

The Water Trimer Reaction $\text{OH} + (\text{H}_2\text{O})_3 \rightarrow (\text{H}_2\text{O})_2\text{-OH} + \text{H}_2\text{O}$

Aifang Gao, Guoliang Li, Bin Peng, Jared Weidman, Yaoming Xie, and Henry F. Schaefer III

Supporting Information

Table S1. The optimized geometries (Z-matrix) of the water trimer $(\text{H}_2\text{O})_3$ with the CCSD(T) method (distances in Å and angles in degrees).

Table S2. The optimized geometries (Z-matrix) of the five complexes with the CCSD(T) method (distances in Å and angles in degrees).

Table S3. The optimized geometries (Z-matrix) of the seven transition states with the CCSD(T) method (distances in Å and angles in degrees).

Table S4. The optimized geometries (Z-matrix) of two conformers of the product $(\text{H}_2\text{O})_2\text{OH}$ with the CCSD(T) method (distances in Å and angles in degrees).

Table S1. The optimized geometries (Z-matrix) of the water trimer (H₂O)₃ with the CCSD(T) method (distances in Å and angles in degrees).

	cc-pVDZ	cc-pVTZ	cc-pVQZ
O	R1 = 0.967152598798065	R1 = 0.959235188141124	R1 = 0.957407797684201
H 1 R1	R2 = 0.979159791114356	R2 = 0.972183904005455	R2 = 0.970368330383760
H 1 R2 2 A1	A1 = 102.346847264227748	A1 = 104.653593293955140	A1 = 105.296831616503169
H 1 R3 2 A2 3 T1	R3 = 2.798015986298458	R3 = 2.795472008601075	R3 = 2.794992851164174
H 4 R4 1 A3 2 T2	A2 = 115.571093446185287	A2 = 126.653201313263594	A2 = 131.176922973294552
H 4 R5 5 A4 1 T3	T1 = -80.987193669314195	T1 = -85.328405978221667	T1 = -87.722765601342630
O 1 R6 4 A5 2 T4	R4 = 0.978860976833781	R4 = 0.971718618331569	R4 = 0.969827675116188
H 7 R7 1 A6 2 T5	A3 = 17.889626691463071	A3 = 19.191517134163366	A3 = 20.095212690665218
H 7 R8 8 A7 1 T6	T2 = -91.238996364539759	T2 = -74.948887269931959	T2 = -69.699772006855767
	R5 = 0.967050441851343	R5 = 0.959171833728753	R5 = 0.957417709322551
	A4 = 102.792388173081818	A4 = 104.923830524040312	A4 = 105.464424782643476
	T3 = -110.287990677583494	T3 = -130.645746154949194	T3 = -136.407251785952894
	R6 = 2.791657574199025	R6 = 2.789037977963074	R6 = 2.790220241192305
	A5 = 59.861861733700934	A5 = 59.823459376657844	A5 = 59.863961957361489
	T4 = -94.691214795942940	T4 = -97.668743701665576	T4 = -99.283982543796299
	R7 = 0.978976740413913	R7 = 0.972077380319586	R7 = 0.970305530350375
	A6 = 76.893769523076074	A6 = 78.118776947189545	A6 = 78.653145412845802
	T5 = -107.772970055064462	T5 = -118.907353285457916	T5 = -123.912572088591546
	R8 = 0.967378717441062	R8 = 0.959540978823563	R8 = 0.957744284692813
	A7 = 102.380197926300426	A7 = 104.577322769094607	A7 = 105.144429898514602
	T6 = 112.599233367926189	T6 = 119.705030816794562	T6 = 121.976703052034338

Table S2. The optimized geometries (Z-matrix) of the five complexes with the CCSD(T) method (distances in Å and angles in degrees).

CPI	cc-pVDZ	cc-pVTZ	cc-pVQZ
O	R1 = 0.979124951304948	R1 = 0.971902074075598	R1 = 0.969831804533138
H 1 R1	R2 = 0.967727756785880	R2 = 0.960051970033241	R2 = 0.958192328587773
H 1 R2 2 A1	A1 = 102.861035946994519	A1 = 104.885732845262751	A1 = 105.412656888387218
O 1 R3 3 A2 2 T1	R3 = 2.729358992506742	R3 = 2.723785762074466	R3 = 2.729924954806438
H 4 R4 1 A3 2 T2	A2 = 114.441894671034746	A2 = 118.575566536645013	A2 = 121.132999617010157
H 4 R5 5 A4 1 T3	T1 = 85.707396212259880	T1 = 89.569989528449028	T1 = 91.717619548581411
O 1 R6 4 A5 3 T4	R4 = 0.985651407696979	R4 = 0.978348463019297	R4 = 0.976107746339321
H 7 R7 1 A6 3 T5	A3 = 13.644204010510833	A3 = 14.008626811636944	A3 = 14.177242070348123
H 7 R8 8 A7 1 T6	T2 = 179.161223224215604	T2 = -176.825737179138173	T2 = -178.483650650837490
H 4 R9 7 A8 1 T7	R5 = 0.967805807341881	R5 = 0.959913201312414	R5 = 0.958276420435852
O 10 R10 6 A9 5 T8	A4 = 103.368981789746897	A4 = 105.540323022173766	A4 = 105.871474762872225
	T3 = -116.037497978375981	T3 = -129.243184637474371	T3 = -129.268912095045010
	R6 = 2.775715588604965	R6 = 2.769917119476642	R6 = 2.769510433499927
	A5 = 62.507183233989679	A5 = 62.790806752924780	A5 = 62.823802297980833
	T4 = 98.377216217851341	T4 = 102.279242218836913	T4 = 103.860914300298305
	R7 = 0.975117398746941	R7 = 0.967749239800233	R7 = 0.965863674765605
	A6 = 79.711304011488991	A6 = 81.489514687144464	A6 = 82.574195886506743
	T5 = 108.020462482176342	T5 = 115.540812923777167	T5 = 118.848730707677191
	R8 = 0.967047319216683	R8 = 0.959223531034588	R8 = 0.957450647934658
	A7 = 103.018518906502791	A7 = 105.126639002947769	A7 = 105.719088151849689
	T6 = -118.369577661297384	T6 = -129.892389672022915	T6 = -135.552633973011126
	R9 = 1.889244916772000	R9 = 1.895536774547542	R9 = 1.892258606130886
	A8 = 125.206217677026586	A8 = 112.594037119558763	A8 = 110.812753811445759
	T7 = -103.215123243257025	T7 = -103.611636499487517	T7 = -107.293270902519382
	R10 = 0.984942619597847	R10 = 0.978009883852047	R10 = 0.977051076846343
	A9 = 157.700392000928247	A9 = 160.781991318487002	A9 = 159.485822888587933
	T8 = 134.632648061095324	T8 = 137.150626586384021	T8 = 143.500366622275067

CP2a	cc-pVDZ	cc-pVTZ	cc-pVQZ
O	R1 = 0.984930080283060	R1 = 0.978414231217641	R1 = 0.976469733671164
H 1 R1	R2 = 0.967028113789323	R2 = 0.959172290995967	R2 = 0.957390523865166
H 1 R2 2 A1	A1 = 102.893761554293647	A1 = 105.165671040703714	A1 = 105.788228832812806
O 1 R3 3 A2 2 T1	R3 = 3.849089523132092	R3 = 3.834597877400073	R3 = 3.830079624706634
H 4 R4 1 A3 2 T2	A2 = 124.492503559213517	A2 = 131.678248602563315	A2 = 135.301226804785045
H 4 R5 5 A4 1 T3	T1 = 52.920842897558487	T1 = 54.076975382409046	T1 = 54.516484522639196
O 1 R6 4 A5 3 T4	R4 = 0.979053591123210	R4 = 0.973003683961590	R4 = 0.971294122570931
H 7 R7 1 A6 3 T5	A3 = 53.276555634588306	A3 = 53.829786688889889	A3 = 54.496853990789745
H 7 R8 8 A7 1 T6	T2 = -178.383596542871572	T2 = 177.403227389996999	T2 = 175.540600046378387
O 7 R9 1 A8 3 T7	R5 = 0.967036417135755	R5 = 0.959277701877323	R5 = 0.957531001172511
H 10 R10 7 A9 9 T8	A4 = 102.788253129718171	A4 = 104.877400463880917	A4 = 105.452986008355055
	T3 = 124.010302045596276	T3 = 132.290971817250579	T3 = 136.372833840281288
	R6 = 2.737162016466796	R6 = 2.728629642269366	R6 = 2.732533406822448
	A5 = 45.626885552994274	A5 = 45.709452274944582	A5 = 45.859464323124548
	T4 = 76.080898196839073	T4 = 75.536149643207452	T4 = 74.619153093177658
	R7 = 0.982891856494464	R7 = 0.976418017150701	R7 = 0.974510393044819
	A6 = 96.228098985248536	A6 = 96.883756122886069	A6 = 97.153022059954296
	T5 = 120.968529637760668	T5 = 127.775285979402881	T5 = 131.752689890535919
	R8 = 0.967353208760859	R8 = 0.959611457583299	R8 = 0.957846607984624
	A7 = 102.423262352992197	A7 = 104.535174684007742	A7 = 105.079764960547379
	T6 = -116.823551452976176	T6 = -121.310671630037291	T6 = -123.072582548300105
	R9 = 3.953840245715078	R9 = 3.942089831049103	R9 = 3.955958182212046
	A8 = 43.296145307851319	A8 = 43.372871386201389	A8 = 43.244502232772554
	T7 = 119.132866727808704	T7 = 124.690501752154219	T7 = 127.911351087068482
	R10 = 1.000293247341222	R10 = 0.992243734511707	R10 = 0.989959401324965
	A9 = 50.540063065902807	A9 = 50.411741470867739	A9 = 50.637794279249356
	T8 = -95.120103823052574	T8 = -95.175768195515431	T8 = -94.839434964636794

CP2b	cc-pVDZ	cc-pVTZ	cc-pVQZ
O	R1 = 0.999970993982013	R1 = 0.991710163754109	R1 = 0.98929
H 1 R1	R2 = 1.883390031449714	R2 = 1.875027075066050	R2 = 1.88194
H 1 R2 2 A1	A1 = 98.532765507563212	A1 = 98.305737081590479	A1 = 98.8120
O 1 R3 2 A2 3 T1	R3 = 2.845336410984757	R3 = 2.830522201464524	R3 = 2.83379
H 4 R4 1 A3 2 T2	A2 = 94.097255813051220	A2 = 93.754768834681343	A2 = 94.0870
O 1 R5 4 A4 5 T3	T1 = -0.826658502084383	T1 = 0.356979443816977	T1 = 0.7900
H 6 R6 1 A5 4 T4	R4 = 0.967203056483265	R4 = 0.959404254813498	R4 = 0.95763
H 6 R7 1 A6 4 T5	A3 = 104.839893037777784	A3 = 109.884469338800301	A3 = 111.9040
O 6 R8 1 A7 4 T6	T2 = -113.303883879247238	T2 = -119.229729694594980	T2 = -123.6450
H 9 R9 6 A8 1 T7	R5 = 2.713742253700275	R5 = 2.706244666074668	R5 = 2.70939
H 9 R10 6 A9 1 T8	A4 = 87.471176935770671	A4 = 86.884077182134220	A4 = 86.7330
	T3 = -113.230188170992946	T3 = -118.106122306549437	T3 = -122.3470
	R6 = 0.966585377949417	R6 = 0.958589362303592	R6 = 0.95682
	A5 = 119.027593038872510	A5 = 125.877899116677398	A5 = 129.3100
	T4 = -116.986019641025408	T4 = -129.346351288864582	T4 = -133.7470
	R7 = 0.984484449340256	R7 = 0.977545490229156	R7 = 0.97549
	A6 = 101.251619731392296	A6 = 102.530119939269667	A6 = 103.4700
	T5 = -4.543416812161798	T5 = -9.123697938571745	T5 = -8.9900
	R8 = 2.743572124070696	R8 = 2.735483161476703	R8 = 2.73760
	A7 = 93.206664896122419	A7 = 93.677924696498550	A7 = 93.9380
	T6 = -4.908399077211763	T6 = -6.504727978440633	T6 = -5.6720
	R9 = 0.967094248100667	R9 = 0.959353822798317	R9 = 0.95756
	A8 = 117.138343600423212	A8 = 122.918939754583718	A8 = 125.4910
	T7 = -98.612429107479187	T7 = -101.794802420927752	T7 = -105.2660
	R10 = 0.983023682323958	R10 = 0.976494284603477	R10 = 0.97457
	A9 = 95.687464376984892	A9 = 95.399423631128897	A9 = 95.7930
	T8 = 8.406190236337501	T8 = 9.301333192892514	T8 = 7.8770

CP2c	cc-pVDZ	cc-pVTZ
O	R1 = 1.000383715537280	R1 = 0.992348472716062
H 1 R1	R2 = 1.726311530353464	R2 = 1.730351934167598
O 2 R2 1 A1	A1 = 169.574242504567252	A1 = 169.675225101268097
H 3 R3 2 A2 1 T1	R3 = 0.984740278366588	R3 = 0.978277925183975
O 3 R4 2 A3 1 T2	A2 = 103.964957347665134	A2 = 104.671387730525296
H 5 R5 3 A4 2 T3	T1 = -2.271445472638540	T1 = -5.215991695536086
O 5 R6 3 A5 2 T4	R4 = 2.735603884092700	R4 = 2.729349367893243
H 7 R7 5 A6 3 T5	A3 = 97.442582716500240	A3 = 97.382621217871431
H 3 R8 2 A7 1 T6	T2 = -4.312015078443794	T2 = -5.760239927588600
H 5 R9 3 A8 2 T7	R5 = 0.982587098544583	R5 = 0.975718754418677
H 7 R10 5 A9 3 T8	A4 = 97.077199417040390	A4 = 97.606893320761714
	T3 = 0.252777184588760	T3 = -1.104239000431168
	R6 = 2.762314754291930	R6 = 2.752868801713722
	A5 = 88.695793034924051	A5 = 88.333766844996461
	T4 = 1.686963019862158	T4 = -2.352225635501202
	R7 = 0.979092875909836	R7 = 0.972794490319046
	A6 = 98.637275030122794	A6 = 99.580007859663411
	T5 = -3.819499837255085	T5 = 3.779750428888155
	R8 = 0.967156010418420	R8 = 0.959278594784451
	A7 = 114.748625289139028	A7 = 118.740634003081780
	T6 = -113.687658556027415	T6 = -121.939507886238701
	R9 = 0.966964933895760	R9 = 0.959310539768373
	A8 = 115.885187676153478	A8 = 118.341346439198873
	T7 = 108.452743477747845	T7 = 110.474165025170535
	R10 = 0.966867094832772	R10 = 0.958830821858516
	A9 = 119.354755623556727	A9 = 129.613240547325347
	T8 = 106.052304723712382	T8 = 122.595610916439156

CP2d	cc-pVDZ	cc-pVTZ
O	B1 = 0.983991039718487	B1 = 0.977249596744550
H 1 B1	B2 = 0.966343150665979	B2 = 0.958491547182441
H 1 B2 2 A1	A1 = 103.638636175190413	A1 = 105.788211241738267
O 1 B3 3 A2 2 D1	B3 = 2.709460219801790	B3 = 2.703819571774110
H 4 B4 1 A3 3 D2	A2 = 121.796994817618042	A2 = 127.230482151635428
O 1 B5 4 A4 5 D3	D1 = 112.387267433927818	D1 = 119.424837867537278
H 6 B6 1 A5 4 D4	B4 = 0.999659689180964	B4 = 0.991532602593637
H 6 B7 1 A6 4 D5	A3 = 7.094773204423986	A3 = 7.270482571132755
O 6 B8 1 A7 4 D6	D2 = 58.198543692026405	D2 = 44.551532476612252
H 9 B9 6 A8 1 D7	B5 = 2.750193276834648	B5 = 2.740258058081792
H 9 B10 6 A9 1 D8	A4 = 92.764861296398905	A4 = 93.464701959577226
	D3 = 171.257586623628157	D3 = 167.671320100237921
	B6 = 0.967102503055434	B6 = 0.959287546070851
	A5 = 114.024045882169915	A5 = 120.626261026954410
	D4 = -89.046936294970550	D4 = -95.734557330610514
	B7 = 0.982484456021712	B7 = 0.975571033596009
	A6 = 96.077534354934173	A6 = 95.886699407644798
	D5 = 17.521439957193980	D5 = 15.064167553393093
	B8 = 2.762014165183971	B8 = 2.754873892014967
	A7 = 87.597970111830918	A7 = 86.546358754239691
	D6 = 14.206008914317684	D6 = 14.638019420013123
	B9 = 0.966550885416392	B9 = 0.958690759904041
	A8 = 122.688457573035251	A8 = 131.518121976786489
	D7 = -122.404659142165798	D7 = -134.792121469641529
	B10 = 0.978610349731134	B10 = 0.972470574715901
	A9 = 98.460593146153172	A9 = 99.973725000642290
	D8 = -11.030003063706383	D8 = -14.062703049520541

Table S3. The optimized geometries (Z-matrix) of the seven transition states with the CCSD(T) method (distances in Å and angles in degrees).

TS1	cc-pVDZ	cc-pVTZ	cc-pVTZ
O	B1 = 0.983673328806322	B1 = 0.9761901063	B1 = 0.9743909823
H 1 B1	B2 = 0.966217149169664	B2 = 0.9589208810	B2 = 0.9574457324
H 1 B2 2 A1	A1 = 103.934537986370430	A1 = 105.4210843545	A1 = 105.7898656906
O 2 B3 1 A2 3 D1	B3 = 1.793520266583632	B3 = 1.7998242776	B3 = 1.8061490563
H 4 B4 2 A3 1 D2	A2 = 158.100863822496564	A2 = 159.0899879632	A2 = 159.2831047363
H 4 B5 2 A4 1 D3	D1 = 117.943766697651995	D1 = 120.5133869624	D1 = 123.1311725227
O 5 B6 4 A5 2 D4	B4 = 0.979511308044798	B4 = 0.9717807280	B4 = 0.9695035349
H 7 B7 5 A6 4 D5	A3 = 87.858735749683518	A3 = 89.9250566374	A3 = 91.0571174954
H 7 B8 5 A7 4 D6	D2 = 3.602374407809257	D2 = 7.5242864946	D2 = 9.0569827354
H 1 B9 2 A8 4 D7	B5 = 0.967613325957235	B5 = 0.9597773506	B5 = 0.9580099609
O 10 B10 1 A9 2	A4 = 113.887096146905321	A4 = 119.0647136338	A4 = 120.4495259857
D8	D3 = 106.531653824611141	D3 = 114.3775164042	D3 = 117.4404536396
	B6 = 1.859794490111393	B6 = 1.8608596781	B6 = 1.8754777368
	A5 = 153.560140711320059	A5 = 151.2892357437	A5 = 149.5340051999
	D4 = 9.394676646319075	D4 = 9.5923723456	D4 = 6.7433844658
	B7 = 0.973933106321345	B7 = 0.9657455218	B7 = 0.9638845536
	A6 = 90.842475736115375	A6 = 96.0597727438	A6 = 97.7590576039
	D5 = -7.939947811324408	D5 = -14.3589512739	D5 = -13.3868839402
	B8 = 0.966985605555022	B8 = 0.9587439803	B8 = 0.9570885102
	A7 = 118.433882261854151	A7 = 135.9941935253	A7 = 142.1038377383
	D6 = -113.059505182260096	D6 = -133.6542653545	D6 = -141.6580718513
	B9 = 1.874277522256421	B9 = 1.8811770956	B9 = 1.8819118476
	A8 = 122.427124176682298	A8 = 128.1374743488	A8 = 128.2119197417
	D7 = -88.988615445576954	D7 = -79.1011633639	D7 = -78.8822414957
	B10 = 0.984191554574542	B10 = 0.9778626501	B10 = 0.9768884924
	A9 = 166.693914745207962	A9 = 165.4019006871	A9 = 166.4884268792
	D8 = 85.600417063243668	D8 = 100.6651298308	D8 = 103.8782066422

TS2a	cc-pVDZ	cc-pVTZ
O	R1 = 0.995016777714190	R1 = 0.989037708910158
H 1 R1	R2 = 1.104164997542990	R2 = 1.098820245078721
H 1 R2 2 A1	A1 = 102.251632388455420	A1 = 103.962267687690627
O 3 R3 1 A2 2 T1	R3 = 1.248341444123708	R3 = 1.245187056124402
H 4 R4 3 A3 1 T2	A2 = 136.249538917263692	A2 = 138.425616131715543
O 2 R5 1 A4 3 T3	T1 = -73.433559985407172	T1 = -71.360573641934224
H 6 R6 2 A5 1 T4	R4 = 0.974749218830211	R4 = 0.967065489383878
H 6 R7 2 A6 1 T5	A3 = 99.181559962226842	A3 = 101.279643990543050
O 8 R8 6 A7 2 T6	T2 = -53.102602564242723	T2 = -53.135190152488221
H 9 R9 8 A8 6 T7	R5 = 1.731526280506570	R5 = 1.732924152504327
H 9 R10 8 A9 6 T8	A4 = 175.703971190530126	A4 = 175.473541728028607
	T3 = 10.448249259269636	T3 = 6.680773057957360
	R6 = 0.967568903367457	R6 = 0.959718024054811
	A5 = 111.606718489645374	A5 = 115.734744425523004
	T4 = 123.962202206191648	T4 = 129.149799060927251
	R7 = 0.983154580107675	R7 = 0.976395609815869
	A6 = 100.661668146033065	A6 = 100.754090503932360
	T5 = 15.751500107459412	T5 = 16.757477409703508
	R8 = 1.781794334883902	R8 = 1.786745165382484
	A7 = 162.965871303074152	A7 = 162.236531348862400
	T6 = 12.331434454454481	T6 = 5.742313545612884
	R9 = 0.967450013775728	R9 = 0.959644771182486
	A8 = 113.201485927357211	A8 = 118.700358018938758
	T7 = -119.316323891067583	T7 = -118.069679479617122
	R10 = 0.980157431730499	R10 = 0.973636614222099
	A9 = 93.115152219887833	A9 = 95.385228585577195
	T8 = -14.248501838295342	T8 = -7.959379332189320

TS2b	cc-pVDZ	cc-pVTZ
O	R1 = 0.994856100906863	R1 = 0.989077043538856
H 1 R1	R2 = 1.115730487999070	R2 = 1.102625224192560
H 1 R2 2 A1	A1 = 101.653392479536222	A1 = 103.822691962078537
O 1 R3 2 A2 3 T1	R3 = 3.885017646892514	R3 = 3.785941966652331
H 4 R4 1 A3 2 T2	A2 = 48.204471139742452	A2 = 48.959557205339273
H 4 R5 5 A4 1 T3	T1 = -21.535195605339364	T1 = -22.425641508598250
O 1 R6 4 A5 6 T4	R4 = 0.979760904370452	R4 = 0.973231704835759
H 7 R7 1 A6 4 T5	A3 = 41.777693937225550	A3 = 44.039731383543227
H 7 R8 8 A7 1 T6	T2 = 181.720717468801325	T2 = -178.600609155260486
O 7 R9 1 A8 6 T7	R5 = 0.967426603408265	R5 = 0.959368857163931
H 10 R10 7 A9 9 T8	A4 = 103.075684028876069	A4 = 105.121459828408831
	T3 = -116.543738294985829	T3 = -124.833705407421647
	R6 = 2.726528826512448	R6 = 2.720064120110679
	A5 = 45.060486656548754	A5 = 46.156906067979619
	T4 = -101.816025711455424	T4 = -104.347598817783847
	R7 = 0.982525189182209	R7 = 0.976238187889390
	A6 = 100.727531929943339	A6 = 99.175623585991687
	T5 = 3.302962787893843	T5 = 1.753411477596475
	R8 = 0.967501044983773	R8 = 0.959764605291855
	A7 = 102.456174935364686	A7 = 104.784324660636898
	T6 = 113.084288806466745	T6 = 119.631112536904638
	R9 = 3.524234864759490	R9 = 3.593211183301981
	A8 = 38.203614082167135	A8 = 37.498626176629429
	T7 = -16.221898240760041	T7 = -14.986224095727001
	R10 = 0.974559120820654	R10 = 0.967072613606873
	A9 = 111.639665717806196	A9 = 111.623388890416805
	T8 = 159.799032234461151	T8 = 161.113180684891830

TS2c	cc-pVDZ	cc-pVTZ
O	R1 = 0.994658281034145	R1 = 0.988645641156167
H 1 R1	R2 = 1.104221696984123	R2 = 1.100424830334134
H 1 R2 2 A1	A1 = 102.302462455632238	A1 = 103.942998867980194
O 3 R3 1 A2 2 T1	R3 = 1.246338681240623	R3 = 1.241794870977106
H 4 R4 3 A3 1 T2	A2 = 137.008720676249709	A2 = 138.881898800850593
O 2 R5 1 A4 3 T3	T1 = -72.534032705430434	T1 = -70.489151273820596
H 6 R6 2 A5 1 T4	R4 = 0.974921401822908	R4 = 0.967251163302770
H 6 R7 2 A6 1 T5	A3 = 99.050626014688063	A3 = 101.223181709583841
O 8 R8 6 A7 2 T6	T2 = -50.874256304741721	T2 = -51.634577524598441
H 9 R9 8 A8 6 T7	R5 = 1.732861613615646	R5 = 1.735268418276758
H 9 R10 8 A9 6 T8	A4 = 174.335868058636152	A4 = 175.957798131392508
	T3 = -15.408959272599180	T3 = 2.272548458239709
	R6 = 0.967271654522780	R6 = 0.959474055918331
	A5 = 111.108971450914567	A5 = 115.723239564308884
	T4 = -62.591786532260294	T4 = -93.210503015748898
	R7 = 0.982701973219522	R7 = 0.975624853950394
	A6 = 101.928324170750059	A6 = 101.675447417934279
	T5 = 46.554251267061730	T5 = 20.068527430657774
	R8 = 1.794494909615020	R8 = 1.802651142945835
	A7 = 161.411001006910567	A7 = 160.645339439305019
	T6 = -11.106138368831481	T6 = 6.560480528027716
	R9 = 0.967079445108525	R9 = 0.959282027354102
	A8 = 117.757245210703218	A8 = 123.701393699237087
	T7 = -99.849837100536732	T7 = -120.896936319570059
	R10 = 0.979859197771288	R10 = 0.973407708484601
	A9 = 93.432557429293539	A9 = 95.663994428479057
	T8 = 6.420914294534779	T8 = -8.775071247007341

TS3a (Cs)	cc-pVDZ	cc-pVTZ
O	R1 = 3.427559693095440	R1 = 3.431717503653837
O 1 R1	R2 = 0.968188168538088	R2 = 0.960969441353294
H 2 R2 1 A1	A1 = 119.182712684349426	A1 = 125.112243477300765
H 2 R3 1 A2 3 T1	R3 = 1.168397294359298	R3 = 1.164437377342735
O 2 R4 1 A3 3 T2	A2 = 50.054100676248659	A2 = 50.368907410666992
H 5 R5 2 A4 1 T3	T1 = -86.613527035183225	T1 = -85.826886830977173
O 2 R4 1 A3 3 T4	R4 = 2.404121332060328	R4 = 2.394686238278469
H 7 R5 2 A4 1 T5	A3 = 45.209756366748422	A3 = 44.886649673973011
H 2 R3 1 A2 3 T6	T2 = -85.214650820216619	T2 = -84.382708035929156
H 7 R6 2 A5 1 T7	R5 = 1.138547359208855	R5 = 1.136001850848374
H 5 R6 2 A5 1 T8	A4 = 95.724137699679474	A4 = 96.255853171018913
	T3 = 0.358793664858616	T3 = -0.164195747252768
	T4 = 85.214650820216619	T4 = 84.382708035929156
	T5 = -0.358793664858616	T5 = 0.164195747252768
	T6 = 86.613527035183225	T6 = 85.826886830977173
	R6 = 0.967666859565242	R6 = 0.959898862136848
	A5 = 111.763829666141149	A5 = 115.501584109640305
	T7 = 109.605179580461936	T7 = 114.697478696347943
	T8 = -109.605179580461936	T8 = -114.697478696347943

TS3b	cc-pVDZ	cc-pVTZ
O	R1 = 2.432561121440929	R1 = 2.421833860237584
O 1 R1	R2 = 2.404643014566217	R2 = 2.393445850757753
O 2 R2 1 A2	A2 = 90.697023248226387	A2 = 91.454573326396073
O 3 R3 2 A3 1 T3	R3 = 2.404459003741164	R3 = 2.395276409531863
H 2 R4 3 A4 4 T4	A3 = 89.979761817355708	A3 = 89.240966592849929
H 3 R5 4 A5 1 T5	T3 = -1.935986390743361	T3 = -2.191385464497677
H 3 R6 2 A6 1 T6	R4 = 1.141253079061886	R4 = 1.137142953568381
H 4 R7 3 A7 2 T7	A4 = 95.936355901757580	A4 = 96.650746915463046
H 2 R8 1 A8 4 T8	T4 = -2.042259856484876	T4 = -3.417520893264141
H 3 R9 2 A9 1 T9	R5 = 1.168739744184791	R5 = 1.163790891563551
H 4 R10 3 A10 2	A5 = 95.325764775272205	A5 = 95.189765941480886
T10	T5 = 0.718474785070231	T5 = -0.436186504999630
	R6 = 1.171101201424591	R6 = 1.165460665321734
	A6 = 94.649934626212982	A6 = 94.494472247919774
	T6 = -2.761428633297020	T6 = -3.133882950536064
	R7 = 1.136628291168470	R7 = 1.133516791150804
	A7 = 95.971806890287368	A7 = 96.561260117794774
	T7 = 1.816897816944269	T7 = 1.056864077921369
	R8 = 0.967527873177083	R8 = 0.959465924218787
	A8 = 108.323655816158990	A8 = 113.183628528859046
	T8 = 117.077232311135774	T8 = 124.544912806956063
	R9 = 0.967847136977838	R9 = 0.960601262949774
	A9 = 110.394672458898697	A9 = 114.773144590625080
	T9 = 106.018705128016862	T9 = 109.810437408942178
	R10 = 0.967893298899293	R10 = 0.960070981050012
	A10 = 110.501637984102970	A10 = 114.700533314044947
	T10 = -107.591600684543025	T10 = -113.272932541762529

TS3c (Cs)	cc-pVDZ	cc-pVTZ
O	R1 = 3.422201002592645	R1 = 3.438257215619261
O 1 R1	R2 = 0.967838036983058	R2 = 0.960552409473676
H 2 R2 1 A1	A1 = 107.411402892059712	A1 = 114.643195689643591
H 2 R3 1 A2 3 T1	R3 = 1.170261292790297	R3 = 1.164261176982789
O 2 R4 1 A3 3 T2	A2 = 50.566080282573616	A2 = 50.469555798369996
H 5 R5 2 A4 1 T3	T1 = -97.317540918861368	T1 = -95.382477976468479
O 2 R4 1 A3 3 T4	R4 = 2.404939987548732	R4 = 2.394356561945327
H 7 R5 2 A4 1 T5	A3 = 45.262621376609005	A3 = 44.734134436855520
H 2 R3 1 A2 3 T6	T2 = -99.246170789859946	T2 = -99.239006436936450
H 7 R6 2 A5 1 T7	R5 = 1.137467992065135	R5 = 1.133758618867728
H 5 R6 2 A5 1 T8	A4 = 95.698073356126429	A4 = 96.740906385665753
	T3 = -0.028609880965809	T3 = 0.520436303389754
	T4 = 99.246170789859946	T4 = 99.239006436936450
	T5 = 0.028609880965809	T5 = -0.520436303389754
	T6 = 97.317540918861368	T6 = 95.382477976468479
	R6 = 0.967344368678850	R6 = 0.959373239821044
	A5 = 114.452361937686305	A5 = 119.202047568551777
	T7 = -111.088253669218005	T7 = -117.451768391542970
	T8 = 111.088253669218005	T8 = 117.451768391542970

Table S4. The optimized geometries (Z-matrix) of two conformers of the product (H₂O)₂OH with the CCSD(T) method (distances in Å and angles in degrees).

(H ₂ O) ₂ OH-a	cc-pVDZ	cc-pVTZ	cc-pVQZ
O	R1 = 2.024360157460766	R1 = 2.035505079696688	R1 = 2.046381178373274
H 1 R1	R2 = 0.974919053458221	R2 = 0.968251919919354	R2 = 0.966552648256915
O 2 R2 1 A1	A1 = 148.830892972360346	A1 = 147.530464679984192	A1 = 146.406100427744406
H 3 R3 2 A2 1 T1	R3 = 1.878097389951483	R3 = 1.891090691915692	R3 = 1.900336848146418
O 1 R4 3 A3 2 T2	A2 = 88.528832708125890	A2 = 90.362037663552400	A2 = 91.483551929447728
H 1 R5 5 A4 3 T3	T1 = -3.466201739782615	T1 = 5.204129696537604	T1 = 7.949111848855162
H 3 R6 2 A5 1 T4	R4 = 2.765400372599386	R4 = 2.770686905872201	R4 = 2.773633410144801
H 5 R7 1 A6 3 T5	A3 = 58.760981018777173	A3 = 58.607665843614733	A3 = 58.550951075613852
	T2 = -175.090709910803554	T2 = 174.743898774909781	T2 = 171.472402996653869
	R5 = 0.994205037225581	R5 = 0.985484425910817	R5 = 0.983383678459623
	A4 = 14.819274565736491	A4 = 15.259752386725982	A4 = 15.718668491041845
	T3 = -178.783526883529788	T3 = -173.034132566403969	T3 = -171.894317606696575
	R6 = 0.967278517327261	R6 = 0.959411658092615	R6 = 0.957642888831807
	A5 = 102.729198770792010	A5 = 104.884699452887432	A5 = 105.465194180533587
	T4 = 112.578335651810832	T4 = 131.219499017922800	T4 = 138.194404272493529
	R7 = 0.967259945456131	R7 = 0.959324147084962	R7 = 0.957531663011315
	A6 = 116.880954620886627	A6 = 125.737033992558381	A6 = 129.215262669343275
	T5 = 97.869655111693319	T5 = 102.754900495572784	T5 = 105.093996620059301

(H ₂ O) ₂ OH-b	cc-pVDZ	cc-pVTZ	cc-pVTZ
O	B1 = 2.764129686726911	B1 = 2.766899094295976	B1 = 2.769957677517637
O 1 B1	B2 = 2.791095023303573	B2 = 2.780778498713625	B2 = 2.775812966894010
O 2 B2 1 A1	A1 = 63.018558387748961	A1 = 62.981520395086513	A1 = 62.937389643177134
H 1 B3 2 A2 3 D1	B3 = 0.993860466905565	B3 = 0.985209182843146	B3 = 0.983128096787533
H 3 B4 2 A3 1 D2	A2 = 14.686450532311277	A2 = 15.175200710943166	A2 = 15.555467216886500
H 3 B6 2 A5 1 D4	D1 = -178.670904421945522	D1 = -179.925865827435331	D1 = -179.141036036348453
H 2 B5 1 A4 3 D3	B4 = 0.974866373694762	B4 = 0.968085583119179	B4 = 0.966287476783400
H 2 B7 1 A6 3 D5	A3 = 79.106783050648232	A3 = 80.295471853466211	A3 = 81.469613446890222
	D2 = 4.354663039234600	D2 = 1.579999633907437	D2 = 0.611204721885249
	B6 = 0.967024144324823	B6 = 0.959058216035591	B6 = 0.957188357288054
	A5 = 120.547577271772894	A5 = 134.818712627378176	A5 = 143.042298365715482
	D4 = -94.014788810725321	D4 = -99.877825075047724	D4 = -104.151067217165220
	B5 = 0.978052730395386	B5 = 0.970547588389802	B5 = 0.968426700835339
	A4 = 82.097197603548750	A4 = 83.835348956144315	A4 = 85.016041008958425
	D3 = 0.519153770109417	D3 = -4.165450425653830	D3 = -5.406671448650377
	B7 = 0.966919054507927	B7 = 0.958975049351411	B7 = 0.957237032791377
	A6 = 119.047199981147372	A6 = 128.332465632729850	A6 = 131.553276509059430
	D5 = -100.254292284359721	D5 = -108.980868248011006	D5 = -112.373261087828652