

Computational Supporting Information for:

Gold-Catalyzed Proto- and Deutero-deboronation

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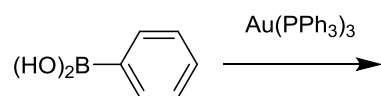
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Computational Details:

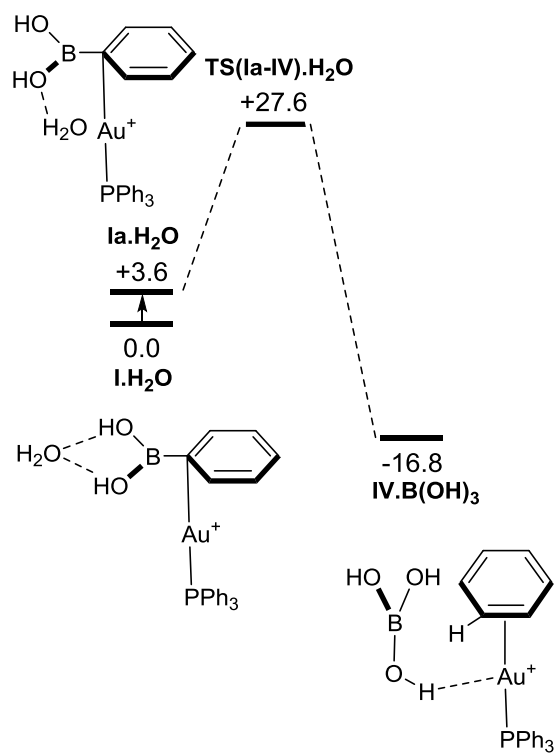
Calculations were run with Gaussian 03 Revision D.01¹ with PCM solvent corrections run with Gaussian 09, Revision A.02.² Geometry optimisations were performed using the BP86 functional³ with Au and P centres described with the Stuttgart RECPs and associated basis sets⁴ (with added d-orbital polarisation on P ($\zeta = 0.387$))⁵ and 6-31G** basis sets for all other atoms.⁶ All stationary points were fully characterized *via* analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). Frequency calculations also provided a free energy in the gas-phase, computed at 298.15 K and 1 atm. For transition states IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by each transition state. Energies reported in the text are based on the gas-phase free energies and incorporate a correction for dispersion effects using Grimme's D3 parameter set⁷ (i.e. BP86-D3) as well as solvation (PCM approach) in THF.

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Protodeboronation with One Water Molecule



Structure	ΔE	ΔG_{Gas}	ΔG_{disp}	$\Delta G_{\text{disp+solv}}$
I.H₂O	+0.0	+0.0	+0.0	+0.0
Ia.H₂O	+6.4	+7.6	+4.0	+3.6
TS(Ia-IV).H₂O	+32.3	+32.9	+29.9	+27.6
IV.B(OH)₃	-15.3	-16.3	-17.2	-16.8



I.H₂O

SCF Energy = -1321.94937757
Enthalpy 0K = -1321.534762
Enthalpy 298K = -1321.502037
Free Energy 298K = -1321.606222
Dispersion Correction = -0.07536666
SCRF PCM Energy (THF) = -1321.99967757
Lowest Frequencies = 4.9212 17.2214 cm-1

54

C 3.21051 -2.80301 1.19021
C 3.23015 -3.48746 -0.03915
C 3.20515 -2.77966 -1.25479
C 3.18497 -1.37678 -1.24666
C 3.19210 -0.64127 -0.01142
C 3.18887 -1.40056 1.20938
Au 0.94611 -0.33566 -0.01205
P -1.33251 0.08621 0.00506
C -1.74580 1.63170 -0.91436
B 3.48362 0.93178 0.00363
O 3.59239 1.54193 1.23032
O 3.62088 1.55846 -1.21135
C -1.97899 0.27989 1.72157
C -2.28935 -1.28241 -0.77985
O 4.25666 4.01220 0.03658
H 3.21626 -0.81503 -2.18574
H 3.22134 -0.85704 2.15907
H 3.21909 -3.32097 -2.20565
H 3.22934 -3.36268 2.13035
H 3.26639 -4.58178 -0.04976
H 3.81415 2.49645 1.12376
H 3.83502 2.51246 -1.08770
H 5.18357 4.31534 0.04876
H 3.71916 4.82548 0.03970
C -1.16790 0.91126 2.68917
C -1.65430 1.10065 3.99068
C -2.94317 0.65627 4.33226
C -3.74819 0.02243 3.37194
C -3.27128 -0.16912 2.06518
H -0.15812 1.24554 2.42454
H -1.02300 1.58696 4.74078
H -3.31749 0.79803 5.35085
H -4.74936 -0.32970 3.63895
H -3.89716 -0.67246 1.32166
C -1.92159 -2.61534 -0.49351
C -2.65233 -3.67496 -1.04882
C -3.74268 -3.41090 -1.89596
C -4.10476 -2.08594 -2.18610
C -3.38195 -1.01731 -1.63070
H -1.06614 -2.82080 0.16004
H -2.36631 -4.70745 -0.82563
H -4.30697 -4.23994 -2.33407

H -4.95066 -1.87916 -2.84890
H -3.66401 0.01407 -1.86340
C -1.04475 1.92196 -2.10513
C -1.37213 3.06668 -2.84597
C -2.38924 3.92783 -2.39899
C -3.08101 3.64424 -1.21036
C -2.76407 2.49734 -0.46436
H -0.24518 1.25533 -2.44791
H -0.82940 3.28816 -3.77021
H -2.64006 4.82301 -2.97659
H -3.87010 4.31628 -0.85907
H -3.30237 2.28138 0.46374

I.H₂O (para position)

SCF Energy = -1321.94408903
Enthalpy 0K = -1321.529490
Enthalpy 298K = -1321.497670
Free Energy 298K = -1321.600279
Dispersion Correction = -0.07150054
SCRF PCM Energy (THF) = -1321.99420289
Lowest Frequencies = -32.4658 2.7999 cm-1
54

Au 0.22637 -1.14594 -0.00127
P -1.60679 0.27311 0.00064
C -1.41966 1.65654 -1.20502
C -1.88983 1.02942 1.65904
C -3.14523 -0.63890 -0.45074
C -0.77462 1.44766 2.41714
C -0.96884 2.05827 3.66423
C -2.27014 2.24568 4.16155
C -3.37933 1.82460 3.41065
C -3.19550 1.21583 2.15853
H 0.24015 1.29211 2.03338
H -0.10343 2.38039 4.25157
H -2.41874 2.71520 5.13887
H -4.39259 1.96537 3.79931
H -4.06179 0.88254 1.57881
C -3.35291 -1.92856 0.08592
C -4.52921 -2.62886 -0.21607
C -5.49586 -2.05126 -1.05756
C -5.28784 -0.77122 -1.59536
C -4.11452 -0.05989 -1.29536
H -2.59606 -2.38153 0.73655
H -4.68795 -3.62848 0.20003
H -6.41000 -2.60288 -1.29776
H -6.03797 -0.32243 -2.25373
H -3.95339 0.93530 -1.72090
C -0.83369 1.39065 -2.46165
C -0.71978 2.41736 -3.40954
C -1.18016 3.71021 -3.10555
C -1.75695 3.97692 -1.85351
C -1.87951 2.95411 -0.89905
H -0.46718 0.38451 -2.69464
H -0.26533 2.20937 -4.38310
H -1.08445 4.51158 -3.84473
H -2.11195 4.98411 -1.61436
H -2.32512 3.16649 0.07762
C 2.38659 -2.22853 1.23442
C 1.86250 -2.73572 0.00213
C 2.40140 -2.24676 -1.23096
C 3.42824 -1.28919 -1.21624
C 3.96062 -0.79939 0.00031
C 3.41376 -1.27052 1.21739
B 5.16232 0.24070 -0.00062

O 5.61983 0.67386 1.21920
O 5.66007 0.62497 -1.22070
O 7.65671 2.22090 0.00028
H 3.84990 -0.92859 -2.15974
H 3.82430 -0.89646 2.16061
H 2.03786 -2.66105 -2.17688
H 2.01295 -2.62896 2.18237
H 1.23136 -3.63380 0.00458
H 6.37754 1.29292 1.10848
H 6.41317 1.24969 -1.11042
H 8.58422 1.92078 0.01942
H 7.70139 3.19449 -0.01979

Ia.H₂O

SCF Energy = -1321.93915956
Enthalpy 0K = -1321.524877
Enthalpy 298K = -1321.492402
Free Energy 298K = -1321.594086
Dispersion Correction = -0.08112568
SCRF PCM Energy (THF) = -1321.99002404
Lowest Frequencies = 7.9491 17.6733 cm-1

54

C -3.37775 -0.01207 -0.22388
C -3.11580 -1.05931 -1.17738
C -3.25767 -2.41974 -0.83217
C -3.65327 -2.77088 0.46420
C -3.88884 -1.77315 1.43501
C -3.75048 -0.42342 1.10284
Au -1.06542 0.01946 -0.06129
P 1.26401 -0.04184 -0.02624
C 2.00679 1.51372 -0.68198
C 1.94488 -1.43182 -1.03225
C 1.89682 -0.26795 1.69218
B -3.56820 1.50498 -0.66259
O -3.62725 2.45572 0.34583
O -1.19053 2.17686 1.71275
O -3.70422 1.94158 -1.95249
H -3.97512 0.34942 1.84444
H -2.87995 -0.80355 -2.21746
H -4.20164 -2.05729 2.44438
H -3.07158 -3.19279 -1.58328
H -3.78446 -3.82551 0.72615
H -3.75460 1.24111 -2.62495
H -3.83369 3.33877 -0.01853
H -1.29811 1.81375 2.61093
H -2.09982 2.41423 1.41277
C 3.12233 3.91349 -1.61520
C 2.05176 3.94425 -0.70461
C 1.48517 2.74955 -0.23671
C 3.08153 1.47945 -1.59436
C 3.63510 2.68395 -2.05819
H 3.55587 4.84945 -1.98121
H 1.65212 4.90303 -0.35939
H 0.64925 2.77051 0.47240
H 3.48262 0.52297 -1.94278
H 4.46798 2.65776 -2.76765
C 2.98832 -3.48631 -2.64123
C 3.58004 -3.19613 -1.40159
C 3.06426 -2.16906 -0.59427
C 1.34679 -1.72956 -2.27576
C 1.87310 -2.75106 -3.07910
H 3.39321 -4.28856 -3.26585
H 4.44625 -3.76980 -1.05777
H 3.52823 -1.94738 0.37167

H 0.47147 -1.16103 -2.60996
H 1.40955 -2.97763 -4.04435
C 2.85633 -0.70238 4.29695
C 1.70263 -1.37289 3.85447
C 1.21867 -1.15479 2.55655
C 3.05286 0.40553 2.13700
C 3.52771 0.18465 3.44033
H 3.22916 -0.86904 5.31231
H 1.17704 -2.06255 4.52238
H 0.31507 -1.67105 2.21153
H 3.57470 1.10217 1.47375
H 4.42346 0.71031 3.78520

TS(Ia-IV).H₂O

SCF Energy = -1321.89792496

Enthalpy 0K = -1321.485773

Enthalpy 298K = -1321.454183

Free Energy 298K = -1321.553729

Dispersion Correction = -0.08023957

SCRF PCM Energy (THF) = -1321.95189901

Lowest Frequencies = -253.4503 8.3277 cm⁻¹

54

C 3.01127 0.29964 0.00460
C 3.58676 0.80420 -1.20584
C 4.68179 1.67745 -1.19412
C 5.22956 2.09652 0.03131
C 4.67476 1.65097 1.24512
C 3.57888 0.78152 1.22831
Au 0.89858 0.10578 0.00225
P -1.46709 0.06297 0.00069
C -2.14715 -1.19776 -1.16588
C -2.15911 1.69688 -0.50141
C -2.15555 -0.32178 1.66992
B 3.37574 -1.77362 -0.17936
O 4.67627 -2.00248 0.20323
O 2.50888 -2.28153 1.09203
O 2.87355 -2.18175 -1.39415
H 3.16143 0.45424 2.18931
H 3.19266 0.46328 -2.16948
H 5.09730 1.98798 2.19709
H 5.11240 2.03101 -2.13652
H 6.09060 2.77278 0.04151
H 1.96854 -1.87169 -1.57946
H 5.27401 -2.09850 -0.55879
H 1.75551 -1.62870 1.21418
H 3.07670 -2.30262 1.89437
C -3.13121 -3.16549 -2.91704
C -2.11478 -3.48835 -2.00083
C -1.61859 -2.50783 -1.13024
C -3.16794 -0.87703 -2.08350
C -3.65487 -1.86382 -2.95684
H -3.51238 -3.92978 -3.60122
H -1.70497 -4.50260 -1.96758
H -0.82804 -2.76386 -0.41525
H -3.57877 0.13641 -2.11912
H -4.44574 -1.61081 -3.66964
C -3.18089 4.17541 -1.34095
C -3.86389 3.42778 -0.36749
C -3.35787 2.18872 0.05616
C -1.47078 2.45230 -1.47599
C -1.98550 3.68761 -1.89559
H -3.57766 5.14274 -1.66418
H -4.79255 3.80974 0.06758
H -3.88875 1.61260 0.82047

H -0.53387 2.07585 -1.90308
H -1.44920 4.27199 -2.64950
C -3.17682 -0.81666 4.24101
C -2.07904 0.04630 4.07762
C -1.56394 0.29193 2.79671
C -3.25707 -1.18609 1.83492
C -3.76270 -1.43064 3.12252
H -3.57426 -1.01111 5.24195
H -1.62256 0.52691 4.94856
H -0.70964 0.96720 2.66895
H -3.71510 -1.66804 0.96573
H -4.61711 -2.10273 3.24876

IV.B(OH)₃

SCF Energy = -1321.97382523

Enthalpy 0K = -1321.559083

Enthalpy 298K = -1321.526633

Free Energy 298K = -1321.632187

Dispersion Correction = -0.07676504

SCRF PCM Energy (THF) = -1322.02357739

Lowest Frequencies = 5.2848 15.8698 cm⁻¹

54

C 3.19340 -1.07955 -0.60608

C 3.16447 -1.16552 0.82356

C 3.02089 -2.43436 1.44955

C 2.92119 -3.59041 0.66882

C 2.94796 -3.50818 -0.74230

C 3.07530 -2.26944 -1.37912

Au 0.97671 -0.53843 0.04482

P -1.25574 0.09963 -0.00531

C -1.42592 1.91849 -0.24550

C -2.12650 -0.33868 1.55876

C -2.14703 -0.73380 -1.38671

B 3.43852 2.71536 0.00648

O 4.52209 3.52748 0.22121

O 3.16683 2.26182 -1.27945

O 2.62482 2.30900 1.05215

H 3.11693 -2.20706 -2.47061

H 3.38681 -0.27580 1.42361

H 2.88209 -4.42285 -1.33953

H 3.02126 -2.49940 2.54159

H 2.83399 -4.56795 1.15297

H 1.84005 1.82973 0.71652

H 4.59414 3.80744 1.15052

H 3.43715 -0.12431 -1.08864

H 3.79288 2.65230 -1.91641

C -1.69771 4.67664 -0.69267

C -0.66934 3.96179 -1.33021

C -0.52682 2.58421 -1.10801

C -2.45655 2.63593 0.39746

C -2.58753 4.01505 0.16919

H -1.80160 5.75261 -0.86326

H 0.02958 4.47709 -1.99596

H 0.28348 2.03380 -1.59995

H -3.14679 2.12470 1.07556

H -3.38481 4.57214 0.67061

C -3.44124 -0.91880 3.97048

C -4.09693 -1.12765 2.74666

C -3.44482 -0.83924 1.53674

C -1.46518 -0.13372 2.78955

C -2.12674 -0.42078 3.99170

H -3.95276 -1.14858 4.91022

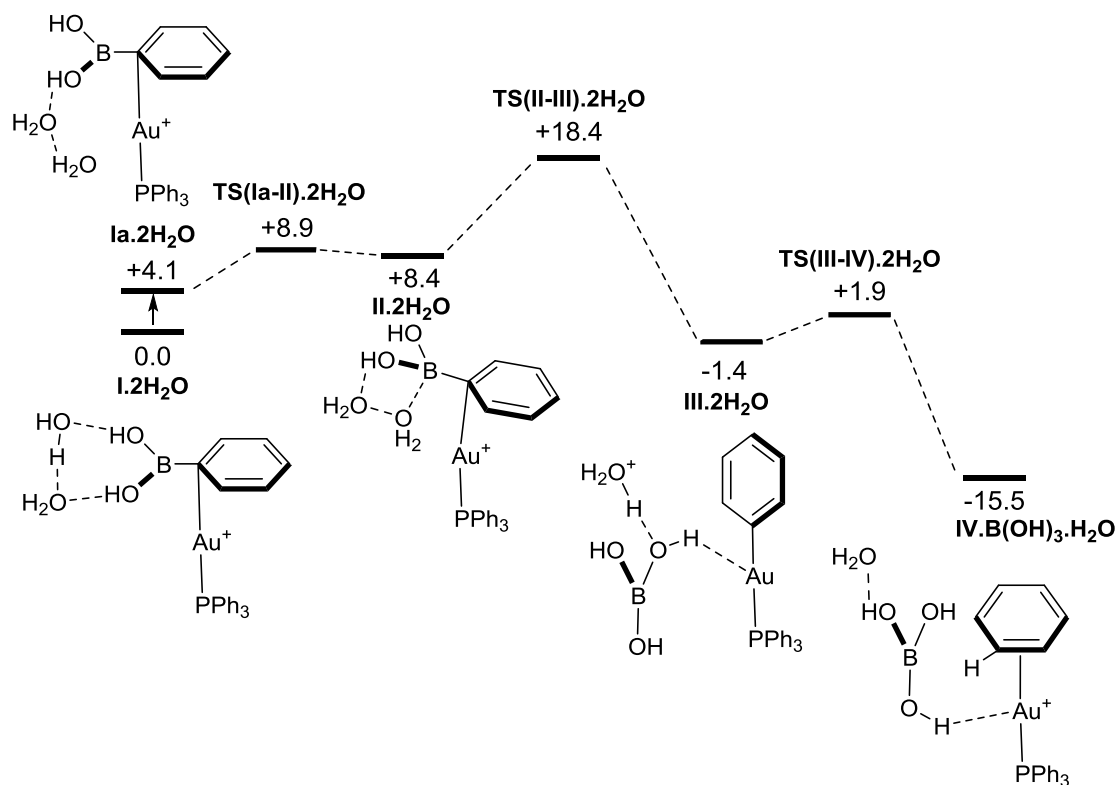
H -5.11885 -1.51860 2.72941

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H -0.43768 0.24733 2.80669
H -1.61364 -0.26144 4.94502
C -3.52118 -2.06475 -3.44141
C -2.61585 -2.77267 -2.63146
C -1.92429 -2.11090 -1.60740
C -3.05412 -0.02307 -2.19905
C -3.73821 -0.69466 -3.22555
H -4.05446 -2.58230 -4.24471
H -2.44377 -3.83993 -2.80144
H -1.21397 -2.66167 -0.98016
H -3.22302 1.04558 -2.03557
H -4.44025 -0.14233 -3.85760

Protodeboronation with Two Water Molecules

Structure	ΔE	ΔG_{Gas}	ΔG_{disp}	$\Delta G_{\text{disp+solv}}$
I.2H₂O	+0.0	+0.0	+0.0	+0.0
Ia.2H₂O	+6.1	+7.8	+2.7	+4.1
TS(Ia-II).2H₂O	+11.0	+14.3	+8.2	+8.9
II.2H₂O	+10.9	+13.0	+7.7	+8.4
TS(II-III).2H₂O	+20.2	+22.0	+17.9	+18.4
III.2H₂O	+0.3	+1.5	-3.0	-1.4
TS(III-IV).2H₂O	+3.2	+0.7	+0.4	+1.9
IV.B(OH)₃.H₂O	-17.0	-17.2	-17.4	-15.5



I.2H₂O

SCF Energy = -1398.38841848

Enthalpy 0K = -1397.949691

Enthalpy 298K = -1397.914195

Free Energy 298K = -1398.024750

Dispersion Correction = -0.07829912

SCRF PCM Energy (THF) = -1398.44157060

Lowest Frequencies = 6.3782 14.6687 cm⁻¹

57

C 2.27056 -4.20462 -0.01324

C 2.44755 -3.51388 -1.22686

C 2.71237 -2.13690 -1.21560

C 2.81217 -1.40813 0.01877

C 2.59661 -2.14330 1.23539

C 2.33317 -3.52213 1.21477

Au 0.69002 -0.63118 -0.00554

B 3.41930 0.08229 0.06643

O 3.80483 0.59818 -1.14958

P -1.45078 0.25191 -0.01357

C -2.04372 0.60034 1.69846

C -2.67581 -0.89368 -0.78346

C -1.54137 1.83718 -0.95623

O 3.49614 0.66246 1.29632

H 2.89811 -1.59902 -2.15069

H 2.70083 -1.60957 2.18556

H 2.39458 -4.05377 -2.17734

H 2.19556 -4.06702 2.15382

H 2.08376 -5.28353 -0.02566

H 3.90234 1.58274 1.34932

H 4.24389 1.48005 -1.12220

O 5.29460 3.02596 -1.23216

H 6.22959 2.76805 -1.34127

H 5.10532 3.62903 -1.97482

O 4.55007 3.10754 1.44037

H 4.84449 3.34432 0.52925

H 3.89960 3.78616 1.69429

C -1.70318 4.19251 -2.47984

C -0.92232 3.11559 -2.93450

C -0.83470 1.94060 -2.17435

C -2.32213 2.91847 -0.49904

C -2.39847 4.09405 -1.26406

H -1.76738 5.11001 -3.07318

H -0.37832 3.19101 -3.88130

H -0.21920 1.10395 -2.52414

H -2.86399 2.84581 0.44900

H -3.00396 4.93282 -0.90683

C -2.90480 1.19871 4.30414

C -3.83275 0.77561 3.33857

C -3.40794 0.47415 2.03470

C -1.11056 1.01882 2.67152

C -1.54507 1.32007 3.97052

H -3.24016 1.42632 5.32075
H -4.89057 0.67325 3.59973
H -4.13185 0.13293 1.28798
H -0.04806 1.09771 2.41360
H -0.81957 1.63938 4.72514
C -4.55060 -2.68242 -1.86758
C -3.50745 -3.16550 -1.05870
C -2.56728 -2.27631 -0.51934
C -3.72087 -0.40919 -1.59692
C -4.65533 -1.30837 -2.13624
H -5.27913 -3.37938 -2.29325
H -3.42155 -4.23698 -0.85316
H -1.74804 -2.65281 0.10370
H -3.80198 0.66036 -1.81408
H -5.46410 -0.93169 -2.77002

Ia.2H₂O

SCF Energy = -1398.37861805
Enthalpy 0K = -1397.939668
Enthalpy 298K = -1397.904566
Free Energy 298K = -1398.012330
Dispersion Correction = -0.08636747
SCRF PCM Energy (THF) = -1398.42957272
Lowest Frequencies = 6.4662 16.4450 cm⁻¹

57

C -2.76558 -1.86548 -0.79965
C -2.94288 -2.92140 0.11635
C -3.55872 -2.67331 1.34950
C -3.98407 -1.37051 1.68661
C -3.81310 -0.31598 0.78651
C -3.20742 -0.52612 -0.50102
Au -0.95664 -0.15036 -0.09899
P 1.37176 -0.01253 -0.00215
C 2.20588 -1.45427 -0.79960
B -3.30102 0.57278 -1.64703
O -1.12052 2.01477 1.50834
C 1.95738 0.03706 1.74821
C 2.01919 1.50458 -0.82971
O -3.03617 0.34569 -2.97366
O -3.71049 1.85749 -1.31691
O -3.63255 2.92057 1.24613
H -4.16073 0.68588 1.05686
H -2.35588 -2.10080 -1.78903
H -4.46665 -1.18702 2.65145
H -2.61397 -3.93073 -0.14737
H -3.71637 -3.49634 2.05399
H -2.81935 -0.57403 -3.20153
H -3.76817 2.40658 -2.12321
H -1.04183 1.61916 2.39580
H -2.03949 2.41798 1.47921
H -3.86313 3.85768 1.37588
H -3.75253 2.73066 0.28368
C 3.47066 -3.60302 -2.09816
C 2.32408 -3.01891 -2.66411
C 1.68780 -1.95131 -2.01500
C 3.35740 -2.03943 -0.23434
C 3.98356 -3.11463 -0.88601
H 3.96155 -4.44181 -2.60132
H 1.92236 -3.39950 -3.60845
H 0.78811 -1.49903 -2.44795
H 3.76094 -1.66281 0.71049
H 4.87429 -3.57017 -0.44242
C 2.84058 0.03019 4.41667
C 1.74591 -0.76682 4.03903
C 1.30043 -0.76237 2.70905
C 3.05419 0.83727 2.12863
C 3.49134 0.82985 3.46341

H 3.18343 0.03027 5.45600
H 1.23653 -1.38926 4.78144
H 0.44397 -1.37970 2.41294
H 3.55821 1.46802 1.38991
H 4.34112 1.45381 3.75709
C 2.97237 3.85392 -2.03292
C 1.89744 3.91390 -1.12875
C 1.41103 2.74415 -0.52689
C 3.09904 1.44120 -1.73410
C 3.57082 2.62030 -2.33402
H 3.34305 4.76990 -2.50370
H 1.43255 4.87655 -0.89285
H 0.57308 2.78346 0.17968
H 3.56808 0.48151 -1.97092
H 4.40797 2.57104 -3.03725

TS(Ia-II).2H₂O

SCF Energy = -1398.37084511

Enthalpy 0K = -1397.932233

Enthalpy 298K = -1397.898508

Free Energy 298K = -1398.002041

Dispersion Correction = -0.08801258

SCRF PCM Energy (THF) = -1398.42275278

Lowest Frequencies = -76.9476 10.3173 cm⁻¹

57

C -2.61077 -1.61931 -1.25266

C -2.52784 -2.97609 -0.81896

C -2.94854 -3.32243 0.46694

C -3.45283 -2.32660 1.33414

C -3.52395 -0.99059 0.92704

C -3.11963 -0.58555 -0.38439

Au -0.69079 -0.61881 -0.38178

P 1.46749 0.11280 0.07035

C 2.72279 -1.16460 -0.36285

B -3.43489 0.88474 -0.98855

O -2.60493 2.01861 0.45833

C 1.68208 0.51507 1.85697

C 1.86014 1.63480 -0.89310

O -2.79470 1.34370 -2.13836

O -4.78870 1.28039 -0.86411

O -4.87763 2.05780 1.72633

H -3.94680 -0.24222 1.60698

H -2.46346 -1.39497 -2.31705

H -3.80272 -2.60754 2.33293

H -2.16592 -3.74131 -1.51274

H -2.90612 -4.36510 0.79627

H -1.85379 1.09823 -2.19050

H -4.97297 1.96941 -1.53128

H -1.99769 1.46974 0.99364

H -3.39582 2.21045 1.07100

H -5.37068 2.85317 1.99724

H -5.22451 1.79614 0.83213

C 4.63898 -3.07972 -1.10011

C 3.50431 -2.87895 -1.90519

C 2.54318 -1.92653 -1.53816

C 3.86065 -1.36642 0.44554

C 4.81521 -2.32602 0.07148

H 5.38415 -3.82893 -1.38464

H 3.36381 -3.46913 -2.81591

H 1.65405 -1.77544 -2.16105

H 3.99867 -0.78475 1.36212

H 5.69640 -2.48482 0.70055

C 2.03448 1.04572 4.59184

C 1.29211 -0.07735 4.18649

C 1.11039 -0.34349 2.82194

C 2.42605 1.64213 2.26333

C 2.59846 1.90221 3.63277

H 2.16961 1.25476 5.65750
H 0.85018 -0.74394 4.93346
H 0.52773 -1.21644 2.50547
H 2.86306 2.31395 1.51821
H 3.17382 2.77812 3.94777
C 2.42968 3.98556 -2.31943
C 1.18508 3.83612 -1.68304
C 0.89352 2.66289 -0.97242
C 3.10911 1.78446 -1.53056
C 3.38804 2.96259 -2.24240
H 2.65008 4.89952 -2.87952
H 0.43508 4.63049 -1.74502
H -0.08109 2.55556 -0.48177
H 3.85641 0.98699 -1.47703
H 4.35626 3.07650 -2.73943

II.2H₂O

SCF Energy = -1398.37106210
Enthalpy 0K = -1397.932425
Enthalpy 298K = -1397.898256
Free Energy 298K = -1398.004032
Dispersion Correction = -0.086789
SCRFC PCM Energy (THF) = -1398.42311415
Lowest Frequencies = 6.5432 15.0559 cm⁻¹

57

C -2.61794 -1.57870 -1.25617
C -2.52585 -2.95209 -0.88764
C -2.90164 -3.35434 0.39619
C -3.36446 -2.39695 1.32762
C -3.44190 -1.04466 0.98110
C -3.08803 -0.58040 -0.32842
Au -0.70189 -0.55118 -0.34317
P 1.48531 0.11875 0.06741
C 2.69100 -1.21058 -0.35245
B -3.45920 0.91799 -0.87130
O -2.85083 1.98257 0.43430
C 1.74011 0.55365 1.84116
C 1.92393 1.60318 -0.93479
O -2.86182 1.37283 -2.06390
O -4.87603 1.16250 -0.83530
O -5.07015 2.02130 1.66479
H -3.84109 -0.32848 1.70882
H -2.49238 -1.29953 -2.30991
H -3.67796 -2.72113 2.32539
H -2.19262 -3.68748 -1.62667
H -2.85431 -4.41116 0.67633
H -1.90238 1.21486 -2.10854
H -5.10128 1.75275 -1.57914
H -2.17276 1.51708 0.96507
H -3.66456 2.14892 1.06085
H -5.54696 2.84963 1.85650
H -5.38594 1.70487 0.76874
C 4.52916 -3.20755 -1.07125
C 3.40265 -2.96998 -1.87783
C 2.48029 -1.97665 -1.52001
C 3.82061 -1.44921 0.45735
C 4.73609 -2.44966 0.09253
H 5.24390 -3.98842 -1.34865
H 3.23825 -3.56301 -2.78269
H 1.59766 -1.79655 -2.14439
H 3.98279 -0.86399 1.36766
H 5.61094 -2.63675 0.72267
C 2.15212 1.13015 4.55852
C 1.34790 0.03794 4.18857
C 1.13634 -0.25068 2.83282
C 2.54642 1.64960 2.21213
C 2.74826 1.93307 3.57284

H 2.31071 1.35711 5.61726
H 0.88117 -0.58695 4.95623
H 0.50553 -1.09924 2.54345
H 3.00924 2.27951 1.44623
H 3.37197 2.78505 3.86028
C 2.56053 3.90150 -2.41885
C 1.31208 3.80403 -1.77987
C 0.98899 2.65703 -1.04117
C 3.17637 1.70155 -1.57515
C 3.48880 2.85340 -2.31573
H 2.80706 4.79441 -3.00148
H 0.58523 4.61782 -1.86238
H 0.01330 2.58579 -0.54670
H 3.90028 0.88431 -1.50202
H 4.45974 2.92705 -2.81503

TS(II-III).2H₂O

SCF Energy = -1398.35615267

Enthalpy 0K = -1397.919320

Enthalpy 298K = -1397.885774

Free Energy 298K = -1397.989662

Dispersion Correction = -0.08486521

SCRF PCM Energy (THF) = -1398.40843130

Lowest Frequencies = -231.5949 8.2537 cm⁻¹

57

C 3.22860 1.58941 -1.08246

C 4.20879 2.55572 -0.82319

C 4.80155 2.62621 0.45040

C 4.40799 1.73469 1.46497

C 3.42504 0.77313 1.20170

C 2.81601 0.64569 -0.08789

Au 0.72738 0.25446 -0.05677

P -1.61580 0.00525 0.04027

C -2.46664 1.64199 -0.00502

B 3.27333 -1.20757 -0.92951

O 2.69716 -2.17317 0.13432

C -2.16379 -0.83578 1.59033

C -2.28620 -0.98741 -1.36753

O 2.71434 -1.24575 -2.19698

O 4.67350 -1.33699 -0.83603

O 4.70940 -2.60291 1.48704

H 3.13849 0.08785 2.00894

H 2.79930 1.52393 -2.08840

H 4.86587 1.79767 2.45755

H 4.51512 3.25366 -1.60932

H 5.57244 3.37708 0.65301

H 1.75151 -1.09543 -2.20110

H 5.10898 -1.04748 -1.65679

H 1.90337 -1.76317 0.55843

H 3.48039 -2.44948 0.84395

H 5.02997 -3.52545 1.50600

H 5.20377 -2.14641 0.75411

C -3.73368 4.14552 -0.15190

C -2.54616 3.91920 -0.86816

C -1.90905 2.67195 -0.79382

C -3.65744 1.87132 0.71532

C -4.28638 3.12411 0.63811

H -4.22573 5.12161 -0.20506

H -2.11071 4.71616 -1.47875

H -0.97737 2.49827 -1.34467

H -4.08682 1.08040 1.33819

H -5.20858 3.30164 1.19998

C -2.97809 -2.02838 4.00152

C -1.93546 -1.08549 4.00350

C -1.52360 -0.49179 2.80166

C -3.20934 -1.78168 1.58965

C -3.61170 -2.37526 2.79749

H -3.29487 -2.49434 4.93976
H -1.44050 -0.81423 4.94123
H -0.71031 0.24337 2.80242
H -3.70350 -2.05663 0.65267
H -4.42269 -3.11015 2.79472
C -3.24976 -2.55039 -3.49791
C -2.13742 -2.98594 -2.75653
C -1.65189 -2.20616 -1.69736
C -3.40273 -0.55409 -2.11068
C -3.87911 -1.33816 -3.17465
H -3.62309 -3.15613 -4.32936
H -1.64462 -3.93062 -3.00668
H -0.78530 -2.54902 -1.12008
H -3.89586 0.39091 -1.86373
H -4.74451 -0.99701 -3.75116

III.2H₂O

SCF Energy = -1398.38797460
Enthalpy 0K = -1397.951106
Enthalpy 298K = -1397.917319
Free Energy 298K = -1398.022341
Dispersion Correction = -0.08546931
SCRF PCM Energy (THF) = -1398.43865132
Lowest Frequencies = 8.3030 22.3586 cm⁻¹

57

C 3.43633 -1.10989 1.34931
C 4.79645 -1.46683 1.40763
C 5.42202 -2.05532 0.28773
C 4.66469 -2.30854 -0.87509
C 3.30539 -1.94726 -0.92497
C 2.66274 -1.32990 0.17967
Au 0.68916 -0.75222 0.09076
P -1.60199 -0.08858 -0.00048
C -2.51897 -0.44975 1.56154
B 2.73886 2.71730 -0.06097
O 2.80819 1.55804 -0.89390
C -2.54204 -0.89128 -1.37145
C -1.77121 1.73883 -0.28651
O 1.59280 3.33608 0.30192
O 3.98522 3.14404 0.33551
O 5.13393 0.85846 -0.84752
H 2.74209 -2.14647 -1.84323
H 2.97460 -0.64968 2.23006
H 5.13766 -2.78147 -1.74233
H 5.37017 -1.29232 2.32470
H 6.47748 -2.34383 0.33232
H 0.76971 3.03351 -0.13966
H 3.95241 3.98704 0.82291
H 2.12489 0.83909 -0.69942
H 3.98733 1.10268 -0.92561
H 5.46118 1.53555 -0.21320
H 5.27265 -0.04951 -0.44648
C -3.84611 -0.96720 3.98492
C -2.47403 -0.66535 3.98919
C -1.80771 -0.41160 2.78101
C -3.89582 -0.75684 1.55946
C -4.55384 -1.01423 2.77231
H -4.36288 -1.17390 4.92725
H -1.91922 -0.63807 4.93217
H -0.73398 -0.19073 2.78126
H -4.44829 -0.80626 0.61582
H -5.62094 -1.25716 2.76781
C -3.95888 -2.22008 -3.40310
C -2.92020 -2.88121 -2.72624
C -2.20829 -2.21970 -1.71477
C -3.58410 -0.22837 -2.05358
C -4.28848 -0.89647 -3.06786

H -4.50929 -2.73572 -4.19613
H -2.65887 -3.91075 -2.98968
H -1.39327 -2.73283 -1.19138
H -3.84051 0.80545 -1.80083
H -5.09515 -0.37990 -3.59731
C -1.93504 4.51234 -0.77841
C -1.16141 3.69448 -1.62332
C -1.07146 2.31330 -1.37630
C -2.54544 2.56291 0.55242
C -2.62382 3.94514 0.30410
H -2.00142 5.58766 -0.96945
H -0.63382 4.12929 -2.47848
H -0.49067 1.67426 -2.05265
H -3.08723 2.12819 1.39786
H -3.22853 4.57753 0.96150

TS(III-IV).2H₂O

SCF Energy = -1398.38331629

Enthalpy 0K = -1397.949834

Enthalpy 298K = -1397.915788

Free Energy 298K = -1398.023634

Dispersion Correction = -0.0788076

SCRF PCM Energy (THF) = -1398.43406196

Lowest Frequencies = -402.7930 5.4487 cm⁻¹

57

C 3.24725 -1.53628 1.29924

C 4.21145 -2.54955 1.39310

C 4.66650 -3.19307 0.22807

C 4.16139 -2.82021 -1.02986

C 3.19508 -1.80789 -1.12213

C 2.71056 -1.13275 0.03884

Au 0.71897 -0.43293 0.00583

P -1.59926 0.01234 -0.01498

C -2.29549 0.32927 1.66707

B 2.99934 2.56677 0.21597

O 3.56595 1.37819 -0.31570

C -2.50802 -1.44566 -0.69447

C -2.06431 1.46005 -1.06384

O 1.70284 2.64058 0.60887

O 3.88383 3.61621 0.28999

O 5.96783 1.92401 -0.73285

H 2.81411 -1.52331 -2.10991

H 2.90297 -1.04147 2.21516

H 4.51921 -3.32162 -1.93512

H 4.60669 -2.84333 2.37123

H 5.41875 -3.98555 0.30088

H 1.20154 1.80012 0.44612

H 3.46082 4.43253 0.61273

H 3.07631 0.34600 -0.17187

H 4.60605 1.45281 -0.50719

H 5.86593 2.87074 -0.49401

H 6.64516 1.56603 -0.12792

C -3.32199 0.87637 4.22680

C -2.09226 1.43014 3.83146

C -1.57519 1.15553 2.55736

C -3.52926 -0.22546 2.06534

C -4.03738 0.05056 3.34517

H -3.72002 1.08580 5.22453

H -1.53108 2.07122 4.51840

H -0.61425 1.58682 2.25558

H -4.08705 -0.87422 1.38306

H -4.99364 -0.38422 3.65221

C -3.85547 -3.71394 -1.66246

C -2.75915 -3.86719 -0.79653

C -2.08174 -2.73784 -0.31478

C -3.60700 -1.29332 -1.56439

C -4.27677 -2.43029 -2.04513

H -4.37868 -4.59679 -2.04272
H -2.42609 -4.86689 -0.50095
H -1.22305 -2.85937 0.35573
H -3.93480 -0.29473 -1.86939
H -5.12834 -2.30996 -2.72198
C -2.75551 3.60646 -2.74163
C -1.70163 2.74840 -3.10013
C -1.35090 1.67965 -2.26260
C -3.12008 2.32294 -0.70448
C -3.46080 3.39437 -1.54605
H -3.02436 4.44346 -3.39354
H -1.14896 2.91418 -4.03021
H -0.52455 1.01371 -2.53743
H -3.66925 2.16287 0.22863
H -4.27913 4.06419 -1.26410

IV. B(OH)₃·H₂O

SCF Energy = -1398.4155973

Enthalpy 0K = -1397.976097

Enthalpy 298K = -1397.941035

Free Energy 298K = -1398.052214

Dispersion Correction = -0.07863389

SCRF PCM Energy (THF) = -1398.46562571

Lowest Frequencies = 5.9571 12.9421 cm⁻¹

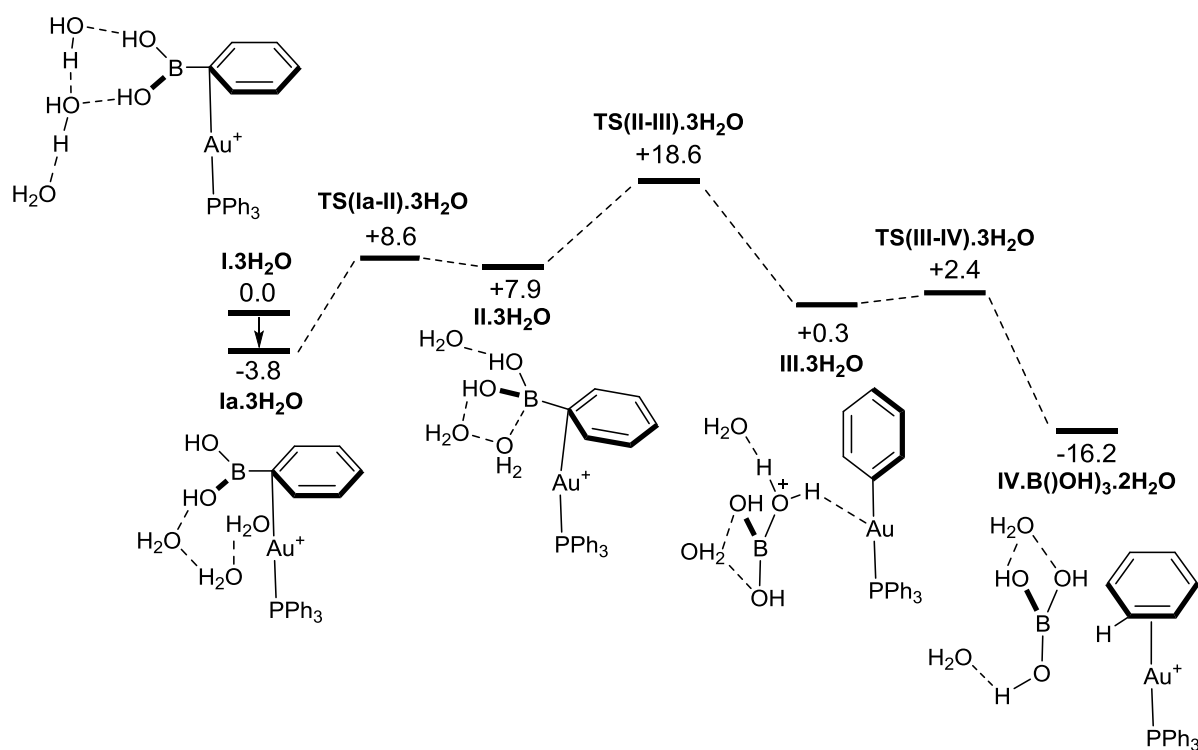
57

C -2.16159 2.42110 1.18699
C -1.47370 3.63149 1.47749
C -1.19941 4.53949 0.44963
C -1.58680 4.25713 -0.88058
C -2.25263 3.06630 -1.18771
C -2.56053 2.13108 -0.15788
Au -0.53420 0.94902 0.19546
P 1.32918 -0.41907 -0.06875
C 1.89724 -1.13186 1.53438
B -3.66159 -1.74205 0.48402
O -4.02388 -0.75059 -0.39115
C 2.72685 0.55053 -0.77940
C 0.98288 -1.82390 -1.20677
O -2.41102 -1.74875 1.08762
O -4.56284 -2.75800 0.78637
O -6.40489 -1.74072 -1.05734
H -2.57174 2.85695 -2.21315
H -2.50819 1.78176 2.00679
H -1.37450 4.98246 -1.67203
H -1.19318 3.85840 2.51035
H -0.69227 5.48217 0.67753
H -1.86465 -1.02013 0.72021
H -4.17746 -3.42372 1.38238
H -3.20898 1.26532 -0.36146
H -4.94133 -0.94524 -0.75996
H -6.14556 -2.47123 -0.45162
H -7.15911 -1.31260 -0.61180
C 2.72133 -2.25305 3.97200
C 1.38142 -2.37077 3.56256
C 0.96138 -1.81027 2.34812
C 3.24177 -1.01407 1.94220
C 3.64805 -1.57731 3.16307
H 3.04168 -2.68779 4.92388
H 0.65783 -2.89732 4.19241
H -0.08484 -1.91183 2.03815
H 3.96663 -0.48724 1.31460
H 4.69167 -1.48525 3.47914
C 4.87185 2.05015 -1.79707
C 4.03536 2.60400 -0.81237
C 2.96024 1.86038 -0.30544
C 3.56545 -0.00482 -1.76757
C 4.63602 0.75042 -2.27292

H 5.70585 2.63520 -2.19675
H 4.21628 3.61823 -0.44332
H 2.30358 2.29479 0.45713
H 3.38232 -1.01581 -2.14387
H 5.28431 0.32007 -3.04230
C 0.50544 -3.91762 -3.01382
C -0.13898 -2.68111 -3.18948
C 0.09500 -1.63342 -2.28738
C 1.62684 -3.06647 -1.02722
C 1.38470 -4.10924 -1.93543
H 0.31620 -4.73578 -3.71558
H -0.83110 -2.53414 -4.02417
H -0.41561 -0.67222 -2.41622
H 2.30421 -3.22159 -0.18171
H 1.88170 -5.07404 -1.79530

Protodeboronation with Three Water Molecules

Structure	ΔE	ΔG_{Gas}	ΔG_{disp}	$\Delta G_{\text{disp+solv}}$
I.3H ₂ O	+0.0	+0.0	+0.0	+0.0
Ia.3H ₂ O	-5.5	+0.0	-6.0	-3.8
TS(Ia-II).3H ₂ O	+9.4	+13.6	+7.4	+8.6
II.3H ₂ O	+9.3	+12.9	+6.8	+7.9
TS(II-III).3H ₂ O	+20.8	+23.7	+18.6	+18.6
III.3H ₂ O	+1.5	+2.7	+0.9	+0.3
TS(III-IV).3H ₂ O	+3.0	+2.9	+1.4	+2.4
IV.B(OH) ₃ .2H ₂ O	-18.7	-16.2	-18.5	-16.2



I.3H₂O

SCF Energy = -1474.83002578

Enthalpy 0K = -1474.366821

Enthalpy 298K = -1474.328580

Free Energy 298K = -1474.447274

Dispersion Correction = -0.08037501

SCRF PCM Energy (THF) = -1474.88332939

Lowest Frequencies = 3.3942 11.9804 cm⁻¹

60

C 1.03041 -4.26694 0.75483

C 0.98096 -4.71170 -0.57785

C 1.48590 -3.91060 -1.61985

C 2.06451 -2.66747 -1.32866

C 2.15993 -2.18860 0.02215

C 1.60763 -3.02211 1.05500

Au 0.31318 -0.88949 -0.01769

P -1.53740 0.50065 -0.02213

C -2.84810 -0.08049 -1.18467

B 3.08740 -0.92424 0.40319

O 3.10055 -0.57374 1.72045

O 3.76205 -0.35547 -0.64820

C -1.11243 2.22727 -0.52023

C -2.30844 0.59617 1.65189

O 4.54729 1.55250 2.36853

O 5.76546 1.46412 -0.05665

H 2.50076 -2.05588 -2.12483

H 1.70234 -2.68623 2.09274

H 1.44027 -4.26529 -2.65426

H 0.63717 -4.89623 1.55928

H 0.54708 -5.69052 -0.80780

H 3.66640 0.22324 1.98107

H 4.41556 0.35558 -0.41841

H 6.58151 0.93478 0.00187

H 5.96300 2.21328 -0.69695

H 5.07702 1.71256 1.54255

H 3.97048 2.33168 2.46157

O 6.26566 3.46836 -1.75939

H 6.95747 4.10632 -1.50635

H 6.47468 3.21895 -2.67785

C -4.87332 -1.02693 -2.88600

C -4.10761 -1.93531 -2.13488

C -3.09299 -1.46698 -1.28821

C -3.61475 0.83061 -1.94006

C -4.62581 0.35167 -2.78914

H -5.65991 -1.39538 -3.55180

H -4.29549 -3.01057 -2.21386

H -2.48799 -2.17472 -0.71018

H -3.42036 1.90548 -1.87244

H -5.21777 1.05964 -3.37744

C -0.48381 4.82838 -1.37673

C -1.41594 4.63573 -0.34447

C -1.73418 3.33767 0.08715
C -0.16851 2.42239 -1.55168
C 0.13899 3.72191 -1.97959
H -0.23909 5.84200 -1.70945
H -1.89811 5.49636 0.12951
H -2.45731 3.19110 0.89555
H 0.32455 1.55944 -2.01365
H 0.86913 3.87031 -2.78136
C -3.41999 0.79722 4.22346
C -4.25493 0.82124 3.09458
C -3.70491 0.72049 1.80647
C -1.47029 0.56477 2.78755
C -2.02888 0.66937 4.06960
H -3.85423 0.87030 5.22541
H -5.33894 0.91323 3.21380
H -4.35935 0.72848 0.92916
H -0.38692 0.44967 2.66649
H -1.37792 0.64069 4.94892

Ia.3H₂O

SCF Energy = -1474.83879342
Enthalpy 0K = -1474.373441
Enthalpy 298K = -1474.336875
Free Energy 298K = -1474.447289
Dispersion Correction = -0.0899592
SCRFC PCM Energy (THF) = -1474.88854670
Lowest Frequencies = 7.4608 21.8039 cm⁻¹

60

C -2.96358 -1.88220 1.25089
C -2.91586 -1.37433 -0.09222
C -2.58446 -2.30511 -1.13803
C -2.34418 -3.65979 -0.85484
C -2.42505 -4.12210 0.46993
C -2.72354 -3.23521 1.52283
Au -0.75909 -0.64691 -0.04550
P 1.43601 0.10256 -0.02765
C 1.59219 1.93438 -0.21150
C 2.38137 -0.65935 -1.41758
C 2.30257 -0.34734 1.53620
B -3.48526 0.07084 -0.46215
O -3.45395 0.45302 -1.77582
O -3.98975 0.86654 0.55680
O -2.41694 4.17877 0.17762
O -2.18484 2.25649 2.08454
O -4.34533 2.92690 -1.02232
H -3.23967 -1.19898 2.06013
H -2.58380 -1.94434 -2.17167
H -2.78564 -3.60641 2.55035
H -2.11404 -4.35575 -1.66714
H -2.25734 -5.18236 0.68570
H -3.79486 1.38090 -1.86824
H -4.34464 1.71135 0.12852
H -1.55472 4.14549 -0.27881
H -2.30462 3.57060 0.96715
H -2.49480 2.44624 2.98898
H -2.85937 1.63964 1.68970
H -3.59484 3.51978 -0.65357
H -5.11580 3.49521 -1.19873
C 1.85097 4.72718 -0.39564
C 0.94574 4.16304 0.52237
C 0.80530 2.76841 0.61375
C 2.50021 2.49864 -1.13035
C 2.62341 3.89556 -1.22079
H 1.95323 5.81467 -0.46480
H 0.34847 4.81111 1.17253
H 0.08654 2.33692 1.32091
H 3.10722 1.85406 -1.77316
H 3.32762 4.33047 -1.93664
C 3.78873 -1.76278 -3.58348
C 2.45792 -1.34345 -3.75360

C 1.75021 -0.79697 -2.67339
C 3.71633 -1.08046 -1.24692
C 4.41451 -1.63228 -2.33327
H 4.33629 -2.19671 -4.42582
H 1.96733 -1.44884 -4.72616
H 0.70896 -0.47989 -2.80296
H 4.20605 -0.98489 -0.27297
H 5.44901 -1.96282 -2.19857
C 3.65602 -1.11970 3.87297
C 3.97456 0.09656 3.24743
C 3.30134 0.48803 2.07904
C 1.97885 -1.56661 2.16922
C 2.65933 -1.95082 3.33347
H 4.18112 -1.41841 4.78550
H 4.74708 0.74665 3.66955
H 3.54790 1.43980 1.59838
H 1.19368 -2.20780 1.75239
H 2.40649 -2.89608 3.82357

TS(Ia-II).3H₂O

SCF Energy = -1474.81511190

Enthalpy 0K = -1474.351717

Enthalpy 298K = -1474.315022

Free Energy 298K = -1474.425584

Dispersion Correction = -0.09021561

SCRF PCM Energy (THF) = -1474.86658413

Lowest Frequencies = -52.5687 8.0087 cm-1

60

C -3.04359 -1.87878 0.80221

C -2.86537 -0.98511 -0.30266

C -2.36491 -1.56220 -1.52598

C -2.08412 -2.95549 -1.62671

C -2.29873 -3.79033 -0.52724

C -2.78096 -3.24746 0.68474

Au -0.50518 -0.62663 -0.45005

P 1.60618 0.18002 0.05032

C 1.70168 0.73744 1.81027

C 2.02054 1.62611 -1.01477

C 2.94153 -1.07083 -0.18361

B -3.42731 0.53568 -0.33281

O -2.89152 1.31113 -1.36644

O -4.78911 0.66314 0.05996

O -2.61472 1.34179 1.26170

O -4.53835 0.34051 2.71748

O -5.13547 3.09660 -1.32201

H -3.44520 -1.48676 1.74338

H -2.35630 -0.94010 -2.42918

H -2.96022 -3.90853 1.53908

H -1.73340 -3.36674 -2.57865

H -2.10528 -4.86459 -0.60705

H -3.42365 2.12573 -1.49576

H -5.14468 1.51874 -0.27690

H -1.72355 0.96988 1.41923

H -3.21033 1.02955 2.02159

H -5.08187 0.87781 3.32108

H -4.96412 0.40211 1.81540

H -5.21803 3.98691 -0.93429

H -5.72325 3.09731 -2.09981

C 1.82815 1.50634 4.51068

C 1.28258 0.25797 4.16249

C 1.21273 -0.12697 2.81602

C 2.24829 1.98845 2.16029

C 2.30772 2.36799 3.51180

H 1.87659 1.80708 5.56184

H 0.90789 -0.41554 4.93960

H 0.78448 -1.09912 2.54514

H 2.62222 2.66351 1.38457

H 2.73063 3.34081 3.78101

C 2.62353 3.86700 -2.59464

C 1.28435 3.53618 -2.32912

C 0.97576 2.41578 -1.54254
C 3.36625 1.95339 -1.28715
C 3.66205 3.07578 -2.07582
H 2.85894 4.73758 -3.21478
H 0.47524 4.14537 -2.74383
H -0.07084 2.14763 -1.35326
H 4.17702 1.32971 -0.89702
H 4.70540 3.32701 -2.29012
C 4.98394 -2.94321 -0.64085
C 5.04003 -2.10493 0.48396
C 4.02155 -1.16650 0.71793
C 2.88279 -1.91790 -1.31150
C 3.90620 -2.84874 -1.53835
H 5.77814 -3.67536 -0.81661
H 5.87652 -2.18072 1.18555
H 4.06511 -0.51989 1.59980
H 2.03827 -1.84849 -2.00647
H 3.85885 -3.50531 -2.41259

II.3H₂O

SCF Energy = -1474.81512590

Enthalpy 0K = -1474.351579

Enthalpy 298K = -1474.314232

Free Energy 298K = -1474.426713

Dispersion Correction = -0.09007119

SCRFCM Energy (THF) = -1474.86665773

Lowest Frequencies = 8.3913 15.8684 cm⁻¹

60

C -3.03564 -1.88688 0.80194

C -2.85944 -0.97203 -0.28591

C -2.37590 -1.52965 -1.52464

C -2.10772 -2.92302 -1.65565

C -2.31970 -3.77797 -0.57127

C -2.78734 -3.25541 0.65525

Au -0.50034 -0.62390 -0.45300

P 1.61236 0.17731 0.05105

C 1.71406 0.70513 1.81997

C 2.01739 1.64312 -0.99053

C 2.95100 -1.06475 -0.20968

B -3.40620 0.56027 -0.27653

O -2.85749 1.34127 -1.30820

O -4.79458 0.66508 0.05731

O -2.67008 1.29790 1.27679

O -4.59920 0.32769 2.69742

O -5.14100 3.08579 -1.35195

H -3.42814 -1.51184 1.75394

H -2.37086 -0.88933 -2.41510

H -2.96609 -3.93201 1.49749

H -1.76869 -3.31819 -2.61863

H -2.13598 -4.85199 -0.67406

H -3.38988 2.15425 -1.44286

H -5.15003 1.51276 -0.29815

H -1.77635 0.93383 1.44085

H -3.28296 0.98530 2.03207

H -5.13619 0.88363 3.29016

H -5.01136 0.39373 1.78616

H -5.28857 3.97750 -0.98753

H -5.68629 3.04320 -2.15897

C 1.85018 1.42840 4.53264

C 1.30416 0.18568 4.16539

C 1.22951 -0.17646 2.81284

C 2.26120 1.95039 2.18912

C 2.32543 2.30714 3.54664

H 1.90252 1.71130 5.58856

H 0.93318 -0.50128 4.93245

H 0.80105 -1.14422 2.52703

H 2.63190 2.63862 1.42349

H 2.74883 3.27552 3.83068

C 2.60595 3.91370 -2.53295

C 1.26907 3.57284 -2.26862

C 0.96747 2.43758 -1.50077
C 3.36084 1.98046 -1.26188
C 3.64945 3.11765 -2.03178
H 2.83572 4.79599 -3.13849
H 0.45612 4.18597 -2.66981
H -0.07763 2.16208 -1.31297
H 4.17545 1.35327 -0.88557
H 4.69104 3.37676 -2.24531
C 4.99754 -2.92222 -0.70738
C 5.05600 -2.10263 0.43101
C 4.03547 -1.17173 0.68521
C 2.88995 -1.89301 -1.35132
C 3.91541 -2.81645 -1.59831
H 5.79335 -3.64863 -0.89892
H 5.89597 -2.18723 1.12742
H 4.08089 -0.53968 1.57748
H 2.04212 -1.81483 -2.04133
H 3.86622 -3.45851 -2.48316

TS(II-III).3H₂O

SCF Energy = -1474.79685094

Enthalpy 0K = -1474.335297

Enthalpy 298K = -1474.298774

Free Energy 298K = -1474.409486

Dispersion Correction = -0.08858198

SCRF PCM Energy (THF) = -1474.85003108

Lowest Frequencies = -237.1497 8.2181 cm-1

60

C 3.08659 1.39298 1.25377
C 2.64612 0.76405 0.04602
C 3.09081 1.36005 -1.17705
C 3.93926 2.47456 -1.19496
C 4.37095 3.04224 0.01794
C 3.94399 2.50085 1.24381
Au 0.55640 0.33438 0.00677
P -1.76293 -0.00933 -0.04028
C -2.35045 -0.94105 1.44635
C -2.28399 -0.97836 -1.52330
C -2.72520 1.56664 -0.07159
B 3.17669 -1.21989 -0.06818
O 2.72662 -1.69021 -1.29643
O 4.54227 -1.23654 0.30236
O 2.41180 -1.85973 1.11575
O 4.11268 -1.50903 2.88451
O 5.42196 -1.60325 -2.29947
H 2.76927 0.98699 2.22185
H 2.77641 0.90594 -2.12449
H 4.27555 2.95077 2.18551
H 4.26435 2.90804 -2.14717
H 5.03882 3.91019 0.00781
H 3.47258 -1.73335 -1.93243
H 5.11669 -1.27474 -0.49790
H 1.51890 -1.43616 1.19817
H 3.00712 -1.75852 2.00666
H 4.45341 -2.31741 3.31292
H 4.70790 -1.33151 2.10239
H 5.89330 -2.42070 -2.54521
H 5.80191 -0.90548 -2.86423
C -3.19152 -2.29683 3.76245
C -2.36356 -1.16578 3.87376
C -1.93778 -0.49082 2.72090
C -3.18053 -2.07430 1.33685
C -3.59675 -2.74902 2.49710
H -3.51914 -2.82518 4.66322
H -2.04767 -0.80966 4.85945
H -1.29230 0.39087 2.80911
H -3.49974 -2.42963 0.35240
H -4.24062 -3.62958 2.40794
C -3.04684 -2.51839 -3.74635
C -1.75137 -2.64382 -3.21806

C -1.36400 -1.87399 -2.11049
C -3.58303 -0.84777 -2.05909
C -3.95958 -1.61990 -3.16885
H -3.34381 -3.11555 -4.61425
H -1.03610 -3.33621 -3.67295
H -0.34642 -1.95818 -1.71132
H -4.29257 -0.13940 -1.61950
H -4.96632 -1.51466 -3.58508
C -4.16214 3.97714 -0.22161
C -4.66876 2.90358 0.52853
C -3.95450 1.69705 0.60734
C -2.21419 2.64943 -0.81953
C -2.93543 3.84965 -0.89526
H -4.72049 4.91685 -0.27656
H -5.62144 3.00375 1.05794
H -4.34774 0.86594 1.20124
H -1.25276 2.55272 -1.33692
H -2.53547 4.68798 -1.47404

III.3H₂O

SCF Energy = -1474.82759315
Enthalpy 0K = -1474.365920
Enthalpy 298K = -1474.328778
Free Energy 298K = -1474.443004
Dispersion Correction = -0.08324320
SCRf PCM Energy (THF) = -1474.88175917
Lowest Frequencies = 6.3558 12.2665 cm⁻¹

60

C 2.60621 -2.68971 -1.09063
C 2.22787 -1.91876 0.04587
C 3.02447 -2.05555 1.21739
C 4.13390 -2.91607 1.25234
C 4.47929 -3.66604 0.11644
C 3.71547 -3.54986 -1.05683
Au 0.40867 -0.93266 0.09319
P -1.73069 0.08520 0.11843
C -1.78662 1.55554 -1.02170
C -2.25795 0.71723 1.77433
C -3.07988 -1.02554 -0.48080
B 3.97330 1.55948 -0.22541
O 4.73262 1.11016 0.79981
O 3.81883 2.84096 -0.69301
O 3.20543 0.60346 -0.96293
O 1.77171 1.88394 -2.47669
O 5.72697 3.72113 1.12342
H 2.01993 -2.61861 -2.01430
H 2.77073 -1.48251 2.11615
H 3.98079 -4.13369 -1.94479
H 4.72717 -3.00378 2.16884
H 5.34333 -4.33815 0.14423
H 5.23529 1.85422 1.20441
H 4.41365 3.45425 -0.19823
H 2.89141 -0.28144 -0.53534
H 2.48270 1.06792 -1.65732
H 0.79013 1.86105 -2.36558
H 2.07646 2.77381 -2.19763
H 5.57159 4.30573 1.88860
H 6.63863 3.91343 0.83360
C -1.76361 3.73350 -2.82110
C -1.41167 2.44620 -3.27134
C -1.41462 1.36174 -2.37552
C -2.14121 2.84464 -0.58140
C -2.12778 3.92744 -1.48036
H -1.76403 4.57621 -3.51933
H -1.14559 2.28254 -4.32086
H -1.16639 0.35581 -2.73585
H -2.43426 3.00418 0.46090
H -2.41147 4.92427 -1.12793
C -2.96953 1.69836 4.31231
C -1.61433 1.57340 3.96466

C -1.25635 1.07986 2.70080
C -3.61815 0.83900 2.12842
C -3.96853 1.32969 3.39579
H -3.24795 2.07372 5.30203
H -0.83490 1.84691 4.68287
H -0.20030 0.96023 2.43198
H -4.39997 0.53726 1.42417
H -5.02463 1.41679 3.66956
C -5.10961 -2.79157 -1.29657
C -5.22976 -1.41630 -1.55677
C -4.21882 -0.53063 -1.15157
C -2.95781 -2.40925 -0.22826
C -3.97480 -3.28685 -0.63311
H -5.89880 -3.47883 -1.61706
H -6.11100 -1.03048 -2.07889
H -4.31309 0.53893 -1.36610
H -2.06641 -2.79599 0.27862
H -3.87558 -4.35893 -0.43702

TS(III-IV).3H₂O

SCF Energy = -1474.82527440

Enthalpy 0K = -1474.366620

Enthalpy 298K = -1474.329838

Free Energy 298K = -1474.442584

Dispersion Correction = -0.08278903

SCRF PCM Energy (THF) = -1474.87698276

Lowest Frequencies = -643.7813 6.2006 cm-1

60

C 2.53312 -2.66969 -1.20024

C 2.32907 -1.77524 -0.10599

C 2.99605 -2.07964 1.11812

C 3.81838 -3.20778 1.24090

C 3.99544 -4.06782 0.14318

C 3.35569 -3.79748 -1.07953

Au 0.45224 -0.80784 0.00862

P -1.70456 0.10884 0.11609

C -1.81746 1.66015 -0.89970

C -2.23353 0.57345 1.82423

C -3.00198 -1.01652 -0.56049

B 3.97905 1.50469 -0.21307

O 4.73539 0.98955 0.79178

O 3.87185 2.82733 -0.59182

O 3.19198 0.60737 -0.97725

O 1.87005 2.14771 -2.47370

O 5.83178 3.55384 1.24842

H 2.04942 -2.46431 -2.16243

H 2.88153 -1.40814 1.97589

H 3.50207 -4.46572 -1.93448

H 4.32472 -3.41819 2.18866

H 4.64003 -4.94804 0.23825

H 5.25889 1.70038 1.22560

H 4.48946 3.38608 -0.06325

H 2.73563 -0.39876 -0.54788

H 2.55882 1.11698 -1.64439

H 0.90840 2.24658 -2.29829

H 2.30890 2.93242 -2.07723

H 5.71526 4.11109 2.04013

H 6.74320 3.72428 0.94525

C -1.88959 3.97607 -2.50836

C -1.44416 2.75605 -3.05301

C -1.40196 1.60224 -2.25191

C -2.26640 2.88152 -0.36285

C -2.29999 4.03466 -1.16837

H -1.92283 4.87387 -3.13327

H -1.13939 2.69948 -4.10315

H -1.07138 0.64981 -2.68354

H -2.59167 2.93461 0.68066

H -2.65378 4.97927 -0.74336

C -2.96529 1.31891 4.43447

C -1.61208 1.32746 4.05714

C -1.24343 0.95161 2.75673
C -3.59135 0.56148 2.20668
C -3.95161 0.93491 3.51089
H -3.25091 1.60306 5.45209
H -0.84152 1.61495 4.77936
H -0.18733 0.93986 2.46328
H -4.36212 0.24923 1.49496
H -5.00521 0.91896 3.80663
C -4.96293 -2.79671 -1.50042
C -5.12590 -1.41350 -1.68284
C -4.14915 -0.52003 -1.21532
C -2.83661 -2.40754 -0.38482
C -3.81957 -3.29263 -0.85183
H -5.72528 -3.48963 -1.86987
H -6.01365 -1.02694 -2.19310
H -4.27575 0.55655 -1.36864
H -1.93900 -2.79373 0.11141
H -3.68752 -4.37046 -0.71590

IV. B(OH)₃·2H₂O

SCF Energy = -1474.85979658

Enthalpy 0K = -1474.394919

Enthalpy 298K = -1474.357101

Free Energy 298K = -1474.473087

Dispersion Correction = -0.08399455

SCRF PCM Energy (THF) = -1474.90948165

Lowest Frequencies = 7.9963 14.0903 cm⁻¹

60

C 2.01781 2.64119 0.43340

C 1.86286 2.66455 -0.98910

C 1.10786 3.70542 -1.59757

C 0.53441 4.70657 -0.80764

C 0.68427 4.68477 0.59789

C 1.40955 3.66256 1.21724

Au 0.30390 1.08601 -0.10452

P -1.37262 -0.50363 0.07354

C -1.20110 -1.82257 -1.20216

C -3.05649 0.22711 -0.12180

C -1.35052 -1.33208 1.72541

B 3.90692 -0.72771 -0.11737

O 3.94981 0.05752 1.01989

O 4.60569 -1.93124 -0.24272

O 3.12854 -0.29862 -1.17019

O 3.55362 -2.49127 -2.70230

O 5.78007 -1.72416 2.28764

H 2.71748 1.92362 0.88378

H 1.00908 3.73302 -2.68710

H 1.54450 3.65897 2.30329

H -0.02633 5.51947 -1.27960

H 0.23763 5.48043 1.20233

H 4.53775 -0.33982 1.69796

H 5.12672 -2.13483 0.56709

H 2.43468 1.94984 -1.59191

H 3.18205 -0.96703 -1.91196

H 4.20282 -2.39120 -3.42234

H 4.09195 -2.70191 -1.90069

H 6.72502 -1.50147 2.37787

H 5.57835 -2.30699 3.04252

C -0.87767 -3.86978 -3.09447

C 0.25056 -3.20395 -2.58639

C 0.09174 -2.17835 -1.64205

C -2.33462 -2.48671 -1.71759

C -2.16579 -3.51113 -2.66245

H -0.75487 -4.66493 -3.83681

H 1.26071 -3.45800 -2.92321

H 0.97158 -1.64768 -1.26062

H -3.34017 -2.20048 -1.39324

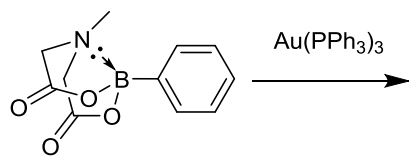
H -3.04464 -4.02408 -3.06555

C -5.61425 1.31844 -0.52228

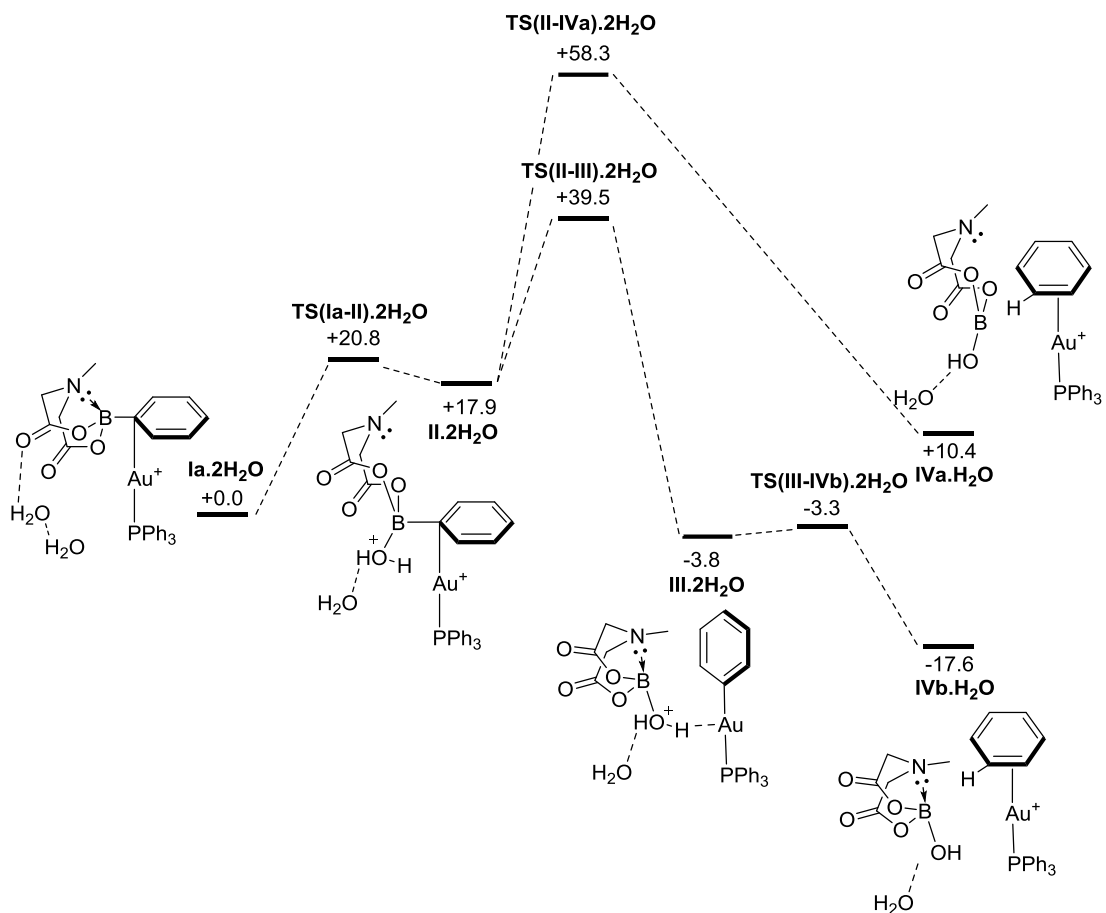
C -4.52560 1.78816 -1.27706

C -3.24704 1.24859 -1.07705
C -4.14855 -0.24265 0.63688
C -5.42485 0.30669 0.43258
H -6.61006 1.74592 -0.67527
H -4.67077 2.58066 -2.01777
H -2.39503 1.62075 -1.65720
H -4.00363 -1.02619 1.38711
H -6.27068 -0.05654 1.02453
C -1.37399 -2.52424 4.26993
C -1.53006 -3.31685 3.12188
C -1.51970 -2.72612 1.84729
C -1.18519 -0.53670 2.88039
C -1.20236 -1.13415 4.14852
H -1.38356 -2.98905 5.26082
H -1.66140 -4.39951 3.21416
H -1.64004 -3.34680 0.95409
H -1.04410 0.54592 2.78491
H -1.07765 -0.51471 5.04224

Protodeboronation MIDA



Structure	ΔE	ΔG_{Gas}	ΔG_{disp}	$\Delta G_{\text{disp+solv}}$
Ia.2H ₂ O	+0.0	+0.0	+0.0	+0.0
TS(Ia-II).2H ₂ O	+18.5	+16.6	+19.6	+20.8
II.2H ₂ O	+15.4	+13.3	+16.9	+17.9
TS(II-III).2H ₂ O	+39.0	+35.1	+38.3	+39.5
III.2H ₂ O	-6.3	+6.6	-2.9	-3.8
TS(III-IVb).2H ₂ O	-2.0	-4.4	-2.9	-3.3
TS(II-IVa).2H ₂ O	+52.7	+46.8	+55.1	+58.3
IVa.H ₂ O	+0.3	-4.6	+5.6	+10.4
IVb.H ₂ O	-22.5	-24.5	-19.3	-17.6



Ia.2H₂O

SCF Energy = -1797.14788511
Enthalpy 0K = -1796.610245
Enthalpy 298K = -1796.568630
Free Energy 298K = -1796.690641
Dispersion Correction = -0.11605808
SCRF PCM Energy (THF)= -1797.20465573
Lowest Frequencies = 8.3589 16.8247 cm-1
C -1.32358 0.11656 -3.97741
C -1.45812 -1.05404 -3.22068
C -1.95803 -0.99249 -1.88832
C -2.30019 0.27178 -1.29499
C -2.12719 1.43726 -2.09102
C -1.67412 1.36065 -3.41377
Au 0.07022 -0.65170 -0.71082
B -2.93390 0.34105 0.17861
O -2.81380 -0.95736 0.87221
P 2.03437 0.16307 0.22479
C 2.39355 -0.56782 1.88218
C 2.00355 1.99493 0.46276
C 3.49552 -0.20685 -0.84574
O -2.47250 1.48171 0.98670
H -2.22766 -1.92138 -1.37121
H -2.34356 2.42138 -1.65970
H -1.21004 -2.02673 -3.65743
H -1.57232 2.27430 -4.00824
H -0.95659 0.06487 -5.00705
C -3.38386 2.46643 1.18084
C -3.91856 -1.34633 1.52097
C 5.69546 -0.70296 -2.52477
C 4.46050 -0.32592 -3.08011
C 3.36034 -0.08266 -2.24550
C 4.73441 -0.58632 -0.28999
C 5.83004 -0.83362 -1.13346
H 6.55135 -0.89973 -3.17795
H 4.35236 -0.22793 -4.16495
H 2.39316 0.20140 -2.67622
H 4.84196 -0.69436 0.79366
H 6.78950 -1.13165 -0.69930
C 2.99906 -1.74136 4.36003
C 3.32541 -0.39601 4.12380
C 3.02432 0.19606 2.88699
C 2.05566 -1.91803 2.12024
C 2.36583 -2.49824 3.35989
H 3.23287 -2.19817 5.32694
H 3.81209 0.19813 4.90362
H 3.27187 1.24717 2.70889
H 1.54391 -2.50399 1.34695
H 2.10445 -3.54477 3.54675
C 1.90200 4.76232 0.93716
C 0.76879 3.96748 1.18215

C 0.81521 2.58673 0.94163
C 3.14051 2.79171 0.21629
C 3.08284 4.17525 0.45390
H 1.86383 5.84106 1.11921
H -0.15925 4.41374 1.55346
H -0.07585 1.97576 1.12000
H 4.06217 2.33890 -0.16244
H 3.96483 4.79352 0.25897
C -4.99653 -0.25909 1.43900
O -4.04164 -2.42214 2.09007
C -4.73194 2.06427 0.54851
O -3.16774 3.52226 1.73649
H -4.86263 2.61316 -0.39866
H -5.58268 2.29898 1.20584
N -4.62166 0.59806 0.25478
H -4.95908 0.34325 2.36207
H -6.00577 -0.68370 1.33324
C -5.38279 0.17967 -0.96591
H -5.22211 -0.89505 -1.13801
H -5.00306 0.73918 -1.83205
H -6.45751 0.37648 -0.82646
H -2.81522 -3.55663 1.25225
O -2.36489 -4.09947 0.55756
H -2.39301 -5.01340 0.89286
H -0.85117 -3.55663 0.11035
O 0.04115 -3.22015 -0.21761
H 0.23845 -3.73578 -1.02054

TS(Ia-II).2H₂O

SCF Energy = -1797.11837154
Enthalpy 0K = -1796.582402
Enthalpy 298K = -1796.541183
Free Energy 298K = -1796.664161
Dispersion Correction = -0.11137048
SCRF PCM Energy (THF)= -1797.17317804
Lowest Frequencies = -204.9528 4.6057 cm-1
C -1.14120 -3.63275 -1.10796
C -1.02175 -3.04503 0.17170
C -1.68265 -1.80794 0.45081
C -2.48624 -1.15973 -0.54959
C -2.59109 -1.79159 -1.80411
C -1.93487 -3.00957 -2.07998
Au 0.43170 -0.94705 0.10940
B -3.20110 0.22264 -0.23272
O -3.14895 0.78220 1.07837
P 2.45156 0.19623 0.05165
C 2.70221 1.11987 -1.52628
C 3.88006 -0.95510 0.24645
C 2.54197 1.43522 1.41208
H -1.73775 -1.45464 1.48991
H -3.21037 -1.32919 -2.58078
H -0.49572 -3.57454 0.97335
H -2.05116 -3.47523 -3.06420
H -0.64097 -4.58182 -1.32152
C -3.76297 0.33239 2.21394
C 2.72213 3.26927 3.53064
C 1.97845 2.08769 3.68907
C 1.88509 1.17036 2.63261
C 3.28464 2.62444 1.25120
C 3.37285 3.53630 2.31484
H 2.78815 3.98697 4.35420
H 1.46117 1.88373 4.63143
H 1.29550 0.25433 2.75161
H 3.78191 2.84178 0.30069
H 3.94707 4.45940 2.18903
C 3.02952 2.58797 -3.89680
C 4.03624 1.70660 -3.47320
C 3.87880 0.96994 -2.28720
C 1.68507 2.00309 -1.95349
C 1.85626 2.73688 -3.13582
H 3.15728 3.15977 -4.82120
H 4.94998 1.58963 -4.06399
H 4.66660 0.28532 -1.95906
H 0.76795 2.11314 -1.36276
H 1.07166 3.42565 -3.46489
C 6.05469 -2.71978 0.46514
C 4.93150 -3.08369 -0.29749
C 3.84181 -2.20757 -0.40432
C 5.00696 -0.59048 1.01170

C 6.09037 -1.47738 1.11834
H 6.90038 -3.40860 0.55460
H 4.90034 -4.05384 -0.80302
H 2.96015 -2.49459 -0.98881
H 5.03663 0.37470 1.52644
H 6.96200 -1.19530 1.71685
C -4.93236 -0.64091 1.98552
O -3.40579 0.68767 3.31879
H -5.74065 -0.36178 2.69187
H -4.58422 -1.64446 2.28860
H -2.14382 2.29508 -1.07413
O -1.63963 1.41897 -0.88928
H -1.45049 1.08047 -1.78672
H -3.96022 3.25015 -1.68562
O -3.02936 3.56156 -1.54217
H -3.10581 4.25819 -0.86485
O -4.06641 0.80418 -1.22044
C -5.25544 1.34101 -0.86834
C -6.06791 0.50580 0.13302
O -5.64666 2.39886 -1.34645
H -6.34007 1.16922 0.97416
N -5.33470 -0.68179 0.58435
H -7.01945 0.23850 -0.36184
C -5.91082 -1.95572 0.12927
H -6.90583 -2.16572 0.57248
H -5.22921 -2.78070 0.39087
H -6.01357 -1.93765 -0.96771

II.2H₂O

SCF Energy = -1797.12333142
Enthalpy 0K = -1796.587295
Enthalpy 298K = -1796.546473
Free Energy 298K = -1796.669494
Dispersion Correction = -0.11024827
SCRF PCM Energy (THF)= -1797.17855672
Lowest Frequencies = 5.4425 7.4882 cm-1
C -1.09435 -3.54522 -0.34322
C -1.00459 -2.78124 0.84432
C -1.61745 -1.48711 0.90522
C -2.33773 -0.95793 -0.22112
C -2.40608 -1.75902 -1.37686
C -1.80112 -3.03203 -1.43957
Au 0.55249 -0.88223 0.40579
B -3.05157 0.48406 -0.11329
O -3.63687 0.83962 1.16740
P 2.58074 0.16522 -0.00711
C 2.34190 1.66829 -1.05559
C 3.76733 -0.93545 -0.88997
C 3.38818 0.72016 1.55264
H -1.70590 -0.97821 1.87465
H -2.97424 -1.38783 -2.23606
H -0.55550 -3.21526 1.74437
H -1.89440 -3.63161 -2.35127
H -0.63962 -4.53926 -0.38663
C -4.66185 0.34435 1.91548
C 4.67050 1.48120 3.93172
C 3.93775 0.28282 3.88377
C 3.29367 -0.09917 2.69844
C 4.12219 1.92401 1.60100
C 4.76156 2.29883 2.79361
H 5.16636 1.78070 4.86015
H 3.86095 -0.35146 4.77213
H 2.71589 -1.02970 2.66166
H 4.18807 2.56803 0.71858
H 5.32827 3.23418 2.83201
C 1.91294 3.97078 -2.60939
C 2.86533 3.02088 -3.00919
C 3.08440 1.86775 -2.23608
C 1.38181 2.62480 -0.65231
C 1.17357 3.77397 -1.42901
H 1.74513 4.86615 -3.21578
H 3.44314 3.17345 -3.92593
H 3.82762 1.12972 -2.55221
H 0.80774 2.47491 0.26928
H 0.43274 4.51562 -1.11408
C 5.54828 -2.58285 -2.30409
C 4.16789 -2.66699 -2.55432
C 3.27494 -1.84955 -1.84641
C 5.15268 -0.85216 -0.63756

C 6.03794 -1.67892 -1.34730
H 6.24252 -3.22792 -2.85138
H 3.78507 -3.37583 -3.29501
H 2.19694 -1.92329 -2.03043
H 5.53738 -0.15403 0.11231
H 7.11206 -1.61746 -1.14743
C -5.54966 -0.77505 1.34823
O -4.85522 0.76999 3.03980
H -6.55610 -0.60908 1.79271
H -5.16873 -1.71423 1.79194
H -2.41688 2.56263 -0.32935
O -1.88309 1.60255 -0.16475
H -1.32296 1.45578 -0.95436
H -4.01602 3.33483 -1.04442
O -3.17028 3.67891 -0.60015
H -3.47535 4.07898 0.23736
O -3.86693 0.84927 -1.29283
C -5.13018 1.28116 -1.14465
C -6.16366 0.20881 -0.79550
O -5.43818 2.45949 -1.34981
H -7.00160 0.69174 -0.25051
N -5.57209 -0.93770 -0.10483
H -6.57636 -0.12411 -1.76638
C -6.18136 -2.21894 -0.49252
H -7.24769 -2.31425 -0.19122
H -5.62022 -3.04504 -0.02509
H -6.11771 -2.34233 -1.58600

TS(II-III).2H₂O

SCF Energy = -1797.08577607

Enthalpy 0K = -1796.553625

Enthalpy 298K = -1796.513043

Free Energy 298K = -1796.634684

Dispersion Correction = -0.1109752

SCRF PCM Energy (THF)= -1797.14063533

Lowest Frequencies = -105.7575 6.2439 cm⁻¹

C -3.65850 3.62500 -0.39878

C -2.93662 3.30113 -1.56055

C -1.90455 2.35409 -1.50074

C -1.57164 1.68196 -0.28612

C -2.33015 2.02490 0.87006

C -3.35126 2.98782 0.81583

Au 0.29310 0.78409 -0.08503

B -2.78619 -0.44272 -0.87700

O -4.00428 -0.05242 -1.36854

P 2.50455 -0.06801 0.11654

C 2.96080 -1.18819 -1.28622

C 2.78345 -1.03724 1.66647

C 3.76955 1.27929 0.11401

H -1.34351 2.13119 -2.41500

H -2.10933 1.53883 1.82577

H -3.16945 3.79791 -2.50815

H -3.89497 3.25867 1.72789

H -4.45073 4.38031 -0.43828

C -5.31034 -0.33055 -0.93450

C 5.65279 3.36473 0.19859

C 4.39258 3.53430 0.79644

C 3.44935 2.49721 0.75260

C 5.03381 1.11226 -0.48869

C 5.97115 2.15681 -0.44334

H 6.38510 4.17757 0.22757

H 4.13967 4.47773 1.29012

H 2.46266 2.63390 1.21016

H 5.28191 0.17601 -0.99869

H 6.95053 2.02587 -0.91411

C 3.62390 -2.81311 -3.48601

C 3.90762 -3.24580 -2.18115

C 3.57987 -2.43708 -1.07963

C 2.67000 -0.75768 -2.60057

C 3.00682 -1.56716 -3.69509

H 3.88435 -3.44477 -4.34111

H 4.38978 -4.21445 -2.01571

H 3.80638 -2.77720 -0.06446

H 2.19230 0.21514 -2.76604

H 2.78783 -1.22475 -4.71152

C 3.14337 -2.56673 3.99943

C 1.89304 -2.54908 3.35887

C 1.70929 -1.78323 2.19797

C 4.03647 -1.05343 2.31385

C 4.21141 -1.81830 3.47805
H 3.28355 -3.15859 4.90936
H 1.05799 -3.12592 3.76918
H 0.73134 -1.75423 1.70366
H 4.86857 -0.46378 1.91628
H 5.18402 -1.82528 3.97987
C -5.73706 0.17852 0.44445
O -6.06973 -0.86317 -1.71015
H -6.78453 -0.17217 0.56874
H -5.74949 1.28286 0.37450
H -1.82202 -2.14298 -1.86488
O -1.79127 -0.78092 -1.86754
H -0.90317 -0.45860 -1.52718
H -2.60502 -3.36004 -0.86817
O -1.96285 -3.24323 -1.70657
H -2.37301 -3.65839 -2.49201
O -2.68006 -1.21225 0.32212
C -3.62142 -2.10538 0.69576
C -4.65683 -1.61848 1.69481
O -3.58633 -3.26548 0.25611
H -5.56266 -2.25583 1.58922
N -4.86821 -0.18146 1.57218
H -4.23628 -1.83484 2.69630
C -5.36721 0.42218 2.81771
H -6.37944 0.06579 3.10939
H -5.41238 1.51580 2.69260
H -4.66656 0.20197 3.63934

III.2H₂O

SCF Energy = -1797.15794869
Enthalpy 0K = -1796.622100
Enthalpy 298K = -1796.582039
Free Energy 298K = -1796.701092
Dispersion Correction = -0.1102852
SCRF PCM Energy (THF)= -1797.21606422
Lowest Frequencies = 6.7912 17.7285 cm⁻¹
C 3.04174 4.47215 -0.16730
C 2.98535 3.47538 0.82240
C 1.89015 2.58575 0.86980
C 0.82179 2.67810 -0.06806
C 0.90760 3.69072 -1.05480
C 1.99841 4.57860 -1.10057
Au -0.76395 1.37291 0.03569
B 3.72242 -0.64461 -0.04451
O 3.87682 -0.29991 1.35714
P -2.48202 -0.28895 0.12621
C -1.90939 -1.75314 -0.86676
C -4.10761 0.22005 -0.58518
C -2.80886 -0.93181 1.82472
H 1.84955 1.84388 1.67631
H 0.10698 3.80094 -1.79456
H 3.77789 3.39929 1.57565
H 2.02999 5.35903 -1.86864
H 3.88546 5.16897 -0.20071
C 5.17406 -0.13765 1.75807
C -3.35440 -1.80347 4.44036
C -3.01869 -0.45950 4.20595
C -2.74195 -0.02190 2.90227
C -3.14253 -2.28208 2.06257
C -3.41430 -2.71238 3.37097
H -3.56462 -2.14424 5.45893
H -2.96515 0.24827 5.03890
H -2.47229 1.02473 2.72050
H -3.18112 -2.99581 1.23327
H -3.67136 -3.76042 3.55395
C -0.86744 -3.86026 -2.42843
C -2.10634 -3.28792 -2.75067
C -2.62845 -2.23512 -1.97604
C -0.65963 -2.33826 -0.53878
C -0.14175 -3.39022 -1.31581
H -0.46636 -4.67854 -3.03444
H -2.67536 -3.65746 -3.60960
H -3.59377 -1.79109 -2.23795
H -0.10696 -1.99518 0.34467
H 0.82081 -3.84091 -1.04839
C -6.54017 1.03745 -1.73141
C -5.33755 1.63631 -2.14156
C -4.12203 1.23403 -1.56762
C -5.31725 -0.37709 -0.17190

C -6.52911 0.03451 -0.74742
H -7.48869 1.35847 -2.17310
H -5.34560 2.42489 -2.90039
H -3.18401 1.71136 -1.87389
H -5.31449 -1.14907 0.60418
H -7.46694 -0.42599 -0.42153
C 6.12299 -0.41305 0.57428
O 5.52211 0.20089 2.86435
H 6.98950 -1.02165 0.87239
H 6.49105 0.54825 0.17941
H 2.11108 0.11485 -1.48573
O 3.19326 0.44766 -0.85587
H 2.98160 1.26300 -0.31480
H 0.83089 -1.06180 -1.73782
O 1.10760 -0.14197 -1.99436
H 0.43085 0.46346 -1.52029
O 2.95496 -1.85878 -0.32871
C 3.73223 -2.96621 -0.47055
C 5.21225 -2.58521 -0.30107
O 3.31133 -4.08300 -0.68295
H 5.52864 -2.85781 0.71962
N 5.28170 -1.08619 -0.47148
H 5.85721 -3.10926 -1.02178
C 5.66547 -0.71692 -1.87358
H 6.70742 -1.01506 -2.06650
H 5.54401 0.36697 -2.00158
H 4.99621 -1.23553 -2.57589

TS(III-Ivb).2H₂O

SCF Energy = -1797.15101693

Enthalpy 0K = -1796.618361

Enthalpy 298K = -1796.577930

Free Energy 298K = -1796.697724

Dispersion Correction = -0.11363022

SCRF PCM Energy (THF)= -1797.20839586

Lowest Frequencies = -706.4125 8.1139 cm⁻¹

C -2.62318 -4.90399 -0.24260

C -2.56437 -4.09180 0.90330

C -1.94076 -2.83723 0.83996

C -1.36292 -2.35365 -0.37321

C -1.44392 -3.20510 -1.51704

C -2.06596 -4.45932 -1.45518

Au 0.32846 -1.09115 -0.18868

B -3.20999 0.79132 -0.06526

O -3.26992 0.17310 1.24808

P 2.25688 0.22267 0.12337

C 2.00612 1.91901 -0.58587

C 3.77575 -0.46587 -0.66667

C 2.65133 0.46889 1.90972

H -1.92103 -2.20630 1.73497

H -1.01918 -2.87234 -2.47183

H -3.00455 -4.43729 1.84443

H -2.11657 -5.09314 -2.34670

H -3.10871 -5.88436 -0.19286

C -4.52510 -0.17898 1.64964

C 3.29037 0.73563 4.63230

C 2.81147 -0.49131 4.14220

C 2.48756 -0.62731 2.78462

C 3.12905 1.70078 2.40276

C 3.44714 1.82853 3.76455

H 3.53654 0.84113 5.69344

H 2.68272 -1.34196 4.81854

H 2.10724 -1.58205 2.40370

H 3.24447 2.55774 1.73156

H 3.81570 2.78567 4.14649

C 1.47155 4.46218 -1.67707

C 2.66766 3.79772 -1.98832

C 2.93853 2.52685 -1.44851

C 0.80124 2.59325 -0.27010

C 0.53533 3.86144 -0.81341

H 1.26616 5.44877 -2.10387

H 3.39691 4.26477 -2.65768

H 3.87079 2.01258 -1.70175

H 0.07369 2.13455 0.40905

H -0.40272 4.36768 -0.56021

C 6.05612 -1.51371 -1.93265

C 4.77661 -1.86325 -2.39469

C 3.63658 -1.34450 -1.76218

C 5.06241 -0.12225 -0.19924

C 6.19769 -0.64685 -0.83583
H 6.94469 -1.92498 -2.42160
H 4.66477 -2.54887 -3.24034
H 2.63636 -1.63289 -2.10588
H 5.17680 0.53941 0.66549
H 7.19443 -0.38281 -0.46908
C -5.55268 0.24434 0.58095
O -4.78898 -0.75947 2.67703
H -6.44581 0.70653 1.02694
H -5.86533 -0.64792 0.01409
H -1.99565 0.38861 -1.72067
O -2.66910 -0.10610 -1.08234
H -2.04080 -1.03628 -0.69739
H -0.56542 1.78770 -2.01742
O -0.91155 1.02729 -2.54167
H -0.17274 0.38130 -2.51438
O -2.54904 2.09402 -0.12241
C -3.40999 3.14187 -0.01313
C -4.84943 2.61613 0.12718
O -3.08143 4.30840 -0.01175
H -5.13365 2.65638 1.19195
N -4.82048 1.17949 -0.33716
H -5.56507 3.21841 -0.45169
C -5.24904 1.06449 -1.76939
H -6.31676 1.31654 -1.86128
H -5.06437 0.03817 -2.11374
H -4.65175 1.75921 -2.37852

TS(II-Iva).2H₂O

SCF Energy = -1797.06397858

Enthalpy 0K = -1796.532534

Enthalpy 298K = -1796.491493

Free Energy 298K = -1796.616096

Dispersion Correction = -0.10284839

SCRF PCM Energy (THF)= -1797.11556275

Lowest Frequencies = 12.8698 19.1322 cm⁻¹

C 1.02451 -2.18343 2.47583

C 0.93819 -2.35787 1.06265

C 1.55691 -1.40754 0.19544

C 2.26516 -0.28239 0.74099

C 2.33317 -0.15568 2.14388

C 1.72456 -1.09508 3.00483

Au -0.74143 -0.85439 0.29312

B 3.57657 0.56011 -0.33639

O 3.92903 -0.28274 -1.41772

P -2.79684 0.13964 -0.14774

C -3.58459 0.79469 1.38513

C -3.96671 -1.07403 -0.89438

C -2.63000 1.54726 -1.32511

H 1.66105 -1.63636 -0.87134

H 2.89073 0.68492 2.57077

H 0.54387 -3.29589 0.65494

H 1.81013 -0.97760 4.08968

H 0.56915 -2.92640 3.13781

C 4.48943 -1.54234 -1.42155

C -2.40086 3.63491 -3.18747

C -1.58383 2.49764 -3.30682

C -1.69284 1.45412 -2.37671

C -3.44801 2.69004 -1.20272

C -3.32904 3.73052 -2.13786

H -2.30954 4.45082 -3.91113

H -0.85433 2.42512 -4.11912

H -1.04858 0.57203 -2.46446

H -4.16704 2.77055 -0.38161

H -3.96181 4.61816 -2.04164

C -4.74602 1.87026 3.70429

C -5.54120 1.17504 2.77947

C -4.96625 0.63504 1.61735

C -2.78397 1.48938 2.31814

C -3.36843 2.02863 3.47254

H -5.19842 2.28607 4.60987

H -6.61297 1.04847 2.96061

H -5.58800 0.09000 0.90058

H -1.70894 1.60780 2.14082

H -2.74723 2.56746 4.19461

C -5.76491 -2.94767 -1.96247

C -4.93630 -3.30763 -0.88534

C -4.03423 -2.37643 -0.35223

C -4.79744 -0.71294 -1.97485

C -5.69448 -1.65471 -2.50487
H -6.46260 -3.67890 -2.38213
H -4.98713 -4.31664 -0.46482
H -3.38338 -2.65914 0.48309
H -4.74156 0.29241 -2.40311
H -6.33637 -1.37503 -3.34583
C 6.01691 -1.54931 -1.47450
O 3.79421 -2.54228 -1.45248
H 6.33690 -1.18833 -2.48097
H 6.32949 -2.60041 -1.38786
H 2.99083 2.55497 -0.31774
O 2.71272 1.68711 -0.79913
H 2.13425 0.87187 0.06700
H 4.45730 3.49360 0.79659
O 3.53502 3.77689 0.54710
H 3.65751 4.59312 0.02864
O 4.56845 0.98386 0.62628
C 5.76815 1.51650 0.27364
C 6.69420 0.66122 -0.59632
O 6.07259 2.64673 0.64993
H 6.45115 0.92265 -1.64797
N 6.58375 -0.77548 -0.36883
H 7.71990 1.03266 -0.41991
C 7.78076 -1.37082 0.23655
H 8.67112 -1.36723 -0.43108
H 7.56919 -2.41271 0.52641
H 8.03819 -0.81917 1.15551

IVa.H₂O

SCF Energy = -1797.14742261
Enthalpy 0K = -1796.611260
Enthalpy 298K = -1796.568952
Free Energy 298K = -1796.697977
Dispersion Correction = -0.09984743
SCRF PCM Energy (THF)= -1797.19644040
Lowest Frequencies = 7.6037 8.7369 cm⁻¹
C -1.40842 4.75537 -0.75726
C -0.57912 4.20639 0.22557
C 0.38930 3.22141 -0.12270
C 0.48421 2.79007 -1.48415
C -0.37836 3.34923 -2.46689
C -1.30714 4.32847 -2.10123
Au -0.80407 1.18167 -0.25965
B 3.27840 -0.59413 -0.77906
O 2.64351 0.27214 0.13065
P -2.06123 -0.70365 0.22802
C -3.80926 -0.26243 0.62230
C -1.40060 -1.62161 1.68524
C -2.10312 -1.88317 -1.19061
H 1.15131 2.90007 0.60200
H -0.28691 3.03093 -3.50965
H -0.64195 4.55209 1.26180
H -1.95342 4.77651 -2.86247
H -2.13293 5.53030 -0.48821
C 3.21459 0.84400 1.24611
C -2.11552 -3.67810 -3.34901
C -0.90961 -3.08833 -2.93205
C -0.89474 -2.18806 -1.85665
C -3.31403 -2.47481 -1.60560
C -3.31423 -3.37252 -2.68558
H -2.12104 -4.37307 -4.19459
H 0.02494 -3.32139 -3.45177
H 0.05389 -1.73638 -1.54240
H -4.25102 -2.23393 -1.09450
H -4.25503 -3.82884 -3.00864
C -6.48961 0.40404 1.13656
C -5.87425 -0.63369 1.85494
C -4.53510 -0.97181 1.60159
C -4.42704 0.78482 -0.09497
C -5.76640 1.11164 0.16104
H -7.53242 0.66612 1.34047
H -6.43476 -1.18204 2.61834
H -4.05765 -1.77742 2.16784
H -3.85829 1.34280 -0.84760
H -6.24320 1.92418 -0.39588
C -0.48322 -2.97128 3.97114
C -0.46098 -1.56634 3.93066
C -0.91410 -0.88910 2.78947
C -1.41921 -3.03107 1.72398

C -0.95900 -3.70064 2.86957
H -0.12636 -3.49779 4.86189
H -0.08716 -0.99632 4.78694
H -0.88921 0.20592 2.75398
H -1.78579 -3.60153 0.86494
H -0.97359 -4.79461 2.89867
C 4.44214 0.14197 1.85597
O 2.72709 1.85543 1.72289
H 4.35600 -0.95574 1.74091
H 4.43046 0.35651 2.94040
H 3.10338 -2.07754 -2.06130
O 2.53523 -1.50452 -1.42284
H 1.31069 2.13794 -1.78615
H 4.99591 -2.69047 -2.39627
O 4.15480 -2.91667 -2.87637
H 4.05105 -3.87805 -2.75339
O 4.65382 -0.38009 -1.01774
C 5.74715 -1.06023 -0.57840
C 6.47501 -0.36341 0.57202
O 6.13200 -2.10605 -1.08654
H 6.85420 -1.16785 1.24479
N 5.66269 0.65263 1.21495
H 7.37108 0.11662 0.13434
C 6.40577 1.61334 2.03445
H 6.85956 1.16409 2.94625
H 5.72572 2.42137 2.34699
H 7.20985 2.06607 1.43136

IVb.H₂O

SCF Energy = -1797.18381608
Enthalpy 0K = -1796.645847
Enthalpy 298K = -1796.604002
Free Energy 298K = -1796.729743
Dispersion Correction = -0.10770479
SCRF PCM Energy (THF)= -1797.23783125
Lowest Frequencies = 5.0595 12.4375 cm⁻¹
C 0.97300 -4.80608 -0.09675
C 0.34458 -4.10102 0.93465
C -0.63549 -3.11621 0.63286
C -0.96348 -2.84190 -0.73445
C -0.29454 -3.56175 -1.76798
C 0.65701 -4.53437 -1.44739
Au 0.55148 -1.15178 -0.10716
B -3.62074 0.06374 -0.31691
O -2.74944 -0.41611 0.78760
P 2.00560 0.65089 0.02912
C 1.34467 2.17211 -0.77502
C 3.62989 0.27711 -0.76461
C 2.35898 1.08611 1.78852
H -1.22454 -2.66087 1.43970
H -0.56107 -3.36940 -2.81188
H 0.57586 -4.32425 1.98060
H 1.15058 -5.09941 -2.24421
H 1.70882 -5.58041 0.14195
C -3.41499 -0.96079 1.82464
C 2.96226 1.69056 4.46464
C 2.84098 0.35018 4.05926
C 2.53595 0.04496 2.72541
C 2.47828 2.43081 2.19572
C 2.78026 2.72680 3.53504
H 3.19320 1.92667 5.50805
H 2.97565 -0.45855 4.78418
H 2.43059 -0.99941 2.41056
H 2.33070 3.24121 1.47534
H 2.86960 3.77100 3.85032
C 0.30621 4.54007 -1.86607
C 1.67079 4.24027 -2.01204
C 2.19712 3.05816 -1.46674
C -0.02919 2.46703 -0.64244
C -0.54532 3.65465 -1.18265
H -0.09619 5.46584 -2.28966
H 2.33131 4.92709 -2.55056
H 3.26060 2.82690 -1.58202
H -0.69671 1.77111 -0.12295
H -1.61084 3.87911 -1.06326
C 6.06912 -0.25663 -2.05274
C 4.86422 -0.70816 -2.61845
C 3.64552 -0.44721 -1.97614
C 4.83899 0.72887 -0.19667

C 6.05535 0.45872 -0.84473
H 7.01988 -0.46780 -2.55197
H 4.87398 -1.27054 -3.55731
H 2.70620 -0.80783 -2.41052
H 4.83253 1.28158 0.74783
H 6.99306 0.80677 -0.40060
C -4.93244 -0.74035 1.67283
O -2.89533 -1.57170 2.74240
H -5.39357 -0.40231 2.61367
H -5.39954 -1.69502 1.38097
H -3.95808 -0.36973 -2.20902
O -3.68145 -0.83704 -1.37421
H -1.83396 -2.21571 -0.97605
H -3.85057 1.61197 -2.91873
O -4.44670 0.92810 -3.28363
H -4.25921 0.89892 -4.23927
O -3.34413 1.47744 -0.68098
C -4.04904 2.38366 0.03610
C -5.00981 1.67538 1.00620
O -3.92562 3.58975 -0.06199
H -4.58123 1.72966 2.02087
N -5.09100 0.24518 0.55969
H -5.99684 2.16245 1.02119
C -6.28811 -0.00343 -0.30093
H -7.21337 0.10751 0.28641
H -6.20929 -1.01712 -0.71691
H -6.28076 0.71425 -1.13519