

Supporting Information

On the Mechanism of Reduction of $M(H_2O)_m^{n+}$ by Borohydride: The Case of $Ag(H_2O)_2^+$

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Cartesian coordinates of all relevant reactants, intermediates, and transition states.

BH₄⁻

B	-0.000101000	-0.000004000	0.000000000
H	0.418762000	0.550268000	-1.035719000
H	0.416781000	0.619712000	0.996555000
H	0.410560000	-1.175016000	0.040550000
H	-1.245600000	0.005058000	-0.001386000

[BH₃(OH)]⁻

B	-0.163705000	-0.531111000	0.365637000
H	-0.148133000	0.168736000	1.414355000
H	-1.163864000	-1.295655000	0.435586000
H	-0.301402000	0.220142000	-0.615309000
O	1.134454000	-1.312754000	0.188089000
H	1.215953000	-1.884072000	0.964529000

[BH₂(OH)₂]⁻

B	-0.016958000	0.051752000	0.583665000
H	0.528010000	1.201638000	0.650637000
H	-0.172826000	-0.276548000	-0.611045000
O	0.820022000	-1.011246000	1.216938000
H	0.789351000	-0.825843000	2.169445000
O	-1.343645000	0.148327000	1.332289000
H	-1.489875000	1.092874000	1.476947000

[BH(OH)₃]⁻

B	-0.062260000	0.136122000	0.515236000
H	-0.190778000	-0.136646000	-0.705138000
O	0.791909000	-0.934970000	1.089712000
H	0.735732000	-0.802003000	2.052518000
O	-1.355703000	0.201342000	1.256417000
H	-1.576170000	1.145203000	1.287123000

O	0.546906000	1.518503000	0.676561000
H	1.353157000	1.523265000	0.139839000

[B(OH)₄]⁻

B	-0.066988000	0.194128000	0.483929000
O	0.563759000	-1.040844000	1.043297000
H	0.252560000	-1.088431000	1.959891000
O	-1.402053000	0.331722000	1.143609000
H	-1.618856000	1.273876000	1.075200000
O	0.676409000	1.464400000	0.750140000
H	1.334156000	1.524071000	0.040888000
O	-0.105808000	0.022330000	-1.000897000
H	-0.236075000	-0.927748000	-1.140973000

H₂O

H	0.000000000	0.765495000	-0.476696000
O	0.000000000	0.000000000	0.119174000
H	0.000000000	-0.765495000	-0.476696000

H₂

H	0.000000000	0.000000000	0.375975000
H	0.000000000	0.000000000	-0.375975000

TS1

B	-1.271976000	-0.138546000	-0.003006000
H	-0.076626000	1.751846000	0.109994000
H	-1.591359000	0.200215000	1.115323000
H	-1.025348000	-1.315499000	-0.172921000
H	-1.773180000	0.454428000	-0.929032000
O	1.129357000	-0.115432000	-0.114459000
H	0.591916000	0.918974000	-0.008507000
H	1.199622000	-0.393776000	0.815842000

TS2A

B	-1.351502000	0.429057000	0.096492000
H	-2.319352000	0.687183000	-0.615241000
H	-0.051440000	1.532762000	-0.699257000
H	-1.232384000	1.090255000	1.121186000
O	-0.740220000	-0.794156000	-0.061578000
O	1.653799000	0.089728000	0.136955000
H	2.127455000	-0.247187000	-0.641930000
H	0.666251000	1.081695000	-0.430122000
H	0.258352000	-0.654562000	0.179893000

TS3A

B	0.802282000	-0.117036000	0.459892000
H	-0.330113000	-1.452774000	-0.032985000
H	0.815102000	-0.504955000	1.614631000
O	0.050699000	0.974834000	0.014286000
O	-2.280962000	-0.238766000	-0.015100000
H	-2.612316000	-0.258366000	-0.928556000
H	-1.188428000	-1.060224000	-0.049402000
H	-0.935069000	0.738560000	0.063991000
O	2.019432000	-0.359331000	-0.234735000
H	1.926064000	0.109036000	-1.082749000

TS4A

B	0.655673000	-0.004241000	-0.067354000
H	-0.500523000	0.106601000	1.410344000
O	-0.250219000	-0.543430000	-0.973814000
O	-2.475722000	0.154774000	0.279607000
H	-2.920253000	-0.669378000	0.540672000
H	-1.401780000	0.152868000	1.018403000
H	-1.184989000	-0.243222000	-0.734472000
O	1.667174000	-0.858442000	0.471234000
H	1.298229000	-1.754983000	0.452273000
O	1.029421000	1.359650000	-0.142046000
H	1.665718000	1.528904000	0.569701000

TS2B

B	1.010929000	0.675985000	0.153790000
H	1.042152000	1.288517000	1.226340000
H	-3.611247000	-0.092025000	1.076900000
H	1.118257000	1.390455000	-0.856493000
O	1.158037000	-0.690928000	0.097601000
O	-1.100904000	0.005600000	-0.288540000
H	-1.190093000	0.283037000	-1.216012000
H	-2.929775000	-0.062060000	0.713473000
H	0.058996000	-0.705222000	-0.185645000

TS3B

B	-0.669070000	0.069172000	0.472782000
H	-0.431113000	-0.262331000	1.631330000
H	4.005579000	-0.812932000	0.814377000
O	-0.393005000	1.314465000	-0.045647000
O	1.494320000	-0.210048000	-0.271419000
H	1.384126000	-0.662236000	-1.125096000
H	3.305960000	-0.646581000	0.514796000
H	0.599521000	0.989631000	-0.279736000
O	-1.579365000	-0.776403000	-0.213365000
H	-1.694321000	-1.575519000	0.323865000

TS4B

B	0.593895000	0.057311000	-0.140859000
H	-4.227660000	-0.115665000	-0.197595000
O	0.286105000	1.356960000	-0.578994000
O	-1.524837000	-0.061793000	0.585651000
H	-1.566148000	-0.101391000	1.554119000
H	-3.480116000	-0.099663000	0.017812000
H	-0.684625000	1.356770000	-0.411898000
O	1.679694000	-0.034532000	0.758067000
H	1.863044000	-0.984265000	0.838110000
O	0.284061000	-1.151557000	-0.827722000

H	-0.674153000	-1.214970000	-0.592263000
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[BH₂(O)...H₂O...H₂]⁻

B	-1.916453000	-0.007364000	0.648231000
H	-3.130668000	-0.072827000	0.938838000
H	2.483866000	1.947625000	-2.507914000
H	-1.355009000	-1.127340000	0.540695000
O	-1.283486000	1.122461000	0.471467000
O	1.204575000	0.768654000	-0.108027000
H	1.216941000	-0.200601000	-0.091618000
H	2.122925000	1.656438000	-1.899231000
H	0.203719000	0.964610000	0.123951000

[BH(OH)(O)...H₂O...H₂]⁻

B	1.150418000	0.713494000	0.299376000
H	-3.227373000	-2.644192000	-1.703822000
H	0.382347000	1.569082000	0.752414000
O	0.837056000	-0.522604000	-0.007109000
O	-1.610325000	-1.251245000	0.364054000
H	-1.983972000	-0.413162000	0.676092000
H	-2.785346000	-2.282187000	-1.195590000
H	-0.612850000	-0.992837000	0.202682000
O	2.472624000	1.255359000	0.144033000
H	2.991575000	0.511142000	-0.213912000

[B(OH)₂(O)...H₂O...H₂]⁻

B	1.195700000	0.256161000	0.109603000
H	-3.843637000	-1.770090000	1.979487000
O	0.631018000	0.242767000	1.290088000
O	-1.958683000	0.246226000	0.882692000
H	-1.862127000	0.248707000	-0.084036000
H	-3.332903000	-1.270967000	1.704676000
H	-0.963424000	0.242661000	1.149712000
O	2.628340000	0.262685000	-0.116694000
H	3.010018000	0.254179000	0.775161000
O	0.489494000	0.266587000	-1.142710000

H	1.145301000	0.274323000	-1.856905000
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Ag(H₂O)₂⁺

Ag	0.218577000	-1.522749000	3.086410000
O	1.596950000	-3.162389000	2.695666000
H	1.325028000	-3.966484000	2.219764000
H	2.534503000	-3.005979000	2.486398000
O	-1.103443000	0.143678000	3.553024000
H	-1.698753000	0.534253000	2.889647000
H	-1.544201000	0.220746000	4.417354000

Ag(H₂O)(BH₄)

Ag	0.041994000	-0.179685000	3.083687000
O	1.993744000	-0.194461000	1.941603000
H	1.954523000	0.167112000	1.040568000
H	2.739579000	0.249719000	2.378225000
H	-0.776176000	-0.060986000	4.813657000
B	-1.907859000	-0.135806000	4.192997000
H	-1.875111000	-0.237916000	2.906836000
H	-2.461896000	0.916793000	4.417156000
H	-2.414971000	-1.163475000	4.582345000

Ag(BH₄)₂⁻

Ag	0.370886000	-0.245612000	-0.001864000
B	2.299705000	1.075003000	0.000721000
H	2.337941000	-0.198697000	0.010693000
H	1.125835000	1.571263000	-0.010431000
H	2.846158000	1.437435000	-1.028310000
H	2.833267000	1.452826000	1.030987000
H	-0.991830000	-1.177876000	1.069985000
B	-1.554129000	-1.572860000	-0.002962000
H	-0.986122000	-1.183133000	-1.074960000
H	-1.505714000	-2.792132000	0.000107000
H	-2.678658000	-1.099193000	-0.007368000

Ag(H₂O)[BH(OH)₃]

B	-1.129333000	-0.779059000	0.844037000
H	-1.151358000	-0.956937000	2.049987000
H	-1.338539000	-1.844030000	0.240646000
H	-2.338851000	0.026345000	0.936862000
O	-0.072198000	-0.015356000	0.246722000
H	0.227522000	0.678121000	0.851582000
Ag	-3.086742000	-0.612722000	-0.478490000
O	-4.360556000	-1.093140000	-2.286315000
H	-4.756419000	-0.313912000	-2.711656000
H	-3.880223000	-1.565897000	-2.987479000

Ag(H₂O)(H)

H	-4.544275000	-1.243456000	1.982779000
Ag	-4.067901000	-0.792333000	0.523706000
O	-3.377646000	-0.110525000	-1.552080000
H	-3.851207000	0.683517000	-1.853373000
H	-2.434017000	0.123799000	-1.567252000

BH(OH)₂

B	-0.989160000	-0.867566000	0.480042000
H	-1.378085000	-1.960776000	0.167288000
O	-0.853366000	0.079398000	-0.494032000
H	-0.534560000	0.924431000	-0.130267000
O	-0.676840000	-0.535996000	1.780112000
H	-0.808447000	-1.273194000	2.394764000

B(OH)₃

B	-0.179869000	-0.972623000	-1.653618000
O	0.727326000	0.032866000	-1.396099000
H	0.296924000	0.813438000	-1.013518000
O	-1.514446000	-0.787374000	-1.363654000
H	-2.041658000	-1.568765000	-1.592572000
O	0.248091000	-2.163254000	-2.200991000
H	1.205551000	-2.161026000	-2.356316000

TS6

Ag	-0.449622000	-0.099603000	-0.011074000
O	1.464664000	-1.197470000	-0.051021000
H	2.135170000	-0.505977000	-0.424439000
H	1.782923000	-1.244080000	0.868035000
H	-2.024273000	0.250264000	1.090531000
B	-2.595642000	0.692777000	0.034560000
H	-1.870920000	0.730921000	-1.022634000
H	-2.884782000	1.849469000	0.272672000
H	-3.522007000	-0.059557000	-0.205817000
H	2.108012000	1.628427000	0.270402000
B	3.194933000	1.091845000	0.031951000
H	4.049148000	1.924993000	-0.255452000
H	3.084871000	0.362244000	-0.990362000
H	3.560334000	0.401294000	0.993168000

TS7

B	-1.782969000	1.134022000	-0.022232000
H	-0.877612000	-1.614876000	-0.027548000
H	-2.480689000	2.112200000	0.139011000
H	-1.176579000	1.199861000	-1.097517000
H	-0.994997000	1.089716000	0.975052000
O	-2.644612000	-0.153702000	-0.067934000
H	-1.722802000	-1.044200000	-0.037985000
H	-3.184297000	-0.221477000	0.737495000
Ag	0.309523000	-0.245832000	-0.003958000
O	2.524316000	0.515564000	-0.066504000
H	2.604876000	1.444339000	0.207555000
H	3.161735000	0.023537000	0.476622000

TS8

B	-1.869245000	0.115125000	0.599629000
H	0.091515000	-1.938738000	-0.621176000
H	-2.835668000	0.130670000	1.344528000

H	-0.829518000	-0.147990000	1.284581000
O	-2.068716000	-0.989024000	-0.445909000
H	-0.778864000	-1.608101000	-0.602358000
H	-2.721090000	-1.627842000	-0.114969000
Ag	0.827106000	-0.415429000	0.045931000
O	-1.574966000	1.396145000	-0.092499000
H	-2.361197000	1.780205000	-0.506618000
O	0.975663000	1.870391000	-0.074848000
H	1.291681000	2.224627000	-0.921220000
H	-0.040455000	1.916601000	-0.113635000

TS9

B	-0.124550000	0.001646000	0.234211000
H	0.262221000	-0.138747000	1.590796000
O	1.395334000	-0.368660000	-0.190169000
H	1.789686000	0.445292000	-0.558538000
H	1.154421000	-0.250930000	1.004184000
O	-0.376577000	1.350487000	-0.034516000
H	-1.288215000	1.471498000	-0.341653000
O	-1.083002000	-0.941701000	-0.129695000
H	-0.781408000	-1.856356000	-0.030808000

Ag(BH₄)[BH(OH)₃]⁻

B	-1.194736000	-0.831846000	0.773019000
H	-1.036615000	-1.202193000	1.936013000
H	-1.482279000	-1.846255000	0.088473000
H	-2.244390000	-0.021513000	0.923437000
O	-0.063614000	-0.121408000	0.146247000
H	0.250748000	0.552843000	0.764188000
Ag	-3.258517000	-0.799885000	-0.409433000
B	-5.123101000	-1.084700000	-1.783367000
H	-5.062412000	-1.553878000	-0.599023000
H	-4.088604000	-0.436821000	-2.151397000
H	-5.233341000	-2.036690000	-2.538187000
H	-6.055421000	-0.298052000	-1.800897000

TS10

B	-2.456186000	1.112405000	-0.069220000
H	-0.777494000	-1.437179000	-0.165450000
H	-3.004246000	1.696303000	0.860354000
H	-2.808115000	1.494879000	-1.173992000
H	-1.209824000	1.225152000	0.049658000
O	-2.802412000	-0.421291000	0.047079000
H	-1.660595000	-0.991010000	-0.078911000
H	-3.038848000	-0.585868000	0.973368000
Ag	0.492153000	-0.196631000	-0.035168000
B	2.682091000	0.629625000	0.129144000
H	1.977669000	0.338656000	1.151683000
H	2.089893000	0.460807000	-0.987756000
H	2.943259000	1.817820000	0.210367000
H	3.646875000	-0.117721000	0.137324000

Ag(BH₄)[BH₂(OH)₂]⁻

B	-1.359511000	-0.406186000	0.384544000
H	-1.496529000	-1.017753000	-0.711888000
H	-2.528590000	-0.040708000	0.932364000
O	-0.597132000	0.812077000	0.080158000
H	-0.454742000	1.281028000	0.917644000
Ag	-3.613387000	-0.768255000	-0.335981000
B	-5.569673000	-1.375731000	-1.432951000
H	-4.993374000	-2.135414000	-0.584708000
H	-5.007961000	-0.242972000	-1.607792000
H	-5.545012000	-1.954615000	-2.505777000
H	-6.681993000	-1.144751000	-0.990212000
O	-0.802598000	-1.255751000	1.455081000
H	0.020944000	-1.640774000	1.118071000

TS11

B	-2.278466000	0.441496000	0.586422000
H	-0.254408000	-1.465657000	-0.728023000

H	-2.814219000	0.466273000	1.704224000
H	-1.064885000	0.748369000	0.662557000
O	-2.338807000	-1.085165000	0.145559000
H	-1.135952000	-1.299412000	-0.348845000
H	-2.365699000	-1.607134000	0.965072000
Ag	0.830416000	-0.191833000	-0.117160000
B	2.873003000	0.849199000	0.355202000
H	2.308366000	0.051393000	1.174126000
H	2.218252000	1.060861000	-0.720208000
H	2.963351000	1.924711000	0.921328000
H	3.932086000	0.337521000	0.031017000
O	-2.902870000	1.244556000	-0.448076000
H	-3.855717000	1.070633000	-0.442726000

Ag(BH₄)[BH(OH)₃]⁻

B	1.759604000	1.955690000	-0.510133000
O	0.419311000	1.431332000	-1.118279000
H	0.539031000	1.444439000	-2.081298000
Ag	-1.521513000	2.009115000	-0.429114000
B	-3.698601000	2.511706000	0.102015000
H	-3.411308000	2.070733000	-1.055496000
H	-2.708943000	2.656938000	0.908255000
H	-4.163793000	3.627340000	-0.047478000
H	-4.434364000	1.693424000	0.624314000
O	1.916987000	1.358088000	0.806701000
H	1.994103000	0.397871000	0.672966000
O	2.736598000	1.487678000	-1.536549000
H	3.519079000	2.052530000	-1.474531000
H	1.737163000	3.186798000	-0.392248000

TS12

B	2.080120000	0.323911000	0.068151000
H	-0.215227000	-1.768569000	-0.005891000
H	0.904282000	0.759983000	0.145793000
O	2.008305000	-1.203574000	-0.239434000

H	0.705289000	-1.496686000	-0.107019000
H	2.182863000	-1.260799000	-1.196312000
Ag	-1.142457000	-0.251584000	0.024476000
B	-2.990941000	1.170464000	-0.045290000
H	-2.341561000	0.844039000	-1.093817000
H	-2.539065000	0.674418000	1.041804000
H	-2.896759000	2.380383000	0.061931000
H	-4.123746000	0.740786000	-0.183029000
O	2.717584000	0.542091000	1.351543000
H	3.641029000	0.249920000	1.271237000
O	2.810307000	0.841274000	-1.113594000
H	2.642904000	1.790778000	-1.187482000

Ag(BH₄)[B(OH)₄]⁻

B	1.443389000	1.782779000	-0.392310000
O	0.297962000	0.792016000	-0.694250000
H	0.380265000	0.603409000	-1.643527000
Ag	-1.553274000	1.987722000	-0.348377000
B	-3.696305000	2.772350000	-0.011695000
H	-3.183316000	2.644055000	-1.178165000
H	-2.942483000	2.435652000	0.962239000
H	-3.939086000	3.958787000	0.126143000
H	-4.662139000	2.028851000	0.021094000
O	2.061953000	1.432024000	0.889195000
H	2.371206000	0.516234000	0.838283000
O	2.315182000	1.678417000	-1.581717000
H	2.701026000	2.554441000	-1.723798000
O	0.876175000	3.144481000	-0.253839000
H	0.976286000	3.402223000	0.675714000

TS13

B	2.210744000	0.203974000	0.015236000
H	-0.404045000	-1.785548000	0.263677000
O	1.853223000	-1.317202000	0.056177000
H	0.509539000	-1.497774000	0.171076000

H	2.089853000	-1.640667000	-0.830389000
Ag	-1.329425000	-0.299757000	0.026663000
B	-3.139298000	1.165911000	-0.116616000
H	-2.682736000	0.520691000	-1.121352000
H	-2.549927000	0.923785000	0.987520000
H	-2.977200000	2.349745000	-0.357855000
H	-4.298438000	0.813364000	0.021105000
O	2.794330000	0.606640000	1.287165000
H	3.738141000	0.393141000	1.261867000
O	3.129636000	0.299698000	-1.141298000
H	2.848764000	1.076706000	-1.646669000
O	0.965630000	0.966637000	-0.200785000
H	0.909227000	1.639535000	0.494683000

Ag[B(OH)₄][BH₃(OH)]⁻

Ag	1.135437000	-0.017129000	-0.336633000
B	2.680779000	1.801279000	-0.360247000
H	2.829622000	0.465583000	-0.595372000
H	1.628716000	2.075571000	0.247016000
H	3.628426000	1.929110000	0.414215000
B	-0.926307000	-2.079178000	0.371732000
O	-2.279347000	-2.189801000	0.929067000
H	-2.384461000	-1.490160000	1.589992000
O	-0.544181000	-3.376599000	-0.204287000
H	-1.228512000	-4.003259000	0.074458000
O	-0.843109000	-1.010232000	-0.723235000
O	0.057798000	-1.572775000	1.383712000
H	-0.935755000	-1.462661000	-1.574852000
H	0.640432000	-2.313821000	1.604964000
O	2.754219000	2.554089000	-1.622501000
H	3.645293000	2.456396000	-1.985569000

TS15

B	-3.344190000	1.281455000	-0.086416000
H	-1.952145000	-1.455693000	-0.027696000

H	-3.798665000	1.988392000	0.806785000
H	-3.679426000	1.616821000	-1.210773000
H	-2.086064000	1.276184000	0.002292000
O	-3.846302000	-0.190526000	0.153501000
H	-2.779943000	-0.899346000	0.039731000
H	-4.065430000	-0.262301000	1.095944000
Ag	-0.612099000	-0.307175000	-0.071781000
B	2.323953000	0.184767000	0.049136000
O	3.026354000	-1.105107000	-0.002801000
H	3.972498000	-0.899280000	0.031328000
O	3.332432000	1.250515000	0.096954000
H	2.874100000	2.099925000	0.175457000
O	1.359524000	0.245180000	1.211707000
O	1.380030000	0.335950000	-1.130863000
H	1.656510000	-0.411745000	1.858092000
H	1.712070000	-0.234908000	-1.839067000

Ag[B(OH)₄][BH₂(OH)₂]⁻

Ag	1.146203000	-0.067107000	-0.525253000
B	2.682219000	1.813311000	-0.442518000
H	2.692539000	0.559664000	-1.031138000
H	1.618239000	2.106103000	0.134306000
B	-0.885171000	-2.049607000	0.389988000
O	-2.214465000	-2.113463000	1.005385000
H	-2.311247000	-1.344044000	1.584998000
O	-0.510793000	-3.392362000	-0.071790000
H	-1.181735000	-3.994861000	0.282489000
O	-0.845950000	-1.086144000	-0.800510000
O	0.132612000	-1.438909000	1.310736000
H	-0.947048000	-1.618322000	-1.603669000
H	0.717613000	-2.151380000	1.606917000
O	2.864628000	2.757848000	-1.546788000
H	3.738713000	2.584724000	-1.931559000
O	3.835455000	1.664012000	0.464237000
H	3.814223000	2.405154000	1.087904000

TS16

B	3.181662000	0.702751000	0.599508000
H	1.497367000	-1.706456000	-0.401707000
H	3.618543000	0.987547000	1.712727000
H	1.923255000	0.797290000	0.581675000
O	3.487024000	-0.803360000	0.309350000
H	2.340203000	-1.306017000	-0.088637000
H	4.042051000	-0.759625000	-0.491382000
Ag	0.280387000	-0.461178000	-0.102653000
B	-2.585237000	0.319106000	0.058132000
O	-3.398974000	-0.760277000	-0.517778000
H	-4.321309000	-0.473534000	-0.441748000
O	-3.486413000	1.409189000	0.451137000
H	-2.963267000	2.088447000	0.901326000
O	-1.520663000	0.774278000	-0.925896000
O	-1.734416000	-0.171535000	1.206479000
H	-1.840916000	0.565357000	-1.815529000
H	-2.149681000	-0.979138000	1.542447000
O	3.802170000	1.468261000	-0.502037000
H	4.503613000	2.019769000	-0.132710000

Ag[B(OH)₄][BH(OH)₃]⁻

Ag	1.136098000	-0.019463000	0.141861000
B	3.538255000	1.942649000	-0.499899000
H	3.568114000	1.795607000	0.732998000
B	-0.799706000	-2.343729000	0.488906000
O	-2.139247000	-2.248102000	1.060533000
H	-2.670262000	-1.727115000	0.441382000
O	-0.298516000	-3.729982000	0.489398000
H	-1.055662000	-4.287617000	0.720611000
O	-0.770311000	-1.713838000	-0.859303000
O	0.207865000	-1.542985000	1.361584000
H	-0.297024000	-2.323253000	-1.445194000
H	0.836058000	-2.194110000	1.712026000

O	3.854563000	3.312294000	-0.940796000
H	3.401729000	3.934571000	-0.353723000
O	4.371409000	1.017851000	-1.268532000
H	5.085419000	1.548975000	-1.652640000
O	2.045910000	1.622423000	-0.862026000
H	2.039765000	1.497618000	-1.828819000

TS17

B	-2.958077000	0.566125000	0.065780000
H	-1.133362000	-1.958306000	-0.385743000
H	-1.706002000	0.651341000	0.283137000
O	-3.136611000	-0.817953000	-0.613232000
H	-1.963803000	-1.453891000	-0.470304000
H	-3.822271000	-1.269570000	-0.089483000
Ag	0.006314000	-0.660549000	-0.003912000
B	2.758270000	0.457130000	0.032826000
O	3.714554000	-0.603985000	-0.306194000
H	4.592278000	-0.194051000	-0.290186000
O	3.512521000	1.676277000	0.338648000
H	2.884260000	2.404039000	0.453923000
O	1.869502000	0.019878000	1.190076000
O	1.738004000	0.667063000	-1.061996000
H	2.354926000	-0.658376000	1.682343000
H	2.120825000	0.311102000	-1.877146000
O	-3.776706000	0.489456000	1.276008000
H	-4.133618000	1.376686000	1.428866000
O	-3.401195000	1.663346000	-0.789008000
H	-2.651496000	1.967902000	-1.319010000

Ag[B(OH)₄]₂⁻

Ag	1.027207000	-0.243420000	-0.298514000
B	3.060180000	1.926957000	-0.612750000
B	-1.107563000	-2.204617000	0.419931000
O	-2.423490000	-2.266786000	1.066764000
H	-2.443179000	-1.593146000	1.761812000

O	-0.835313000	-3.496880000	-0.226902000
H	-1.539341000	-4.094961000	0.065231000
O	-1.040706000	-1.100743000	-0.638862000
O	-0.030582000	-1.796160000	1.384153000
H	-1.179160000	-1.528515000	-1.497298000
H	0.503945000	-2.584746000	1.558090000
O	3.022972000	2.462140000	-1.982302000
H	3.679488000	3.174179000	-2.007852000
O	4.204514000	2.511149000	0.096324000
H	4.008869000	2.481617000	1.043981000
O	1.776340000	2.139669000	0.134737000
H	1.260288000	2.785411000	-0.369773000
O	3.155346000	0.399083000	-0.690998000
H	3.494655000	0.186942000	-1.573621000

TS18

B	-2.280868000	0.816350000	-0.018126000
H	-1.408197000	-2.359274000	0.369667000
O	-3.060186000	-0.474225000	0.198553000
H	-1.931623000	-1.670807000	0.304016000
H	-3.527368000	-0.360157000	1.041305000
Ag	-0.011420000	-1.254559000	-0.031186000
B	2.359417000	0.793938000	-0.023148000
O	3.053350000	1.015460000	1.275799000
H	3.545125000	1.845533000	1.195907000
O	3.159401000	1.103641000	-1.200608000
O	1.091127000	1.503262000	-0.154260000
O	2.111821000	-0.765167000	0.035280000
H	0.590714000	1.473233000	0.682917000
H	2.523303000	-1.046515000	0.868988000
O	-1.585414000	1.162753000	1.251572000
H	-1.729015000	2.111862000	1.389492000
O	-3.157213000	1.948082000	-0.359662000
H	-3.368948000	1.871462000	-1.301691000
O	-1.339270000	0.454421000	-1.111427000

H	-0.561924000	1.057513000	-1.074364000
H	3.823009000	0.404192000	-1.286086000

Ag[BH₃(OH)]₂⁻

B	-1.217035000	-0.824432000	0.723514000
H	-1.090857000	-1.221567000	1.880917000
H	-1.542120000	-1.826977000	0.024676000
H	-2.224895000	0.029138000	0.852858000
O	-0.039975000	-0.173814000	0.115388000
H	0.308821000	0.469190000	0.748002000
Ag	-3.230621000	-0.770618000	-0.508421000
B	-5.250112000	-1.149454000	-1.678466000
H	-5.187308000	-1.460532000	-0.455432000
H	-4.217847000	-0.397733000	-2.045818000
H	-6.175396000	-0.346932000	-1.796101000
O	-5.333287000	-2.380430000	-2.487049000
H	-5.540673000	-2.131017000	-3.398131000

TS20

B	-2.866178000	1.034213000	-0.021430000
H	-1.093953000	-1.452957000	-0.106837000
H	-3.397621000	1.640034000	0.903219000
H	-3.282863000	1.344902000	-1.125925000
H	-1.621572000	1.205053000	0.034411000
O	-3.140141000	-0.505277000	0.185016000
H	-1.993260000	-1.035154000	0.014552000
H	-3.313571000	-0.635248000	1.130705000
Ag	0.118225000	-0.152875000	-0.109812000
B	2.300809000	0.743098000	0.188054000
H	1.556019000	0.585315000	1.197571000
H	1.619064000	0.626977000	-0.943189000
H	2.614735000	1.931706000	0.157471000
O	3.405748000	-0.234500000	0.250874000
H	4.058411000	0.006154000	-0.421038000

Ag[BH₃(OH)][BH₂(OH)₂]⁻

B	-1.298356000	-0.655707000	0.685645000
H	-1.476303000	-1.492032000	-0.279981000
H	-2.366245000	0.076011000	0.914027000
O	-0.188624000	0.197018000	0.231805000
H	-0.014568000	0.841680000	0.935561000
Ag	-3.341402000	-0.798932000	-0.469105000
B	-5.373541000	-1.314773000	-1.535036000
H	-5.127415000	-1.829314000	-0.406025000
H	-4.527606000	-0.327155000	-1.822320000
H	-6.425319000	-0.688608000	-1.418266000
O	-5.338961000	-2.368070000	-2.565725000
H	-5.699352000	-2.001886000	-3.385070000
O	-1.091347000	-1.344054000	1.971278000
H	-0.338275000	-1.944927000	1.860073000

TS21

B	-2.628373000	0.457809000	0.605832000
H	-0.627754000	-1.496664000	-0.680693000
H	-3.142820000	0.521604000	1.731437000
H	-1.414712000	0.771883000	0.647030000
O	-2.689878000	-1.086196000	0.223823000
H	-1.507241000	-1.316255000	-0.287540000
H	-2.695832000	-1.577441000	1.062631000
Ag	0.450108000	-0.179104000	-0.164894000
B	2.540537000	0.751262000	0.477071000
H	1.881208000	0.099838000	1.334710000
H	1.801719000	1.047823000	-0.587923000
H	2.731424000	1.872263000	0.943885000
O	-3.275479000	1.218533000	-0.445929000
H	-4.227986000	1.045937000	-0.412863000
O	3.736557000	-0.025468000	0.097868000
H	4.316489000	0.548573000	-0.421288000

Ag[BH₂(OH)₂]₂⁻

B	-1.354213000	-0.663834000	0.704273000
H	-1.500767000	-1.529093000	-0.247905000
H	-2.444227000	0.039154000	0.913393000
O	-0.266785000	0.207302000	0.234033000
H	-0.119393000	0.880633000	0.916646000
Ag	-3.363941000	-0.899031000	-0.468757000
B	-5.344613000	-1.281797000	-1.650977000
H	-5.055657000	-1.905568000	-0.551115000
H	-4.411917000	-0.428996000	-2.000968000
O	-5.463419000	-2.355136000	-2.649225000
H	-5.677138000	-1.938043000	-3.498526000
O	-1.132197000	-1.322698000	2.001607000
H	-0.348720000	-1.886813000	1.908953000
O	-6.531175000	-0.426918000	-1.484242000
H	-7.260190000	-0.997598000	-1.195138000

TS22

B	-2.749350000	0.740946000	0.502187000
H	-1.080590000	-1.673955000	-0.391919000
H	-3.179354000	1.109065000	1.603007000
H	-1.504060000	0.893616000	0.433946000
O	-3.017988000	-0.831099000	0.474015000
H	-1.922984000	-1.306500000	-0.007329000
H	-3.024375000	-1.126237000	1.400435000
Ag	0.157590000	-0.427707000	-0.142392000
B	2.375624000	0.359429000	0.102431000
H	1.667781000	-0.041142000	1.108178000
H	1.700354000	0.323712000	-1.021477000
O	-3.361705000	1.332664000	-0.668697000
H	-4.324119000	1.311496000	-0.562545000
O	3.502140000	-0.588087000	0.055638000
H	4.073472000	-0.316988000	-0.680165000
O	2.736653000	1.778330000	0.227371000
H	3.182985000	1.892806000	1.080566000

Ag[BH₂(OH)₂][BH₃(OH)]⁻

B	-1.817630000	-1.191524000	-0.023318000
H	-2.519129000	-2.308723000	0.017030000
H	-2.554096000	-0.160281000	-0.233448000
O	-0.884720000	-1.440495000	-1.136230000
H	-0.366233000	-0.631336000	-1.265864000
Ag	-4.143671000	-1.408747000	-0.315782000
B	-6.408876000	-1.353185000	-0.944556000
H	-5.905704000	-1.435664000	0.285106000
H	-5.536378000	-1.603382000	-1.825585000
H	-7.186855000	-2.305450000	-0.936331000
O	-1.196194000	-0.947237000	1.287261000
H	-0.616785000	-1.702227000	1.475718000
O	-6.990199000	-0.022951000	-1.200667000
H	-7.767436000	0.081891000	-0.634827000

TS23

B	-2.926457000	1.273158000	-0.013081000
H	-1.549641000	-1.444589000	-0.181100000
H	-3.360744000	1.911087000	0.938793000
H	-3.284963000	1.686369000	-1.102755000
H	-1.669182000	1.249211000	0.047567000
O	-3.432389000	-0.216061000	0.131285000
H	-2.395405000	-0.895677000	-0.046082000
H	-3.637385000	-0.354005000	1.069675000
Ag	-0.179950000	-0.323932000	-0.079467000
B	2.120210000	0.228401000	0.051733000
H	1.341684000	0.123384000	1.087378000
H	1.475734000	0.043140000	-1.065011000
O	3.124058000	-0.830257000	0.261518000
H	3.739490000	-0.792467000	-0.487502000
O	2.649762000	1.593568000	-0.077050000
H	3.097820000	1.812532000	0.754689000

TS24

B	-2.749350000	0.740946000	0.502187000
H	-1.080590000	-1.673955000	-0.391919000
H	-3.179354000	1.109065000	1.603007000
H	-1.504060000	0.893616000	0.433946000
O	-3.017988000	-0.831099000	0.474015000
H	-1.922984000	-1.306500000	-0.007329000
H	-3.024375000	-1.126237000	1.400435000
Ag	0.157590000	-0.427707000	-0.142392000
B	2.375624000	0.359429000	0.102431000
H	1.667781000	-0.041142000	1.108178000
H	1.700354000	0.323712000	-1.021477000
O	-3.361705000	1.332664000	-0.668697000
H	-4.324119000	1.311496000	-0.562545000
O	3.502140000	-0.588087000	0.055638000
H	4.073472000	-0.316988000	-0.680165000
O	2.736653000	1.778330000	0.227371000
H	3.182985000	1.892806000	1.080566000

Ag[BH₂(OH)₂](H)⁻

Ag	0.628265000	-0.129093000	0.402833000
H	-0.983351000	-0.643885000	-0.080929000
B	-1.893765000	-1.701008000	-0.438831000
H	-1.880617000	-1.604615000	-1.662453000
H	2.142337000	0.360302000	0.857441000
O	-3.172837000	-1.352205000	0.119481000
H	-3.146278000	-1.609177000	1.055879000
O	-1.376485000	-2.931627000	0.156342000
H	-0.429246000	-3.003046000	-0.035088000

TS25

B	2.555059000	0.495688000	0.028427000
H	0.655436000	-1.948221000	0.018538000
H	1.324061000	0.719078000	0.169260000
O	2.728767000	-1.020977000	-0.317737000
H	1.534210000	-1.523861000	-0.130801000

H	2.854026000	-1.029709000	-1.284265000
Ag	-0.474221000	-0.585139000	0.095517000
B	-2.558091000	0.511049000	-0.062592000
H	-1.794519000	0.339648000	-1.091339000
H	-2.015062000	0.043776000	1.041304000
O	3.204181000	0.792360000	1.286636000
H	4.161241000	0.687972000	1.154450000
O	3.125170000	1.148981000	-1.170195000
H	2.780200000	2.050650000	-1.224615000
O	-2.744538000	1.935728000	0.242843000
H	-3.089982000	2.363346000	-0.555986000
O	-3.777869000	-0.243899000	-0.387817000
H	-4.391760000	-0.132363000	0.355147000

Ag[BH(OH)₃](H)⁻

B	2.298882000	-0.333485000	0.007837000
H	0.882927000	-0.463246000	-0.390047000
O	2.248922000	-0.099499000	1.426174000
H	1.857392000	-0.881134000	1.844585000
Ag	-0.808493000	-0.620020000	-0.811409000
O	2.778424000	0.785896000	-0.757735000
H	2.294317000	1.574426000	-0.469279000
O	2.883921000	-1.594270000	-0.362753000
H	2.826725000	-1.678279000	-1.326624000
H	-2.410186000	-0.771360000	-1.211569000

Ag[BH₂(OH)₂](OH)⁻

Ag	-1.874139000	1.872862000	0.469884000
B	-4.390687000	2.003180000	0.106981000
H	-3.216901000	2.601139000	-0.307066000
H	-4.247081000	1.005927000	0.817515000
O	-5.045309000	1.594929000	-1.139940000
H	-5.236046000	2.404763000	-1.640180000
O	-5.014623000	3.158080000	0.787127000
H	-5.761691000	2.816945000	1.301011000

O	-0.031491000	1.270232000	1.201670000
H	-0.175612000	0.385190000	1.576262000

TS26

Ag	-1.215743000	-0.285951000	-0.031386000
B	2.024542000	-0.233360000	0.395391000
H	0.889788000	-0.773763000	0.214071000
H	2.114138000	0.210656000	1.551993000
O	2.129970000	1.007123000	-0.513482000
H	2.128981000	0.671088000	-1.425405000
O	3.038913000	-1.239693000	0.040204000
H	3.895706000	-0.919640000	0.360878000
H	-2.501009000	-1.275366000	-0.253056000
O	-0.194758000	1.877134000	0.224100000
H	-0.039693000	1.896712000	1.183271000
H	0.736316000	1.640285000	-0.140144000

TS27

Ag	0.597166000	-0.164667000	-0.109609000
B	-1.775093000	0.101982000	0.170599000
H	-1.012501000	-0.100163000	-0.923814000
H	-1.119422000	0.135050000	1.245458000
O	-2.703203000	-1.032828000	0.286081000
H	-3.239044000	-1.048593000	-0.522809000
O	-2.400617000	1.397268000	-0.167160000
H	-2.911332000	1.678080000	0.607752000
H	2.120803000	-1.592802000	0.190450000
O	2.800790000	0.624468000	0.177803000
H	2.535117000	-0.756782000	0.255097000
H	2.859291000	1.003398000	1.072715000

TS28

B	2.044679000	-0.020912000	-0.230752000
H	-0.661324000	0.973464000	1.154891000
H	1.036454000	-0.171282000	-0.946600000

O	1.609207000	0.329355000	1.210802000
H	0.184632000	0.667527000	1.121248000
H	1.652092000	-0.519138000	1.685801000
Ag	-1.577231000	-0.009742000	-0.062964000
O	2.830249000	1.079578000	-0.783426000
H	3.610201000	1.179983000	-0.211437000
O	2.804624000	-1.292319000	-0.032440000
H	2.860607000	-1.739988000	-0.887896000
H	-2.728815000	-0.761037000	-0.962413000

TS29

Ag	-1.410516000	-0.258699000	0.006468000
B	1.783454000	-0.302343000	0.024383000
H	0.621702000	-0.837148000	0.096609000
O	1.916979000	0.558331000	-1.187938000
H	2.071951000	-0.026519000	-1.945136000
O	2.830062000	-1.335241000	-0.038877000
H	2.627897000	-2.000059000	0.635856000
H	-2.814516000	-1.107076000	-0.031794000
O	-0.192350000	1.865922000	-0.033574000
H	0.439972000	1.625967000	0.695883000
H	0.395515000	1.623476000	-0.791254000
O	1.858682000	0.582487000	1.225814000
H	2.727503000	1.019931000	1.190535000

Ag(H)₂⁻

H	0.699566000	-0.667403000	-0.546862000
Ag	-0.810494000	-1.122758000	-1.175232000
H	-2.319915000	-1.576479000	-1.805454000

OH⁻

O	0.561552000	0.485968000	-1.608050000
H	0.729995000	0.736781000	-0.681458000

Ag(BH₄)(H)⁻

Ag	0.412190000	-0.219536000	-0.001707000
H	-1.001368000	-1.185730000	1.053485000
B	-1.571236000	-1.584698000	-0.003019000
H	-0.995656000	-1.190950000	-1.058481000
H	-1.534440000	-2.808537000	0.000035000
H	-2.702889000	-1.117287000	-0.007330000
H	1.771927000	0.716830000	-0.000095000

TS32

B	1.901696000	0.073952000	-0.306558000
O	1.118371000	-0.191980000	1.000165000
H	1.335225000	-1.106058000	1.249923000
Ag	-0.901207000	-0.010398000	0.070021000
B	-3.143263000	0.075329000	-0.451510000
H	-2.486317000	-1.022526000	-0.452382000
H	-2.471229000	1.121929000	-0.153736000
H	-3.544864000	0.236744000	-1.590352000
H	-4.005200000	-0.038104000	0.403074000
O	2.643202000	1.326524000	-0.211905000
H	3.152945000	1.290026000	0.615857000
O	2.748480000	-1.134659000	-0.441719000
H	3.432156000	-0.942806000	-1.099719000
H	1.071430000	0.204021000	-1.245648000

Ag[BH₃(OH)](H)⁻

Ag	0.356713000	-0.176266000	0.188393000
H	-0.915873000	-1.297891000	0.945528000
B	-1.605430000	-1.658913000	-0.122027000
H	-0.993065000	-1.380368000	-1.169526000
H	-1.618657000	-2.887462000	0.016248000
H	1.639762000	0.851144000	0.049320000
O	-2.934966000	-0.999993000	-0.133234000
H	-3.438802000	-1.331962000	0.622564000

TS33

B	2.518957000	0.861857000	0.049317000
H	0.308456000	-1.266133000	0.491345000
H	3.215694000	1.261420000	-0.887129000
H	2.964993000	1.194946000	1.142922000
H	1.348307000	1.268722000	-0.087269000
O	2.494389000	-0.710821000	0.004286000
H	1.181315000	-1.012545000	0.280139000
H	2.582527000	-0.959254000	-0.928879000
Ag	-0.890890000	0.001724000	0.001927000
H	-2.279348000	0.809084000	-0.382585000

TS34

B	-2.222223000	-0.224223000	0.562259000
H	0.288099000	1.402059000	-0.447655000
H	-2.708496000	-0.148132000	1.695739000
H	-1.110601000	-0.785109000	0.567912000
O	-1.977324000	1.236673000	0.048233000
H	-0.597497000	1.291603000	-0.227014000
H	-2.396050000	1.218510000	-0.831652000
Ag	1.276726000	-0.058790000	-0.016524000
O	-3.131204000	-0.878314000	-0.417510000
H	-4.026630000	-0.849237000	-0.054667000
H	2.524409000	-1.112324000	0.216892000

Ag₂(BH₄)(H)₂⁻

H	-0.167976000	1.877642000	-2.453410000
Ag	-1.296975000	0.842877000	-1.807080000
H	-2.734812000	-0.120876000	-1.327546000
Ag	-2.239597000	-1.243831000	-0.134646000
H	-1.100344000	-2.176325000	1.113606000
B	-2.065299000	-2.934250000	1.477042000
H	-3.163064000	-2.705745000	0.885433000
H	-2.236306000	-2.720981000	2.665250000
H	-1.727519000	-4.071598000	1.196345000

Ag₂(H)₄²⁻

H	0.139798000	-0.744903000	-0.973236000
Ag	-1.317953000	-1.029994000	-1.918539000
H	-2.457535000	-1.003611000	-3.202910000
H	0.516875000	-1.943049000	2.028099000
Ag	-0.624834000	-1.914938000	0.745469000
H	-2.083679000	-2.198285000	-0.198812000

Ag₂(H₂O)(H)₂⁻

H	-0.722843000	1.601102000	-0.935061000
Ag	-1.741866000	0.398486000	-0.461483000
H	-3.033107000	-0.757712000	0.147928000
Ag	-2.400319000	-2.263543000	-0.210293000
O	-1.640740000	-4.346657000	-0.649295000
H	-1.244951000	-4.436299000	-1.533214000
H	-0.969331000	-4.670402000	-0.024724000

Ag₂[BH(OH)₃]₂(H)₂²⁻

B	2.992678000	-1.065381000	-0.292318000
H	1.791019000	-0.493446000	-0.464816000
O	2.718932000	-2.425073000	0.242757000
H	1.748500000	-2.533580000	0.265737000
Ag	-0.229517000	-0.794239000	-0.390357000
O	3.795838000	-0.266629000	0.647311000
H	3.540128000	-0.611376000	1.515880000
O	3.693146000	-1.072220000	-1.590254000
H	3.187974000	-1.689405000	-2.140156000
H	-0.401402000	-2.401335000	0.141319000
B	-5.353213000	2.041680000	-1.310443000
H	-4.087561000	1.330172000	-1.151703000
O	-6.326880000	1.128777000	-0.759349000
H	-6.090200000	0.971843000	0.167525000
Ag	-2.387411000	0.907878000	-0.983245000
O	-5.494572000	2.243817000	-2.732678000
H	-5.498145000	1.370525000	-3.153419000

O	-5.211608000	3.264319000	-0.556946000
H	-4.443452000	3.739650000	-0.908722000
H	-0.634524000	0.871935000	-0.947482000