Supplementary Information (SI) for RSC Advances.
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Electronic Supporting Information (ESI)

Computational Study of H_2 Generation from BH_3 and BH_3^- with HO· radical

Trinh Le Huyen[1,2], Pham Cam Nam[1,2*]

[1] Faculty of Chemical Engineering, University of Science and Technology, The University of Danang, Danang 550000, Viet Nam

[2]Strategic Materials & Advanced Research Team – DUT (SMART-DUT), The University of Danang- University of Science and Technology, Danang 550000, Viet Nam

Table S1. Cartesian coordinates of all species related to all reactions were calculated at the M06-2X/6-311++G(d,p) level of theory.

BH_3^- - G			
5	0.000000000	0.000000000	0.000000000
1	0.000000000	1.204785000	0.000000000
1	-1.043374000	-0.602392000	0.000000000
1	1.043374000	-0.602392000	0.000000000
Zero-point correction=		0.023846 (Hartree/Particle)	
Thermal correction to Energy=		0.026894	
Thermal correction to Enthalpy=		0.027839	
Thermal correction to Gibbs Free Energy=		0.005552	
Sum of electronic and zero-point Energies=		-26.564603	
Sum of electronic and thermal Energies=		-26.561555	
Sum of electronic and thermal Enthalpies=		-26.560611	
Sum of electronic and thermal Free Energies=		-26.582897	

BH_3 – G			
5	0.000000000	0.000000000	0.000000000
1	0.000000000	1.187546000	0.000000000
1	1.028445000	-0.593773000	0.000000000
1	-1.028445000	-0.593773000	0.000000000
Zero-point correction=		0.026751 (Hartree/Particle)	
Thermal correction to Energy=		0.029634	
Thermal correction to Enthalpy=		0.030578	
Thermal correction to Gibbs Free Energy=		0.009211	
Sum of electronic and zero-point Energies=		-26.565431	
Sum of electronic and thermal Energies=		-26.562549	
Sum of electronic and thermal Enthalpies=		-26.561604	
Sum of electronic and thermal Free Energies=		-26.582971	

BH_3^- - W			
5	0.000000000	0.000000000	0.000000000
1	0.000000000	1.204785000	0.000000000
1	-1.043374000	-0.602392000	0.000000000
1	1.043374000	-0.602392000	0.000000000
Zero-point correction=		0.023105 (Hartree/Particle)	
Thermal correction to Energy=		0.026372	
Thermal correction to Enthalpy=		0.027317	
Thermal correction to Gibbs Free Energy=		0.004651	
Sum of electronic and zero-point Energies=		-26.662083	
Sum of electronic and thermal Energies=		-26.658815	
Sum of electronic and thermal Enthalpies=		-26.657871	
Sum of electronic and thermal Free Energies=		-26.680537	

BH_3 – W			
5	0.000000000	0.000000000	0.000000000
1	0.000000000	1.187546000	0.000000000
1	-1.028445000	-0.593773000	0.000000000
1	1.028445000	-0.593773000	0.000000000
Zero-point correction=		0.026640 (Hartree/Particle)	
Thermal correction to Energy=		0.029524	
Thermal correction to Enthalpy=		0.030469	
Thermal correction to Gibbs Free Energy=		0.009100	
Sum of electronic and zero-point Energies=		-26.566296	
Sum of electronic and thermal Energies=		-26.563411	
Sum of electronic and thermal Enthalpies=		-26.562467	
Sum of electronic and thermal Free Energies=		-26.583836	

LM1-G			
5	0.642010000	0.147213000	0.000218000
1	1.317650000	-0.708970000	0.672996000
1	1.317634000	-0.710367000	-0.672619000
1	1.067392000	1.257058000	-0.001081000
8	-0.706734000	-0.150888000	-0.000123000
1	-1.258854000	0.633322000	0.000596000
Zero-point correction=		0.040523 (Hartree/Particle)	
Thermal correction to Energy=		0.043984	
Thermal correction to Enthalpy=		0.044928	
Thermal correction to Gibbs Free Energy=		0.017139	
Sum of electronic and zero-point Energies=		-102.361275	
Sum of electronic and thermal Energies=		-102.357813	
Sum of electronic and thermal Enthalpies=		-102.356869	
Sum of electronic and thermal Free Energies=		-102.384658	

TS1-G			
5	-0.562121000	0.290320000	-0.201397000
1	-1.081092000	1.205547000	0.349804000
1	-1.524610000	-0.875475000	-0.183907000
1	-1.526662000	-0.858692000	0.621387000
8	0.716523000	-0.149495000	-0.054216000
1	1.210784000	0.272984000	0.653429000
Zero-point correction=		0.038476 (Hartree/Particle)	
Thermal correction to Energy=		0.042123	
Thermal correction to Enthalpy=		0.043067	
Thermal correction to Gibbs Free Energy=		0.014872	
Sum of electronic and zero-point Energies=		-102.341914	
Sum of electronic and thermal Energies=		-102.338268	
Sum of electronic and thermal Enthalpies=		-102.337324	
Sum of electronic and thermal Free Energies=		-102.365519	

TS2-G

5	0.664847000	-0.097686000	-0.005165000
1	0.996558000	-0.288533000	1.150375000
1	1.263725000	-0.711740000	-0.834839000
1	0.871334000	1.225578000	-0.147579000
8	-0.789724000	-0.092101000	-0.006662000
1	-0.138057000	0.999933000	-0.088836000

Zero-point correction= 0.036188 (Hartree/Particle)
Thermal correction to Energy= 0.039517
Thermal correction to Enthalpy= 0.040462
Thermal correction to Gibbs Free Energy= 0.012772
Sum of electronic and zero-point Energies= -102.284690
Sum of electronic and thermal Energies= -102.281360
Sum of electronic and thermal Enthalpies= -102.280416
Sum of electronic and thermal Free Energies= -102.308105

$BH_2O^{\bullet}$-G

5	0.607726000	-0.000014000	0.000000000
1	1.194161000	1.049613000	0.000001000
1	1.194649000	-1.049291000	0.000001000
8	-0.678430000	-0.000031000	0.000000000

Zero-point correction= 0.020448 (Hartree/Particle)
Thermal correction to Energy= 0.023549
Thermal correction to Enthalpy= 0.024493
Thermal correction to Gibbs Free Energy= -0.002090
Sum of electronic and zero-point Energies= -101.205069
Sum of electronic and thermal Energies= -101.201968
Sum of electronic and thermal Enthalpies= -101.201024
Sum of electronic and thermal Free Energies= -101.227608

$OHBH^{\bullet}$-G

5	-0.769398000	-0.188149000	0.000000000
1	-1.527323000	0.738332000	0.000000000
8	0.557729000	-0.077225000	0.000000000
1	0.912484000	0.820213000	0.000000000

Zero-point correction= 0.024051 (Hartree/Particle)
Thermal correction to Energy= 0.027066
Thermal correction to Enthalpy= 0.028010
Thermal correction to Gibbs Free Energy= 0.001696
Sum of electronic and zero-point Energies= -101.199512
Sum of electronic and thermal Energies= -101.196498
Sum of electronic and thermal Enthalpies= -101.195554
Sum of electronic and thermal Free Energies= -101.221868

LM1-W

5	0.642303000	0.147847000	-0.000010000
1	1.327407000	-0.706873000	0.665009000
1	1.327405000	-0.706909000	-0.664955000
1	1.062088000	1.259601000	-0.000011000
8	-0.708439000	-0.152420000	-0.000005000
1	-1.260904000	0.634303000	0.000048000

Zero-point correction= 0.040364 (Hartree/Particle)
Thermal correction to Energy= 0.043838
Thermal correction to Enthalpy= 0.044782
Thermal correction to Gibbs Free Energy= 0.016971
Sum of electronic and zero-point Energies= -102.365846
Sum of electronic and thermal Energies= -102.362373
Sum of electronic and thermal Enthalpies= -102.361429
Sum of electronic and thermal Free Energies= -102.389239

TS1-W

5	-0.565004000	0.291539000	-0.205744000
1	-1.086972000	1.191439000	0.366743000
1	-1.532463000	-0.902220000	-0.174668000
1	-1.507581000	-0.847154000	0.618053000
8	0.720827000	-0.141384000	-0.059832000
1	1.185417000	0.231311000	0.697250000

Zero-point correction= 0.038937 (Hartree/Particle)
Thermal correction to Energy= 0.042535
Thermal correction to Enthalpy= 0.043480
Thermal correction to Gibbs Free Energy= 0.015355
Sum of electronic and zero-point Energies= -102.347216
Sum of electronic and thermal Energies= -102.343617
Sum of electronic and thermal Enthalpies= -102.342673
Sum of electronic and thermal Free Energies= -102.370798

TS2-W

5	0.661033000	-0.095968000	-0.008096000
1	0.962180000	-0.220990000	1.173286000
1	1.280301000	-0.765885000	-0.777637000
1	0.880235000	1.208199000	-0.183639000
8	-0.786421000	-0.092740000	-0.006094000
1	-0.136516000	1.000437000	-0.122775000

Zero-point correction= 0.035957 (Hartree/Particle)
Thermal correction to Energy= 0.039260
Thermal correction to Enthalpy= 0.040204
Thermal correction to Gibbs Free Energy= 0.012572
Sum of electronic and zero-point Energies= -102.288182
Sum of electronic and thermal Energies= -102.284879
Sum of electronic and thermal Enthalpies= -102.283935
Sum of electronic and thermal Free Energies= -102.311568

$BH_2O^{\bullet}$-W

5	0.605636000	-0.000001000	0.000000000
1	1.200083000	1.047041000	0.000001000
1	1.200124000	-1.047014000	0.000001000
8	-0.678549000	-0.000003000	0.000000000

Zero-point correction= 0.020102 (Hartree/Particle)
Thermal correction to Energy= 0.023234
Thermal correction to Enthalpy= 0.024178
Thermal correction to Gibbs Free Energy= -0.002448
Sum of electronic and zero-point Energies= -101.207867
Sum of electronic and thermal Energies= -101.204735
Sum of electronic and thermal Enthalpies= -101.203791
Sum of electronic and thermal Free Energies= -101.230416

$OHBH^{\bullet}$-W

5	0.122801000	0.780371000	0.000000000
1	-0.851550000	1.471318000	0.000000000
8	0.122801000	-0.549476000	0.000000000
1	-0.744868000	-0.977364000	0.000000000

Zero-point correction= 0.023856 (Hartree/Particle)
Thermal correction to Energy= 0.026878
Thermal correction to Enthalpy= 0.027822
Thermal correction to Gibbs Free Energy= 0.001504
Sum of electronic and zero-point Energies= -101.205156
Sum of electronic and thermal Energies= -101.202134
Sum of electronic and thermal Enthalpies= -101.201190
Sum of electronic and thermal Free Energies= -101.227508

LM2-G

5	-0.741554000	0.013263000	-0.000023000
1	-1.234578000	-1.115715000	0.000008000
1	-1.143698000	0.630751000	1.007503000
1	-1.143761000	0.630698000	-1.007409000
8	0.763105000	-0.121954000	0.000016000
1	1.124966000	0.763581000	-0.000114000

Zero-point correction= 0.041549 (Hartree/Particle)
Thermal correction to Energy= 0.045064

TS3-G

5	0.713688000	-0.083453000	-0.018109000
1	1.365775000	-0.815349000	0.685122000
1	1.272577000	0.555334000	-0.856684000
1	-0.038146000	2.240566000	0.512089000
8	-0.645361000	-0.271281000	-0.004435000
1	-1.005753000	0.606963000	-0.214497000

Zero-point correction= 0.036926 (Hartree/Particle)
Thermal correction to Energy= 0.040451

Thermal correction to Enthalpy=	0.046009		
Thermal correction to Gibbs Free Energy=	0.018563		
Sum of electronic and zero-point Energies=	-102.457462		
Sum of electronic and thermal Energies=	-102.453947		
Sum of electronic and thermal Enthalpies=	-102.453002		
Sum of electronic and thermal Free Energies=	-102.480448		

Thermal correction to Enthalpy=	0.041395		
Thermal correction to Gibbs Free Energy=	0.013829		
Sum of electronic and zero-point Energies=	-102.397887		
Sum of electronic and thermal Energies=	-102.394362		
Sum of electronic and thermal Enthalpies=	-102.393418		
Sum of electronic and thermal Free Energies=	-102.420984		

TS4-G

5	-0.532344000	0.384780000	-0.259485000
1	-0.871703000	1.127351000	0.673923000
1	-1.671363000	-0.666127000	-0.233836000
1	-1.900890000	-1.005622000	0.536634000
8	0.749996000	-0.178269000	-0.060244000
1	1.105708000	0.046651000	0.802656000

Zero-point correction=	0.035259 (Hartree/Particle)
Thermal correction to Energy=	0.038926
Thermal correction to Enthalpy=	0.039870
Thermal correction to Gibbs Free Energy=	0.012083
Sum of electronic and zero-point Energies=	-102.344725
Sum of electronic and thermal Energies=	-102.341058
Sum of electronic and thermal Enthalpies=	-102.340114
Sum of electronic and thermal Free Energies=	-102.367901

$BH_2O^{\bullet-}$-G

5	0.590038000	-0.000018000	-0.000003000
1	1.296031000	-1.039881000	0.000004000
1	1.295952000	1.039979000	0.000004000
8	-0.692771000	-0.000001000	0.000001000

Zero-point correction=	0.020446 (Hartree/Particle)
Thermal correction to Energy=	0.023375
Thermal correction to Enthalpy=	0.024319
Thermal correction to Gibbs Free Energy=	-0.001400
Sum of electronic and zero-point Energies=	-101.290599
Sum of electronic and thermal Energies=	-101.287670
Sum of electronic and thermal Enthalpies=	-101.286726
Sum of electronic and thermal Free Energies=	-101.312446

OH-$BH^{\bullet-}$-G

5	0.829925000	-0.219392000	0.000001000
1	1.311326000	0.946697000	-0.000004000
8	-0.574221000	-0.085645000	-0.000001000
1	-0.867186000	0.835423000	0.000005000

Zero-point correction=	0.021680 (Hartree/Particle)
Thermal correction to Energy=	0.024722
Thermal correction to Enthalpy=	0.025666
Thermal correction to Gibbs Free Energy=	-0.000212
Sum of electronic and zero-point Energies=	-101.192042
Sum of electronic and thermal Energies=	-101.189000
Sum of electronic and thermal Enthalpies=	-101.188056
Sum of electronic and thermal Free Energies=	-101.213934

LM2-W

5	0.738969000	-0.017429000	0.000029000
1	1.226001000	1.112792000	0.000063000
1	1.146391000	-0.623690000	1.002218000
1	1.146472000	-0.623667000	-1.002150000
8	-0.757385000	0.121498000	-0.000029000
1	-1.154629000	-0.750272000	-0.000041000

Zero-point correction=	0.042073 (Hartree/Particle)
Thermal correction to Energy=	0.045526
Thermal correction to Enthalpy=	0.046470
Thermal correction to Gibbs Free Energy=	0.019158
Sum of electronic and zero-point Energies=	-102.559273
Sum of electronic and thermal Energies=	-102.555820
Sum of electronic and thermal Enthalpies=	-102.554876
Sum of electronic and thermal Free Energies=	-102.582188

TS3-W

5	-0.321288000	0.678209000	0.042289000
1	-0.986861000	1.220349000	-0.783455000
1	0.188591000	1.270738000	0.942071000
1	3.423986000	0.446774000	-0.357311000
8	-0.175503000	-0.660297000	-0.077073000
1	0.384748000	-1.046534000	0.603832000

Zero-point correction=	0.036643 (Hartree/Particle)
Thermal correction to Energy=	0.040833
Thermal correction to Enthalpy=	0.041777
Thermal correction to Gibbs Free Energy=	0.012298
Sum of electronic and zero-point Energies=	-102.510926
Sum of electronic and thermal Energies=	-102.506736
Sum of electronic and thermal Enthalpies=	-102.505792
Sum of electronic and thermal Free Energies=	-102.535271

LM3-W

5	-0.776498000	0.220636000	0.000012000
1	-1.800351000	-0.406437000	0.001380000
1	-0.810929000	1.423972000	-0.000931000
1	2.183178000	1.058229000	0.001547000
8	0.386539000	-0.427142000	-0.000136000
1	1.218281000	0.238189000	-0.000968000

Zero-point correction=	0.036638 (Hartree/Particle)
Thermal correction to Energy=	0.040276
Thermal correction to Enthalpy=	0.041220
Thermal correction to Gibbs Free Energy=	0.013548
Sum of electronic and zero-point Energies=	-102.526925
Sum of electronic and thermal Energies=	-102.523287
Sum of electronic and thermal Enthalpies=	-102.522343
Sum of electronic and thermal Free Energies=	-102.550015

TS3a-W

5	0.768414000	0.212413000	-0.000321000
1	0.802054000	1.423720000	0.001189000
1	1.814554000	-0.390341000	-0.000419000
1	-2.086462000	1.041391000	-0.000356000
8	-0.385780000	-0.431959000	0.000254000
1	-1.285972000	0.318838000	-0.000840000

Zero-point correction=	0.033614 (Hartree/Particle)
Thermal correction to Energy=	0.037190
Thermal correction to Enthalpy=	0.038135
Thermal correction to Gibbs Free Energy=	0.010546
Sum of electronic and zero-point Energies=	-102.529382
Sum of electronic and thermal Energies=	-102.525806
Sum of electronic and thermal Enthalpies=	-102.524862
Sum of electronic and thermal Free Energies=	-102.552450

TS4-W

5	-0.580772000	0.362594000	-0.246423000
1	-1.006788000	0.985481000	0.719769000
1	-1.569293000	-0.812637000	-0.270842000
1	-1.569007000	-0.977028000	0.545464000
8	0.748073000	-0.122744000	-0.073844000
1	1.064370000	-0.026837000	0.828475000

Zero-point correction=	0.037135 (Hartree/Particle)
Thermal correction to Energy=	0.040662
Thermal correction to Enthalpy=	0.041606
Thermal correction to Gibbs Free Energy=	0.014131
Sum of electronic and zero-point Energies=	-102.443663
Sum of electronic and thermal Energies=	-102.440136
Sum of electronic and thermal Enthalpies=	-102.439192
Sum of electronic and thermal Free Energies=	-102.466667

OHB$H^{\bullet-}$-W

$BH_2O^{\bullet-}$-W

5	0.822142000	-0.213828000	-0.000002000
1	1.326341000	0.917654000	-0.000003000
8	-0.570465000	-0.084956000	0.000001000
1	-0.873333000	0.831128000	0.000002000

Zero-point correction= 0.022840 (Hartree/Particle)
Thermal correction to Energy= 0.025844
Thermal correction to Enthalpy= 0.026789
Thermal correction to Gibbs Free Energy= 0.000991
Sum of electronic and zero-point Energies= -101.301032
Sum of electronic and thermal Energies= -101.298028
Sum of electronic and thermal Enthalpies= -101.297084
Sum of electronic and thermal Free Energies= -101.322881

5	0.599128000	0.000002000	0.000001000
1	1.280069000	-1.034377000	0.000002000
1	1.280065000	1.034374000	0.000002000
8	-0.694472000	-0.000001000	-0.000001000

Zero-point correction= 0.020905 (Hartree/Particle)
Thermal correction to Energy= 0.023833
Thermal correction to Enthalpy= 0.024777
Thermal correction to Gibbs Free Energy= -0.000940
Sum of electronic and zero-point Energies= -101.394971
Sum of electronic and thermal Energies= -101.392043
Sum of electronic and thermal Enthalpies= -101.391099
Sum of electronic and thermal Free Energies= -101.416816

Table S2. Calculated equilibrium constants (K_c) for pre-reactive complex formation and unimolecular rate constants (k_2) for the subsequent product-forming step obtained at the M06-2X/6-311++G(d,p) level under the high-pressure limit approximation, including tunneling corrections using the Eckart and Wigner methods.

$(BH_3 + HO^{\bullet})$-G → LM1-G → TS1-G → $(OHBH^{\bullet} + H_2)$-G						
T(K)	*Kc (cm^3 $molecule^{-1}$)*	*k_2 (s^{-1})*	*κ_{Eck}*	*k_{Eck} (cm^3 $molecule^{-1}$ s^{-1})*	*κ_{Wig}*	*k_{Wig} (cm^3 $molecule^{-1}$ s^{-1})*
280	8.30E+12	2.40E+03	1.7	3.30E+16	1.5	2.90E+16
290	3.70E+11	5.30E+03	1.6	3.20E+15	1.4	2.90E+15
298.15	3.50E+10	9.80E+03	1.6	5.40E+14	1.4	4.80E+14
300	2.10E+10	1.10E+04	1.6	3.60E+14	1.4	3.30E+14
310	1.40E+09	2.20E+04	1.5	4.70E+13	1.4	4.30E+13
320	1.10E+08	4.30E+04	1.5	7.00E+12	1.4	6.50E+12
330	1.00E+07	8.00E+04	1.4	1.20E+12	1.3	1.10E+12
340	1.10E+06	1.40E+05	1.4	2.20E+11	1.3	2.00E+11
350	1.30E+05	2.50E+05	1.4	4.50E+10	1.3	4.20E+10
$(BH_3^- + HO^{\bullet})$-G → LM2-G → TS3-G → $(OHBH^{\bullet} + H_2)$-G						
T(K)	*Kc (cm^3 $molecule^{-1}$)*	*k_2 (s^{-1})*	*κ_{Eck}*	*k_{Eck} (cm^3 $molecule^{-1}$ s^{-1})*	*κ_{Wig}*	*k_{Wig} (cm^3 $molecule^{-1}$ s^{-1})*
280	8.10E+59	4.30E-17	1.4	4.9E+43	1.3	4.60E+43
290	8.40E+56	4.60E-16	1.4	5.2E+41	1.3	4.90E+41
298.15	4.40E+54	2.80E-15	1.3	1.6E+40	1.3	1.50E+40
300	1.40E+54	4.10E-15	1.3	7.5E+39	1.3	7.20E+39
310	3.40E+51	3.20E-14	1.3	1.4E+38	1.3	1.40E+38
320	1.20E+49	2.20E-13	1.3	3.4E+36	1.2	3.30E+36
330	6.20E+46	1.40E-12	1.3	1.1E+35	1.2	1.00E+35
340	4.20E+44	7.50E-12	1.3	4.1E+33	1.2	3.80E+33
350	3.90E+42	3.70E-11	1.2	1.7E+32	1.2	1.70E+32

Table S3. Calculated kinetic parameters and detailed transition state theory (TST) results for the BH_3 + atmospheric oxidant reactions in the solution phase at 298.15 K and 1 atm.

//***//
Input parameters
//***//

Phase solution
Method TST/WIG/DIFF/AB
Reaction symmetry 1

Solvent water
Reaction distance (Angstrom) 1.39
React1 radius (Angstrom) 1.18
React2 radius (Angstrom) 0.5

pKa 9.0
Molar fraction f0
Diffusion constants in M-1 s-1.
(Viscosity in Pa s).

T(K)	visc	kd
280.00	1.43E-03	4.3E+09
290.00	1.08E-03	5.9E+09
298.15	8.90E-04	7.3E+09
300.00	8.54E-04	7.7E+09
310.00	6.94E-04	9.8E+09
320.00	5.77E-04	1.2E+10
330.00	4.90E-04	1.5E+10
340.00	4.22E-04	1.8E+10
350.00	3.69E-04	2.1E+10

Rate constants in (M^{-1} s^{-1}) of reaction BH_3 + $HO^{\bullet}$ → LM1 → TS1 → $OHBH^{\bullet}$ + H_2 in the Aqueous Solution

pH	T(K)	kwig	kapp	kf
1	280.00	5.9E+36	4.3E+09	4.3E+01
	290.00	6.0E+35	5.9E+09	5.9E+01
	298.15	1.0E+35	7.3E+09	7.3E+01
	300.00	7.1E+34	7.7E+09	7.7E+01
	310.00	9.6E+33	9.8E+09	9.8E+01
	320.00	1.5E+33	1.2E+10	1.2E+02
	330.00	2.6E+32	1.5E+10	1.5E+02
	340.00	4.9E+31	1.8E+10	1.8E+02
	350.00	1.0E+31	2.1E+10	2.1E+02
2	280.00	5.9E+36	4.3E+09	4.3E+02
	290.00	6.0E+35	5.9E+09	5.9E+02
	298.15	1.0E+35	7.3E+09	7.3E+02
	300.00	7.1E+34	7.7E+09	7.7E+02
	310.00	9.6E+33	9.8E+09	9.8E+02
	320.00	1.5E+33	1.2E+10	1.2E+03
	330.00	2.6E+32	1.5E+10	1.5E+03
	340.00	4.9E+31	1.8E+10	1.8E+03

	350.00	1.0E+31	2.1E+10	2.1E+03
3	280.00	5.9E+36	4.3E+09	4.3E+03
	290.00	6.0E+35	5.9E+09	5.9E+03
	298.15	1.0E+35	7.3E+09	7.3E+03
	300.00	7.1E+34	7.7E+09	7.7E+03
	310.00	9.6E+33	9.8E+09	9.8E+03
	320.00	1.5E+33	1.2E+10	1.2E+04
	330.00	2.6E+32	1.5E+10	1.5E+04
	340.00	4.9E+31	1.8E+10	1.8E+04
	350.00	1.0E+31	2.1E+10	2.1E+04
4	280.00	5.9E+36	4.3E+09	4.3E+04
	290.00	6.0E+35	5.9E+09	5.9E+04
	298.15	1.0E+35	7.3E+09	7.3E+04
	300.00	7.1E+34	7.7E+09	7.7E+04
	310.00	9.6E+33	9.8E+09	9.8E+04
	320.00	1.5E+33	1.2E+10	1.2E+05
	330.00	2.6E+32	1.5E+10	1.5E+05
	340.00	4.9E+31	1.8E+10	1.8E+05
	350.00	1.0E+31	2.1E+10	2.1E+05
5	280.00	5.9E+36	4.3E+09	4.3E+05
	290.00	6.0E+35	5.9E+09	5.9E+05
	298.15	1.0E+35	7.3E+09	7.3E+05
	300.00	7.1E+34	7.7E+09	7.7E+05
	310.00	9.6E+33	9.8E+09	9.8E+05
	320.00	1.5E+33	1.2E+10	1.2E+06
	330.00	2.6E+32	1.5E+10	1.5E+06
	340.00	4.9E+31	1.8E+10	1.8E+06
	350.00	1.0E+31	2.1E+10	2.1E+06
6	280.00	5.9E+36	4.3E+09	4.3E+06
	290.00	6.0E+35	5.9E+09	5.9E+06
	298.15	1.0E+35	7.3E+09	7.3E+06
	300.00	7.1E+34	7.7E+09	7.7E+06
	310.00	9.6E+33	9.8E+09	9.8E+06
	320.00	1.5E+33	1.2E+10	1.2E+07
	330.00	2.6E+32	1.5E+10	1.5E+07
	340.00	4.9E+31	1.8E+10	1.8E+07
	350.00	1.0E+31	2.1E+10	2.1E+07
7	280.00	5.9E+36	4.3E+09	4.2E+07
	290.00	6.0E+35	5.9E+09	5.8E+07
	298.15	1.0E+35	7.3E+09	7.3E+07
	300.00	7.1E+34	7.7E+09	7.6E+07
	310.00	9.6E+33	9.8E+09	9.7E+07
	320.00	1.5E+33	1.2E+10	1.2E+08
	330.00	2.6E+32	1.5E+10	1.5E+08
	340.00	4.9E+31	1.8E+10	1.8E+08
	350.00	1.0E+31	2.1E+10	2.1E+08
8	280.00	5.9E+36	4.3E+09	3.9E+08
	290.00	6.0E+35	5.9E+09	5.3E+08
	298.15	1.0E+35	7.3E+09	6.7E+08
	300.00	7.1E+34	7.7E+09	7.0E+08
	310.00	9.6E+33	9.8E+09	8.9E+08
	320.00	1.5E+33	1.2E+10	1.1E+09
	330.00	2.6E+32	1.5E+10	1.3E+09
	340.00	4.9E+31	1.8E+10	1.6E+09

	350.00	1.0E+31	2.1E+10	1.9E+09
9	280.00	5.9E+36	4.3E+09	2.1E+09
	290.00	6.0E+35	5.9E+09	2.9E+09
	298.15	1.0E+35	7.3E+09	3.7E+09
	300.00	7.1E+34	7.7E+09	3.9E+09
	310.00	9.6E+33	9.8E+09	4.9E+09
	320.00	1.5E+33	1.2E+10	6.1E+09
	330.00	2.6E+32	1.5E+10	7.4E+09
	340.00	4.9E+31	1.8E+10	8.8E+09
	350.00	1.0E+31	2.1E+10	1.0E+10
10	280.00	5.9E+36	4.3E+09	3.9E+09
	290.00	6.0E+35	5.9E+09	5.3E+09
	298.15	1.0E+35	7.3E+09	6.7E+09
	300.00	7.1E+34	7.7E+09	7.0E+09
	310.00	9.6E+33	9.8E+09	8.9E+09
	320.00	1.5E+33	1.2E+10	1.1E+10
	330.00	2.6E+32	1.5E+10	1.3E+10
	340.00	4.9E+31	1.8E+10	1.6E+10
	350.00	1.0E+31	2.1E+10	1.9E+10
11	280.00	5.9E+36	4.3E+09	4.2E+09
	290.00	6.0E+35	5.9E+09	5.8E+09
	298.15	1.0E+35	7.3E+09	7.3E+09
	300.00	7.1E+34	7.7E+09	7.6E+09
	310.00	9.6E+33	9.8E+09	9.7E+09
	320.00	1.5E+33	1.2E+10	1.2E+10
	330.00	2.6E+32	1.5E+10	1.5E+10
	340.00	4.9E+31	1.8E+10	1.8E+10
	350.00	1.0E+31	2.1E+10	2.1E+10
12	280.00	5.9E+36	4.3E+09	4.3E+09
	290.00	6.0E+35	5.9E+09	5.9E+09
	298.15	1.0E+35	7.3E+09	7.3E+09
	300.00	7.1E+34	7.7E+09	7.7E+09
	310.00	9.6E+33	9.8E+09	9.8E+09
	320.00	1.5E+33	1.2E+10	1.2E+10
	330.00	2.6E+32	1.5E+10	1.5E+10
	340.00	4.9E+31	1.8E+10	1.8E+10
	350.00	1.0E+31	2.1E+10	2.1E+10
13	280.00	5.9E+36	4.3E+09	4.3E+09
	290.00	6.0E+35	5.9E+09	5.9E+09
	298.15	1.0E+35	7.3E+09	7.3E+09
	300.00	7.1E+34	7.7E+09	7.7E+09
	310.00	9.6E+33	9.8E+09	9.8E+09
	320.00	1.5E+33	1.2E+10	1.2E+10
	330.00	2.6E+32	1.5E+10	1.5E+10
	340.00	4.9E+31	1.8E+10	1.8E+10
	350.00	1.0E+31	2.1E+10	2.1E+10
14	280.00	5.9E+36	4.3E+09	4.3E+09
	290.00	6.0E+35	5.9E+09	5.9E+09
	298.15	1.0E+35	7.3E+09	7.3E+09
	300.00	7.1E+34	7.7E+09	7.7E+09
	310.00	9.6E+33	9.8E+09	9.8E+09
	320.00	1.5E+33	1.2E+10	1.2E+10
	330.00	2.6E+32	1.5E+10	1.5E+10
	340.00	4.9E+31	1.8E+10	1.8E+10

	350.00	1.0E+31	2.1E+10	2.1E+10

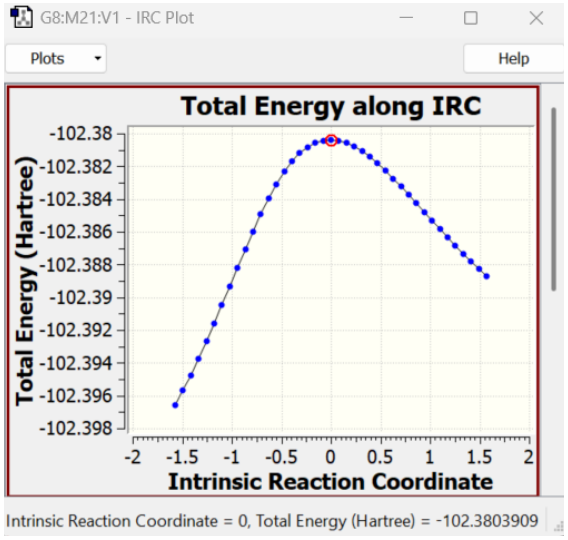
Rate constants in (M^{-1} s^{-1}) of reaction $^{BH}_{3}^{-}$ + **HO˙ →TS3 → LM3 →TS3a → OHBH˙ + H_2** in the aqueous solution

pH	T(K)	kwig	kapp	kf
1	280.00	6.7E+69	4.9E+09	4.9E+01
	290.00	4.9E+67	6.7E+09	6.7E+01
	298.15	1.2E+66	8.4E+09	8.4E+01
	300.00	5.1E+65	8.8E+09	8.8E+01
	310.00	7.1E+63	1.1E+10	1.1E+02
	320.00	1.3E+62	1.4E+10	1.4E+02
	330.00	3.0E+60	1.7E+10	1.7E+02
	340.00	8.5E+58	2.0E+10	2.0E+02
	350.00	3.0E+57	2.4E+10	2.4E+02
2	280.00	6.7E+69	4.9E+09	4.9E+02
	290.00	4.9E+67	6.7E+09	6.7E+02
	298.15	1.2E+66	8.4E+09	8.4E+02
	300.00	5.1E+65	8.8E+09	8.8E+02
	310.00	7.1E+63	1.1E+10	1.1E+03
	320.00	1.3E+62	1.4E+10	1.4E+03
	330.00	3.0E+60	1.7E+10	1.7E+03
	340.00	8.5E+58	2.0E+10	2.0E+03
	350.00	3.0E+57	2.4E+10	2.4E+03
3	280.00	6.7E+69	4.9E+09	4.9E+03
	290.00	4.9E+67	6.7E+09	6.7E+03
	298.15	1.2E+66	8.4E+09	8.4E+03
	300.00	5.1E+65	8.8E+09	8.8E+03
	310.00	7.1E+63	1.1E+10	1.1E+04
	320.00	1.3E+62	1.4E+10	1.4E+04
	330.00	3.0E+60	1.7E+10	1.7E+04
	340.00	8.5E+58	2.0E+10	2.0E+04
	350.00	3.0E+57	2.4E+10	2.4E+04
4	280.00	6.7E+69	4.9E+09	4.9E+04
	290.00	4.9E+67	6.7E+09	6.7E+04
	298.15	1.2E+66	8.4E+09	8.4E+04
	300.00	5.1E+65	8.8E+09	8.8E+04
	310.00	7.1E+63	1.1E+10	1.1E+05
	320.00	1.3E+62	1.4E+10	1.4E+05
	330.00	3.0E+60	1.7E+10	1.7E+05
	340.00	8.5E+58	2.0E+10	2.0E+05
	350.00	3.0E+57	2.4E+10	2.4E+05
5	280.00	6.7E+69	4.9E+09	4.9E+05
	290.00	4.9E+67	6.7E+09	6.7E+05
	298.15	1.2E+66	8.4E+09	8.4E+05
	300.00	5.1E+65	8.8E+09	8.8E+05
	310.00	7.1E+63	1.1E+10	1.1E+06
	320.00	1.3E+62	1.4E+10	1.4E+06
	330.00	3.0E+60	1.7E+10	1.7E+06
	340.00	8.5E+58	2.0E+10	2.0E+06

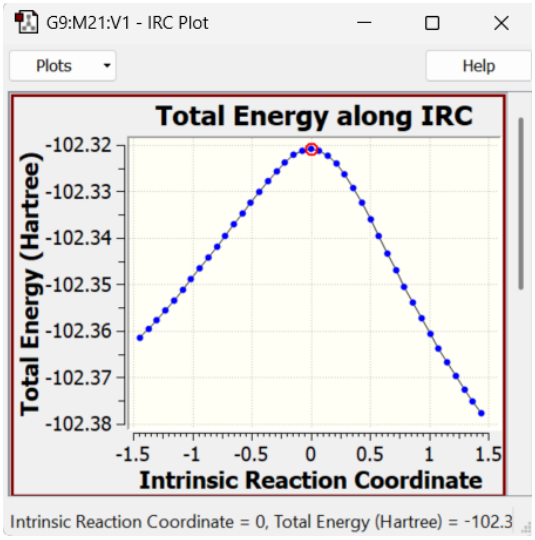
	350.00	3.0E+57	2.4E+10	2.4E+06
6	280.00	6.7E+69	4.9E+09	4.9E+06
	290.00	4.9E+67	6.7E+09	6.7E+06
	298.15	1.2E+66	8.4E+09	8.3E+06
	300.00	5.1E+65	8.8E+09	8.8E+06
	310.00	7.1E+63	1.1E+10	1.1E+07
	320.00	1.3E+62	1.4E+10	1.4E+07
	330.00	3.0E+60	1.7E+10	1.7E+07
	340.00	8.5E+58	2.0E+10	2.0E+07
	350.00	3.0E+57	2.4E+10	2.4E+07
7	280.00	6.7E+69	4.9E+09	4.8E+07
	290.00	4.9E+67	6.7E+09	6.6E+07
	298.15	1.2E+66	8.4E+09	8.3E+07
	300.00	5.1E+65	8.8E+09	8.7E+07
	310.00	7.1E+63	1.1E+10	1.1E+08
	320.00	1.3E+62	1.4E+10	1.4E+08
	330.00	3.0E+60	1.7E+10	1.7E+08
	340.00	8.5E+58	2.0E+10	2.0E+08
	350.00	3.0E+57	2.4E+10	2.3E+08
8	280.00	6.7E+69	4.9E+09	4.4E+08
	290.00	4.9E+67	6.7E+09	6.1E+08
	298.15	1.2E+66	8.4E+09	7.6E+08
	300.00	5.1E+65	8.8E+09	8.0E+08
	310.00	7.1E+63	1.1E+10	1.0E+09
	320.00	1.3E+62	1.4E+10	1.3E+09
	330.00	3.0E+60	1.7E+10	1.5E+09
	340.00	8.5E+58	2.0E+10	1.8E+09
	350.00	3.0E+57	2.4E+10	2.2E+09
9	280.00	6.7E+69	4.9E+09	2.4E+09
	290.00	4.9E+67	6.7E+09	3.3E+09
	298.15	1.2E+66	8.4E+09	4.2E+09
	300.00	5.1E+65	8.8E+09	4.4E+09
	310.00	7.1E+63	1.1E+10	5.6E+09
	320.00	1.3E+62	1.4E+10	6.9E+09
	330.00	3.0E+60	1.7E+10	8.4E+09
	340.00	8.5E+58	2.0E+10	1.0E+10
	350.00	3.0E+57	2.4E+10	1.2E+10
10	280.00	6.7E+69	4.9E+09	4.4E+09
	290.00	4.9E+67	6.7E+09	6.1E+09
	298.15	1.2E+66	8.4E+09	7.6E+09
	300.00	5.1E+65	8.8E+09	8.0E+09
	310.00	7.1E+63	1.1E+10	1.0E+10
	320.00	1.3E+62	1.4E+10	1.3E+10
	330.00	3.0E+60	1.7E+10	1.5E+10
	340.00	8.5E+58	2.0E+10	1.8E+10
	350.00	3.0E+57	2.4E+10	2.2E+10
11	280.00	6.7E+69	4.9E+09	4.8E+09
	290.00	4.9E+67	6.7E+09	6.6E+09
	298.15	1.2E+66	8.4E+09	8.3E+09
	300.00	5.1E+65	8.8E+09	8.7E+09

	310.00	7.1E+63	1.1E+10	1.1E+10
	320.00	1.3E+62	1.4E+10	1.4E+10
	330.00	3.0E+60	1.7E+10	1.7E+10
	340.00	8.5E+58	2.0E+10	2.0E+10
	350.00	3.0E+57	2.4E+10	2.3E+10
12	280.00	6.7E+69	4.9E+09	4.9E+09
	290.00	4.9E+67	6.7E+09	6.7E+09
	298.15	1.2E+66	8.4E+09	8.3E+09
	300.00	5.1E+65	8.8E+09	8.8E+09
	310.00	7.1E+63	1.1E+10	1.1E+10
	320.00	1.3E+62	1.4E+10	1.4E+10
	330.00	3.0E+60	1.7E+10	1.7E+10
	340.00	8.5E+58	2.0E+10	2.0E+10
	350.00	3.0E+57	2.4E+10	2.4E+10
13	280.00	6.7E+69	4.9E+09	4.9E+09
	290.00	4.9E+67	6.7E+09	6.7E+09
	298.15	1.2E+66	8.4E+09	8.4E+09
	300.00	5.1E+65	8.8E+09	8.8E+09
	310.00	7.1E+63	1.1E+10	1.1E+10
	320.00	1.3E+62	1.4E+10	1.4E+10
	330.00	3.0E+60	1.7E+10	1.7E+10
	340.00	8.5E+58	2.0E+10	2.0E+10
	350.00	3.0E+57	2.4E+10	2.4E+10
14	280.00	6.7E+69	4.9E+09	4.9E+09
	290.00	4.9E+67	6.7E+09	6.7E+09
	298.15	1.2E+66	8.4E+09	8.4E+09
	300.00	5.1E+65	8.8E+09	8.8E+09
	310.00	7.1E+63	1.1E+10	1.1E+10
	320.00	1.3E+62	1.4E+10	1.4E+10
	330.00	3.0E+60	1.7E+10	1.7E+10
	340.00	8.5E+58	2.0E+10	2.0E+10
	350.00	3.0E+57	2.4E+10	2.4E+10

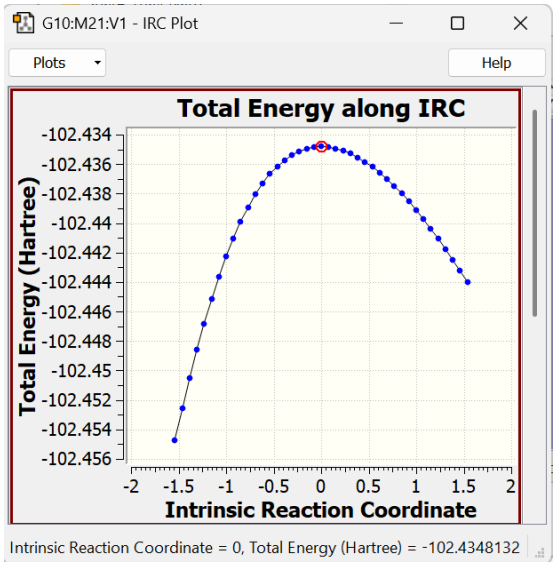
Fig S1. Intrinsic reaction coordinate (IRC) profiles connecting the pre-reactive complexes and the first transition states along all reaction pathways.



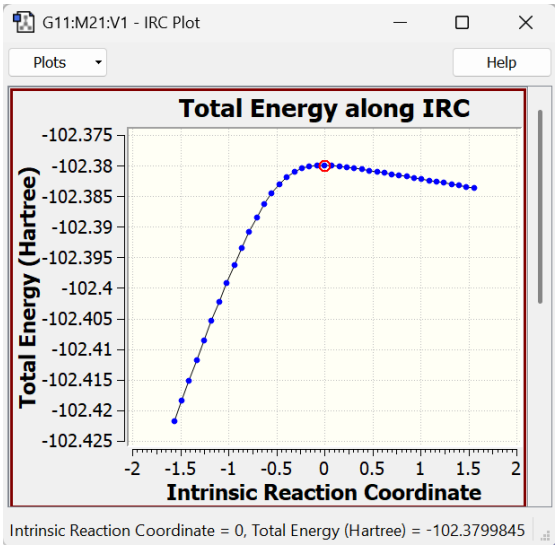
IRC-TS1-G



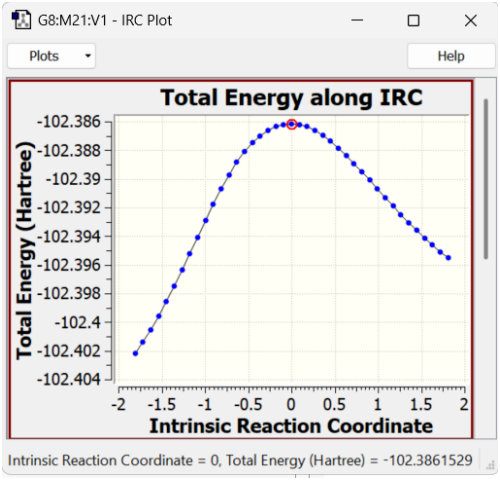
IRC-TS2-G

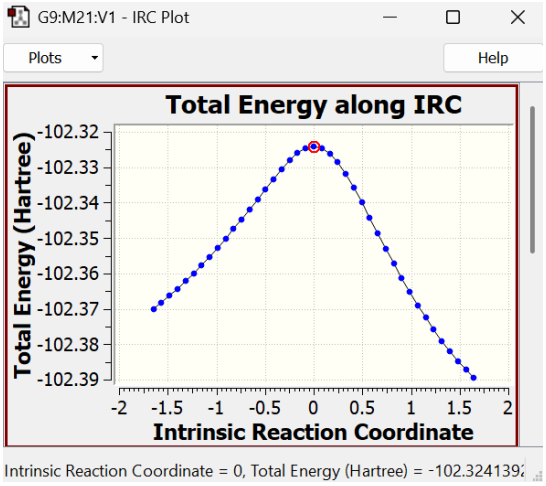


IRC-TS3-G



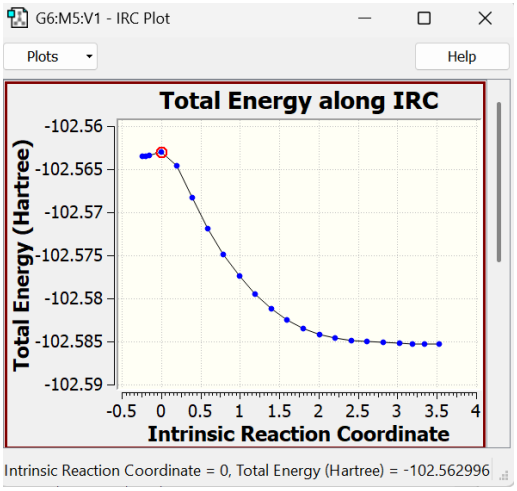
IRC-TS4-G



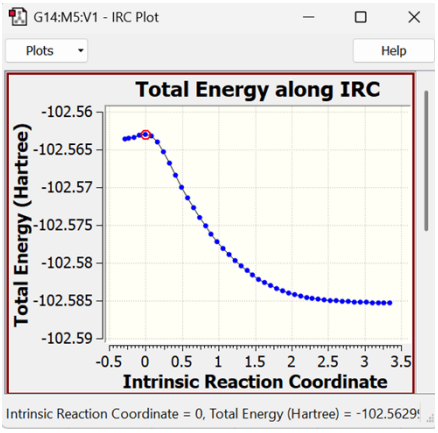


TS1-W

TS2-W



IRC-TS3-W



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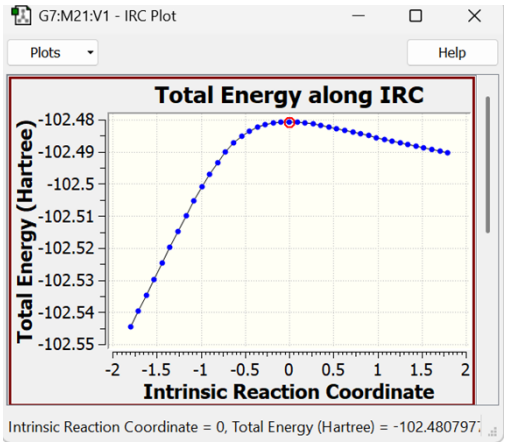

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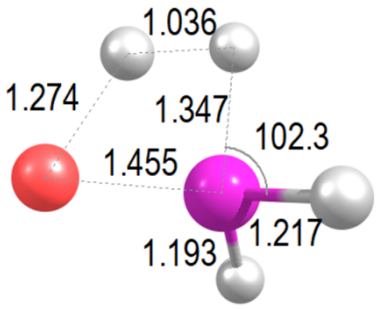
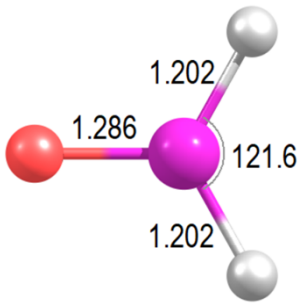
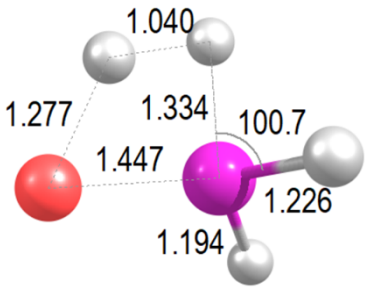


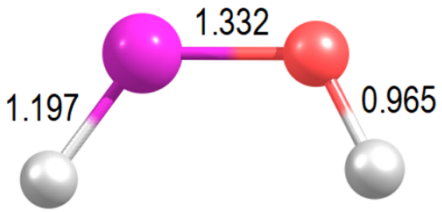
TS2-G



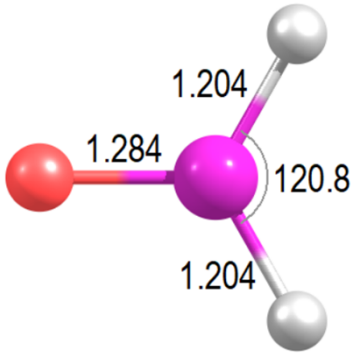
$BH_2O^{\bullet}$-G



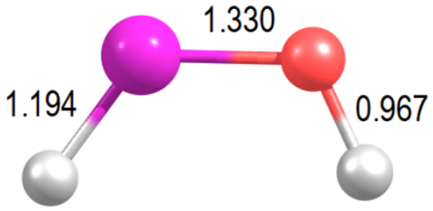
TS2-W



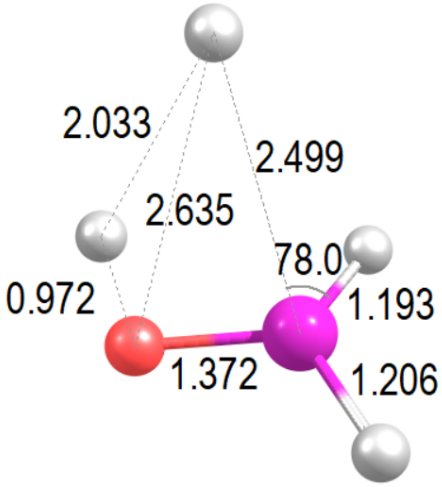
$OHBH^{\bullet}$-G



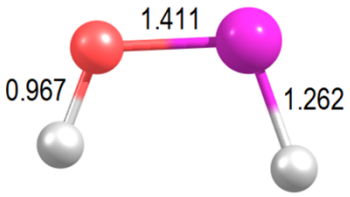
$BH_2O^{\bullet}$-W



$OHBH^{\bullet}$-W



TS3-G



$OH\text{-}BH^{\bullet-}$-G

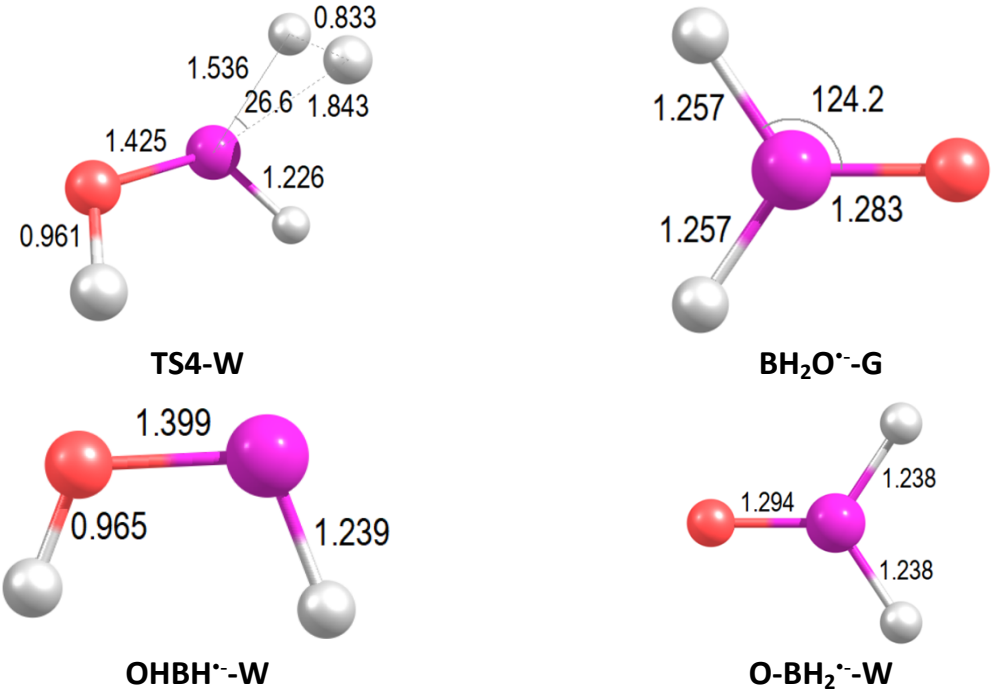


Fig. S2 Optimized geometries of stationary points for the BH_3 + HO• and BH_3^- + HO• reaction in the gas phase and aqueous solution (PCM) at the M06-2X/6-311++G(d,p) level. Selected bond lengths (Å) and bond angles (°) are indicated. Gas-phase structures are labeled with the suffix "G", whereas those in aqueous solution are denoted by "W".