$^-$ Trans Structure S_0 State

E_h = -722.8313

Cartesian Coordinates:

O	-0.23283	-0.70222	-5.83566
C	-0.21679	-0.65442	-4.42066
C	-0.57851	-1.75072	-2.30499
C	-0.19607	-0.59317	-1.57741
C	0.17856	0.54172	-2.34924
C	0.16481	0.50073	-3.73827
H	-0.88826	-2.68754	-4.22173
H	-0.86758	-2.62619	-1.73157
H	0.47479	1.43864	-1.82010
H	0.45879	1.39134	-4.30145
N	-0.21918	-0.66344	-0.20585
N	0.15198	0.45707	0.37782
C	0.16393	0.49380	1.71405
C	0.57476	1.73251	2.32242
C	-0.19675	-0.59299	2.59365
C	0.62780	1.89443	3.66897
H	0.84432	2.54357	1.64985
C	-0.14957	-0.44859	3.94146
H	-0.50668	-1.52843	2.14229
C	0.26633	0.80828	4.58532
H	0.93800	2.82934	4.12560
H	-0.41862	-1.25934	4.61230
O	0.30806	0.93369	5.81169
C	-0.58976	-1.78407	-3.69518
H	0.05419	0.16788	-6.13503

8.12 F_{OC} -0.0075 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8047

Cartesian Coordinates:

N	0.83473	1.47607	-0.10330
N	0.36207	1.37746	1.14213
C	-1.22317	0.77587	-1.22655
C	-1.89244	0.55207	-2.42268
C	-1.27166	0.75615	-3.65468
C	0.04603	1.21953	-3.67571
H	1.75431	1.84103	-2.52431
H	-1.72539	0.59304	-0.28337
H	-2.92732	0.20499	-2.38660
H	0.53677	1.38087	-4.63497
C	0.73210	1.47380	-2.49766
C	0.13845	1.25093	-1.20457
C	0.53459	0.25191	1.80637
C	0.06754	0.20184	3.17984
C	1.15186	-0.94423	1.26209
C	0.11111	-0.93817	3.90687
H	-0.34115	1.11937	3.59241
C	1.20792	-2.08498	1.98148
H	1.56295	-0.87862	0.26080
C	0.65346	-2.18280	3.34537
H	-0.25591	-0.98246	4.92716
H	1.66304	-2.99118	1.59092
O	0.65418	-3.25123	3.95903
O	-1.94356	0.50152	-4.88565
H	-2.63176	-0.14356	-4.68829

8.13 F_{OC} -0.0075 au OH−AB−OH Rotation Inversion TS Structure S_0 State

E_h = -722.7683

Cartesian Coordinates:

N	-0.91094	1.47711	-0.50287
N	-0.49845	0.98702	0.61296
C	-0.22333	-0.62149	-1.68515
C	-0.06212	-1.30227	-2.88811
C	-0.29801	-0.66237	-4.10298
C	-0.71131	0.67007	-4.10932
H	-1.22662	2.37758	-2.88940
H	-0.05171	-1.12552	-0.74212
H	0.24714	-2.35005	-2.87425
H	-0.89112	1.16978	-5.05950
C	-0.88847	1.34439	-2.90546
C	-0.63936	0.72832	-1.66015
C	-0.03971	0.52170	1.73385
C	0.94615	-0.55563	1.81462
C	-0.47023	1.05801	3.02472
C	1.43447	-1.01869	2.99056
H	1.31210	-0.96534	0.87591
C	-0.01351	0.58568	4.21066
H	-1.20103	1.86220	2.99461
C	0.98080	-0.49147	4.28487
H	2.18006	-1.80847	3.03304
H	-0.35833	0.98877	5.15840
O	1.41369	-0.93066	5.35334
O	-0.13386	-1.33091	-5.33344
H	0.16067	-2.22481	-5.12264

8.14 F_{OC} -0.0075 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.7677

Cartesian Coordinates:

O	-0.43802	-1.74434	-5.13010
C	-0.47138	-1.68444	-3.72231
C	-1.20174	-2.62786	-1.63033
C	-0.57532	-1.59756	-0.89968
C	0.11907	-0.61504	-1.63489
C	0.17516	-0.66713	-3.02561
H	-1.67628	-3.45940	-3.56609
H	-1.71855	-3.39787	-1.06425
H	0.63402	0.16994	-1.09534
H	0.73523	0.09683	-3.57210
N	-0.59569	-1.69963	0.51093
N	-0.24672	-0.66517	1.17692
C	0.10648	0.44724	1.75796
C	0.45418	0.47894	3.17235
C	0.16526	1.73692	1.08063
C	0.86951	1.60738	3.80591
H	0.38310	-0.46307	3.70906
C	0.54106	2.87918	1.71038
H	-0.14805	1.76872	0.03957
C	0.96699	2.89302	3.11355
H	1.14007	1.59786	4.85767
H	0.55646	3.83850	1.19771
O	1.37807	3.92914	3.65582
C	-1.16793	-2.66832	-3.02015
H	0.07336	-0.98025	-5.42213

8.15 F_{OC} -0.0075 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8101

Cartesian Coordinates:

O	-0.42462	-1.62101	-4.43668
C	-0.43017	-1.66364	-3.02935
C	-1.57199	-2.18594	-0.97309
C	-0.49719	-1.69950	-0.20495
C	0.63800	-1.23166	-0.90467
C	0.67111	-1.22377	-2.29139
H	-2.40531	-2.49714	-2.94289
H	-2.43761	-2.57709	-0.44778
H	1.48727	-0.86259	-0.34164
H	1.56245	-0.85858	-2.80366
N	-0.49214	-1.91176	1.18577
N	-0.08141	-1.05081	2.03944
C	0.13683	0.28321	1.84338
C	0.94173	0.93960	2.82551
C	-0.41245	1.10018	0.80620
C	1.32233	2.24767	2.69602
H	1.27530	0.34232	3.66946
C	-0.08005	2.41987	0.69270
H	-1.14404	0.67507	0.12848
C	0.88350	3.06788	1.57765
H	1.96061	2.71718	3.43841
H	-0.53887	3.04985	-0.06626
O	1.26858	4.24322	1.38346
C	-1.54956	-2.15253	-2.36820
H	0.28627	-1.02141	-4.69052

8.16 F_{OC} -0.0100 au OH−AB−O$^-$ Trans Structure S_0 State

E_h = -722.8330

Cartesian Coordinates:

O	-0.22897	-0.69045	-5.84695
C	-0.21712	-0.65537	-4.42069
C	-0.58106	-1.75809	-2.30688
C	-0.19845	-0.60045	-1.56844
C	0.17765	0.53859	-2.34514
C	0.16391	0.49769	-3.73340
H	-0.88993	-2.69187	-4.22281
H	-0.87083	-2.63542	-1.73639
H	0.47359	1.43436	-1.81393
H	0.45890	1.39108	-4.29488
N	-0.22202	-0.67219	-0.20787
N	0.15219	0.45796	0.38168
C	0.16385	0.49374	1.71090
C	0.57638	1.73773	2.32063
C	-0.19765	-0.59608	2.59483
C	0.62975	1.90074	3.66354
H	0.84541	2.54727	1.64619
C	-0.15016	-0.45068	3.93986
H	-0.50741	-1.53150	2.14410
C	0.26690	0.81097	4.58179
H	0.93940	2.83397	4.12350
H	-0.41787	-1.25800	4.61498
O	0.30961	0.93817	5.80237
C	-0.59093	-1.78721	-3.69676
H	0.06060	0.18696	-6.12197

8.17 F_{OC} -0.0100 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8105

Cartesian Coordinates:

N	0.81303	1.41492	-0.13918
N	0.32652	1.32435	1.10718
C	-1.19268	0.58311	-1.27600
C	-1.85502	0.36740	-2.47432
C	-1.26739	0.68372	-3.70277
C	0.02676	1.21280	-3.71217
H	1.72832	1.83550	-2.54819
H	-1.67620	0.33476	-0.33796
H	-2.85915	-0.06005	-2.44922
H	0.48781	1.47172	-4.66629
C	0.72510	1.41807	-2.53189
C	0.14339	1.13924	-1.23910
C	0.52442	0.23308	1.81065
C	0.03277	0.21562	3.18079
C	1.20320	-0.95751	1.32316
C	0.09764	-0.89483	3.94765
H	-0.40964	1.13382	3.55474
C	1.28244	-2.06764	2.08353
H	1.64267	-0.90907	0.33279
C	0.68578	-2.14177	3.43479
H	-0.28426	-0.91605	4.96315
H	1.78614	-2.96836	1.74351
O	0.69126	-3.19337	4.06995
O	-1.97704	0.50712	-4.93623
H	-2.87711	0.81264	-4.77244

8.18 F_{OC} -0.0100 au OH−AB−O^- Rotation Inversion TS Structure

S_0 State

E_h = -722.7706

Cartesian Coordinates:

N	-0.82667	1.52153	-0.51816
N	-0.44192	1.01866	0.60666
C	-0.19741	-0.60462	-1.67759
C	-0.08940	-1.30633	-2.87376
C	-0.34846	-0.68507	-4.09410
C	-0.71302	0.66267	-4.11190
H	-1.14625	2.40536	-2.91112
H	-0.01244	-1.10041	-0.73255
H	0.19554	-2.36167	-2.84912
H	-0.90325	1.15504	-5.06554
C	-0.83775	1.36259	-2.91643
C	-0.58404	0.75961	-1.66116
C	-0.00790	0.54536	1.72755
C	1.02713	-0.49172	1.81025
C	-0.51288	1.02136	3.02057
C	1.48733	-0.97280	2.98660
H	1.44794	-0.84556	0.87144
C	-0.08628	0.52511	4.20499
H	-1.27375	1.79658	2.98800
C	0.94918	-0.51694	4.28058
H	2.26817	-1.72680	3.03847
H	-0.48253	0.87777	5.15249
O	1.34844	-0.98585	5.34355
O	-0.23061	-1.38511	-5.32033
H	0.02781	-2.28581	-5.08726

8.19 F_{OC} -0.0100 au OH−AB−O$^-$ Inversion TS Structure S_0 State

E_h = -722.7689

Cartesian Coordinates:

O	-0.32679	-1.83023	-5.13032
C	-0.41139	-1.72695	-3.72787
C	-1.23517	-2.60424	-1.63673
C	-0.64115	-1.54949	-0.91167
C	0.05971	-0.57229	-1.65157
C	0.17770	-0.67062	-3.03643
H	-1.61446	-3.50378	-3.55934
H	-1.76550	-3.36379	-1.06973
H	0.53316	0.24426	-1.11973
H	0.73909	0.09080	-3.58610
N	-0.70429	-1.62471	0.49462
N	-0.32835	-0.61626	1.17282
C	0.05921	0.47118	1.76789
C	0.49226	0.46023	3.16214
C	0.06916	1.77832	1.11691
C	0.95847	1.56817	3.79117
H	0.44102	-0.49189	3.68194
C	0.49282	2.89864	1.74881
H	-0.32017	1.83214	0.10275
C	1.03125	2.86766	3.11642
H	1.29088	1.53466	4.82417
H	0.47424	3.87354	1.26760
O	1.51154	3.87917	3.63753
C	-1.13960	-2.68647	-3.02104
H	0.21469	-1.08445	-5.42879

8.20 F_{OC} -0.0100 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8100

Cartesian Coordinates:

O	-0.37764	-1.57772	-4.42764
C	-0.40308	-1.65213	-3.01295
C	-1.56395	-2.20606	-0.97467
C	-0.50827	-1.70293	-0.18753
C	0.63148	-1.21571	-0.87287
C	0.68369	-1.20260	-2.25774
H	-2.37038	-2.50958	-2.95636
H	-2.43072	-2.61172	-0.46242
H	1.46740	-0.83815	-0.29587
H	1.57818	-0.82526	-2.75595
N	-0.51761	-1.91548	1.19820
N	-0.11297	-1.05306	2.05480
C	0.10845	0.27593	1.85913
C	0.93530	0.93727	2.82159
C	-0.45397	1.08393	0.82111
C	1.34317	2.23215	2.65233
H	1.26583	0.35408	3.67626
C	-0.09578	2.39173	0.67106
H	-1.21655	0.65855	0.17799
C	0.91362	3.02947	1.51277
H	1.99959	2.70615	3.37547
H	-0.56504	3.02147	-0.08196
O	1.34089	4.17920	1.26374
C	-1.52321	-2.16161	-2.36997
H	0.24016	-0.86931	-4.64314

8.21 F_{OC} +0.0025 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8624

Cartesian Coordinates:

O	-0.25731	-0.77723	-5.80918
C	-0.22022	-0.66527	-4.43694
C	-0.56600	-1.71390	-2.29738
C	-0.18008	-0.54429	-1.62068
C	0.18755	0.57059	-2.39555
C	0.16702	0.50867	-3.78480
H	-0.88711	-2.68691	-4.20083
H	-0.85040	-2.57607	-1.70271
H	0.48751	1.48002	-1.88984
H	0.45481	1.38160	-4.36929
N	-0.19732	-0.59656	-0.21315
N	0.16108	0.48426	0.36417
C	0.16900	0.50898	1.73809
C	0.57110	1.72038	2.35659
C	-0.19079	-0.57341	2.58982
C	0.61741	1.86141	3.72298
H	0.84532	2.54524	1.70255
C	-0.14925	-0.44661	3.95424
H	-0.49994	-1.50478	2.12649
C	0.25848	0.78195	4.62133
H	0.92885	2.79959	4.17600
H	-0.42619	-1.27957	4.59721
O	0.29362	0.88955	5.87751
C	-0.58796	-1.78026	-3.68519
H	0.01655	0.05450	-6.21317

8.22 F_{OC} +0.0025 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8055

Cartesian Coordinates:

N	0.80777	1.46746	-0.08893
N	0.32181	1.37051	1.12964
C	-1.21565	0.73736	-1.24553
C	-1.86614	0.48702	-2.45614
C	-1.24305	0.73613	-3.67291
C	0.06412	1.23810	-3.67475
H	1.74323	1.87059	-2.50335
H	-1.71697	0.52300	-0.30868
H	-2.87982	0.08536	-2.43870
H	0.54923	1.42820	-4.62766
C	0.72927	1.48330	-2.48840
C	0.11877	1.23942	-1.21977
C	0.49097	0.22359	1.79590
C	0.06416	0.20024	3.16778
C	1.06391	-0.98249	1.25505
C	0.16843	-0.91912	3.93291
H	-0.35943	1.12151	3.55985
C	1.16523	-2.11019	2.01099
H	1.39567	-0.95933	0.22288
C	0.73752	-2.15934	3.40902
H	-0.17071	-0.93675	4.96545
H	1.56968	-3.02973	1.59648
O	0.84299	-3.18870	4.10719
O	-1.84663	0.49759	-4.90429
H	-2.73559	0.15549	-4.75790

8.23 F_{OC} +0.0025 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.7931

Cartesian Coordinates:

N	-0.99112	1.40219	-0.47394
N	-0.55187	0.93701	0.61623
C	-0.22547	-0.66639	-1.71658
C	-0.02049	-1.30755	-2.93745
C	-0.26369	-0.63294	-4.13470
C	-0.72717	0.68327	-4.10483
H	-1.31803	2.32569	-2.84185
H	-0.04792	-1.19513	-0.78768
H	0.32516	-2.34071	-2.95868
H	-0.91524	1.19589	-5.04272
C	-0.94293	1.30722	-2.88302
C	-0.68324	0.65446	-1.66891
C	-0.05597	0.47776	1.75276
C	0.86579	-0.62661	1.85803
C	-0.40873	1.09539	3.00797
C	1.37342	-1.05478	3.05586
H	1.17910	-1.11239	0.93789
C	0.07246	0.66433	4.21357
H	-1.09640	1.93649	2.95413
C	1.00358	-0.44751	4.32496
H	2.07822	-1.88229	3.09750
H	-0.22257	1.15015	5.14162
O	1.45203	-0.84880	5.42868
O	-0.07428	-1.21576	-5.36941
H	0.25233	-2.11605	-5.25728

8.24 F_{OC} +0.0025 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.7926

Cartesian Coordinates:

O	-0.60930	-1.81235	-5.13121
C	-0.54709	-1.70671	-3.75852
C	-1.14374	-2.63375	-1.61836
C	-0.48850	-1.59125	-0.94631
C	0.15488	-0.61588	-1.71723
C	0.13140	-0.67408	-3.11027
H	-1.71034	-3.49096	-3.52160
H	-1.62235	-3.40185	-1.01737
H	0.69576	0.18034	-1.21994
H	0.64864	0.08559	-3.69513
N	-0.46929	-1.68487	0.49289
N	-0.14258	-0.65768	1.15481
C	0.19290	0.47693	1.74883
C	0.39799	0.49606	3.17587
C	0.34803	1.75594	1.09529
C	0.73267	1.62728	3.86665
H	0.27956	-0.45550	3.68925
C	0.65648	2.90190	1.77705
H	0.18271	1.80179	0.02242
C	0.88046	2.92022	3.21546
H	0.89189	1.60228	4.94284
H	0.75126	3.85173	1.25591
O	1.17406	3.96474	3.84609
C	-1.18883	-2.69132	-3.00508
H	-0.13834	-1.07503	-5.53687

8.25 F_{OC} +0.0025 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8296

Cartesian Coordinates:

O	-0.61721	-1.81894	-4.47507
C	-0.51931	-1.75873	-3.10096
C	-1.58004	-2.10217	-0.96432
C	-0.42801	-1.67927	-0.28243
C	0.68964	-1.31658	-1.05231
C	0.64636	-1.36145	-2.44271
H	-2.53642	-2.44005	-2.87343
H	-2.43954	-2.41678	-0.38048
H	1.59833	-0.99542	-0.55503
H	1.52781	-1.08351	-3.01814
N	-0.36428	-1.87485	1.12409
N	0.06440	-1.02419	1.97107
C	0.27007	0.33172	1.78119
C	0.92682	0.96918	2.87269
C	-0.18137	1.18434	0.72647
C	1.17659	2.31639	2.90780
H	1.23734	0.32523	3.69256
C	0.03188	2.53858	0.76298
H	-0.73003	0.76842	-0.10885
C	0.73980	3.20542	1.84757
H	1.69606	2.76948	3.74913
H	-0.33873	3.17302	-0.03829
O	0.93444	4.44542	1.87065
C	-1.63645	-2.12663	-2.35418
H	0.20041	-1.50003	-4.87458

8.26 F_{OC} +0.0050 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8793

Cartesian Coordinates:

O	-0.26541	-0.80182	-5.80603
C	-0.22223	-0.67136	-4.44395
C	-0.56261	-1.70303	-2.29486
C	-0.17465	-0.52774	-1.63124
C	0.19122	0.58122	-2.41321
C	0.16737	0.50925	-3.80163
H	-0.88849	-2.69014	-4.19089
H	-0.84563	-2.56057	-1.69299
H	0.49292	1.49552	-1.91727
H	0.45334	1.37621	-4.39449
N	-0.18957	-0.57311	-0.21929
N	0.16581	0.49901	0.36130
C	0.17138	0.51658	1.74556
C	0.57082	1.72027	2.37090
C	-0.18863	-0.56727	2.58826
C	0.61405	1.85186	3.74286
H	0.84665	2.55027	1.72414
C	-0.14965	-0.44836	3.95766
H	-0.49685	-1.49635	2.11920
C	0.25484	0.77148	4.63388
H	0.92535	2.78968	4.19799
H	-0.42872	-1.28856	4.59130
O	0.28813	0.87186	5.89899
C	-0.58839	-1.78098	-3.68090
H	0.00469	0.01796	-6.23701

8.27 F_{OC} +0.0050 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8125

Cartesian Coordinates:

N	0.79690	1.46298	-0.08842
N	0.30924	1.36636	1.12659
C	-1.22605	0.73934	-1.25209
C	-1.87062	0.48670	-2.46590
C	-1.24153	0.74178	-3.67923
C	0.06851	1.24180	-3.67528
H	1.74305	1.86371	-2.49562
H	-1.72923	0.52352	-0.31668
H	-2.88170	0.07998	-2.45644
H	0.55466	1.43282	-4.62683
C	0.72806	1.47980	-2.48674
C	0.10838	1.23534	-1.22364
C	0.47754	0.21437	1.79333
C	0.06407	0.19665	3.16641
C	1.04445	-0.99320	1.25614
C	0.18776	-0.91738	3.94089
H	-0.36419	1.11754	3.55543
C	1.16104	-2.11708	2.02351
H	1.35837	-0.98243	0.21817
C	0.76335	-2.15571	3.42646
H	-0.14320	-0.92805	4.97718
H	1.55713	-3.03821	1.60416
O	0.89159	-3.17646	4.14394
O	-1.82774	0.50949	-4.90989
H	-2.73107	0.19555	-4.78931

8.28 F_{OC} +0.0050 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8069

Cartesian Coordinates:

N	-0.96376	1.40630	-0.47716
N	-0.53206	0.93913	0.61227
C	-0.19507	-0.66620	-1.72712
C	-0.00388	-1.30468	-2.95182
C	-0.27561	-0.63242	-4.14606
C	-0.75168	0.68011	-4.10726
H	-1.33573	2.31486	-2.83602
H	0.00377	-1.19557	-0.80281
H	0.35263	-2.33339	-2.98088
H	-0.96186	1.18897	-5.04208
C	-0.95157	1.30026	-2.88232
C	-0.66535	0.64892	-1.67303
C	-0.04178	0.47352	1.75522
C	0.86820	-0.63408	1.87402
C	-0.39768	1.09891	3.00147
C	1.36326	-1.05927	3.08280
H	1.18687	-1.12864	0.96063
C	0.06919	0.66857	4.21666
H	-1.07600	1.94688	2.93663
C	0.98786	-0.44721	4.34417
H	2.06261	-1.89143	3.12981
H	-0.23147	1.16530	5.13812
O	1.42245	-0.84797	5.46151
O	-0.10647	-1.20421	-5.38083
H	0.23011	-2.10374	-5.29374

8.29 F_{OC} +0.0050 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.8047

Cartesian Coordinates:

O	-0.61909	-1.86815	-5.13766
C	-0.55248	-1.73229	-3.77508
C	-1.11930	-2.64110	-1.61894
C	-0.48745	-1.57294	-0.96518
C	0.12733	-0.59225	-1.75154
C	0.10039	-0.67114	-3.14360
H	-1.66709	-3.54195	-3.50760
H	-1.57699	-3.41176	-1.00517
H	0.64911	0.22664	-1.27052
H	0.59403	0.09262	-3.74203
N	-0.47363	-1.65447	0.47729
N	-0.14328	-0.63508	1.14478
C	0.19919	0.49809	1.74842
C	0.37548	0.50182	3.17621
C	0.38638	1.77831	1.11180
C	0.70823	1.62421	3.88668
H	0.23520	-0.45387	3.67690
C	0.69510	2.91580	1.81338
H	0.25033	1.83779	0.03562
C	0.88318	2.92066	3.25482
H	0.84427	1.58555	4.96658
H	0.81550	3.86644	1.29910
O	1.17042	3.95750	3.90958
C	-1.16689	-2.72162	-3.00321
H	-0.16963	-1.13523	-5.57515

8.30 F_{OC} +0.0050 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8390

Cartesian Coordinates:

O	-0.65578	-1.88416	-4.48439
C	-0.53735	-1.79240	-3.12017
C	-1.57841	-2.09473	-0.96683
C	-0.41743	-1.66635	-0.30371
C	0.69226	-1.31786	-1.08964
C	0.63573	-1.38640	-2.47960
H	-2.55458	-2.45965	-2.86080
H	-2.43243	-2.40042	-0.37018
H	1.60913	-0.99477	-0.60853
H	1.51235	-1.12358	-3.06831
N	-0.34316	-1.85643	1.10581
N	0.09021	-1.01240	1.95472
C	0.29925	0.34890	1.77069
C	0.91826	0.97581	2.88818
C	-0.12196	1.21375	0.71366
C	1.14186	2.32721	2.95887
H	1.21705	0.32016	3.70378
C	0.06820	2.57173	0.78304
H	-0.62390	0.80595	-0.15422
C	0.71393	3.23128	1.90917
H	1.63195	2.77244	3.82266
H	-0.27460	3.21160	-0.02609
O	0.86975	4.47665	1.97691
C	-1.64976	-2.14043	-2.35415
H	0.15800	-1.59730	-4.91551

8.31 F_{OC} +0.0075 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.8996

Cartesian Coordinates:

O	-0.27451	-0.82902	-5.80305
C	-0.22468	-0.67858	-4.45153
C	-0.55900	-1.69098	-2.29180
C	-0.16848	-0.50911	-1.64117
C	0.19559	0.59336	-2.43310
C	0.16779	0.50956	-3.82020
H	-0.89054	-2.69418	-4.17876
H	-0.84056	-2.54335	-1.68206
H	0.49944	1.51318	-1.94868
H	0.45181	1.36973	-4.42255
N	-0.18086	-0.54705	-0.22737
N	0.17173	0.51706	0.35887
C	0.17430	0.52541	1.75283
C	0.57068	1.72101	2.38728
C	-0.18613	-0.56077	2.58628
C	0.61031	1.84156	3.76474
H	0.84803	2.55676	1.74858
C	-0.15014	-0.45113	3.96074
H	-0.49320	-1.48700	2.11021
C	0.25106	0.75916	4.64753
H	0.92102	2.77871	4.22330
H	-0.43156	-1.29913	4.58424
O	0.28133	0.85154	5.92220
C	-0.58914	-1.78198	-3.67560
H	-0.00855	-0.02286	-6.26266

8.32 F_{OC} +0.0075 au OH−AB−O^- Rotation TS Structure S_0 State

E_h = -722.8228

Cartesian Coordinates:

N	0.78403	1.45137	-0.09346
N	0.29563	1.35423	1.12041
C	-1.24203	0.73899	-1.26468
C	-1.88170	0.49436	-2.48179
C	-1.24469	0.75851	-3.69148
C	0.07167	1.24875	-3.67978
H	1.74418	1.84598	-2.48849
H	-1.74824	0.52143	-0.33140
H	-2.89267	0.08888	-2.48309
H	0.55954	1.44224	-4.62945
C	0.72637	1.47048	-2.48825
C	0.09597	1.22318	-1.23055
C	0.46357	0.20008	1.79054
C	0.06108	0.19025	3.16483
C	1.03191	-1.00913	1.26407
C	0.20678	-0.91559	3.95238
H	-0.37594	1.11003	3.54789
C	1.16695	-2.12565	2.04792
H	1.33265	-1.01443	0.22207
C	0.79439	-2.15119	3.45359
H	-0.11835	-0.91644	4.99182
H	1.56236	-3.04727	1.62845
O	0.94681	-3.16108	4.19393
O	-1.81664	0.54577	-4.92116
H	-2.72486	0.23549	-4.82824

8.33 F_{OC} +0.0075 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8236

Cartesian Coordinates:

N	-0.90553	1.42670	-0.48655
N	-0.49009	0.95275	0.60467
C	-0.15538	-0.66082	-1.73800
C	0.00759	-1.30289	-2.96485
C	-0.30118	-0.63782	-4.15644
C	-0.78340	0.67345	-4.11044
H	-1.33899	2.30998	-2.83393
H	0.07257	-1.18692	-0.81845
H	0.37102	-2.32841	-3.00062
H	-1.02097	1.17528	-5.04219
C	-0.95245	1.29676	-2.88413
C	-0.63216	0.65160	-1.67878
C	-0.01788	0.47361	1.75549
C	0.88750	-0.63155	1.88999
C	-0.39439	1.09517	2.99408
C	1.36255	-1.05617	3.11184
H	1.22482	-1.12596	0.98334
C	0.04611	0.65841	4.22063
H	-1.06823	1.94584	2.91747
C	0.96237	-0.45251	4.36596
H	2.06444	-1.88621	3.16555
H	-0.27545	1.15579	5.13594
O	1.37679	-0.85540	5.49876
O	-0.16696	-1.20574	-5.38945
H	0.18428	-2.10199	-5.32774

8.34 F_{OC} +0.0075 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.8193

Cartesian Coordinates:

O	-0.62187	-1.93433	-5.14526
C	-0.55650	-1.76318	-3.79379
C	-1.08947	-2.65072	-1.62011
C	-0.49467	-1.54892	-0.98654
C	0.08232	-0.56000	-1.79137
C	0.05621	-0.66497	-3.18163
H	-1.60249	-3.60717	-3.49105
H	-1.52021	-3.42495	-0.99162
H	0.57258	0.28895	-1.32928
H	0.51793	0.10553	-3.79551
N	-0.49372	-1.61421	0.45736
N	-0.15487	-0.60499	1.13284
C	0.20063	0.52346	1.74827
C	0.34329	0.50974	3.17687
C	0.43343	1.80322	1.13161
C	0.68255	1.61913	3.90918
H	0.17014	-0.44841	3.66301
C	0.75100	2.92811	1.85537
H	0.33045	1.87839	0.05280
C	0.90016	2.91677	3.29923
H	0.79087	1.56491	4.99269
H	0.90695	3.87839	1.35004
O	1.19102	3.94210	3.97947
C	-1.13410	-2.76006	-3.00107
H	-0.20332	-1.20319	-5.61606

8.35 F_{OC} +0.0075 au OH−AB−O^- Cis Structure S_0 State

E_h = -722.8503

Cartesian Coordinates:

O	-0.68367	-1.96274	-4.49392
C	-0.55258	-1.83297	-3.14044
C	-1.57781	-2.10363	-0.97450
C	-0.41791	-1.64837	-0.32633
C	0.68148	-1.29916	-1.12549
C	0.61873	-1.39792	-2.51421
H	-2.56041	-2.51629	-2.85504
H	-2.42333	-2.41251	-0.36729
H	1.59951	-0.95841	-0.65875
H	1.48886	-1.13901	-3.11328
N	-0.33915	-1.83060	1.08600
N	0.10037	-0.99627	1.93917
C	0.32230	0.36937	1.76253
C	0.90935	0.98059	2.90371
C	-0.06642	1.24977	0.70633
C	1.11724	2.33363	3.00747
H	1.19274	0.31152	3.71463
C	0.11056	2.60931	0.80668
H	-0.52825	0.85443	-0.18918
C	0.70350	3.25484	1.96855
H	1.58316	2.76716	3.89143
H	-0.20310	3.25776	-0.00730
O	0.83204	4.50230	2.07682
C	-1.65785	-2.17583	-2.35868
H	0.11922	-1.68838	-4.95354

8.36 F_{OC} +0.0100 au OH−AB−O^- Trans Structure S_0 State

E_h = -722.9232

Cartesian Coordinates:

O	-0.28351	-0.85593	-5.80038
C	-0.22724	-0.68611	-4.45946
C	-0.55552	-1.67918	-2.28886
C	-0.16232	-0.49044	-1.64985
C	0.20002	0.60558	-2.45343
C	0.16819	0.50966	-3.83880
H	-0.89279	-2.69859	-4.16611
H	-0.83566	-2.52641	-1.67138
H	0.50606	1.53099	-1.98106
H	0.45027	1.36295	-4.45082
N	-0.17215	-0.52084	-0.23670
N	0.17808	0.53656	0.35688
C	0.17729	0.53461	1.75944
C	0.57070	1.72237	2.40419
C	-0.18362	-0.55436	2.58423
C	0.60653	1.83137	3.78683
H	0.84964	2.56393	1.77387
C	-0.15073	-0.45425	3.96365
H	-0.48937	-1.47756	2.10097
C	0.24692	0.74655	4.66101
H	0.91665	2.76763	4.24927
H	-0.43436	-1.31002	4.57690
O	0.27454	0.83064	5.94572
C	-0.59001	-1.78322	-3.66992
H	-0.02185	-0.06403	-6.28792

8.37 F_{OC} +0.0100 au OH−AB−O$^-$ Rotation TS Structure S_0 State

E_h = -722.8368

Cartesian Coordinates:

N	0.76963	1.42915	-0.10628
N	0.28192	1.32962	1.10862
C	-1.26248	0.73117	-1.28587
C	-1.89870	0.50731	-2.50630
C	-1.25300	0.78764	-3.71196
C	0.07237	1.26097	-3.69039
H	1.74537	1.81768	-2.48420
H	-1.77250	0.50910	-0.35582
H	-2.91158	0.10848	-2.52134
H	0.56192	1.46173	-4.63737
C	0.72340	1.45480	-2.49505
C	0.08202	1.19924	-1.24263
C	0.44956	0.17750	1.78721
C	0.05320	0.18003	3.16199
C	1.02902	-1.03383	1.28203
C	0.22418	-0.91232	3.96928
H	-0.39866	1.09790	3.53352
C	1.18608	-2.13689	2.08981
H	1.32292	-1.06059	0.23820
C	0.83187	-2.14394	3.49611
H	-0.09882	-0.89838	5.01084
H	1.59037	-3.05821	1.67741
O	1.01109	-3.13837	4.26533
O	-1.81429	0.60912	-4.94005
H	-2.72614	0.30029	-4.87695

8.38 F_{OC} +0.0100 au OH−AB−O^- Rotation Inversion TS Structure S_0 State

E_h = -722.8435

Cartesian Coordinates:

N	-0.75916	1.48743	-0.51013
N	-0.39027	0.99280	0.58726
C	-0.12373	-0.65311	-1.74439
C	-0.02830	-1.31604	-2.96655
C	-0.36436	-0.65895	-4.15849
C	-0.80241	0.66920	-4.11455
H	-1.24812	2.34161	-2.84718
H	0.12784	-1.17380	-0.82749
H	0.30537	-2.35110	-3.00264
H	-1.05787	1.16395	-5.04519
C	-0.90084	1.31439	-2.89377
C	-0.55765	0.67539	-1.68932
C	0.02984	0.48343	1.74909
C	0.97335	-0.58278	1.90274
C	-0.43642	1.05086	2.98035
C	1.41653	-1.00724	3.14231
H	1.37870	-1.03827	1.00333
C	-0.04789	0.58860	4.21953
H	-1.14007	1.87595	2.89212
C	0.92264	-0.46643	4.38733
H	2.16224	-1.79795	3.20575
H	-0.44916	1.04164	5.12786
O	1.30689	-0.87435	5.53969
O	-0.30125	-1.24051	-5.38269
H	0.04107	-2.14178	-5.34280

8.39 F_{OC} +0.0100 au OH−AB−O^- Inversion TS Structure S_0 State

E_h = -722.8363

Cartesian Coordinates:

O	-0.61741	-2.00719	-5.15271
C	-0.55645	-1.79821	-3.81364
C	-1.04832	-2.66286	-1.62096
C	-0.50251	-1.52228	-1.00961
C	0.02676	-0.52317	-1.83617
C	0.00314	-0.65744	-3.22354
H	-1.51439	-3.68216	-3.47061
H	-1.44598	-3.44119	-0.97605
H	0.47369	0.36082	-1.39575
H	0.42367	0.12165	-3.85491
N	-0.51923	-1.56818	0.43333
N	-0.17137	-0.56995	1.11906
C	0.19816	0.55183	1.74819
C	0.30250	0.52093	3.17734
C	0.48294	1.82937	1.15413
C	0.65177	1.61487	3.93292
H	0.09011	-0.43765	3.64743
C	0.81290	2.93900	1.90177
H	0.41605	1.92021	0.07365
C	0.92101	2.91090	3.34710
H	0.72826	1.54495	5.01958
H	1.00948	3.88745	1.40717
O	1.22084	3.92244	4.05365
C	-1.08678	-2.80465	-2.99752
H	-0.24053	-1.27592	-5.65839

8.40 F_{OC} +0.0100 au OH−AB−O$^-$ Cis Structure S_0 State

E_h = -722.8635

Cartesian Coordinates:

O	-0.69695	-2.05905	-4.50390
C	-0.56433	-1.88313	-3.16243
C	-1.57855	-2.13572	-0.98864
C	-0.43438	-1.62461	-0.35131
C	0.65077	-1.25446	-1.16095
C	0.59169	-1.39156	-2.54720
H	-2.54838	-2.62449	-2.85704
H	-2.41058	-2.46398	-0.37286
H	1.55987	-0.87465	-0.70707
H	1.45248	-1.12067	-3.15362
N	-0.36087	-1.79375	1.06362
N	0.08663	-0.97319	1.92422
C	0.33656	0.39459	1.75634
C	0.89898	0.98342	2.91944
C	-0.01457	1.29518	0.70462
C	1.10634	2.33528	3.05499
H	1.16049	0.29823	3.72506
C	0.16361	2.65388	0.83525
H	-0.44488	0.91814	-0.21440
C	0.71533	3.27770	2.02806
H	1.55463	2.75170	3.95737
H	-0.11789	3.31471	0.01951
O	0.83226	4.52465	2.17423
C	-1.65868	-2.24159	-2.36874
H	0.08897	-1.77802	-4.98918