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SUPPLEMENTARY MATERIAL ACCOMPANIING THE MANUSCRIPT ENTITLED

"Can alumina particles be formed from Al hydroxide in the circumstellar media? A first-principles chemical study" Sonia Álvarez-Barcia and Jesús R. Flores

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SM_F1. Formation and evolution of $Al_2O \cdot H_2O$. Numbers in brackets are relative energies with respect to 2 AlOH.

PAGE 2

Coordinates of structures (angstroms) optimized at the M06/CEP-31G* for the $(HAlO)_2$ system. See Figures 2 and 3 of the main text and SM_F1.

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Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the $(HAlO)_2 \cdot H_2O$ system. See Figure 4 (a and b), Figure 5 and P1 + H reaction of the main text.

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Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the $(HAlO)_2 \cdot 2H_2O$ systems. See Figures 6-10 of the main text.

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Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the structures in Figures 12-13 of the main text and SM_F2.

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Table SM_T1. Absolute energies, ZPE energies and energy differences relative to 2 AlOH + *n* H_2O, with *n*=0-2.

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Table SM_T2. Absolute energies, ZPE energies and energy differences relative to P1 + H.

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Table SM_T3. Absolutes energies, ZPE energies and energy differences relative to reactants for the reactions shown in fig. 12-13 of the main text. See also SM_F2.

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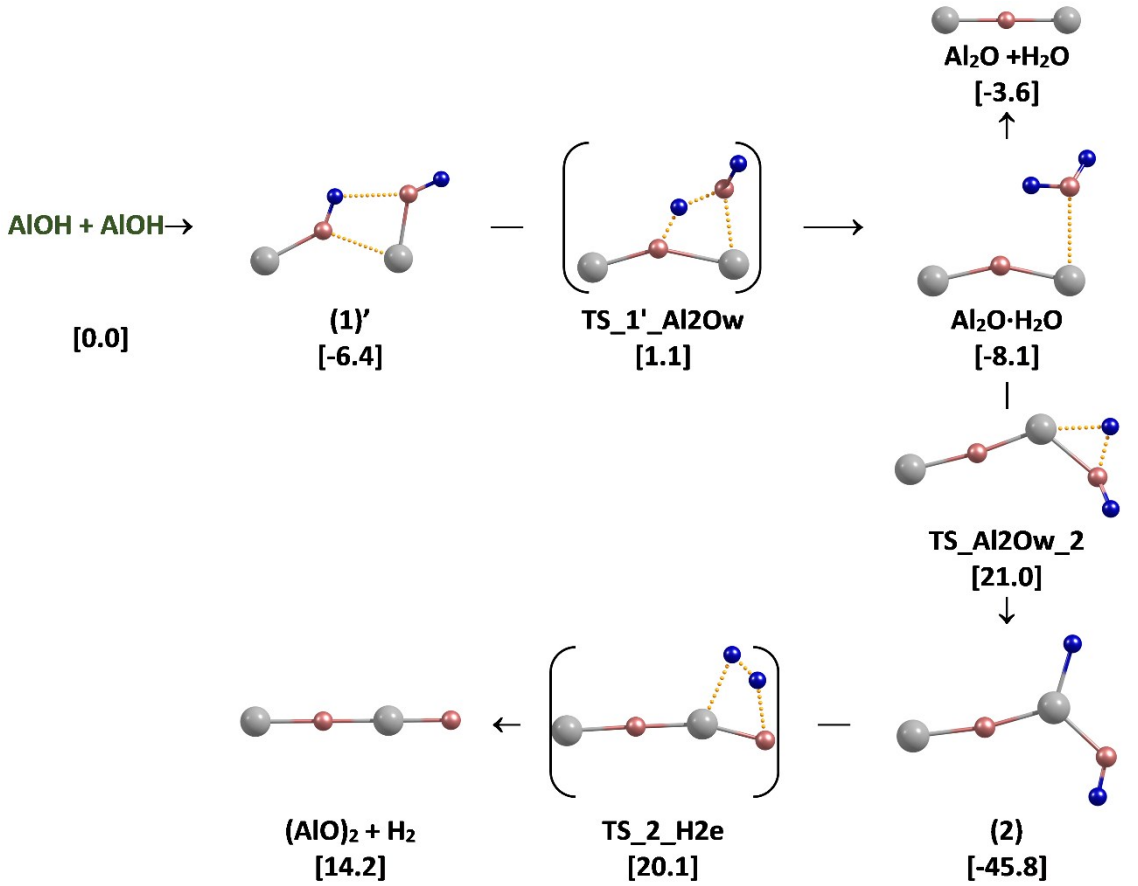
Figure SM_F2. Some structures resulting from the coalescence of $Al(OH)_2$ dimers. Numbers in brackets are relative energies with respect to 2 $Al(OH)_2$. The structure on the left is a minimum on the triplet electronic state and the other are singlets. The most stable of the four has syn isomer (-98.9) and a H migration isomer with a Al-H bond (-100.5 kcal/mol). See also fig. 13 c in the main text.

SM_F1. Formation and evolution of $Al_2O \cdot H_2O$. Numbers in brackets are relative energies with respect to 2 AlOH.



Coordinates of structures (angstroms) optimized at the M06/CEP-31G* for the $(HAlO)_2$ system. See Figures 2 and 3 of the main text and SM_F1. (Standard G09 convergence criteria or stiffer ones have been used. The G09 ultrafine grid has been used for the DFT computations).

(1)

1	0.432451000	-2.494298000	0.005581000
8	0.257527000	-1.541531000	-0.031744000
13	-1.463791000	-0.677270000	-0.196656000
1	-0.338256000	1.705346000	-0.160303000
8	-0.163642000	0.752545000	-0.123060000
13	1.556601000	-0.111869000	0.042110000

TS_1_2

1	0.864789000	-2.724835000	0.023987000
8	0.337969000	-1.914117000	0.011464000
13	-1.871660000	1.760289000	-0.047910000
1	0.966500000	1.388527000	-0.040151000
8	-0.300411000	0.946444000	-0.033133000
13	1.008278000	-0.334648000	-0.012477000

(2)

1	-0.687562000	-2.586709000	1.081466000
8	-0.100799000	-1.934546000	0.675952000
13	-0.635833000	-0.341426000	0.365579000
1	-2.114792000	0.102167000	0.738486000
8	0.470177000	0.725659000	-0.347847000
13	1.875926000	1.424033000	-1.043949000

TS_2_3

1	1.305694000	1.427601000	-0.643542000
8	0.041262000	1.272757000	0.108399000
13	-1.194010000	0.014571000	-0.018637000
1	-2.765654000	0.044662000	-0.163840000
8	-0.024999000	-1.269452000	0.016504000
13	1.296306000	-0.129856000	0.003880000

(3)

1	2.784840000	0.106072000	0.117938000
8	0.269321000	-1.625331000	-0.014012000
13	-1.136648000	-0.598313000	-0.155992000
1	-2.683356000	-0.876113000	-0.264031000
8	-0.167781000	0.855041000	-0.131959000
13	1.238192000	-0.171966000	0.009990000

(1)'

1	-0.028316000	-1.210680000	0.001833000
8	-0.560877000	-0.384478000	0.002164000
13	1.226991000	0.856611000	0.000148000
1	2.861504000	-0.952406000	-0.002053000
8	1.909668000	-0.780038000	-0.000895000
13	-2.274954000	0.026405000	-0.000912000

TS_1'_1"

1	0.395712000	1.848727000	0.053959000
8	0.528836000	0.884832000	-0.015441000
13	-0.770252000	-0.626571000	-0.025096000
1	-2.899689000	0.659511000	-0.460723000
8	-2.283825000	0.170221000	0.095138000
13	2.042859000	-0.215634000	0.007341000

(1)"

1	-0.090126000	-1.348468000	0.432922000
8	-0.231583000	-1.635051000	-0.488871000
13	-0.058068000	-3.328651000	-1.529666000
1	0.674262000	-4.381895000	0.552768000
8	0.484989000	-4.495237000	-0.388183000
13	-0.817490000	-0.660448000	-1.995951000

Al_2O

13	-2.155701000	-0.155783000	0.000000000
8	-0.506436000	0.337541000	0.000000000
13	1.142828000	0.830866000	0.000000000

TS_1'_Al_2Ow

1	0.361308000	-2.402843000	-0.774915000
8	0.390139000	-1.696457000	-0.112145000
13	-1.204683000	1.857287000	0.157585000
1	-0.274978000	-0.650237000	-0.182186000
8	-0.106731000	0.508864000	0.004251000
13	1.686341000	-0.279333000	0.158681000

$Al_2O{\cdot}H_2O$

1	0.291204000	-2.662267000	-0.325096000
8	0.366268000	-1.753917000	-0.662290000
13	-1.102060000	1.992462000	0.317050000
1	-0.451122000	-1.272769000	-0.422075000
8	0.053164000	0.732882000	0.159414000
13	1.679800000	0.049867000	0.099415000

TS_Al_2Ow_2

1	2.012313000	-1.747582000	-0.222468000
8	0.786654000	-1.820887000	-0.729771000
13	-0.959835000	2.365476000	0.440845000
1	0.135003000	-2.540944000	-0.573945000
8	0.085227000	1.022561000	0.190497000
13	1.283329000	-0.160176000	-0.074251000

TS_2_H_2e

1	-1.744942000	-2.222941000	-1.028376000
8	-1.734884000	-1.941704000	0.468423000
13	-0.641970000	-1.029026000	-0.329440000
1	-1.352300000	-1.984916000	-1.810908000
8	0.563882000	0.070670000	-0.695724000
13	1.820374000	1.214791000	-1.043450000

$(AlO)_2$

8	0.000000000	0.000000000	-2.685751000
13	0.000000000	0.000000000	-1.083844000
8	0.000000000	0.000000000	0.589470000
13	0.000000000	0.000000000	2.326539000

Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the $(HAlO)_2 \cdot H_2O$ system. See Figure 4 (a and b), Figure 5 and P1 + H reaction of the main text. (Standard G09 convergence criteria or stiffer ones have been used. The G09 ultrafine grid has been used for the DFT computations)

(1)_w1

1	2.741810000	0.819212000	0.010249000
8	1.833851000	0.481343000	0.008194000
13	1.252606000	-1.379668000	-0.007746000
1	-1.303606000	-0.601133000	-0.011861000
8	-0.352926000	-0.347358000	0.000223000
13	0.187525000	1.471340000	0.007856000
8	-3.137017000	-0.339588000	-0.045749000
1	-3.585313000	-0.256656000	0.810962000
1	-3.325869000	0.491670000	-0.512125000

TS_1w1_2w1

1	0.223438000	-2.759964000	0.161370000
8	0.000878000	-1.819772000	0.137695000
13	-1.762648000	0.776460000	0.142144000
1	0.932299000	1.775247000	-0.347041000
8	-0.018501000	0.892690000	-0.067964000
13	1.136789000	-0.535136000	-0.138372000
8	1.988808000	2.094625000	-0.616810000
1	2.388259000	2.564224000	0.141699000
1	2.345211000	0.932085000	-0.542460000

(2)_w1_a

1	-2.023778000	2.090902000	-0.290296000
8	-1.236111000	1.571289000	-0.495043000
13	2.459722000	0.037754000	-0.137869000
1	-0.685084000	-1.892359000	-0.669037000
8	0.826149000	-0.327226000	0.215583000
13	-0.790364000	0.230772000	0.489182000
8	-1.526995000	-1.453066000	-0.433113000
1	-2.000027000	-2.046367000	0.176938000
1	-1.497107000	0.029000000	1.915918000

(2)_w1_b

1	-2.509102000	1.451778000	-0.000484000
8	-1.629032000	1.050826000	-0.000476000
13	1.895104000	-0.547718000	-0.000343000
1	1.471960000	2.418018000	-0.000787000
8	0.230074000	-1.114026000	0.000248000
13	-1.386882000	-0.673303000	0.000133000
8	1.029951000	1.554324000	0.000654000
1	0.046653000	1.687349000	0.000108000
1	-2.664341000	-1.612879000	0.000476000

TS_2w1b_3w1

1	1.687129000	-0.857748000	-0.047313000
8	0.278806000	-0.818996000	0.042569000
13	0.245897000	1.086392000	0.018809000
1	3.139375000	-0.508050000	0.716949000
8	-1.511784000	0.966192000	-0.012195000
13	-1.458820000	-0.759696000	-0.007770000
8	2.655448000	-0.365952000	-0.120099000
1	2.124010000	0.757459000	-0.066962000
1	-2.562273000	-1.888666000	-0.028368000

(3)_w1

1	-1.649117000	1.372418000	1.403285000
8	0.712693000	1.190316000	-0.461440000
13	1.534207000	-0.309005000	-0.180067000
1	2.953474000	-0.872084000	-0.583639000
8	0.202075000	-0.992280000	0.709338000
13	-0.649074000	0.569240000	0.466814000
8	-1.955196000	-0.458750000	-0.696602000
1	-1.582465000	-1.342294000	-0.473115000
1	-2.905198000	-0.455383000	-0.484601000

TS_3w1_4

1	2.677739000	-0.201127000	0.864553000
8	0.285717000	-1.475679000	-0.409503000
13	-1.113929000	-0.498421000	-0.192980000
1	-2.667240000	-0.748791000	-0.283384000
8	-0.190800000	0.942186000	0.209412000
13	1.357660000	-0.145588000	-0.006591000
8	1.484209000	1.193992000	-1.371105000
1	0.548787000	1.475492000	-0.773610000
1	2.184462000	1.866645000	-1.386149000

(4)

1	-1.457444000	0.311691000	1.960892000
8	0.465220000	1.237216000	0.003363000
13	1.623064000	0.053915000	-0.244410000
1	3.100813000	-0.145340000	-0.710793000
8	0.517765000	-1.224601000	0.310658000
13	-0.920713000	0.237154000	0.470538000
8	-2.014055000	-0.204334000	-0.784207000
1	0.431858000	-2.173066000	0.191680000
1	-2.957231000	-0.243429000	-0.619960000

TS_4_5

1	2.233829000	0.759329000	-1.318406000
8	-0.350221000	1.355967000	0.123970000
13	-1.327823000	-0.019136000	0.293636000
1	-2.642647000	-0.520935000	0.995276000
8	-0.436805000	-0.876389000	-1.037824000

13	1.029804000	0.368379000	-0.370258000
8	1.146545000	-0.772446000	0.987209000
1	-0.271477000	-1.833370000	-1.044787000
1	1.678387000	-0.602235000	1.777170000

(5)

1	2.745049000	-0.013444000	0.008295000
8	-0.000539000	0.886988000	-1.114549000
13	-1.178736000	0.082785000	-0.117249000
1	-2.745312000	0.002112000	0.027200000
8	-0.009470000	-1.440870000	-0.197001000
13	1.177920000	0.072850000	-0.125030000
8	0.010345000	0.408438000	1.405387000
1	-0.013666000	-2.114549000	0.503463000
1	0.021847000	1.266173000	1.859972000

TS_4_open

1	1.578282000	-0.042783000	2.011553000
8	-0.189304000	-1.148451000	0.012436000
13	-1.626717000	-0.294209000	-0.231555000
1	-3.040557000	-0.790951000	-0.729083000
8	-1.207497000	1.311460000	0.230191000
13	1.165709000	-0.204102000	0.486098000
8	2.171892000	0.375293000	-0.770538000
1	-1.718476000	2.129935000	0.198077000
1	2.973120000	0.875427000	-0.566322000

(4)_open

1	1.633934000	-1.944763000	1.452679000
8	0.000000000	0.000000000	0.130115000
13	-0.562380000	1.585535000	0.346172000
1	-1.633934000	1.944763000	1.452679000
8	0.000000000	2.856591000	-0.641654000
13	0.562380000	-1.585535000	0.346172000
8	0.000000000	-2.856591000	-0.641654000
1	0.652195000	2.711183000	-1.340140000
1	-0.652195000	-2.711183000	-1.340140000

TS_4_6

1	3.138478000	0.045368000	0.503158000
8	-2.415690000	0.095540000	0.123962000
13	-0.739288000	-0.121171000	0.113456000
1	0.260923000	0.022699000	1.617574000
8	0.456949000	1.285009000	-0.418468000
13	1.598791000	-0.109773000	0.216419000
8	0.468543000	-1.215200000	-0.484136000
1	0.413838000	2.187940000	-0.063369000
1	-3.065193000	-0.576517000	-0.116591000

(6)

1	2.575456000	0.116602000	-1.402736000
8	-2.520916000	-0.009833000	0.000075000
13	-0.836802000	-0.096847000	-0.000056000
1	2.574902000	0.116843000	1.403159000
8	0.206055000	1.316533000	-0.000124000
13	1.835537000	-0.104819000	0.000079000
8	0.428035000	-1.195001000	-0.000090000
1	0.066509000	2.273414000	0.000137000
1	-3.105805000	-0.778791000	0.000260000

TS_6_open

1	2.726765000	0.138035000	1.405674000
8	-0.207597000	1.555746000	-0.000143000
13	-0.840197000	-0.038618000	-0.000089000
1	2.727872000	0.137662000	-1.404910000
8	-2.497055000	-0.390890000	0.000180000
13	2.029890000	-0.156020000	0.000143000
8	0.528937000	-1.020362000	-0.000262000
1	-2.831396000	-1.297646000	0.000268000
1	-0.683518000	2.396295000	0.000070000

(6)_open

1	-3.180365000	0.092715000	1.404331000
8	2.074896000	-1.239001000	-0.000076000
13	0.899657000	-0.005344000	0.000077000
1	-3.180251000	0.094479000	-1.404381000
8	1.442299000	1.607331000	-0.000043000
13	-2.432470000	-0.015108000	-0.000044000
8	-0.757710000	-0.310096000	0.000093000
1	2.392960000	1.783457000	0.000548000
1	1.818352000	-2.170647000	-0.000705000

TS_6_7

1	-0.614892000	-0.027530000	1.647980000
8	-0.474298000	-1.172584000	-0.553503000
13	-1.627340000	-0.140307000	0.278018000
1	-3.193409000	0.042624000	0.193703000
8	-0.331378000	1.388443000	-0.224311000
13	0.731851000	-0.084613000	0.001535000
8	2.406140000	0.006237000	0.197045000
1	-0.337149000	1.900375000	-1.049998000
1	2.983083000	-0.768278000	0.220268000

(7)

1	-0.357952000	-0.025406000	1.591683000
8	-0.458758000	-1.189174000	-0.547742000
13	-1.597091000	-0.131626000	0.239938000
1	-3.157690000	-0.009098000	0.410955000
8	-0.428590000	1.362442000	-0.246610000

13	0.731147000	-0.101227000	0.100826000
8	2.412749000	0.068863000	0.129742000
1	-0.459661000	1.787683000	-1.120790000
1	3.029382000	-0.663136000	0.005101000

TS_3w1_H_2e

1	2.649235000	0.297020000	0.307404000
8	0.237256000	-1.181346000	-0.913138000
13	-1.158326000	-0.622184000	-0.026642000
1	-2.584574000	-1.231702000	0.252914000
8	-0.378633000	0.871432000	0.426882000
13	1.022854000	0.304276000	-0.452056000
8	2.072152000	1.417527000	-1.451838000
1	1.912036000	2.369389000	-1.579276000
1	2.719744000	1.006979000	-0.470840000

P1

8	0.478755000	-1.262184000	0.000140000
13	1.663096000	0.023301000	-0.000069000
1	3.236820000	0.054846000	-0.000551000
8	0.429024000	1.260768000	0.000089000
13	-0.745112000	-0.028665000	0.000084000
8	-2.431979000	-0.085758000	-0.000257000
1	-2.977016000	0.712275000	0.000589000

TS_4_H_2e

1	-1.560549000	0.079133000	-1.805404000
8	0.534658000	-1.226542000	0.014437000
13	1.750447000	-0.054552000	0.025533000
1	3.310748000	0.101275000	0.047987000
8	0.519974000	1.237856000	0.007914000
13	-0.885367000	-0.205644000	-0.020778000
8	-2.458821000	0.093227000	0.328130000
1	0.432973000	2.201906000	0.049440000
1	-2.195696000	0.163893000	-1.157693000

P2

8	0.457964000	-1.221401000	-0.000079000
13	1.684965000	-0.058818000	0.000036000
1	3.247045000	0.077352000	0.000342000
8	0.463781000	1.238947000	0.000020000
13	-0.966313000	-0.200909000	-0.000047000
8	-2.541858000	0.119354000	0.000102000
1	0.371379000	2.203910000	-0.000541000

TS_6_H_2e

1	1.848732000	0.915745000	1.456237000
8	0.390235000	1.254054000	-0.174385000
13	-0.819675000	-0.011264000	-0.027038000
1	3.068034000	-0.328797000	-0.772489000

8	-2.501928000	0.091360000	-0.006336000
13	1.677116000	-0.133911000	-0.056367000
8	0.349527000	-1.263577000	0.106530000
1	-3.077761000	-0.678986000	0.087505000
1	1.111597000	1.324619000	0.906527000

TS_4o_H_2e

1	2.736457000	-1.733294000	-0.027424000
8	0.079675000	-0.673958000	-0.041741000
13	-1.479134000	-0.073340000	-0.052077000
1	-2.023583000	0.749142000	-1.670573000
8	-3.011192000	0.292816000	0.372765000
13	1.773409000	-0.480214000	0.003824000
8	2.296915000	1.135786000	0.076826000
1	-2.686241000	0.740712000	-1.052761000
1	3.224608000	1.402494000	0.115255000

P2_open

1	2.628789000	-1.742558000	0.000636000
8	-0.014250000	-0.659197000	-0.000269000
13	-1.576311000	-0.067148000	-0.000084000
8	-3.093658000	0.445146000	0.000204000
13	1.684169000	-0.476157000	0.000109000
8	2.211795000	1.138166000	-0.000083000
1	3.137964000	1.412600000	0.000224000

TS_P2_H_2e

8	-0.351342000	-1.335437000	-0.044446000
13	-1.565423000	-0.191601000	0.077913000
1	-2.534491000	0.973123000	-0.908383000
8	-0.552528000	1.206903000	0.170518000
13	0.902395000	0.011066000	0.010823000
8	2.516386000	0.123554000	-0.070505000
1	-1.746273000	1.413682000	-0.689728000

$Al_2O_3(^1A')$

8	1.337055000	-0.455778000	0.000000000
13	0.113273000	-1.619497000	0.000000000
8	-1.227896000	-0.594402000	0.000000000
13	0.000000000	0.789535000	0.000000000
8	-0.293228000	2.398869000	0.000000000

$Al_2O_3(^3B_2)$

8	0.000000000	1.266246000	0.458056000
13	0.000000000	0.000000000	1.683579000
8	0.000000000	-1.266246000	0.458056000
13	0.000000000	0.000000000	-0.728153000
8	0.000000000	0.000000000	-2.468680000

TS_P2o_H_2e

1	-2.333868000	-1.772390000	0.000076000
8	0.101527000	-0.034760000	-0.000096000
13	1.779240000	0.019149000	-0.000015000
8	3.378125000	0.046052000	0.000071000
13	-1.580156000	-0.054428000	-0.000016000
8	-3.140098000	0.409116000	0.000055000
1	-2.970651000	-1.132244000	0.000092000

Al_2O_3_open ($^1\Sigma_g$)

8	0.000000000	0.000000000	3.280238000
13	0.000000000	0.000000000	1.681314000
8	0.000000000	0.000000000	0.000000000
13	0.000000000	0.000000000	-1.681314000
8	0.000000000	0.000000000	-3.280238000

TS_P2_open

1	-3.130519000	-0.924741000	0.000050000
8	-0.185450000	-1.108767000	-0.000014000
13	1.252145000	-0.216587000	-0.000005000
8	2.717576000	0.432872000	0.000014000
13	-1.688108000	-0.293888000	0.000008000
8	-1.218495000	1.348647000	-0.000010000
1	-1.711011000	2.178902000	0.000000000

TS_Al_2O_3_conv

8	-0.314494000	-1.284125000	0.000000000
13	-1.593702000	-0.191601000	-0.000001000
8	-1.246287000	1.392139000	0.000001000
13	1.007574000	-0.132388000	0.000001000
8	2.513239000	0.418469000	-0.000001000

TS_P1_H

8	0.936185000	0.356887000	-1.606235000
13	2.100717000	0.632580000	-0.333092000
1	3.732718000	0.766514000	-0.302531000
8	0.857288000	0.710486000	0.892753000
13	-0.299459000	0.436218000	-0.376189000
8	-1.981571000	0.301896000	-0.386702000
1	-2.484175000	0.145631000	-1.197150000
1	5.098029000	0.877459000	-0.283469000

P1_m2H

8	-0.465548000	-1.266876000	0.000000000
13	-1.694248000	-0.011899000	0.000000000
8	-0.486753000	1.264239000	0.000000000
13	0.720711000	0.013252000	0.000000000
8	2.409317000	0.048224000	0.000000000
1	2.939690000	-0.759739000	0.000000000

TS_P1_OH_H

8	0.695032000	0.390570000	-1.573351000
13	1.976802000	0.530178000	-0.390538000
1	3.546818000	0.469703000	-0.471248000
8	0.839148000	0.763304000	0.919263000
13	-0.425081000	0.623254000	-0.263018000
8	-2.144184000	0.689906000	-0.172947000
1	-2.583389000	0.523931000	-1.351203000
1	-2.669799000	0.396248000	-2.206652000

P1_OH_m2H-H_2

8	0.417387000	0.289202000	-1.564328000
13	1.815150000	0.487153000	-0.526054000
1	3.367540000	0.394932000	-0.760158000
8	0.813734000	0.826866000	0.868998000
13	-0.562288000	0.628069000	-0.171419000
8	-2.269019000	0.741569000	0.137195000
1	-2.776118000	0.295595000	-1.968504000
1	-2.213418000	0.167236000	-2.449916000

P1_OH_m2H

8	-0.421722000	1.261867000	0.000000000
13	-1.636969000	-0.001281000	0.000000000
1	-3.209170000	-0.002278000	0.000000000
8	-0.420027000	-1.262809000	0.000000000
13	0.767819000	0.000376000	0.000000000
8	2.506131000	0.001670000	0.000000000

Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the $(HAlO)_2 \cdot 2H_2O$ systems. See Figures 6-10 of the main text. (Standard G09 convergence criteria or stiffer ones have been used. The G09 ultrafine grid has been used for the DFT computations).

(1)_w2

1	2.803458000	-1.644880000	-0.023370000
8	2.093263000	-0.985996000	-0.017445000
13	2.250188000	0.979537000	0.079229000
1	-0.428228000	1.195056000	0.004594000
8	0.381676000	0.618084000	-0.002470000
13	0.217863000	-1.243452000	-0.083384000
8	-2.113324000	1.665451000	0.002791000
1	-2.480494000	2.176796000	-0.733693000
1	-2.645903000	0.832008000	0.040510000
8	-3.262312000	-0.859858000	0.024017000
1	-3.662430000	-1.210833000	0.835902000
1	-2.465496000	-1.418690000	-0.125076000

TS_1w2_2w2

1	-2.583370000	-1.907874000	0.024330000
8	-1.962707000	-1.165250000	0.017254000
13	-2.090325000	1.059816000	-0.041655000
1	0.997079000	1.277533000	-0.033687000
8	-0.322023000	0.692967000	0.000375000
13	-0.165960000	-1.079567000	0.036860000
8	2.051838000	1.445331000	-0.050178000
1	2.284546000	2.003902000	0.708879000
1	2.571306000	0.275370000	0.004573000
8	2.856042000	-0.841442000	0.044157000
1	3.280196000	-1.102337000	-0.795875000
1	1.796748000	-1.342683000	0.061248000

(2)_w2_a

1	1.848512000	-2.569031000	0.022786000
8	1.480543000	-1.728942000	0.323566000
13	1.567586000	1.786325000	0.249932000
1	-1.408629000	1.363164000	-0.216149000
8	0.297919000	0.782633000	-0.358070000
13	0.179292000	-0.958487000	-0.513095000
8	-2.361266000	1.210192000	0.028277000
1	-2.880002000	1.405980000	-0.767327000
1	-2.011656000	-0.347363000	0.510811000
8	-1.412793000	-1.146819000	0.650784000
1	-1.943633000	-1.958332000	0.605058000
1	-0.349247000	-1.592826000	-1.890510000

(2)_w2_b

1	1.731836000	-0.755850000	-0.062523000
8	0.860570000	-0.293772000	-0.047714000
13	-3.442890000	0.780671000	0.011044000
1	4.104814000	-0.980420000	0.686094000
8	-2.049745000	-0.220249000	-0.004119000
13	-0.625176000	-1.140080000	0.002117000
8	3.585483000	-0.709985000	-0.085810000
1	3.545130000	0.275997000	-0.042189000
1	-0.655829000	-2.725326000	0.057560000
8	2.587368000	1.857104000	0.107569000
1	2.541379000	2.455544000	-0.652987000
1	1.748114000	1.337588000	0.083539000

TS_2w2_3w2

1	-0.301311000	-2.661743000	0.737350000
8	0.290425000	-1.460955000	0.235578000
13	-0.965704000	-0.051015000	0.265383000
1	-1.025229000	-4.131436000	0.511306000
8	0.343104000	1.000037000	-0.303051000
13	1.468925000	-0.299656000	-0.310408000
8	-0.971838000	-3.391393000	1.136989000
1	-2.087461000	-2.768430000	1.267935000

1	3.001375000	-0.441025000	-0.672860000
8	-2.994184000	-2.062686000	1.326129000
1	-3.240774000	-1.917363000	2.259634000
1	-2.530620000	-1.060658000	0.937618000

(3)_w2

1	1.451142000	1.337680000	-0.301084000
8	-0.079674000	0.796540000	-0.729605000
13	-0.176724000	-1.002464000	-0.496528000
1	3.030639000	1.477748000	-0.449330000
8	-1.644536000	-0.787911000	0.460666000
13	-1.544207000	0.913376000	0.220958000
8	2.333900000	1.214189000	0.170562000
1	1.985651000	-0.303313000	0.538377000
1	-2.410094000	2.158888000	0.658075000
8	1.421992000	-1.151699000	0.618229000
1	1.988930000	-1.937421000	0.554473000
1	0.072385000	-2.144391000	-1.576915000

TS_3w2_4w1

1	1.141894000	-1.286225000	0.323064000
8	-0.081918000	-0.808330000	0.716942000
13	-0.065036000	1.040558000	0.447628000
1	2.818950000	-1.475105000	0.461549000
8	-1.576797000	0.858472000	-0.451614000
13	-1.584014000	-0.833487000	-0.197424000
8	2.119847000	-1.269131000	-0.179525000
1	2.006247000	-0.042664000	-0.456087000
1	-2.528966000	-2.036929000	-0.581041000
8	1.505856000	1.002059000	-0.579111000
1	2.112807000	1.754584000	-0.642236000
1	0.150815000	2.129854000	1.588549000

(4)_w1_b

1	0.830946000	-1.217576000	0.723814000
8	-0.058643000	-0.787278000	0.831098000
13	-0.161810000	1.158018000	0.392820000
1	3.235084000	-1.341630000	0.190345000
8	-1.634125000	0.668275000	-0.475119000
13	-1.486792000	-0.992803000	-0.226020000
8	2.344558000	-1.262427000	-0.182264000
1	2.237952000	-0.314900000	-0.460058000
1	-2.209786000	-2.337391000	-0.604084000
8	1.332597000	1.233573000	-0.538912000
1	1.746262000	2.087717000	-0.722195000
1	-0.283726000	2.158842000	1.625360000

TS_4w1_close

1	-0.750938000	1.265222000	0.805369000
8	0.108445000	0.781295000	0.871660000
13	0.132640000	-1.167969000	0.377157000
1	-2.228404000	0.350555000	-0.420407000
8	1.588997000	-0.691420000	-0.522719000
13	1.504278000	0.965402000	-0.227447000
8	-2.319132000	1.279235000	-0.084134000
1	-2.952835000	1.742704000	-0.649402000
1	2.249136000	2.297655000	-0.608228000
8	-1.373133000	-1.219548000	-0.535683000
1	-1.894390000	-2.033635000	-0.501747000
1	0.256078000	-2.185626000	1.595188000

(4)_w1_close

1	0.093869000	-0.303870000	2.180938000
8	0.091615000	-0.702759000	1.298240000
13	-1.289783000	-0.496571000	-0.115100000
1	0.191205000	1.680212000	-0.023502000
8	0.044396000	-0.859081000	-1.178867000
13	1.307884000	-0.487716000	-0.081298000
8	1.200764000	1.484887000	0.010429000
1	1.636078000	2.007448000	-0.683884000
1	2.841495000	-0.865619000	0.004371000
8	-1.359078000	1.294548000	-0.023570000
1	-2.158972000	1.810987000	0.137645000
1	-2.660554000	-1.274195000	0.087755000

(3)_w1w1_sin

1	-1.771866000	1.536484000	0.816949000
8	-0.483480000	0.947744000	-0.687527000
13	-1.116422000	-0.517071000	0.107100000
1	1.771866000	-1.536484000	-0.816949000
8	0.483480000	-0.947744000	0.687527000
13	1.116422000	0.517071000	-0.107100000
8	2.084098000	-0.766754000	-1.354689000
1	3.057122000	-0.769559000	-1.368507000
1	2.297343000	1.505627000	0.296266000
8	-2.084098000	0.766754000	1.354689000
1	-3.057122000	0.769559000	1.368507000
1	-2.297343000	-1.505627000	-0.296266000

TS_3w1w1s_4w1cl

1	-0.763482000	1.103773000	0.836024000
8	-0.308718000	-0.179068000	1.287243000
13	-1.300646000	-0.570054000	-0.197329000
1	0.774085000	1.672065000	-0.530310000
8	0.116257000	-1.097310000	-1.044568000
13	1.127926000	-0.649305000	0.320866000
8	1.630417000	1.229265000	-0.313098000
1	2.160399000	1.230507000	-1.130079000

1	2.519739000	-1.242716000	0.787818000
8	-1.151681000	1.531480000	-0.089263000
1	-1.900142000	2.136060000	0.051374000
1	-2.835447000	-0.922967000	-0.343312000

TS_4w1cl_8

1	-0.145809000	-1.707292000	1.623600000
8	-0.016553000	-1.219533000	0.799008000
13	-1.297791000	-0.285807000	-0.401137000
1	0.829500000	1.302866000	-0.410190000
8	0.233992000	0.296912000	-1.138009000
13	1.404217000	-0.505607000	-0.064470000
8	1.595389000	1.312720000	0.439719000
1	2.364607000	1.891730000	0.317887000
1	2.748303000	-1.319028000	-0.222242000
8	-2.060659000	0.917878000	0.568624000
1	-3.020674000	1.017184000	0.576741000
1	-2.176816000	-1.360895000	-1.187643000

(8)

8	0.023889000	-0.125430000	1.284452000
13	-1.438449000	-0.366822000	0.118684000
1	-2.424830000	-1.548813000	0.492031000
8	1.964364000	1.191658000	-0.269530000
13	1.418349000	-0.401715000	0.080087000
8	-2.103634000	1.156117000	-0.306669000
1	2.878884000	1.401221000	-0.495353000
1	-1.536795000	1.857796000	-0.655923000
8	-0.022527000	-0.893812000	-0.995942000
1	0.058139000	0.659075000	1.853888000
1	-0.040879000	-1.405650000	-1.815237000
1	2.430060000	-1.600911000	0.338087000

TS_8_10

8	1.891382000	1.577349000	0.002971000
13	-1.853572000	-0.476415000	0.138154000
1	-1.789840000	-1.926221000	0.734025000
8	2.212193000	-1.266448000	-0.603594000
13	1.494990000	-0.069833000	0.417982000
8	-3.305115000	0.338842000	-0.152387000
1	2.427064000	-2.134920000	-0.239628000
1	-3.442817000	1.230257000	-0.495625000
8	-0.331848000	0.283510000	-0.262537000
1	2.747967000	1.778933000	-0.394920000
1	-0.185442000	1.170639000	-0.647191000
1	1.171746000	-0.483499000	1.937947000

(10)

8	-2.422669000	0.819284000	-0.052814000
13	1.078602000	0.072094000	-0.106327000
1	-0.166841000	-0.289393000	-1.301458000

8	-0.222730000	-0.654836000	0.992688000
13	-1.567887000	-0.650505000	-0.290008000
8	1.292410000	1.760395000	0.051007000
1	-0.296563000	-0.592866000	1.956912000
1	0.522383000	2.345898000	0.025416000
8	2.427829000	-0.958375000	-0.249434000
1	-3.335829000	0.959382000	-0.332754000
1	3.295732000	-0.601871000	-0.479431000
1	-2.256903000	-2.033554000	-0.647919000

TS_10_11

8	1.414169000	1.051527000	-0.791134000
13	-0.839924000	-0.066436000	-0.052064000
1	0.438667000	-1.147916000	-1.017663000
8	0.423486000	-0.520169000	1.239706000
13	1.735769000	-0.518395000	-0.121935000
8	-1.302999000	1.534916000	0.358179000
1	0.436069000	0.039987000	2.034335000
1	-2.212636000	1.793892000	0.154934000
8	-2.162989000	-1.050060000	-0.518456000
1	1.609248000	1.938295000	-0.460194000
1	-2.008880000	-1.917285000	-0.915744000
1	3.118205000	-1.233885000	0.159950000

(11)

8	-1.629165000	1.441150000	-0.456826000
13	2.005622000	-0.000003000	-0.000005000
1	2.751093000	-1.248809000	0.659541000
8	-1.629258000	-1.441101000	0.456807000
13	-0.821280000	0.000001000	0.000001000
8	0.566647000	0.642379000	1.047755000
1	-2.459429000	-1.459342000	0.948190000
1	0.510634000	1.568177000	1.332454000
8	0.566644000	-0.642437000	-1.047724000
1	-2.459309000	1.459448000	-0.948250000
1	0.510621000	-1.568237000	-1.332411000
1	2.750991000	1.248855000	-0.659568000

TS_11_12

1	-2.730959000	-1.871246000	0.425027000
8	0.656880000	1.695782000	-0.264257000
13	1.111998000	0.141207000	0.379625000
1	0.440680000	-0.027726000	1.845310000
8	-2.126402000	0.973100000	0.065279000
13	-1.773326000	-0.671956000	0.074544000
8	-0.145242000	-1.033926000	-0.552271000
1	-1.365878000	1.575949000	-0.085138000
1	0.217239000	-1.916275000	-0.737419000
8	2.560182000	-0.668004000	-0.083852000
1	1.077906000	2.029855000	-1.068385000
1	3.394938000	-0.626438000	0.397225000

(12)

1	2.809064000	1.864922000	-0.411617000
8	-0.487967000	-1.586797000	-0.225820000
13	-1.324604000	-0.200424000	0.457622000
1	-1.581130000	-0.261301000	2.033788000
8	2.205703000	-0.966663000	0.015060000
13	1.832215000	0.666580000	-0.106581000
8	0.136691000	1.091301000	0.193561000
1	1.406620000	-1.543654000	0.000276000
1	-0.231133000	1.968994000	-0.008986000
8	-2.453033000	0.608373000	-0.580210000
1	-0.828566000	-1.958229000	-1.051519000
1	-3.384950000	0.699531000	-0.346205000

(1)_w1w1

1	2.133755000	-0.255444000	0.223972000
8	1.162788000	-0.144002000	0.324742000
13	0.000000000	0.000000000	1.854806000
1	-2.133755000	0.255444000	0.223972000
8	-1.162788000	0.144002000	0.324742000
13	0.000000000	0.000000000	-1.153404000
8	-3.720021000	0.432351000	-0.766428000
1	-3.974655000	1.338056000	-1.004432000
1	-3.570363000	-0.017817000	-1.614709000
1	3.570363000	0.017817000	-1.614709000
8	3.720021000	-0.432351000	-0.766428000
1	3.974655000	-1.338056000	-1.004432000

TS_1w1w1_2w1w1b

1	-2.170421000	-0.851988000	-0.057792000
8	-1.195199000	-0.895316000	-0.066354000
13	1.713631000	-1.865695000	0.036767000
1	1.986584000	1.050412000	0.048888000
8	1.414955000	-0.128970000	-0.026592000
13	-0.283428000	0.570456000	-0.049794000
8	1.997232000	2.191447000	0.130803000
1	2.325318000	2.571233000	-0.707526000
1	0.765985000	2.188722000	0.066048000
1	-3.964852000	0.828783000	-0.644341000
8	-3.908282000	0.137949000	0.035405000
1	-4.004918000	0.610064000	0.877994000

(2)_w1w1_b

1	-1.946576000	-0.776638000	1.057479000
8	-1.010458000	-0.536777000	1.180145000
13	2.871000000	-0.923463000	-0.075295000
1	0.938998000	2.259707000	0.127141000
8	1.467582000	0.030851000	-0.303271000
13	-0.251813000	0.179675000	-0.175133000
8	-0.034093000	2.183794000	0.197286000
1	-0.421421000	2.770807000	-0.475311000

1	-1.136805000	0.307647000	-1.530899000
1	-2.887104000	-0.537707000	-1.068637000
8	-3.460008000	-0.917187000	-0.375007000
1	-4.300703000	-0.440020000	-0.447414000

(2)_w1w1_a

1	-0.926097000	1.591918000	0.395286000
8	-0.215018000	-0.944340000	-0.380765000
13	1.130108000	0.088895000	-0.607006000
1	2.270582000	-0.053142000	-1.719378000
8	-1.791714000	1.123709000	0.566074000
13	-1.947012000	-0.991616000	-0.130020000
8	0.726154000	1.717019000	-0.085057000
1	-2.501633000	1.779181000	0.653303000
1	1.298841000	2.472332000	-0.272676000
8	2.065346000	-0.807173000	0.975195000
1	1.340247000	-1.442484000	1.163970000
1	2.859650000	-1.326159000	0.757264000

TS_2w1w1_3w1w1

1	2.530576000	0.491873000	0.516999000
8	-0.907949000	1.315022000	-0.172923000
13	-1.087072000	-0.369402000	-0.682500000
1	-1.993142000	-1.042945000	-1.801663000
8	2.894254000	-0.740718000	0.365898000
13	0.804530000	1.099543000	0.150070000
8	0.608872000	-0.696889000	-0.355323000
1	3.530751000	-0.765704000	-0.373882000
1	1.874704000	-0.992663000	-0.031329000
8	-2.210088000	-0.683134000	0.971361000
1	-2.222803000	0.259935000	1.252436000
1	-3.127750000	-0.996580000	0.886927000

(3)_w1w1

1	1.220575000	1.045808000	1.276623000
8	0.275053000	1.237477000	-0.537076000
13	1.199710000	-0.285210000	-0.560180000
1	-1.220575000	-1.045808000	1.276623000
8	-0.275053000	-1.237477000	-0.537076000
13	-1.199710000	0.285210000	-0.560180000
8	-1.691141000	-0.179851000	1.376569000
1	-2.620726000	-0.358435000	1.602865000
1	-2.618588000	0.639896000	-1.182063000
8	1.691141000	0.179851000	1.376569000
1	2.620726000	0.358435000	1.602865000
1	2.618588000	-0.639896000	-1.182063000

TS_3w1w1_4w1a

1	1.640192000	1.990257000	1.064966000
8	-0.333651000	0.892610000	-0.881938000
13	-0.933720000	-0.685098000	-0.367313000
1	-1.673248000	-1.853498000	-1.149647000
8	2.398312000	-0.452178000	-0.289795000
13	1.015016000	0.793949000	0.228667000
8	0.386817000	-0.868209000	0.803192000
1	3.277652000	-0.446084000	0.122078000
1	1.629851000	-1.070793000	0.264884000
8	-2.486228000	0.270826000	0.505633000
1	-2.250172000	1.157896000	0.149303000
1	-3.403121000	0.062761000	0.254075000

(4)_w1_a

1	-1.392401000	-1.425845000	1.635259000
8	0.160893000	-0.896549000	-0.726851000
13	1.080924000	0.534912000	-0.536123000
1	1.916871000	1.533924000	-1.437657000
8	-2.614558000	0.205958000	-0.370411000
13	-1.206281000	-0.514708000	0.329158000
8	-0.074193000	1.114263000	0.732499000
1	-3.491635000	-0.100844000	-0.108337000
1	-0.414825000	1.997047000	0.935747000
8	2.473046000	-0.470052000	0.492373000
1	2.045347000	-1.353959000	0.423414000
1	3.404783000	-0.541930000	0.221245000

TS_4w1_rot_a

1	-1.207617000	-1.399667000	1.624332000
8	0.057917000	-0.870725000	-0.879879000
13	1.111823000	0.446339000	-0.648306000
1	2.047923000	1.323337000	-1.574583000
8	-2.662486000	0.255080000	-0.213517000
13	-1.190193000	-0.485359000	0.298418000
8	0.047088000	1.080865000	0.680928000
1	-3.500667000	-0.007168000	0.187392000
1	-0.214650000	1.973443000	0.947025000
8	2.428128000	-0.395710000	0.643780000
1	1.870029000	-0.911335000	1.261462000
1	3.058599000	-1.027422000	0.252417000

(4)_w1_c

1	-1.188422000	-1.612563000	1.441976000
8	0.110135000	-0.786471000	-0.960802000
13	1.112774000	0.550205000	-0.600883000
1	1.979140000	1.607602000	-1.390401000
8	-2.597615000	0.298865000	-0.184705000
13	-1.152251000	-0.539733000	0.245945000
8	0.042635000	1.014192000	0.807814000
1	-3.463964000	-0.021095000	0.095668000

1	-0.362703000	1.872476000	1.003821000
8	2.364487000	-0.554057000	0.535051000
1	2.279946000	-0.346100000	1.484925000
1	1.912071000	-1.416695000	0.399352000

TS_4w1_rot_b

1	-2.586628000	-1.461541000	-0.572440000
8	0.036235000	-0.025735000	-1.330782000
13	0.621930000	0.880731000	0.044326000
1	1.364029000	2.166249000	0.584246000
8	-1.294783000	1.133852000	0.405134000
13	-1.274554000	-0.610005000	-0.340143000
8	-0.058869000	-1.052120000	1.026888000
1	-1.696713000	1.450499000	1.227617000
1	-0.367043000	-1.198677000	1.935438000
8	2.291396000	-0.392059000	0.025910000
1	1.852172000	-1.102209000	0.550550000
1	2.126468000	-0.685257000	-0.896983000

TS_4w1a_9

1	-1.413191000	-1.447526000	1.618945000
8	0.268110000	-0.890895000	-0.650852000
13	1.145892000	0.641560000	-0.437289000
1	1.854413000	1.719146000	-1.348081000
8	-2.527912000	0.176916000	-0.483532000
13	-1.181870000	-0.513466000	0.345495000
8	-0.134191000	1.119120000	0.754119000
1	-3.405755000	-0.221719000	-0.439368000
1	-0.507738000	1.985966000	0.969634000
8	2.306720000	-0.606597000	0.414128000
1	1.443998000	-1.217940000	-0.001931000
1	3.194169000	-0.871503000	0.123240000

(9)

1	-1.549235000	1.158619000	-1.809407000
8	0.097320000	1.100159000	0.512922000
13	1.298336000	-0.331876000	0.473413000
1	1.548705000	-1.158658000	1.809414000
8	-2.588811000	-0.283539000	0.476340000
13	-1.298464000	0.331882000	-0.473456000
8	-0.097320000	-1.100040000	-0.513245000
1	-3.490364000	0.056456000	0.424361000
1	-0.434426000	-1.992831000	-0.341262000
8	2.589035000	0.283407000	-0.476002000
1	0.434570000	1.992836000	0.340629000
1	3.490623000	-0.056392000	-0.423299000

TS_9_8

8	0.099113000	0.111392000	1.397138000
13	1.457481000	-0.331955000	0.194613000
1	2.917029000	-0.705450000	0.663957000
8	-2.124584000	-0.647249000	0.006539000
13	-0.946264000	0.636986000	-0.115834000
8	0.424637000	-1.189623000	-0.944482000
1	-3.038647000	-0.410946000	-0.203322000
1	-0.101232000	-1.991920000	-0.811307000
8	0.912746000	1.245038000	-0.542261000
1	-0.383953000	-0.565500000	1.899851000
1	1.133931000	1.535219000	-1.439048000
1	-1.668249000	2.016725000	-0.469721000

TS_3w2b_H_2e

1	2.184775000	-0.109771000	0.807348000
8	0.099945000	-0.961814000	-1.155725000
13	-1.349047000	-0.618860000	-0.260452000
1	-2.800543000	-1.242908000	-0.272267000
8	-0.612423000	0.667661000	0.643848000
13	0.878386000	0.323484000	-0.234047000
8	1.840351000	1.589229000	-1.076077000
1	1.582938000	1.904485000	-1.954641000
1	3.162956000	1.625194000	-0.514896000
8	3.859380000	1.254485000	0.205934000
1	4.036231000	1.944956000	0.871708000
1	3.088055000	0.505860000	0.623800000

P1w1_a

8	0.814837000	-0.910199000	-0.925970000
13	1.908420000	0.036073000	0.035767000
1	3.477080000	0.215747000	0.032673000
8	0.633006000	0.727937000	0.990781000
13	-0.502515000	-0.250788000	0.032276000
8	-1.991937000	-0.995926000	0.456728000
1	-2.082865000	-1.945162000	0.606654000
1	-2.419464000	1.213630000	-0.438206000
8	-1.472287000	1.334397000	-0.646202000
1	-1.120461000	2.057409000	-0.088371000

P1w1a_TSH_2e

8	0.586835000	-0.660622000	-1.028522000
13	1.773469000	0.226896000	-0.028918000
1	3.343057000	0.132450000	0.009598000
8	0.564925000	1.180770000	0.731169000
13	-0.697417000	0.224677000	-0.032398000
8	-0.349694000	-1.544876000	0.391108000
1	-1.170594000	-1.941391000	1.719649000
1	-1.299590000	-2.273723000	0.961161000
8	-2.327305000	0.612024000	-0.304308000
1	-2.659630000	1.513849000	-0.208886000

$HAl_2O_3(OH)$

8	0.446031000	-1.058150000	-0.769622000
13	1.607535000	0.260625000	0.000012000
1	3.174514000	0.250757000	0.000087000
8	0.321992000	1.427840000	-0.000005000
13	-0.822489000	0.125022000	-0.000003000
8	0.445991000	-1.058171000	0.769584000
8	-2.497246000	-0.055453000	0.000050000
1	-3.114253000	0.687301000	-0.000261000

TS_3w2_H_2e

1	1.490624000	-1.551756000	0.061446000
8	-0.219656000	-0.967621000	0.431471000
13	0.038291000	0.775029000	0.210454000
1	3.012011000	-1.873105000	0.290749000
8	-1.605994000	1.006113000	-0.309524000
13	-1.866975000	-0.699680000	-0.096246000
8	2.408469000	-1.326698000	-0.233730000
1	2.262061000	0.521287000	-0.427198000
1	-3.100478000	-1.658132000	-0.294280000
8	1.660942000	1.308075000	-0.337266000
1	1.447262000	1.684532000	0.883661000
1	0.711317000	1.738692000	1.593308000

P1w1_b

1	1.653689000	-1.543519000	-0.056433000
8	-0.195093000	-1.044817000	-0.010558000
13	0.131945000	0.690835000	0.004245000
1	3.089751000	-1.728963000	0.524654000
8	-1.564383000	1.068008000	0.018780000
13	-1.898785000	-0.640544000	-0.002199000
8	2.563048000	-1.166510000	-0.062260000
1	2.336039000	0.917705000	-0.024663000
1	-3.212619000	-1.506004000	-0.004888000
8	1.584185000	1.544195000	-0.004120000

TS_4w1b_H_2e

1	0.640737000	-1.471192000	0.332976000
8	-0.202726000	-0.938667000	0.474915000
13	0.137395000	0.923964000	0.071398000
1	3.032695000	-1.724826000	0.212062000
8	-1.564563000	0.984773000	-0.312766000
13	-1.873684000	-0.672516000	-0.067369000
8	2.230019000	-1.431559000	-0.243956000
1	2.296554000	-0.425463000	-0.338688000
1	-3.062823000	-1.688508000	-0.180846000
8	1.741698000	1.204816000	-0.269962000
1	1.367903000	1.694900000	1.073845000
1	0.661261000	1.791370000	1.662418000

P2w1

1	0.740543000	-1.467216000	0.034848000
8	-0.147894000	-0.987448000	0.058868000
13	0.164629000	0.919191000	0.015017000
1	3.071802000	-1.509311000	0.529267000
8	-1.576521000	1.029615000	-0.020740000
13	-1.879263000	-0.651431000	-0.009726000
8	2.398317000	-1.232029000	-0.109421000
1	2.378815000	-0.214181000	-0.087194000
1	-3.102834000	-1.630560000	-0.031270000
8	1.726336000	1.357411000	0.006988000

TS_8_H_2e_a

8	-0.035747000	1.179457000	0.212281000
13	-1.504173000	-0.000027000	0.453369000
1	-2.075510000	-0.000075000	1.925895000
8	2.830508000	0.000024000	-0.672081000
13	1.339308000	0.000007000	-0.000476000
8	-2.597751000	0.000046000	-0.853982000
1	2.890005000	-0.000042000	0.841384000
1	-2.357607000	0.000026000	-1.788775000
8	-0.035747000	-1.179472000	0.212184000
1	0.006726000	2.145884000	0.173392000
1	0.006757000	-2.145901000	0.173364000
1	2.382771000	-0.000071000	1.599910000

TS_8_H_2e_b

8	-0.018303000	0.681873000	1.061478000
13	-1.236166000	-0.167557000	0.061950000
1	-1.558291000	-1.799896000	0.831564000
8	2.216752000	0.883526000	-0.742517000
13	1.463874000	-0.334898000	0.208497000
8	-2.600924000	0.693843000	-0.432978000
1	3.164883000	0.888234000	-0.922077000
1	-3.344673000	0.345011000	-0.939386000
8	0.057632000	-1.187246000	-0.564572000
1	-0.009150000	1.591017000	1.396198000
1	-0.739135000	-1.871677000	0.280007000
1	2.284898000	-1.196745000	1.266602000

TS_9_H_2e_a

1	1.686541000	-0.002779000	-1.937526000
8	-0.033192000	-1.178118000	0.258818000
13	-1.489955000	0.001030000	0.476818000
1	-2.094748000	0.003712000	1.942683000
8	2.960944000	-0.000189000	-0.008819000
13	1.325806000	-0.000232000	-0.060788000
8	-0.032839000	1.179025000	0.255471000
1	2.444150000	-0.002063000	-1.425921000
1	-0.004447000	2.143007000	0.172806000
8	-2.454007000	-0.001862000	-0.932703000

1	-0.005839000	-2.142142000	0.176234000
1	-3.418962000	-0.000961000	-0.918808000

TS_9_H$_2$e_b

1	-0.822850000	1.172546000	-1.636840000
8	0.074493000	1.178935000	0.397903000
13	1.397441000	-0.048458000	0.550688000
1	1.865319000	-0.511351000	2.000951000
8	-2.861114000	-0.180377000	0.055852000
13	-1.219062000	0.134879000	-0.185386000
8	-0.077771000	-1.235743000	-0.096532000
1	-3.578026000	0.455906000	-0.057210000
1	-0.148058000	-2.182282000	-0.283464000
8	2.504921000	0.061840000	-0.760671000
1	-0.211409000	1.429201000	-0.897789000
1	3.451856000	-0.084729000	-0.647002000

TS_11_H$_2$e

8	-2.955850000	0.481653000	0.778278000
13	1.435361000	0.039569000	0.010358000
1	-2.392893000	0.161628000	-1.977940000
8	-0.219484000	-0.395364000	-0.123966000
13	-2.029836000	-0.214199000	-0.481813000
8	1.972677000	1.641766000	-0.115228000
1	-0.753918000	-1.488032000	-0.107525000
1	1.388066000	2.395613000	-0.267558000
8	2.524718000	-1.225393000	0.289225000
1	-2.855525000	0.217948000	1.701868000
1	3.472980000	-1.057688000	0.373519000
1	-1.707012000	-1.980570000	-0.219930000

P3

8	0.036792000	1.181705000	-0.260259000
13	-1.429689000	0.007738000	-0.455164000
1	-2.070713000	0.029619000	-1.904195000
8	2.965442000	-0.006548000	0.382512000
13	1.400941000	-0.001132000	0.033446000
8	0.033281000	-1.173743000	-0.284170000
1	0.060128000	-2.132867000	-0.152184000
8	-2.334155000	-0.015950000	0.991412000
1	0.071590000	2.140620000	-0.128991000
1	-3.298165000	-0.006960000	1.031736000

P4

8	-0.011482000	-1.244518000	0.143645000
13	-1.422584000	-0.212663000	0.427306000
1	-2.096329000	-0.183224000	1.871396000
8	2.835632000	0.089950000	-0.341550000
13	1.194742000	-0.088695000	-0.001621000
8	0.124210000	1.249988000	0.391886000
1	3.424630000	-0.637580000	-0.580813000

1	0.156023000	2.208701000	0.268260000
8	-2.351725000	0.175311000	-0.969310000
1	-3.295458000	0.363898000	-0.890118000

P8

8	-3.147912000	-0.063249000	-0.682789000
13	1.350988000	-0.009128000	-0.026512000
1	-2.360426000	0.423854000	1.970884000
8	-0.307273000	-0.291087000	0.103469000
13	-1.923703000	0.046328000	0.498968000
8	2.504553000	-1.262044000	-0.058753000
1	2.237686000	-2.188610000	0.005827000
8	1.908368000	1.592713000	-0.148264000
1	-2.951638000	-0.288690000	-1.602065000
1	2.857783000	1.759171000	-0.225880000

TS_P3_H_2e1

8	-0.014045000	-1.142074000	-0.324019000
13	1.261551000	0.113568000	-0.171452000
1	1.258469000	1.172572000	-1.639200000
8	-3.018350000	-0.214244000	0.197907000
13	-1.448416000	0.102709000	0.089618000
8	-0.076793000	1.251920000	0.124905000
1	0.511509000	1.483471000	-1.044022000
8	2.753541000	-0.340156000	0.453350000
1	-0.046577000	-2.108151000	-0.407889000
1	3.551023000	0.196939000	0.537819000

$Al_2O_2(OH)_2$_b

8	-0.031509000	1.227799000	0.000009000
13	-1.218174000	-0.090433000	-0.000002000
8	2.994118000	0.161333000	-0.000021000
13	1.426759000	-0.195489000	0.000013000
8	0.019001000	-1.235421000	0.000019000
8	-2.890285000	-0.051649000	-0.000056000
1	0.044159000	2.193613000	-0.000038000
1	-3.486362000	0.706880000	0.000302000

TS_P3_H_2e2

8	0.076042000	1.168077000	0.002466000
13	-1.352030000	0.000000000	-0.028488000
1	-2.035748000	0.000000000	-1.792204000
8	3.105302000	0.000000000	0.027635000
13	1.505660000	0.000000000	0.014499000
8	0.076042000	-1.168077000	0.002466000
1	0.085184000	-2.138561000	0.032233000
8	-2.937238000	0.000000000	0.351628000
1	0.085184000	2.138561000	0.032233000
1	-2.692982000	0.000000000	-1.163957000

$Al_2O_2(OH)_2$_c

8	0.000000000	1.165186000	-0.000345000
13	-1.434187000	0.000000000	-0.000079000
8	3.033699000	0.000000000	0.000502000
13	1.434188000	0.000000000	-0.000076000
8	0.000000000	-1.165186000	-0.000345000
1	0.000001000	-2.136663000	-0.000252000
8	-3.033701000	0.000000000	0.000504000
1	0.000000000	2.136663000	-0.000252000

TS_P4_H_2e1

8	0.020276000	-1.196352000	0.308516000
13	-1.240359000	0.008636000	0.192596000
1	-1.255927000	1.176791000	1.591337000
8	2.914018000	-0.035485000	-0.198747000
13	1.235966000	-0.032612000	-0.044516000
8	0.084631000	1.290259000	-0.165576000
1	3.454121000	-0.830482000	-0.098366000
1	-0.543091000	1.500547000	0.962943000
8	-2.823573000	-0.132413000	-0.392432000
1	-3.160811000	-0.943248000	-0.795031000

$Al_2O_2(OH)_2$_a

8	0.240138000	-1.239532000	0.000000000
13	1.178700000	0.223373000	0.000000000
8	-2.838879000	-0.523923000	0.000000000
13	-1.178700000	-0.223373000	0.000000000
8	-0.240138000	1.239532000	0.000000000
1	-3.199927000	-1.420394000	0.000000000
8	2.838879000	0.523923000	0.000000000
1	3.199927000	1.420394000	0.000000000

TS_P4_H_2e2

8	-0.062709000	-1.246180000	0.009307000
13	1.338741000	-0.198608000	-0.018408000
1	2.010449000	0.101788000	-1.799158000
8	-2.949886000	0.129678000	0.021474000
13	-1.287747000	-0.087262000	0.011702000
8	-0.098806000	1.222040000	0.004362000
1	-3.619941000	-0.566369000	0.029393000
1	-0.064959000	2.189521000	0.043598000
8	2.907290000	0.119273000	0.335593000
1	2.644425000	0.192870000	-1.152549000

P5

8	0.016154000	-1.236547000	0.000072000
13	1.425584000	-0.194674000	0.000004000
8	-2.879515000	0.117482000	-0.000093000
13	-1.216063000	-0.083128000	0.000035000
8	-0.032743000	1.227536000	0.000073000

1	-3.544771000	-0.583253000	-0.000202000
1	0.010425000	2.195623000	0.000058000
8	2.997426000	0.141410000	-0.000098000

TS_P5_H_2e

8	0.083475000	-1.100404000	0.548590000
13	1.381075000	-0.112551000	-0.080076000
8	-2.795150000	-0.099543000	-0.248394000
13	-1.108189000	-0.005890000	-0.173692000
8	0.216569000	0.899265000	-0.892970000
1	-2.250158000	2.154875000	0.316639000
1	-1.579349000	2.474898000	0.184653000
8	3.049410000	-0.085911000	0.191664000

Al_2O_4·H_2

8	-0.060958000	1.240069000	-0.073442000
13	-1.285977000	0.000115000	-0.079430000
8	2.865650000	0.001147000	-0.300851000
13	1.196591000	-0.000057000	-0.014829000
8	-0.061008000	-1.239877000	-0.076797000
1	1.872471000	-0.004254000	2.191633000
1	1.130336000	-0.009113000	2.310093000
8	-2.973782000	0.000236000	0.041546000

Al_2O_4 ($^1A_1$)

8	0.000000000	1.231360000	0.010838000
13	0.000000000	0.000000000	-1.253172000
8	0.000000000	0.000000000	2.936100000
13	0.000000000	0.000000000	1.242906000
8	0.000000000	-1.231360000	0.010838000
8	0.000000000	0.000000000	-2.941093000

Al_2O_4 ($^3B_{1u}$)

8	0.000000000	1.263505000	0.000000000
13	0.000000000	0.000000000	1.195684000
8	0.000000000	-1.263505000	0.000000000
13	0.000000000	0.000000000	-1.195684000
8	0.000000000	0.000000000	-2.932840000
8	0.000000000	0.000000000	2.932840000

Al_2O_2-O_2 (^1A)

8	0.000000000	1.276857000	0.825435000
13	0.000000000	0.000000000	1.961560000
8	0.000000000	-1.276857000	0.825435000
13	0.000000000	0.000000000	-0.440370000
8	-0.706663000	0.158324000	-2.061402000
8	0.706663000	-0.158324000	-2.061402000

Al_2O_2-O_2 ($^3A_2$)

8	0.000000000	1.266030000	0.794740000
13	0.000000000	0.000000000	2.018599000
8	0.000000000	-1.266030000	0.794740000
13	0.000000000	0.000000000	-0.390867000
8	-0.678056000	0.000000000	-2.117272000
8	0.678056000	0.000000000	-2.117272000

TS_P4_conf1

8	0.249380000	-1.150162000	0.796953000
13	1.549078000	-0.261978000	0.030838000
1	2.994387000	-0.685240000	-0.445851000
8	-2.528795000	0.316720000	0.145381000
13	-0.925079000	-0.197061000	0.026474000
8	0.033966000	-0.064344000	-1.477036000
1	-3.045050000	0.278443000	0.960972000
1	-0.049903000	0.651909000	-2.124827000
8	1.063800000	1.338729000	0.598226000
1	1.441778000	2.194849000	0.356459000

P4_close

8	0.412613000	-1.128682000	-0.859909000
13	1.564211000	-0.095901000	-0.071460000
1	3.117857000	0.112888000	0.071517000
8	-2.459193000	0.085190000	0.041518000
13	-0.785989000	-0.129208000	-0.105005000
8	0.342528000	1.341485000	-0.575512000
1	-3.121223000	-0.582691000	-0.174232000
1	0.289817000	2.244613000	-0.226321000
8	0.363776000	-0.202269000	1.444928000
1	0.318875000	0.385829000	2.214867000

TS_P4_conf2

8	0.462791000	-0.765787000	-1.132742000
13	1.669812000	-0.152687000	-0.100156000
1	3.202274000	0.197405000	-0.077254000
8	-2.419862000	-0.359421000	0.155072000
13	-0.786138000	-0.018083000	-0.165991000
8	-0.150638000	1.624618000	-0.229317000
1	-2.795174000	-1.243721000	0.057964000
1	-0.517689000	2.409443000	0.199239000
8	0.605365000	-0.403860000	1.344863000
1	0.641583000	0.092491000	2.176947000

P6

1	0.747864000	1.003296000	1.956050000
8	0.757357000	0.419500000	1.184759000
13	-0.758539000	-0.046848000	-0.140340000
1	-2.402316000	1.585156000	-0.430661000
8	0.639977000	-0.555766000	-1.104350000

13	1.890367000	-0.061352000	-0.096056000
8	-1.820386000	-1.249126000	0.477717000
1	-1.617223000	-2.182097000	0.331622000
1	3.459621000	0.016960000	-0.046732000
8	-1.439662000	1.508301000	-0.400268000

TS_P6_H_2e

1	2.237706000	-1.354289000	-0.493213000
8	0.914997000	-0.797871000	-0.922967000
13	-0.575016000	-0.289415000	0.145511000
1	-2.432889000	0.376758000	-0.398008000
8	0.607644000	0.885484000	1.005372000
13	1.827673000	0.303147000	0.031932000
8	-1.753632000	0.987036000	-0.851271000
1	-1.830934000	1.867057000	-0.439990000
1	3.015250000	-1.062849000	-0.088123000
8	-1.928218000	-1.075299000	0.657938000

Al_2O_3·H_2O

8	0.938057000	-0.760087000	-1.046044000
13	-0.501982000	-0.348583000	0.026785000
1	-2.321105000	0.813439000	-0.307818000
8	0.692712000	0.612207000	1.132768000
13	1.872547000	0.124784000	0.037567000
8	-1.503211000	1.243988000	-0.674266000
1	-1.320143000	2.021306000	-0.113881000
8	-1.899569000	-1.086778000	0.535681000

TS_P6_ws

1	-0.196208000	1.641008000	0.156889000
8	0.600521000	0.844155000	0.869584000
13	-0.645530000	-0.243477000	-0.071224000
1	-1.877944000	1.902216000	-0.428033000
8	0.714885000	-1.094746000	-0.769218000
13	1.843546000	-0.113617000	0.087714000
8	-2.132794000	-0.887522000	0.455241000
1	-2.264943000	-1.834207000	0.592943000
1	3.415176000	-0.070611000	0.182629000
8	-1.013898000	1.513590000	-0.645457000

P6_w

1	-1.120177000	2.057164000	-0.088058000
8	0.632984000	0.727699000	0.990953000
13	-0.502545000	-0.250831000	0.032242000
1	-2.419166000	1.213865000	-0.438550000
8	0.814809000	-0.910130000	-0.926057000
13	1.908390000	0.036026000	0.035798000
8	-1.992084000	-0.995756000	0.456663000
1	-2.083290000	-1.944918000	0.606715000
1	3.477026000	0.215827000	0.032571000
8	-1.472007000	1.334502000	-0.646209000

TS_P6w_H_2e

1	1.503603000	1.753307000	0.154167000
8	0.579734000	-0.603200000	1.281846000
13	-0.702617000	0.003112000	-0.047643000
1	-1.057323000	2.274399000	0.619699000
8	0.647488000	-0.344246000	-1.339110000
13	1.623629000	-0.391931000	0.006828000
8	-2.271237000	-0.666292000	-0.056259000
1	-2.428790000	-1.591142000	0.171534000
1	2.267287000	1.546126000	0.170866000
8	-0.488226000	1.747732000	0.040314000

$Al_2O_2(OH)_2$_e·H_2

1	-3.707248000	0.206516000	0.386346000
8	-0.664752000	-0.457741000	-1.258112000
13	0.757075000	0.016168000	0.039583000
1	2.463779000	1.456124000	-0.607534000
8	-0.696557000	0.387256000	1.255914000
13	-1.659219000	-0.006536000	-0.024235000
8	1.725498000	-1.370574000	0.360460000
1	1.440285000	-2.219326000	-0.002016000
1	-3.735115000	-0.047419000	-0.329728000
8	1.544083000	1.500920000	-0.314086000

$Al_2O_2(OH)_2$_e

8	-0.798904000	-0.450795000	-1.259904000
13	0.642660000	0.013467000	0.042249000
1	2.332790000	1.458268000	-0.647450000
8	-0.809643000	0.394233000	1.264819000
13	-1.782198000	0.018539000	-0.018822000
8	1.580662000	-1.392653000	0.348982000
1	1.283586000	-2.241695000	-0.004534000
8	1.427586000	1.495133000	-0.310467000

Coordinates of structures (angstroms) optimized at the M06/CEP-31G* level for the structures in Figures 12-13 of the main text and SM_F2. (Standard G09 convergence criteria or stiffer ones have been used. The G09 ultrafine grid has been used for the DFT computations).

(Figure 12) AlOH + H_2O → $HAl(OH)_2$

AlOH

8	0.000000000	0.000000000	-0.957301000
13	0.000000000	0.000000000	0.736589000
1	0.000000000	0.000000000	-1.917255000

AlOH·H_2O

8	0.070480000	-1.216987000	0.360107000
13	-0.371793000	0.490520000	0.540062000
8	-2.051610000	-0.437184000	-0.692045000
1	-1.647256000	-1.328388000	-0.592779000
1	-2.984649000	-0.497180000	-0.427131000
1	0.914837000	-1.589756000	0.650646000

TS

1	1.381241000	-1.166141000	0.936615000
8	0.553717000	-1.082001000	0.444431000
13	-0.484155000	0.278242000	0.453130000
8	-1.978004000	0.093606000	-0.602034000
1	-2.653067000	-0.606200000	-0.748236000
1	-2.051046000	1.050168000	0.337656000

$HAl(OH)_2$

1	1.498033000	-1.337032000	0.000000000
8	1.480400000	-0.370107000	0.000000000
13	-0.000182000	0.469661000	0.000000000
8	-1.429559000	-0.462446000	0.000000000
1	-2.315010000	-0.076935000	0.000000000
1	0.014960000	2.053383000	0.000000000

(Figure 13.a) AlO + H_2O → $Al(OH)_2$

AlO

8	0.000000000	0.000000000	-1.012064000
13	0.000000000	0.000000000	0.622809000

AlO·H_2O

8	0.206895000	-1.045719000	0.426241000
13	-0.496345000	0.439982000	0.433496000
8	-2.077852000	-0.392506000	-0.685483000
1	-1.538855000	-1.222076000	-0.546294000
1	-2.997580000	-0.559226000	-0.412501000

TS

8	0.082605000	-1.027879000	0.352497000
13	-0.391402000	0.555627000	0.523592000
8	-1.913790000	-0.072711000	-0.588645000
1	-1.242615000	-0.913942000	-0.369737000
1	-2.832945000	-0.239491000	-0.316452000

$Al(OH)_2$

1	1.314910000	-1.130078000	0.886996000
8	0.439902000	-1.138242000	0.474650000
13	-0.507560000	0.281653000	0.308929000
8	-2.043024000	0.175425000	-0.430683000
1	-2.384496000	-0.671252000	-0.755987000

(Figure 13.b) Coalescence of OAlOH units

OAlOH

1	0.817825000	-2.114434000	0.402595000
8	-0.040520000	-2.386073000	0.055390000
13	-1.358143000	-1.464219000	-0.423053000
8	-2.642427000	-0.633425000	-0.891989000

$Al_2O_2(OH)_2$_a

8	0.240138000	-1.239532000	0.000000000
13	1.178700000	0.223373000	0.000000000
8	-2.838879000	-0.523923000	0.000000000
13	-1.178700000	-0.223373000	0.000000000
8	-0.240138000	1.239532000	0.000000000
1	-3.199927000	-1.420394000	0.000000000
8	2.838879000	0.523923000	0.000000000
1	3.199927000	1.420394000	0.000000000

$Al_2O_3(OH)$

1	3.437491000	-0.746122000	-0.000975000
8	2.890095000	0.050255000	-0.000249000
13	1.206422000	0.008234000	-0.000108000
8	-0.011136000	1.255931000	0.000798000
8	0.011714000	-1.270360000	-0.000796000
13	-1.188814000	-0.018267000	0.000121000
8	-2.927148000	-0.035773000	0.000315000

(Figure 13.c) Coalescence of $Al(OH)_2$ units

$Al(OH)_2$

1	1.314910000	-1.130078000	0.886996000
8	0.439902000	-1.138242000	0.474650000
13	-0.507560000	0.281653000	0.308929000
8	-2.043024000	0.175425000	-0.430683000
1	-2.384496000	-0.671252000	-0.755987000

$Al_2(OH)_4$

1	-0.684835000	-0.774252000	0.134652000
8	-1.046711000	0.068653000	-0.165221000
13	-2.472402000	0.753032000	0.500327000

8	-3.906513000	-0.391784000	0.734511000
1	-4.506779000	-0.712442000	0.045949000
1	-2.149961000	1.334034000	2.960602000
8	-2.607064000	0.743242000	2.344769000
13	-4.233220000	-0.288807000	2.654967000
8	-2.946930000	2.253620000	-0.177954000
1	-2.406992000	2.636558000	-0.881737000

$Al_2O(OH)_3$

1	-0.432566000	0.315653000	-0.509535000
8	-1.202510000	-0.167507000	-0.182660000
13	-2.561883000	0.720436000	0.387069000
8	-4.008044000	-0.261654000	0.683995000
1	-2.101068000	1.392978000	3.029677000
8	-2.566816000	0.808846000	2.414526000
13	-4.076475000	-0.167886000	2.366690000
8	-2.715322000	2.397127000	0.012038000
1	-2.696520000	2.724413000	-0.895590000

$Al_2(OH)_4$ (T)

1	0.027311000	-1.499741000	-0.007600000
8	-0.883002000	-1.264548000	0.217050000
13	-1.452096000	0.349091000	0.004558000
8	-3.319479000	0.105856000	-0.095634000
1	-3.688465000	-0.738712000	-0.398928000
1	-1.622088000	2.098317000	1.866463000
8	-1.991062000	1.253734000	1.563191000
13	-3.858463000	1.010666000	1.462884000
8	-4.427361000	2.624346000	1.250161000
1	-5.337663000	2.859648000	1.474744000

$Al_2(OH)_4$_b (S)

1	-0.690400000	-1.724814000	-1.717632000
8	-1.288019000	-1.558836000	-0.977046000
13	-1.833822000	-0.027056000	-0.446561000
8	-2.935179000	-0.273207000	1.063989000
1	-3.109684000	-0.966486000	1.729424000
1	-2.294306000	2.916454000	3.012438000
8	-2.119646000	2.055342000	2.608614000
13	-2.980520000	1.592530000	1.204899000
8	-4.423216000	2.444646000	0.852407000
1	-4.877576000	2.340084000	0.006356000

$Al_2(OH)_4$_c (S)

1	-0.012723000	-0.574474000	1.164611000
8	-0.596042000	-0.912765000	0.473795000
13	-2.136483000	-0.313128000	0.101134000
8	-3.074803000	-0.981749000	-1.132153000
1	-2.761655000	-1.726618000	-1.662138000
1	-2.512917000	1.539065000	1.666531000

8	-2.877312000	1.006690000	0.924749000
13	-4.712903000	2.169820000	0.883910000
8	-3.774808000	2.920538000	2.197843000
1	-4.092711000	3.671262000	2.718663000

(Figure13.d.1) $Al(OH)_2$ reactivity. $Al(OH)_2 + H_2$

$Al(OH)_2$

1	1.314910000	-1.130078000	0.886996000
8	0.439902000	-1.138242000	0.474650000
13	-0.507560000	0.281653000	0.308929000
8	-2.043024000	0.175425000	-0.430683000
1	-2.384496000	-0.671252000	-0.755987000

TS

1	-2.324777000	0.124401000	0.000000000
8	-1.440182000	0.512729000	0.000000000
13	-0.003030000	-0.404911000	0.000000000
8	1.484844000	0.418513000	0.000000000
1	1.521406000	1.385417000	0.000000000
1	0.013808000	-2.055632000	0.000000000
1	0.044164000	-3.407549000	0.000000000

$HAl(OH)_2$

1	1.498033000	-1.337032000	0.000000000
8	1.480400000	-0.370107000	0.000000000
13	-0.000182000	0.469661000	0.000000000
8	-1.429559000	-0.462446000	0.000000000
1	-2.315010000	-0.076935000	0.000000000
1	0.014960000	2.053383000	0.000000000

(Figure13.d.2) $Al(OH)_2$ reactivity. $Al(OH)_2 + H_2O$

$Al(OH)_2 \cdot H_2O$

1	1.333346000	-1.068820000	0.691296000
8	0.917717000	-0.201255000	0.782462000
13	-0.776852000	-0.036169000	1.164347000
8	-1.879882000	0.741707000	0.058561000
1	-2.625249000	0.265143000	-0.330113000
8	-0.324744000	1.822139000	1.841611000
1	-0.834738000	2.394334000	1.232007000
1	0.623024000	1.901497000	1.607828000

TS

1	1.348789000	-0.976216000	0.957763000
8	0.542655000	-0.879414000	0.434346000
13	-0.647937000	0.288056000	0.772905000
8	-2.079523000	0.412115000	-0.143761000
1	-2.387202000	-0.293318000	-0.728317000
8	-0.191311000	1.982712000	1.335648000
1	-0.881145000	2.642824000	1.099214000
1	-0.627997000	1.356361000	2.359298000

$Al(OH)_3$

1	1.292665000	-0.839391000	0.970310000
8	0.432311000	-0.885699000	0.532189000
13	-0.614202000	0.453850000	0.532429000
8	-2.122885000	0.353657000	-0.243638000
1	-2.395931000	-0.460037000	-0.688265000
8	-0.150806000	1.892817000	1.309497000
1	-0.736826000	2.661562000	1.315277000

Table SM_T1. Absolute energies, ZPE energies and energy differences relative to 2 AlOH + *n* H_2O, with *n*=0-2.

	E^{CEP} (a)	E^{6311} (b)	ZPE^{CEP} (c)	E_0^{6311}(d)	ΔE^{CEP}	ΔE^{6311}	ΔZPE^{CEP}	ΔE_0^{6311} (e)
2 AlOH	-37.20271	-636.55876	0.02182	-636.53694	0.0	0.0	0.0	0.0
(1)	-37.24736	-636.60610	0.02702	-636.57908	-28.0	-29.7	3.3	-26.4
TS_1_2	-37.16884	-636.51894	0.01999	-636.49895	21.3	25.0	-1.2	23.8
(2)	-37.28812	-636.63376	0.02385	-636.60992	-53.6	-47.1	1.3	-45.8
TS_2_3	-37.18494	-636.52503	0.01839	-636.50663	11.2	21.2	-2.2	19.0
(3)	-37.29383	-636.62908	0.02200	-636.60708	-57.2	-44.1	0.1	-44.0
(1)'	-37.21782	-636.57322	0.02615	-636.54707	-9.5	-9.1	2.7	-6.4
TS_1'_1"	-37.20766	-636.56770	0.02453	-636.54317	-3.1	-5.6	1.7	-3.9
(1)"	-37.20916	-636.56899	0.02524	-636.54374	-4.1	-6.4	2.1	-4.3
$Al_2O + H_2O$	-37.21287	-636.56706	0.02443	-636.54263	-6.4	-5.2	1.6	-3.6
TS_1'_Al_2Ow	-37.20436	-636.55824	0.02313	-636.53511	-1.0	0.3	0.8	1.1
$Al_2O{\cdot}H_2O$	-37.22354	-636.57673	0.02690	-636.54983	-13.1	-11.3	3.2	-8.1
TS_Al_2Ow_2	-37.17373	-636.52327	0.01982	-636.50344	18.2	22.3	-1.3	21.0
TS_2_H_2e	-37.17725	-636.52452	0.01965	-636.50487	16.0	21.5	-1.4	20.1
$(AlO)_2 + H_2$	-37.18858	-636.53061	0.01630	-636.51432	8.9	17.7	-3.5	14.2

2 AlOH + H_2O	-54.35981	-712.97650	0.04242	-712.93409	0.0	0.0	0.0	0.0
(1)_w1	-54.41804	-713.03549	0.05065	-712.98484	-36.5	-37.0	5.2	-31.8
TS_1w1_2w1	-54.36532	-712.97324	0.04387	-712.92937	-3.5	2.0	0.9	3.0
(2)_w1_a	-54.47654	-713.07927	0.04816	-713.03111	-73.2	-64.5	3.6	-60.9
(2)_w1_b	-54.46642	-713.07194	0.04794	-713.02400	-66.9	-59.9	3.5	-56.4
TS_2w1b_3w1	-54.39086	-712.98958	0.04236	-712.94722	-19.5	-8.2	0.0	-8.2
(3)_w1	-54.48919	-713.08220	0.04646	-713.03574	-81.2	-66.3	2.5	-63.8
TS_3w1_4	-54.48159	-713.07436	0.04276	-713.03160	-76.4	-61.4	0.2	-61.2
(4)	-54.51820	-713.11500	0.04461	-713.07039	-99.4	-86.9	1.4	-85.5
TS_4_5	-54.51173	-713.10754	0.04536	-713.06218	-95.3	-82.2	1.8	-80.4
(5)	-54.51862	-713.11382	0.04656	-713.06727	-99.7	-86.2	2.6	-83.6
TS_4_open	-54.51508	-713.11113	0.04417	-713.06696	-97.4	-84.5	1.1	-83.4
(4)_open	-54.51956	-713.11707	0.04389	-713.07318	-100.2	-88.2	0.9	-87.3
TS_4_6	-54.49000	-713.08761	0.04433	-713.04328	-81.7	-69.7	1.2	-68.5
(6)	-54.51309	-713.11061	0.04457	-713.06604	-96.2	-84.2	1.3	-82.8
TS_6_open	-54.51070	-713.10712	0.04383	-713.06329	-94.7	-82.0	0.9	-81.1
TS_6_7	-54.48831	-713.08577	0.04414	-713.04163	-80.6	-68.6	1.1	-67.5
(7)	-54.48885	-713.08657	0.04480	-713.04177	-81.0	-69.1	1.5	-67.6
TS_3w1_H_2e	-54.45051	-713.04535	0.04176	-713.00359	-56.9	-43.2	-0.4	-43.6
P1 + H_2	-54.49141	-713.07989	0.03801	-713.04188	-82.6	-64.9	-2.8	-67.6
TS_4_H_2e	-54.41287	-713.00894	0.04122	-712.96772	-33.3	-20.4	-0.8	-21.1
P2 + H_2	-54.42248	-713.01324	0.03781	-712.97544	-39.3	-23.1	-2.9	-25.9
TS_4o_H_2e	-54.40681	-713.00516	0.03993	-712.96523	-29.5	-18.0	-1.6	-19.5
P2_open + H_2	-54.41729	-713.01047	0.03663	-712.97384	-36.1	-21.3	-3.6	-24.9
TS_6_H_2e	-54.45984	-713.05446	0.04121	-713.01326	-62.8	-48.9	-0.8	-49.7
TS_P2_open + H_2	-54.41543	-713.00619	0.03682	-712.96938	-34.9	-18.6	-3.5	-22.1
P2_open + H_2	-54.41729	-713.01047	0.03663	-712.97384	-36.1	-21.3	-3.6	-24.9
TS_P2_H_2e + H_2	-54.28287	-712.87366	0.03282	-712.84084	48.3	64.5	-6.0	58.5
$Al_2O_3(^1A')$ + 2 H_2	-54.28813	-712.87332	0.02962	-712.84370	45.0	64.7	-8.0	56.7
$Al_2O_3(^3B_2)$ + 2 H_2	-54.31942	-712.90473	0.02983	-712.87490	25.3	45.0	-7.9	37.1
TS_P2o_H_2e + H_2	-54.29942	-712.89590	0.03251	-712.86338	37.9	50.6	-6.2	44.4
Al_2O_3_open($^1\Sigma_g$) + 2 H_2	-54.30837	-712.89955	0.02919	-712.87036	32.3	48.3	-8.3	40.0
TS_Al_2O_3_conv + 2 H_2	-54.27105	-712.85677	0.02916	-712.82762	55.7	75.1	-8.3	66.8
2 AlOH + 2 H_2O	-71.51692	-789.39424	0.06301	-789.33123	0.0	0.0	0.0	0.0
(1)_w2	-71.59631	-789.47271	0.07534	-789.39737	-49.8	-49.2	7.7	-41.5
TS_1w2_2w2	-71.55685	-789.42392	0.06812	-789.35580	-25.1	-18.6	3.2	-15.4
(2)_w2_a	-71.66243	-789.52422	0.07287	-789.45135	-91.3	-81.6	6.2	-75.4
(2)_w2_b	-71.63483	-789.50006	0.07242	-789.42764	-74.0	-66.4	5.9	-60.5
(3)_w2(*)	-71.68335	-789.53615	0.07093	-789.46522	-104.4	-89.0	5.0	-84.1
TS_3w2_4w1(*)	-71.67956	-789.53141	0.06604	-789.46537	-102.1	-86.1	1.9	-84.2
(4)_w1_b	-71.70274	-789.55809	0.07011	-789.48798	-116.6	-102.8	4.5	-98.4
TS_4w1_close	-71.70158	-789.55717	0.06957	-789.48760	-115.9	-102.2	4.1	-98.1
(3)_w1w1_sin	-71.68407	-789.53376	0.07109	-789.46267	-104.9	-87.5	5.1	-82.5
TS_3w1w1s_4w1cl	-71.67980	-789.52928	0.06865	-789.46063	-102.2	-84.7	3.5	-81.2
(4)_w1_close	-71.73511	-789.58943	0.07024	-789.51919	-136.9	-122.5	4.5	-117.9

TS_4w1cl_8	-71.71078	-789.56544	0.06581	-789.49963	-121.6	-107.4	1.8	-105.7
(8)	-71.75879	-789.61715	0.06850	-789.54865	-151.8	-139.9	3.4	-136.4
TS_8_10	-71.70497	-789.56324	0.06695	-789.49630	-118.0	-106.0	2.5	-103.6
(10)	-71.72744	-789.58631	0.06822	-789.51809	-132.1	-120.5	3.3	-117.3
TS_10_11	-71.70927	-789.56617	0.06847	-789.49770	-120.7	-107.9	3.4	-104.5
(11)	-71.75641	-789.61464	0.06831	-789.54633	-150.3	-138.3	3.3	-135.0
TS_11_12	-71.71304	-789.56978	0.06809	-789.50169	-123.1	-110.2	3.2	-107.0
(12)	-71.71610	-789.57280	0.06838	-789.50442	-125.0	-112.0	3.4	-108.7
(1)_w1w1	-71.58791	-789.46408	0.07412	-789.38996	-44.5	-43.8	7.0	-36.9
TS_1w1w1_2w1w1b	-71.53212	-789.39851	0.06691	-789.33160	-9.5	-2.7	2.4	-0.2
(2)_w1w1_b	-71.64289	-789.50494	0.07173	-789.43321	-79.0	-69.5	5.5	-64.0
(2)_w1w1_a	-71.65917	-789.52233	0.07246	-789.44987	-89.3	-80.4	5.9	-74.4
TS_2w1w1_3w1w1	-71.58589	-789.44181	0.06607	-789.37574	-43.3	-29.8	1.9	-27.9
(3)_w1w1	-71.68310	-789.53335	0.07111	-789.46225	-104.3	-87.3	5.1	-82.2
TS_3w1w1_4w1b	-71.67749	-789.52780	0.06741	-789.46040	-100.8	-83.8	2.8	-81.1
(4)_w1_a	-71.71813	-789.57249	0.06921	-789.50328	-126.3	-111.9	3.9	-108.0
TS_4w1_rot_a	-71.71661	-789.57092	0.06893	-789.50200	-125.3	-110.9	3.7	-107.2
4_w1_c	-71.71907	-789.57240	0.06950	-789.50290	-126.9	-111.8	4.1	-107.7
TS_4w1_rot_b	-71.70112	-789.55413	0.07061	-789.48352	-115.6	-100.3	4.8	-95.6
TS_4w1a_9	-71.71091	-789.56549	0.06598	-789.49950	-121.7	-107.5	1.9	-105.6
(9)	-71.75888	-789.61671	0.06867	-789.54804	-151.8	-139.6	3.6	-136.1
TS_3w2b_H_2e	-71.64496	-789.49499	0.06673	-789.42826	-80.3	-63.2	2.3	-60.9
P1w1_a + H_2	-71.69369	-789.53962	0.06297	-789.47665	-110.9	-91.2	0.0	-91.3
P1w1a_TSH_2e + H_2	-71.50288	-789.34419	0.05193	-789.29227	8.8	31.4	-7.0	24.5
$HAl_2O_3(OH)$ + 2 H_2	-71.55111	-789.38376	0.04998	-789.33379	-21.5	6.6	-8.2	-1.6
TS_3w2_H_2e	-71.63408	-789.48764	0.06650	-789.42114	-73.5	-58.6	2.2	-56.4
P1w1_b + H_2	-71.66859	-789.51585	0.06243	-789.45342	-95.2	-76.3	-0.4	-76.7
TS_4w1b_H_2e	-71.60628	-789.46027	0.06581	-789.39445	-56.1	-41.4	1.8	-39.7
P2w1 + H_2	-71.61801	-789.46648	0.06217	-789.40432	-63.4	-45.3	-0.5	-45.9
TS_8_H_2e_a	-71.65028	-789.50864	0.06465	-789.44399	-83.7	-71.8	1.0	-70.8
TS_8_H_2e_b	-71.69130	-789.54738	0.06415	-789.48323	-109.4	-96.1	0.7	-95.4
TS_9_H_2e_a	-71.65062	-789.50906	0.06436	-789.44470	-83.9	-72.0	0.8	-71.2
TS_9_H_2e_b	-71.69118	-789.54756	0.06413	-789.48344	-109.4	-96.2	0.7	-95.5
TS_11_H_2e	-71.67187	-789.52864	0.06354	-789.46509	-97.2	-84.3	0.3	-84.0
P3 + H_2	-71.66121	-789.51428	0.06121	-789.45308	-90.5	-75.3	-1.1	-76.5
P4 + H_2	-71.71655	-789.56659	0.06072	-789.50587	-125.3	-108.2	-1.4	-109.6
P8 + H_2	-71.71980	-789.56920	0.06045	-789.50875	-127.3	-109.8	-1.6	-111.4
TS_P3_H_2e1 + H_2	-71.59235	-789.44278	0.05725	-789.38553	-47.3	-30.5	-3.6	-34.1
$Al_2O_2(OH)_2$_b + 2 H_2	-71.61804	-789.46213	0.05348	-789.40865	-63.5	-42.6	-6.0	-48.6
TS_P3_H_2e2 + H_2	-71.54707	-789.39953	0.05793	-789.34160	-18.9	-3.3	-3.2	-6.5
$Al_2O_2(OH)_2$_c + 2 H_2	-71.55560	-789.40271	0.05443	-789.34828	-24.3	-5.3	-5.4	-10.7
TS_P8_H_2e + H_2	-71.60724	-789.45809	0.05623	-789.40186	-56.7	-40.1	-4.3	-44.3
$Al_2O_2(OH)_2$_d + 2 H_2	-71.61745	-789.46312	0.05291	-789.41022	-63.1	-43.2	-6.3	-49.6
TS_b_d + 2 H_2	-71.61205	-789.45598	0.05271	-789.40327	-59.7	-38.7	-6.5	-45.2
TS_P4_H2e1 + H_2	-71.65936	-789.50691	0.05712	-789.44979	-89.4	-70.7	-3.7	-74.4
$Al_2O_2(OH)_2$_a + 2 H_2	-71.68873	-789.53025	0.05411	-789.47614	-107.8	-85.3	-5.6	-90.9

TS_P4_H_2e2 + H_2	-71.61092	-789.46021	0.05720	-789.40300	-59.0	-41.4	-3.6	-45.0
P5 + 2 H_2	-71.62021	-789.46430	0.05377	-789.41052	-64.8	-44.0	-5.8	-49.8
TS_P5_H_2e + 2 H_2	-71.36505	-789.19291	0.04359	-789.14931	95.3	126.3	-12.2	114.2
Al_2O_4·H_2 + 2 H_2	-71.36684	-789.19517	0.04401	-789.15116	94.2	124.9	-11.9	113.0
Al_2O_4($^1A_1$) + 3 H_2	-71.36115	-789.18903	0.04100	-789.14803	97.7	128.8	-13.8	115.0
Al_2O_4($^3B_{1u}$) + 3 H_2	-71.46263	-789.29152	0.04208	-789.24944	34.1	64.5	-13.1	51.3
Al_2O_2-O_2 (^1A) +3 H_2	-71.38248	-789.20976	0.04234	-789.16742	84.4	115.8	-13.0	102.8
Al_2O_2-O_2 ($^3A_2$) + 3 H_2	-71.41575	-789.24546	0.04287	-789.20259	63.5	93.4	-12.6	80.7
TS_P4_conf1 + H_2	-71.70837	-789.55799	0.06097	-789.49702	-120.1	-102.7	-1.3	-104.0
P4_close + H_2	-71.71418	-789.56462	0.06168	-789.50294	-123.8	-106.9	-0.8	-107.7
TS_P4_conf2 + H_2	-71.70943	-789.55901	0.06091	-789.49810	-120.8	-103.4	-1.3	-104.7
P6 + H_2	-71.71995	-789.56876	0.06085	-789.50791	-127.4	-109.5	-1.4	-110.9
TS_P6_H_2e + H_2	-71.48318	-789.33085	0.05683	-789.27402	21.2	39.8	-3.9	35.9
Al_2O_3·H_2O + 2 H_2	-71.48835	-789.33024	0.05389	-789.27635	17.9	40.2	-5.7	34.4
TS_P6_ws + H_2	-71.68324	-789.52844	0.05891	-789.46953	-104.4	-84.2	-2.6	-86.8
P6_w + H_2	-71.69369	-789.53963	0.06297	-789.47666	-110.9	-91.2	0.0	-91.3
TS_P6w_H_2e + H_2	-71.58504	-789.43315	0.05703	-789.37612	-42.7	-24.4	-3.8	-28.2
$Al_2O_2(OH)_2$_e·H_2 + H_2	-71.59070	-789.43724	0.05623	-789.38101	-46.3	-27.0	-4.3	-31.2
Al2O2(OH)2_e + 2 H_2	-71.57731	-789.42221	0.05244	-789.36976	-37.9	-17.5	-6.6	-24.2

a. E^{CEP}: Energies at the M06/CEP-31G*//M06/CEP-31G* level.

b. E^{6311}: Energies at the M06/6-311++G**//M06/CEP-31G* level.

c. ZPE energies have been computed at the M06/CEP-31G* level and scaled by a factor of 0.95 (ZPE(AlOH) scaled by 0.93).

d. $E_0^{6311} = E^{6311} + ZPE^{CEP}$

e. $\Delta E_0^{6311} = \Delta E^{6311} + \Delta ZPE^{CEP}$.

Table SM_T2. Absolute energies, ZPE energies and energy differences relative to P1 + H.

	E^{CEP} (a)	E^{6311} (b)	ZPE^{CEP} (c)	E_0^{6311}(d)	ΔE^{CEP}	ΔE^{6311}	ΔZPE^{CEP}	ΔE_0^{6311} (e)
P1 + H	-53.82128	-712.40927	0.02850	-712.38077	0.0	0.0	0.0	0.0
TS_P1_H	-53.81454	-712.40302	0.02801	-712.37501	4.2	3.9	-0.3	3.6
P1_m2H + H_2	-53.84815	-712.43785	0.03109	-712.40676	-16.9	-17.9	1.6	-16.3
TS_P1_OH_H	-53.79269	-712.37635	0.02677	-712.34959	17.9	20.7	-1.1	19.6
P1_OH_m2H-H_2	-53.79929	-712.37960	0.02946	-712.35014	13.8	18.6	0.6	19.2
P1_OH_m2H + H_2	-53.79557	-712.37583	0.02725	-712.34859	16.1	21.0	-0.8	20.2

a. E^{CEP}: Energies at the M06/CEP-31G*//M06/CEP-31G* level.

b. E^{6311}: Energies at the M06/6-311++G**//M06/CEP-31G* level.

c. ZPE energies have been computed at the M06/CEP-31G* level and scaled by a factor of 0.95 (ZPE(AlOH) scaled by 0.93).

d. $E_0^{6311} = E^{6311} + ZPE^{CEP}$

e. $\Delta E_0^{6311} = \Delta E^{6311} + \Delta ZPE^{CEP}$.

Table SM_T3. Absolutes energies, ZPE energies and energy differences relative to reactants for the reactions shown in fig. 12-13 of the main text. See also SM_F2.

	E^{CEP} (a)	E^{6311} (b)	ZPE^{CEP} (c)	E_0^{6311}(d)	ΔE^{CEP}	ΔE^{6311}	ΔZPE^{CEP}	ΔE_0^{6311} (e)
(fig. 12) AlOH + H_2O → $HAl(OH)_2$								
AlOH + H_2O	-35.75846	-394.69712	0.03151	-394.66562	0.0	0.0	0.0	0.0
AlOH·H_2O	-35.77379	-394.71132	0.03611	-394.67521	-9.6	-8.9	2.9	-6.0
TS	-35.71802	-394.65092	0.02801	-394.62291	25.4	29.0	-2.2	26.8
$HAl(OH)_2$	-35.83401	-394.76271	0.03252	-394.73019	-47.4	-41.2	0.6	-40.5
(fig 13.a) AlO + H_2O → $Al(OH)_2$								
AlO + H_2O	-35.07140	-394.00441	0.02258	-393.98183	0.0	0.0	0.0	0.0
AlO·H_2O	-35.10023	-394.03042	0.02573	-394.00469	-18.1	-16.3	2.0	-14.3
TS	-35.09784	-394.02716	0.02288	-394.00428	-16.6	-14.3	0.2	-14.1
$Al(OH)_2$	-35.18813	-394.11795	0.02495	-394.09299	-73.2	-71.2	1.5	-69.8
OAlOH + H	-35.05790	-393.98246	0.01480	-393.96766	8.5	13.8	-4.9	8.9
(fig 13.b) Coalescence of OAlOH units								
2 OAlOH	-69.12265	-786.96503	0.02960	-786.93543	0.0	0.0	0.0	0.0
$Al_2O_2(OH)_2$_a	-69.35530	-787.18913	0.03506	-787.15407	-146.0	-140.6	3.4	-137.2
$Al_2O_3(OH)$ + H	-69.15583	-786.98483	0.02425	-786.96058	-20.8	-12.4	-3.4	-15.8
(fig 13.c) Coalescence of $Al(OH)_2$ units								
2 $Al(OH)_2$	-70.37625	-788.23589	0.04991	-788.18598	0.0	0.0	0.0	0.0
$Al_2(OH)_4$	-70.54041	-788.39770	0.05416	-788.34354	-103.0	-101.5	2.7	-98.9
$Al_2O(OH)_3$ + H	-70.40379	-788.25329	0.04400	-788.20929	-17.3	-10.9	-3.7	-14.6
Other possible structures resulting from de coalescence								
$Al_2(OH)_4$ (T)	-70.45556	-788.31481	0.05406	-788.26075	-49.8	-49.5	2.6	-46.9
$Al_2(OH)_{4\_b}$ (S)	-70.49178	-788.34736	0.05259	-788.29477	-72.5	-69.9	1.7	-68.3
$Al_2(OH)_{4\_c}$ (S)	-70.48307	-788.33966	0.05278	-788.28688	-67.0	-65.1	1.8	-63.3
(fig 13.d) $Al(OH)_2$ reactivity								
d.1								
$Al(OH)_2$ + H_2	-36.35484	-395.28851	0.03448	-395.25403	0.0	0.0	0.0	0.0
TS	-36.32404	-395.25648	0.03192	-395.22456	19.3	20.1	-1.6	18.5
$HAl(OH)_2$ + H	-36.33058	-395.26265	0.03252	-395.23014	15.2	16.2	-1.2	15.0
d.2								
$Al(OH)_2$ + H_2O	-52.34523	-470.53569	0.04555	-470.49014	0.0	0.0	0.0	0.0
$Al(OH)_2$·H_2O	-52.37983	-470.56771	0.04999	-470.51773	-21.7	-20.1	2.8	-17.3
TS	-52.34823	-470.53096	0.04216	-470.48880	-1.9	3.0	-2.1	0.8
$Al(OH)_3$ + H	-52.36454	-470.54513	0.03944	-470.50569	-12.1	-5.9	-3.8	-9.8

a. E^{CEP}: Energies at the M06/CEP-31G*//M06/CEP-31G* level.

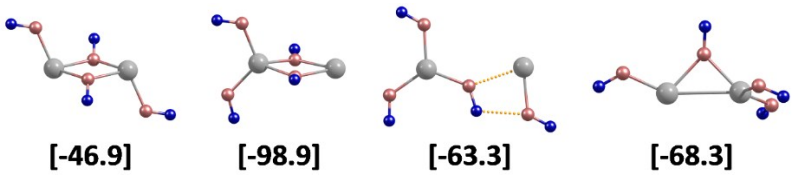
b. E^{6311}: Energies at the M06/6-311++G**//M06/CEP-31G* level.

c. ZPE energies have been computed at the M06/CEP-31G* level and scaled by a factor of 0.95 (ZPE(AlOH) scaled by 0.93).

d. $E_0^{6311} = E^{6311} + ZPE^{CEP}$

e. $\Delta E_0^{6311} = \Delta E^{6311} + \Delta ZPE^{CEP}$.

Figure SM_F2. Some structures resulting from the coalescence of $Al(OH)_2$ dimers. Numbers in brackets are relative energies with respect to 2 $Al(OH)_2$. The structure on the left is a minimum on the triplet electronic state and the other are singlets. The most stable of the four has syn isomer (-98.9) and a H migration isomer with a Al-H bond (-100.5 kcal/mol). See also fig. 13 c in the main text.



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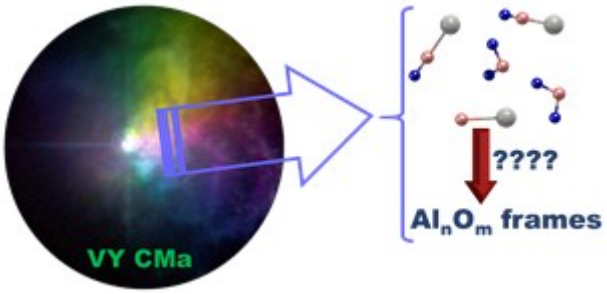

VY Canis Majoris. Image available (free resources) on the following link:

http://hubblesite.org/gallery/album/objects-from/pr2007003c