

Magnesium Oxides Clusters as Promising Candidates for Hydrogen Storage

Juan Pablo Mojica-Sánchez,^{a,b} Tania Isabel Zarate-López,^b José Manuel Flores-Álvarez,^b Juan Reyes-Gómez,^c Kayim Pineda Urbina^{b*} and Zeferino Gómez-Sandoval.^{b*}

^a*Instituto Tecnológico José Mario Molina Pasquel y Henríquez Campus Tamazula de Gordiano, Carretera Tamazula-Santa Rosa No. 329, 49650, Tamazula de Gordiano, Jalisco, México.*

^b*Facultad de Ciencias Químicas, Universidad de Colima, Km. 9 Carretera Colima-Coquimatlán, 28400, Coquimatlán, Colima, México.*

^c*Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo No. 340, Col. Villas San Sebastián, 28045, Colima, Colima, México.*

supplementary material for review

Table S1. XYZ Coordinates of the (MgO)_n, n=1-10 clusters optimized at a def2-TZVP/BP86/D3 level theory.

MgO			
12	-1.152373000	0.840040000	-1.873212000
8	-0.527463000	2.196199000	-0.959723000

(MgO)₂			
12	-1.117157000	-0.981520000	1.113788000
12	0.384615000	-0.484047000	-0.706206000
8	-1.477133000	-0.210904000	-0.570318000
8	0.743498000	-1.254999000	0.978671000

(MgO)₃			
12	0.778375000	1.416144000	0.480002000
12	-1.250266000	0.137816000	-1.182437000

12	0.143498000	-1.405631000	0.864115000
8	1.226426000	-0.054073000	1.501396000
8	-0.405806000	1.753263000	-0.894651000
8	-1.149100000	-1.550828000	-0.444976000

(MgO)₄

12	-1.080274000	0.720685000	-1.759190000
12	1.014149000	-0.711838000	1.876293000
12	-0.433959000	-2.092867000	-0.536808000
12	0.367889000	2.101727000	0.653932000
8	0.483474000	-2.244165000	1.035459000
8	1.124304000	1.108123000	1.987127000
8	-0.549541000	2.253004000	-0.918346000
8	-1.190414000	-1.099266000	-1.869964000

(MgO)₅

12	2.821898000	0.000000000	-0.500763000
12	-2.416216000	0.000000000	-1.149803000
12	1.439698000	0.000000000	2.453795000
12	0.438388000	0.000000000	-2.727920000
12	-1.797669000	0.000000000	2.052807000
8	-2.899622000	0.000000000	0.604636000
8	2.181212000	0.000000000	-2.203999000
8	-1.379394000	0.000000000	-2.645314000
8	-0.278197000	0.000000000	3.054242000
8	2.862193000	0.000000000	1.318658000

(MgO)₆

12	-0.338100000	-1.851390000	-0.866221000
12	0.166119000	-0.548106000	1.993757000
12	1.921500000	-0.762221000	0.010435000
12	-1.933170000	0.765514000	-0.006122000
12	0.326434000	1.854674000	0.870527000
12	-0.177762000	0.551393000	-1.989455000
8	1.695431000	0.597381000	1.344628000
8	-0.572747000	2.016713000	-0.816181000
8	1.150665000	-0.810785000	-1.745447000
8	-1.707088000	-0.594085000	-1.340330000
8	0.561080000	-2.013419000	0.820489000
8	-1.162322000	0.814062000	1.749751000

(MgO)₇

12	0.839085000	-0.873829000	1.599003000
12	-0.774417000	-2.725358000	0.644275000
12	0.332615000	-1.443714000	-1.374330000

12	-1.938745000	-0.375117000	0.392137000
12	-0.019828000	2.159312000	0.925608000
12	-0.450225000	1.674959000	-1.600969000
12	1.910203000	1.251221000	-0.575449000
8	1.074416000	-2.280087000	0.244028000
8	1.437749000	0.897050000	1.297363000
8	0.886555000	0.276751000	-1.938698000
8	-1.061945000	-1.275068000	1.905478000
8	0.807751000	2.850065000	-0.694158000
8	-1.538312000	-1.811114000	-0.891015000
8	-1.585564000	1.439813000	-0.016095000

(MgO)₈

12	-0.200168775	-0.040927983	-0.299438117
8	0.151547852	-1.225535370	-1.763789416
8	1.675595931	-0.004166515	0.356081867
12	1.970255775	-1.357841401	-0.967045221
8	-0.924033603	-0.663137462	1.369905317
12	-1.770508544	-2.359939723	1.468107495
8	-1.467260305	-3.682719889	0.006589754
12	-0.089042738	-3.031629240	-1.124790617
8	1.810426660	-3.231009162	-0.556046802
12	-1.060616734	-4.922491440	1.420059898
8	0.728834841	-5.174495781	2.059472098
12	1.846277322	-3.825389526	1.246595460
8	-1.596295513	-3.673349108	2.871025977
12	0.976007749	-0.862624590	1.938377199
8	1.545711945	-2.503048345	2.705240618
12	0.250996137	-3.759575466	3.370751489

(MgO)₉

8	0.278595379	0.104133951	0.622056344
12	2.019495397	0.837077080	1.468921551
8	3.917841684	0.338138010	0.811313337
12	4.016861466	-0.972671551	-0.787767090
8	2.353454154	-1.775781425	-1.722145458
12	0.513562900	-1.197932548	-0.969968169
12	0.571719396	-1.467074637	1.752008388
8	2.056446763	-0.747800079	2.717473640
8	0.580850042	-2.741861655	0.327682433
12	2.362504767	-3.089610841	-0.271242159
8	4.013617867	-2.521097789	0.506250039
12	3.712654008	-1.265055825	1.915404390
12	0.507106911	1.525066013	-0.704651482
8	1.989138092	2.370333826	0.157349551
8	0.513516820	0.376305016	-2.232448876
12	3.648024237	1.727006520	-0.541322883
12	2.297853031	-0.097495930	-2.727978971
8	3.946273088	0.596995866	-2.053921587

(MgO)₁₀

8	2.512318422	1.825316195	-0.569662386
8	-0.959625529	2.953472539	-0.569659621
8	2.512318479	-1.825316345	-0.569662496
8	-3.105336513	-0.000000071	-0.569648690
8	-0.959625594	-2.953472569	-0.569659637
12	-2.422270015	-1.759907400	-0.461752313
12	0.925247943	-2.847646481	-0.461754699
12	0.925247877	2.847646370	-0.461754695
12	-2.422270042	1.759907370	-0.461752225
12	2.994081583	0.000000015	-0.461764575
12	2.422270033	1.759907339	1.467326283
12	-0.925247882	2.847646353	1.467328771
12	2.422269998	-1.759907284	1.467326212
12	-2.994081490	0.000000007	1.467338505
12	-0.925247924	-2.847646271	1.467328755
8	-2.512318410	-1.825316133	1.575236360
8	0.959625530	-2.953472343	1.575233694
8	0.959625575	2.953472482	1.575233706
8	-2.512318412	1.825316168	1.575236441
8	3.105336373	0.000000059	1.575222610

Table S2. XYZ Coordinates of the (MgO)_n, n=1-10 clusters with H₂ molecules optimized at a def2-TZVP/BP86/D3 level theory.

MgO-(H₂)₉

12	-0.891123000	1.742886000	-2.333839000
8	-0.120010000	1.325045000	-0.816817000
1	0.551989000	0.967758000	1.935630000
1	0.371364000	1.061812000	1.199763000
1	1.543601000	2.875587000	-1.686619000
1	1.930127000	3.403422000	-2.083113000
1	-0.351942000	3.964373000	-3.566345000
1	-1.000123000	3.858239000	-3.944259000
1	1.472783000	-0.079318000	-1.750232000
1	1.943301000	-0.546246000	-2.131137000
1	-2.559001000	0.039818000	-3.402191000
1	-2.710598000	0.573993000	-3.917836000
1	0.868543000	0.930751000	-4.066986000
1	0.541212000	1.259645000	-4.666565000
1	-1.727384000	-1.341535000	-1.141422000
1	-1.276335000	-0.747444000	-0.971777000

1	-2.780590000	1.630078000	-0.521459000
1	-3.485519000	1.773033000	-0.773623000
1	-1.091364000	4.383686000	-0.446903000
1	-0.801121000	3.678525000	-0.407232000

(MgO)₂-(H₂)₁₃

12	-1.165335000	-0.599029000	0.696662000
12	0.901045000	-1.167934000	-0.533123000
8	-0.602198000	-0.147794000	-1.056385000
8	0.341997000	-1.618051000	1.219248000
1	2.186312000	-0.417162000	-2.391588000
1	1.480773000	-0.119723000	-2.349693000
1	2.081807000	-1.816612000	2.640604000
1	2.726568000	-1.858979000	3.047047000
1	-0.803115000	-2.455023000	3.811496000
1	-0.429207000	-2.289355000	3.164258000
1	-2.500447000	-1.398203000	2.374811000
1	-3.011769000	-0.929660000	2.063838000
1	2.437938000	-0.189912000	0.772832000
1	2.830339000	0.136072000	0.205397000
1	-1.417944000	0.024350000	-3.103790000
1	-1.681526000	0.034477000	-3.820882000
1	2.163848000	-2.822434000	0.109044000
1	2.589405000	-2.843046000	-0.528489000
1	-2.576495000	-1.438176000	-0.901908000
1	-0.727316000	0.966837000	2.550604000
1	-0.233670000	0.387033000	2.463446000
1	0.410663000	-2.887503000	-2.252004000
1	-0.075429000	-2.298888000	-2.214692000
1	-0.274962000	-3.807374000	0.920970000
1	-0.490966000	-4.518128000	0.744883000
1	-2.693725000	1.227105000	0.498655000
1	-3.114843000	-1.795016000	-0.488243000
1	-2.223557000	1.105746000	-0.102048000
1	0.167431000	1.957582000	-1.270317000
1	0.485510000	2.651624000	-1.302141000

(MgO)₃-(H₂)₁₂

12	0.316940000	1.292016000	0.744211000
12	-1.066063000	0.016196000	-1.578147000
12	-0.455961000	-1.596316000	0.880844000
8	0.377440000	-0.221775000	1.809060000
8	-0.340017000	1.607149000	-0.966334000
8	-1.247489000	-1.662339000	-0.797896000
1	-0.969200000	1.612149000	-3.169695000
1	-1.284212000	1.231503000	-3.755406000
1	-3.113793000	-0.692418000	-2.120836000
1	-3.315225000	-0.051854000	-2.482116000

1	-2.660665000	-3.222859000	-1.642939000
1	-3.146462000	-3.730811000	-1.935774000
1	-0.420515000	4.461094000	-1.912124000
1	-0.406540000	3.731985000	-1.691037000
1	-0.967578000	3.186967000	1.601845000
1	-1.051780000	3.077263000	0.850972000
1	1.448273000	2.356270000	2.690469000
1	1.272739000	1.610759000	2.746037000
1	-0.902278000	-1.716374000	3.063626000
1	-1.368517000	-2.323242000	3.041817000
1	-0.765007000	-4.023752000	0.969157000
1	-1.013181000	-3.688934000	0.327242000
1	1.677029000	-2.899126000	1.431984000
1	1.627166000	-2.166190000	1.648369000
1	-0.318948000	-1.632194000	-2.945679000
1	-0.131237000	-1.210409000	-3.556320000
1	-3.730494000	-1.374268000	1.172142000
1	-3.233124000	-1.479566000	0.606956000
1	2.388347000	2.436350000	0.089668000
1	1.863828000	2.381149000	-0.463973000

(MgO)₄-(H₂)₁₄

12	-1.477820000	-0.050134000	-1.972956000
12	0.449206000	-0.773920000	2.055621000
12	-0.265993000	-2.558044000	-0.473227000
12	-0.704232000	1.769360000	0.532439000
8	0.425087000	-2.410106000	1.215982000
8	0.112808000	1.029263000	2.000585000
8	-1.461908000	1.582394000	-1.132034000
8	-1.069243000	-1.840170000	-1.953793000
1	-0.975895000	0.821891000	-4.049413000
1	-0.874421000	0.081612000	-4.182644000
1	-3.426096000	-0.834407000	-2.802778000
1	-3.676672000	-0.116774000	-2.806265000
1	-1.265303000	-3.444463000	-4.458852000
1	-1.218280000	-3.037196000	-3.815904000
1	0.149928000	-4.784953000	-0.713708000
1	-0.172382000	-4.630706000	-1.383948000
1	1.423906000	-5.014128000	2.287340000
1	1.177041000	-4.339418000	2.032133000
1	2.452358000	-0.855132000	3.265395000
1	2.400533000	-1.526103000	2.912682000
1	-0.503967000	-2.141439000	3.578237000
1	-0.581680000	-1.562606000	4.066536000
1	0.510182000	0.910725000	5.031070000
1	0.369609000	1.069046000	4.299295000
1	2.260000000	3.119348000	2.565685000
1	1.735789000	2.575394000	2.468106000
1	0.587100000	3.708428000	0.345477000

1	0.215408000	3.669001000	-0.315536000
1	-3.929992000	3.319149000	-1.417412000
1	-3.305234000	2.886375000	-1.373051000
1	-0.712328000	3.097131000	-2.669660000
1	-0.432966000	3.575981000	-3.192256000
1	-3.827523000	0.121197000	0.767556000
1	-3.392655000	0.522299000	0.294887000
1	-1.847759000	2.908113000	2.110320000
1	-2.245556000	3.215750000	1.540451000

(MgO)₅-(H₂)₁₆

12	3.486486000	-0.394389000	-1.582282000
12	-1.684029000	0.599735000	-0.873444000
12	3.143270000	0.654796000	1.522752000
12	0.517698000	-0.435120000	-3.086973000
12	-0.071033000	1.277516000	1.961474000
8	-1.538004000	1.085977000	0.883649000
8	2.322940000	-0.709215000	-2.953005000
8	-1.155427000	0.064921000	-2.541837000
8	1.682120000	1.202286000	2.473119000
8	4.094259000	0.053313000	0.077997000
1	-0.059671000	-2.611674000	-3.881316000
1	0.697482000	-2.594581000	-3.816807000
1	-2.610693000	-1.363770000	-3.542640000
1	-3.078904000	-1.868622000	-3.869096000
1	-3.544838000	-0.658022000	-0.270228000
1	-3.489706000	-0.884261000	-0.992447000
1	3.325752000	-0.679285000	-4.966675000
1	3.665286000	-0.657782000	-5.648861000
1	5.629697000	-0.758899000	-2.318758000
1	5.239614000	-0.898548000	-2.955139000
1	7.035824000	-0.170524000	0.598015000
1	6.288919000	-0.115732000	0.453823000
1	3.961044000	-0.703113000	3.257260000
1	4.360873000	-0.934277000	2.654330000
1	2.495395000	2.649069000	4.969958000
1	2.278153000	2.282644000	4.337380000
1	-1.078514000	1.042986000	4.089002000
1	-0.328954000	1.075309000	4.209114000
1	-1.662600000	-1.627716000	2.461882000
1	-1.743620000	-0.992981000	2.049213000
1	4.930353000	2.063195000	1.945319000
1	4.457515000	2.328627000	2.476317000
1	-0.529532000	3.623544000	2.456135000
1	-1.090822000	3.334179000	2.031986000
1	0.575459000	-1.926120000	0.247818000
1	1.003707000	-1.809782000	-0.362530000
1	0.655308000	0.016004000	-5.360775000
1	-0.049237000	0.255806000	-5.213016000

1	-3.173841000	2.311478000	-0.781326000
1	-3.298609000	2.230439000	-1.526844000
1	-2.440884000	1.965195000	-4.536012000
1	-2.131368000	1.476273000	-4.040435000

(MgO)₆-(H₂)₁₇

12	0.328594000	-2.116951000	-0.597804000
12	0.753834000	-0.504153000	2.196891000
12	2.389753000	-0.565716000	0.082101000
12	-1.660427000	0.258907000	0.236366000
12	0.429393000	1.812685000	0.878857000
12	-0.031072000	0.211373000	-1.880204000
8	2.019736000	0.826897000	1.342955000
8	-0.581248000	1.651341000	-0.742918000
8	1.543057000	-0.880043000	-1.622057000
8	-1.281101000	-1.141494000	-1.031822000
8	1.303425000	-1.963811000	1.057302000
8	-0.807274000	0.593287000	1.935280000
1	-2.905909000	-0.804324000	1.945881000
1	-3.358789000	-1.187030000	1.470551000
1	-1.798005000	-0.374625000	-3.192004000
1	-1.652564000	0.105722000	-3.767553000
1	1.319421000	0.309330000	-3.676942000
1	0.897231000	0.811043000	-4.068521000
1	-0.842873000	-4.117402000	-1.532853000
1	-1.238006000	-3.448073000	-1.552116000
1	4.047896000	-2.711161000	2.201004000
1	3.332883000	-2.626974000	1.951846000
1	2.088366000	-0.104556000	4.177684000
1	2.316438000	0.286869000	3.560271000
1	-0.064054000	3.601766000	2.399839000
1	-0.472923000	2.978047000	2.556089000
1	-2.272433000	3.893362000	-1.705557000
1	-1.808675000	3.331082000	-1.473325000
1	-3.615652000	1.503289000	-0.246190000
1	-3.898667000	0.727056000	-0.469384000
1	4.487010000	-1.445760000	-0.535770000
1	4.011402000	-1.472203000	-1.129534000
1	3.210617000	0.923084000	-2.030374000
1	3.679009000	1.510379000	-1.927066000
1	-4.245217000	-1.772095000	-1.540489000
1	-3.472439000	-1.661388000	-1.447221000
1	2.244883000	3.156612000	0.719477000
1	1.865837000	3.751990000	0.430572000
1	-3.398278000	2.248728000	2.765944000
1	-2.731854000	1.820472000	2.645260000
1	-0.869633000	0.395684000	4.988800000
1	-0.961188000	0.500729000	4.237594000
1	1.865794000	-3.975883000	-0.083505000
1	1.839405000	-4.446732000	-0.705049000

1	0.174753000	-2.146284000	3.913677000
1	0.457795000	-2.463446000	3.280570000

(MgO)₇-(H₂)₁₆

12	0.877584000	-0.544946000	1.251712000
12	-0.391376000	-2.771611000	0.529748000
12	0.530622000	-1.522423000	-1.638896000
12	-1.924522000	-0.659624000	-0.012363000
12	-0.466297000	2.208621000	0.252018000
12	-0.760982000	1.376223000	-2.244738000
12	1.645726000	1.469881000	-1.155136000
8	1.366164000	-2.036773000	0.066808000
8	1.175731000	1.252367000	0.750840000
8	0.807572000	0.183060000	-2.397130000
8	-0.939815000	-1.222476000	1.604819000
8	0.276928000	2.826512000	-1.452985000
8	-1.268111000	-2.151832000	-1.114406000
8	-1.864738000	1.122245000	-0.627077000
1	-3.407208000	-1.169317000	1.608254000
1	-4.009457000	-1.033734000	1.161183000
1	-2.462446000	3.535621000	1.041970000
1	-2.611216000	2.937541000	0.589938000
1	0.197694000	4.340367000	0.209197000
1	0.050735000	4.529623000	0.939933000
1	-0.116668000	4.257098000	-3.085174000
1	-0.307913000	4.679606000	-3.693788000
1	2.856670000	1.166872000	-3.018176000
1	3.415538000	1.651361000	-2.826609000
1	1.274593000	-4.288726000	0.411903000
1	0.875971000	-4.927978000	0.560162000
1	-0.720948000	-3.998766000	2.698408000
1	-0.872285000	-3.246836000	2.692905000
1	-0.136913000	1.040927000	-4.373920000
1	-0.677159000	1.481708000	-4.685919000
1	2.202847000	-0.369264000	3.241401000
1	2.184483000	0.293774000	2.867962000
1	-1.444243000	1.540410000	2.868876000
1	-1.355503000	0.835558000	2.586858000
1	-2.875908000	2.057702000	-2.560152000
1	-2.769699000	2.294816000	-3.277986000
1	-1.963575000	-4.177658000	-0.282478000
1	-1.933685000	-4.725482000	0.253667000
1	3.191481000	2.317117000	0.243601000
1	3.686739000	2.540680000	-0.294069000
1	-2.151634000	-1.111822000	-2.971000000
1	-2.405288000	-0.713149000	-3.571300000
1	-0.047802000	-3.227498000	-3.000989000
1	0.619343000	-3.210543000	-3.368281000

1	3.262023000	-0.894109000	-0.517072000
1	3.852077000	-0.454026000	-0.723862000

(MgO)₈-(H₂)₁₆

12	-0.150419000	0.175987000	-0.090040000
8	0.045125000	-1.036282000	-1.573240000
8	1.762490000	0.022491000	0.493670000
12	1.885823000	-1.342935000	-0.867930000
8	-0.851555000	-0.380649000	1.612733000
12	-1.851269000	-1.991583000	1.716118000
8	-1.729355000	-3.323687000	0.243135000
12	-0.342841000	-2.837863000	-0.958196000
8	1.548713000	-3.205211000	-0.454439000
12	-1.375347000	-4.618909000	1.623748000
8	0.415191000	-5.028182000	2.201990000
12	1.625496000	-3.779863000	1.354407000
8	-1.733695000	-3.322469000	3.112802000
12	1.040838000	-0.757835000	2.108666000
8	1.505774000	-2.449591000	2.829755000
12	0.122969000	-3.577370000	3.554475000
1	3.037976000	0.580730000	-1.455959000
1	3.274035000	0.371640000	-2.149768000
1	3.977604000	-0.934221000	0.493938000
1	4.505802000	-1.421960000	0.246350000
1	3.594529000	-3.654424000	2.424994000
1	3.910864000	-4.184637000	1.978685000
1	0.862586000	-5.149163000	5.210381000
1	0.859741000	-5.433280000	4.500588000
1	0.623223000	-0.330003000	-3.633448000
1	0.882232000	-0.105732000	-4.314326000
1	-0.929615000	-2.577873000	-3.134217000
1	-1.196081000	-3.286799000	-3.218154000
1	1.544348000	-7.765760000	2.516505000
1	1.257374000	-7.064056000	2.431077000
1	-3.125067000	-5.099464000	2.889832000
1	-3.339096000	-5.733075000	2.513148000
1	-3.767721000	-2.068168000	0.539023000
1	-4.103584000	-1.528761000	0.960457000
1	0.308803000	2.549999000	-0.217572000
1	0.902527000	2.121554000	0.007696000
1	0.765410000	0.801935000	3.933538000
1	0.127542000	0.736128000	3.521171000
1	-0.468673000	-2.750276000	5.779823000
1	-1.055336000	-2.800206000	5.290731000
1	3.062177000	-2.741410000	-2.190569000
1	3.407851000	-2.201136000	-2.605073000
1	0.705335000	-5.027086000	-1.675321000

1	0.168718000	-5.428774000	-2.034993000
1	-1.006220000	-6.706850000	0.806374000
1	-1.691259000	-6.680493000	0.477414000
1	-1.945820000	1.249975000	-1.327061000
1	-1.608359000	0.679188000	-1.706822000

(MgO)₉-(H₂)₁₈

8	0.374588000	0.613708000	0.200431000
12	2.113851000	1.089557000	1.199512000
8	3.936657000	0.250711000	0.739198000
12	3.952603000	-1.115852000	-0.806917000
8	2.274121000	-1.666114000	-1.874778000
12	0.501136000	-0.765052000	-1.329525000
12	0.269900000	-0.927880000	1.396910000
8	1.761091000	-0.435802000	2.492326000
8	0.179218000	-2.250306000	0.012385000
12	1.923150000	-2.928335000	-0.399990000
8	3.575899000	-2.595961000	0.520486000
12	3.396557000	-1.248221000	1.878443000
12	0.940807000	1.931651000	-1.127694000
8	2.465663000	2.559991000	-0.149982000
8	0.884582000	0.743286000	-2.627964000
12	4.060210000	1.630200000	-0.665954000
12	2.608978000	-0.044059000	-2.946933000
8	4.276729000	0.391562000	-2.117334000
1	0.509932000	0.435565000	5.087539000
1	0.854873000	0.198456000	4.450026000
1	1.953025000	2.346146000	3.131847000
1	2.111243000	2.896755000	2.633974000
1	2.970329000	5.332634000	0.806991000
1	2.839786000	4.626393000	0.548425000
1	3.782865000	-1.711112000	4.286005000
1	3.142732000	-1.325810000	4.122247000
1	5.391563000	-4.889897000	-0.143859000
1	4.938221000	-4.315129000	0.070105000
1	0.476191000	4.095725000	-0.932695000
1	-0.169616000	3.992599000	-1.321835000
1	2.077910000	1.380331000	-4.678631000
1	2.751038000	1.318522000	-5.029303000
1	2.257996000	-4.837504000	0.868835000
1	1.539477000	-5.047733000	0.742374000
1	2.219264000	-4.076237000	-2.312720000
1	2.081402000	-4.760973000	-2.010217000
1	2.516490000	-1.836059000	-4.314331000
1	2.698577000	-1.450422000	-4.944717000
1	5.746727000	-2.162872000	2.622358000
1	5.400130000	-2.508366000	2.038364000
1	6.049063000	-2.063206000	-1.454227000
1	5.929117000	-1.429512000	-1.859500000
1	5.740796000	1.802433000	0.832455000
1	6.078075000	2.406718000	0.512325000

1	5.367780000	3.231568000	-2.039829000
1	5.288975000	2.538734000	-2.350426000
1	-1.716669000	-1.405065000	2.532151000
1	-1.668709000	-1.876379000	1.937508000
1	-1.348437000	-3.838456000	-0.127041000
1	-1.867517000	-4.396170000	-0.178324000
1	-1.411323000	-1.711117000	-2.162460000
1	-1.346524000	-1.162905000	-2.683604000
1	-0.726767000	1.078522000	-4.117220000
1	-1.299541000	1.181168000	-4.610723000

(MgO)₁₀-(H₂)₁₈

8	2.515069000	1.686204000	-1.112904000
8	-0.964127000	2.780076000	-1.198936000
8	2.564909000	-1.955699000	-0.413041000
8	-3.261043000	-0.053259000	-0.540084000
8	-0.933066000	-2.798538000	-0.133331000
12	-2.501119000	-1.749019000	-0.142171000
12	0.957525000	-2.914530000	-0.085204000
12	0.936714000	2.747315000	-1.150010000
12	-2.415566000	1.630206000	-0.780275000
12	2.931833000	-0.112004000	-0.661616000
12	2.481572000	2.015993000	0.907353000
12	-0.839312000	3.080785000	0.822941000
12	2.539347000	-1.525383000	1.571711000
12	-3.071911000	0.312987000	1.470105000
12	-0.829787000	-2.357971000	1.863589000
8	-2.510002000	-1.457349000	1.865485000
8	1.052184000	-2.647580000	1.943302000
8	1.044297000	3.243920000	0.814750000
8	-2.394268000	2.069566000	1.204137000
8	3.077631000	0.273056000	1.337793000
1	1.942850000	4.428683000	-2.524702000
1	2.429782000	3.856409000	-2.403815000
1	-0.365082000	2.569112000	-3.499084000
1	0.059759000	2.470002000	-4.121494000
1	-0.198490000	-0.692540000	-1.583478000
1	-0.078225000	-0.011704000	-1.896915000
1	0.235836000	-4.121369000	-1.900261000
1	0.945115000	-4.248628000	-2.144823000
1	-1.669530000	5.389919000	0.426894000
1	-1.599747000	4.989448000	-0.216370000
1	-0.298329000	0.494470000	1.944728000
1	0.436026000	0.292972000	1.949849000
1	-1.044589000	-1.531976000	4.197834000
1	-0.333210000	-1.785533000	4.256606000
1	1.796993000	-4.468737000	4.237019000
1	1.608841000	-4.010131000	3.657883000
1	4.291127000	3.092135000	0.006930000

1	4.525511000	3.374209000	0.673259000
1	4.911817000	-0.309214000	-1.917030000
1	4.671376000	0.404610000	-2.016045000
1	4.524454000	-2.915682000	1.824907000
1	4.281355000	-2.888417000	1.103157000
1	-5.573724000	0.322493000	1.447546000
1	-5.254047000	0.208585000	0.764881000
1	-3.924279000	0.999881000	3.667103000
1	-3.625248000	1.587265000	3.285530000
1	-4.963372000	-0.425849000	-1.989353000
1	-5.534829000	-0.557656000	-2.475907000
1	-4.212336000	2.351839000	-2.038715000
1	-3.719549000	2.912574000	-2.172859000
1	1.552955000	-4.832972000	1.044228000
1	1.630244000	-5.275271000	0.428793000
1	-1.369893000	-4.380172000	2.964353000
1	-2.031115000	-4.010897000	2.936499000
1	-4.180528000	-2.963350000	0.787929000
1	-4.412900000	-3.257929000	0.125312000

Table S3. XYZ Coordinates of the $(\text{MgO})_n$, $n=1-10$ clusters with H_2 molecules optimized at a def2-TZVP/BP86 level theory.

$\text{MgO}-(\text{H}_2)_9$

12	-1.035636000	1.492429000	-2.355343000
8	0.208554000	1.563194000	-1.124599000
1	0.353079000	0.819397000	1.802637000
1	0.336273000	1.014752000	1.067354000
1	2.111740000	2.767396000	-1.595195000
1	2.722263000	3.175791000	-1.797017000
1	-1.295189000	3.693951000	-3.205398000
1	-1.847197000	3.554030000	-3.709260000
1	1.692348000	-0.235086000	-1.352805000
1	2.128574000	-0.847488000	-1.472873000
1	-2.909755000	0.517770000	-3.579360000
1	-2.543518000	0.864469000	-4.145156000
1	0.571990000	1.260343000	-4.093774000
1	0.203057000	1.250167000	-4.761102000
1	-1.873215000	-0.918092000	-1.548492000
1	-1.291914000	-0.506706000	-1.257170000
1	-2.650419000	1.987699000	-0.812211000
1	-3.294155000	2.009139000	-1.223497000
1	-0.664942000	4.328366000	0.103031000
1	-0.384848000	3.664014000	-0.143624000

$(\text{MgO})_2-(\text{H}_2)_{13}$

12	-1.154657000	-0.590635000	0.690869000
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12	0.907082000	-1.181130000	-0.530666000
8	-0.577466000	-0.129684000	-1.057987000
8	0.328539000	-1.647175000	1.213551000
1	2.310952000	-0.459131000	-2.367344000
1	1.626478000	-0.119149000	-2.350837000
1	2.103756000	-1.948374000	2.734877000
1	2.735838000	-2.021759000	3.151219000
1	-0.801225000	-2.451474000	3.937549000
1	-0.422201000	-2.317267000	3.290309000
1	-2.546633000	-1.378707000	2.393140000
1	-3.056297000	-0.919756000	2.067381000
1	2.550233000	-0.249354000	0.803689000
1	2.962657000	0.061866000	0.244426000
1	-1.449770000	0.187349000	-3.175740000
1	-1.725790000	0.250668000	-3.882237000
1	2.208316000	-2.893518000	0.000180000
1	2.617856000	-2.869577000	-0.644699000
1	-2.656885000	-1.376810000	-0.936320000
1	-0.796937000	1.030138000	2.577829000
1	-0.300704000	0.452144000	2.526788000
1	0.432627000	-2.887995000	-2.384974000
1	-0.050183000	-2.301089000	-2.322684000
1	-0.165215000	-4.000482000	1.121535000
1	-0.329193000	-4.736333000	1.025255000
1	-2.780516000	1.241829000	0.511195000
1	-3.210139000	-1.728415000	-0.542588000
1	-2.303530000	1.143571000	-0.083290000
1	0.043104000	2.098336000	-1.472874000
1	0.281036000	2.814737000	-1.569059000

(MgO)₃-(H₂)₁₂

12	0.332744000	1.310201000	0.750224000
12	-1.071773000	0.029295000	-1.560703000
12	-0.463971000	-1.577396000	0.891529000
8	0.383548000	-0.207494000	1.814749000
8	-0.327544000	1.621672000	-0.960835000
8	-1.279083000	-1.646067000	-0.776762000
1	-0.949229000	1.633353000	-3.203147000
1	-1.262564000	1.256922000	-3.790469000
1	-3.157828000	-0.670290000	-2.208447000
1	-3.335075000	-0.040007000	-2.596569000
1	-2.719878000	-3.339784000	-1.678376000
1	-3.179246000	-3.868399000	-1.969918000
1	-0.451513000	4.545934000	-2.017482000
1	-0.426838000	3.826848000	-1.774314000
1	-0.901967000	3.255117000	1.680582000
1	-1.008092000	3.157866000	0.932593000
1	1.507891000	2.368327000	2.744798000
1	1.319634000	1.626031000	2.785276000
1	-0.872511000	-1.764696000	3.121391000

1	-1.302601000	-2.396416000	3.104599000
1	-0.707636000	-4.083014000	1.002659000
1	-0.969579000	-3.759402000	0.363250000
1	1.741614000	-2.891976000	1.435609000
1	1.678116000	-2.160377000	1.647644000
1	-0.322519000	-1.647843000	-2.989112000
1	-0.126507000	-1.234831000	-3.600368000
1	-3.995457000	-1.413354000	1.175083000
1	-3.466349000	-1.502472000	0.641264000
1	2.457238000	2.464804000	0.125249000
1	1.940453000	2.415873000	-0.433875000

(MgO)₄-(H₂)₁₄

12	-1.583211000	-0.102284000	-1.919247000
12	0.605026000	-0.933142000	1.958509000
12	-0.179516000	-2.636924000	-0.606549000
12	-0.773095000	1.630965000	0.641546000
8	0.609976000	-2.530777000	1.046076000
8	0.157380000	0.850836000	2.025232000
8	-1.600204000	1.492083000	-0.998536000
8	-1.097396000	-1.875637000	-2.001126000
1	-0.993652000	0.716369000	-4.061574000
1	-0.850600000	-0.027514000	-4.108026000
1	-3.527697000	-0.818699000	-2.911105000
1	-3.767707000	-0.101496000	-2.846547000
1	-1.689992000	-3.721123000	-4.398482000
1	-1.549655000	-3.258080000	-3.812507000
1	0.356743000	-4.842205000	-0.877273000
1	-0.005343000	-4.728926000	-1.534873000
1	1.974826000	-5.033799000	2.205933000
1	1.639963000	-4.413928000	1.920891000
1	2.661325000	-0.607217000	3.020572000
1	2.738226000	-1.331693000	2.809292000
1	-0.086332000	-2.222082000	3.753433000
1	-0.199362000	-1.562414000	4.111725000
1	-0.541248000	1.576884000	5.008948000
1	-0.378191000	1.421374000	4.284235000
1	2.558565000	2.659010000	2.955718000
1	1.976013000	2.218288000	2.749022000
1	0.688040000	3.496883000	0.542373000
1	0.277351000	3.591717000	-0.087855000
1	-3.807788000	3.654765000	-1.650208000
1	-3.272522000	3.137308000	-1.506416000
1	-0.636871000	3.093787000	-2.617506000
1	-0.304100000	3.542677000	-3.129814000
1	-4.534276000	0.598108000	0.590520000
1	-3.949005000	0.866384000	0.195217000
1	-1.807689000	2.926861000	2.244329000
1	-2.215721000	3.203267000	1.667567000

(MgO)₅-(H₂)₁₅

12	3.619337000	-0.082667000	-1.799565000
12	-1.608632000	0.550759000	-0.873318000
12	3.300838000	0.820390000	1.376199000
12	0.608010000	-0.292674000	-3.194630000
12	0.050852000	1.214718000	1.949006000
8	-1.429267000	1.045758000	0.882826000
8	2.440232000	-0.390586000	-3.163849000
8	-1.079085000	0.019507000	-2.547910000
8	1.828798000	1.203310000	2.398489000
8	4.230142000	0.333960000	-0.127157000
1	0.225857000	-2.506514000	-4.138901000
1	0.975920000	-2.393788000	-4.099204000
1	-2.528490000	-1.671655000	-3.486993000
1	-2.968514000	-2.223115000	-3.766106000
1	-3.476580000	-0.711534000	-0.240955000
1	-3.425480000	-0.956689000	-0.956788000
1	3.504745000	-0.265255000	-5.267325000
1	3.849959000	-0.216882000	-5.942119000
1	5.770253000	-0.467910000	-2.525941000
1	5.393609000	-0.609580000	-3.169578000
1	7.239270000	-0.268811000	0.329043000
1	6.502306000	-0.119393000	0.220373000
1	4.025449000	-0.272636000	3.294163000
1	4.625198000	-0.478328000	2.877327000
1	2.478575000	2.601104000	5.105542000
1	2.321010000	2.260312000	4.445231000
1	-0.776064000	-0.041662000	3.851701000
1	-0.031165000	0.057946000	3.959938000
1	-4.136527000	1.287586000	2.415311000
1	-3.474530000	1.231318000	2.047287000
1	4.973258000	2.424377000	1.638063000
1	4.527538000	2.684818000	2.193957000
1	-0.450722000	3.120979000	3.280643000
1	-1.086229000	3.015276000	2.880111000
1	0.749371000	0.374358000	-5.427821000
1	0.009100000	0.500865000	-5.322318000
1	-3.110869000	2.313576000	-0.865226000
1	-3.184633000	2.203058000	-1.612496000
1	-2.820424000	1.622393000	-4.654935000
1	-2.418922000	1.210858000	-4.159675000

(MgO)₆-(H₂)₁₇

12	0.232301000	-1.994468000	-0.640178000
12	0.724490000	-0.599944000	2.214380000
12	2.351977000	-0.526592000	0.071168000
12	-1.762641000	0.311231000	0.362946000

12	0.356988000	1.804945000	1.069028000
12	-0.134324000	0.400311000	-1.781277000
8	1.968881000	0.797804000	1.424047000
8	-0.690645000	1.772705000	-0.547561000
8	1.438937000	-0.710748000	-1.617601000
8	-1.383314000	-1.008771000	-1.001930000
8	1.273997000	-1.989347000	0.982130000
8	-0.850403000	0.506322000	2.056643000
1	-3.885253000	-0.788601000	1.052703000
1	-3.613995000	-1.121478000	0.426791000
1	-1.738052000	-0.182729000	-3.327611000
1	-1.508388000	0.311408000	-3.859332000
1	1.326572000	1.070046000	-3.465649000
1	0.889092000	1.650444000	-3.688327000
1	0.188828000	-4.247763000	-1.235959000
1	-0.453975000	-4.007084000	-1.556823000
1	4.339384000	-2.033898000	0.335140000
1	3.688346000	-2.327280000	0.600325000
1	2.197993000	-0.252834000	4.296273000
1	2.384701000	0.153565000	3.678134000
1	-0.388356000	3.575438000	2.657187000
1	-0.698546000	2.894856000	2.798055000
1	-1.208735000	4.579531000	-1.847177000
1	-1.087828000	3.900087000	-1.530235000
1	-3.092845000	2.062896000	-0.318166000
1	-3.755307000	1.779884000	-0.069019000
1	4.178771000	0.919566000	0.213131000
1	4.576641000	0.617673000	-0.360812000
1	2.702274000	-1.614843000	-3.405409000
1	3.107869000	-1.916516000	-3.972289000
1	-3.588193000	-2.782623000	-2.347232000
1	-3.061839000	-2.340877000	-2.023416000
1	2.175019000	3.289028000	1.221323000
1	1.798604000	3.926752000	1.047011000
1	-3.803403000	1.310552000	3.199298000
1	-3.088101000	1.113161000	3.047274000
1	-0.994370000	0.190346000	5.290734000
1	-1.069198000	0.307913000	4.545983000
1	1.768953000	-4.244470000	1.612543000
1	1.905632000	-4.967758000	1.798850000
1	0.234481000	-2.227372000	4.010194000
1	0.533844000	-2.576073000	3.405131000

(MgO)₇-(H₂)₁₆

12	0.868576000	-0.188366000	1.117660000
12	-0.367788000	-2.472026000	0.471498000
12	0.524765000	-1.264993000	-1.742660000
12	-1.933025000	-0.386738000	-0.128375000
12	-0.508269000	2.540599000	0.018771000
12	-0.808845000	1.623368000	-2.437874000

12	1.600612000	1.788812000	-1.372616000
8	1.376265000	-1.719730000	-0.020533000
8	1.143860000	1.607826000	0.546644000
8	0.772747000	0.435808000	-2.557531000
8	-0.937467000	-0.899369000	1.499837000
8	0.212641000	3.118744000	-1.711418000
8	-1.258854000	-1.910778000	-1.187908000
8	-1.897072000	1.392683000	-0.799854000
1	-3.727824000	-0.879808000	1.285979000
1	-4.209129000	-0.729219000	0.720101000
1	-2.011917000	3.365141000	1.749091000
1	-2.378907000	2.897375000	1.275413000
1	-0.123550000	4.798190000	-0.144239000
1	-0.304061000	5.026544000	0.564316000
1	0.525137000	5.006892000	-3.015176000
1	0.628774000	5.620928000	-3.452352000
1	2.967823000	1.287997000	-3.147852000
1	3.547167000	1.742752000	-2.950396000
1	1.410804000	-4.038714000	0.533401000
1	1.059141000	-4.687083000	0.731187000
1	-0.778200000	-3.774883000	2.678170000
1	-0.924701000	-3.026124000	2.677229000
1	-0.338194000	1.092361000	-4.619511000
1	-0.920891000	1.473506000	-4.930195000
1	2.204483000	-0.081403000	3.164668000
1	2.220838000	0.597024000	2.825856000
1	-2.037410000	-0.250377000	4.325246000
1	-1.766780000	-0.407350000	3.632120000
1	-3.031483000	2.133980000	-2.787761000
1	-2.983045000	2.306009000	-3.529308000
1	-1.821920000	-4.104737000	-0.342775000
1	-1.733608000	-4.646774000	0.187433000
1	3.281989000	2.578551000	0.000369000
1	3.785087000	2.762072000	-0.542548000
1	-2.817141000	-2.695457000	-2.769193000
1	-3.324261000	-2.946357000	-3.276746000
1	0.263209000	-3.036350000	-3.255701000
1	0.952735000	-2.886231000	-3.532239000
1	3.660534000	-2.259595000	-0.091300000
1	4.402287000	-2.423604000	-0.120271000

(MgO)₈-(H₂)₁₆

12	-0.019547000	0.138775000	-0.147826000
8	-0.012661000	-1.090717000	-1.640334000
8	1.901381000	-0.194095000	0.336900000
12	1.825014000	-1.562628000	-1.024963000
8	-0.682912000	-0.385070000	1.589096000
12	-1.820469000	-1.905535000	1.771952000
8	-1.887850000	-3.246070000	0.291269000
12	-0.530401000	-2.846981000	-0.985486000

8	1.352138000	-3.394181000	-0.582911000
12	-1.602539000	-4.575482000	1.665100000
8	0.177711000	-5.150951000	2.147307000
12	1.448655000	-4.008069000	1.225770000
8	-1.759988000	-3.254809000	3.164977000
12	1.196291000	-0.928270000	1.994210000
8	1.519747000	-2.667506000	2.702685000
12	0.090501000	-3.684197000	3.513998000
1	3.374981000	0.360478000	-1.533929000
1	3.642543000	0.256865000	-2.238083000
1	3.806350000	1.021585000	1.196638000
1	4.383406000	1.401692000	1.509802000
1	3.593119000	-4.154981000	2.117681000
1	3.792134000	-4.701473000	1.629416000
1	0.846870000	-5.305386000	5.214739000
1	0.765339000	-5.612767000	4.522097000
1	-0.085360000	-0.360714000	-3.890466000
1	-0.092837000	-0.128821000	-4.613802000
1	-1.111828000	-2.962680000	-3.219286000
1	-1.318666000	-3.688067000	-3.136479000
1	1.075970000	-8.143434000	2.380300000
1	0.861236000	-7.417619000	2.316366000
1	-3.414828000	-4.937338000	3.034042000
1	-3.708107000	-5.552025000	2.686763000
1	-3.951776000	-1.714684000	0.842490000
1	-4.145292000	-1.162887000	1.326818000
1	0.565437000	2.556564000	-0.318321000
1	1.148340000	2.108376000	-0.117040000
1	1.374902000	0.674568000	3.869515000
1	0.686774000	0.726494000	3.553227000
1	-0.383281000	-2.921384000	5.891213000
1	-0.974431000	-2.901572000	5.408109000
1	3.155559000	-2.915463000	-2.297877000
1	3.522009000	-2.331793000	-2.620429000
1	1.875967000	-5.377705000	-1.985370000
1	2.035561000	-5.979135000	-2.416908000
1	-1.494394000	-6.760668000	0.945564000
1	-2.193205000	-6.747532000	0.646251000
1	-1.802695000	1.489412000	-1.268734000
1	-1.565083000	0.901475000	-1.689956000

(MgO)₉-(H₂)₁₇

8	0.376904000	0.611797000	0.181582000
12	2.112731000	1.105607000	1.206317000
8	3.964373000	0.302702000	0.721455000
12	4.016059000	-1.033972000	-0.868075000
8	2.333357000	-1.592462000	-1.957728000
12	0.527658000	-0.734019000	-1.389146000
12	0.300902000	-0.964959000	1.349314000

8	1.78760000	-0.46366700	2.46185900
8	0.24473100	-2.26156100	-0.07041300
12	2.00797800	-2.88703900	-0.51144600
8	3.65118200	-2.55478200	0.43241400
12	3.43428300	-1.23861300	1.82112800
12	0.92615100	1.97736900	-1.11920300
8	2.44105100	2.61071800	-0.11806600
8	0.89247200	0.81610100	-2.65248200
12	4.06146100	1.72136200	-0.65351800
12	2.63581300	0.06480500	-2.99278400
8	4.29700100	0.51880500	-2.13997700
1	0.71103700	-0.13085000	5.38496000
1	0.99076500	-0.21287900	4.68351800
1	1.92188400	2.32732500	3.24282200
1	2.04982300	2.91046800	2.77566000
1	2.70217200	5.64274300	0.50862200
1	2.64657700	4.89950500	0.35933100
1	4.21566200	-1.67973600	4.08116900
1	3.54449600	-1.32018000	4.08225100
1	4.47784900	-5.62362500	0.55943900
1	4.34780700	-4.87617200	0.55576000
1	0.12815500	4.12534300	-1.06054300
1	-0.43831700	3.87945000	-1.50086200
1	2.09140700	1.44708000	-4.85074500
1	2.76695600	1.38318100	-5.19185400
1	2.05800800	-4.56054700	-2.11666400
1	1.91250700	-5.04923700	-1.55705800
1	2.77969200	-1.76579700	-4.44950400
1	2.96955200	-1.37419100	-5.07210100
1	6.18283900	-2.63607200	2.40099700
1	5.68670900	-2.80947000	1.85396700
1	6.20496700	-1.97817700	-1.55389800
1	6.08448500	-1.33875200	-1.94598600
1	5.81577600	1.99969400	0.87082900
1	6.12635100	2.61307700	0.54690000
1	5.48023600	3.40478400	-2.03683200
1	5.38981500	2.71315500	-2.34230800
1	-1.59933000	-1.35010800	2.70574000
1	-1.67160500	-1.84423500	2.13517100
1	-1.39235300	-3.94203600	-0.09340700
1	-1.91908700	-4.49004300	-0.09474800
1	-1.46599800	-1.67883700	-2.25924300
1	-1.39858000	-1.12240100	-2.76981700
1	-0.72962000	1.44361500	-4.24571100
1	-1.26327700	1.65530500	-4.74344000

(MgO)₁₀-(H₂)₁₅

8	2.41792300	1.59020500	-1.20208000
8	-1.08480400	2.66891700	-1.49445900
8	2.45005500	-1.99935700	-0.36597800

8	-3.263925000	-0.227432000	-0.844700000
8	-1.038121000	-3.057563000	-0.165778000
12	-2.547737000	-1.915304000	-0.325771000
12	0.863340000	-3.007846000	-0.059959000
12	0.813027000	2.607978000	-1.344320000
12	-2.563276000	1.523227000	-1.127370000
12	2.900521000	-0.172368000	-0.669043000
12	2.307889000	1.994051000	0.799700000
12	-1.076789000	3.037399000	0.516772000
12	2.334939000	-1.481509000	1.602090000
12	-3.187790000	0.236968000	1.160428000
12	-1.031225000	-2.519698000	1.798486000
8	-2.646800000	-1.516681000	1.667555000
8	0.863376000	-2.637327000	1.963975000
8	0.819201000	3.162260000	0.618511000
8	-2.662152000	2.039491000	0.838686000
8	2.960084000	0.288058000	1.316335000
1	1.544206000	4.066475000	-3.107991000
1	2.123709000	3.608241000	-2.931457000
1	-1.634586000	4.490818000	-2.946201000
1	-1.803765000	5.074071000	-3.401953000
1	0.277650000	-4.443716000	-1.847975000
1	0.994510000	-4.555189000	-2.073765000
1	-0.768415000	5.135277000	1.355362000
1	-1.521659000	5.230801000	1.391177000
1	1.581729000	-3.994409000	4.744773000
1	1.404566000	-3.688074000	4.073761000
1	4.206064000	3.249232000	0.175307000
1	4.296373000	3.497199000	0.885355000
1	4.587482000	-1.268226000	-1.770154000
1	4.866490000	-0.598827000	-1.996482000
1	4.353596000	-2.716508000	2.367768000
1	4.258842000	-2.844387000	1.627363000
1	-5.915909000	0.122659000	0.902359000
1	-5.494493000	-0.012765000	0.285709000
1	-4.365945000	0.937122000	3.257507000
1	-4.085099000	1.538621000	2.887481000
1	-4.759902000	-0.879891000	-2.656320000
1	-5.204682000	-1.108953000	-3.226194000
1	-4.295898000	2.107876000	-2.596494000
1	-3.814074000	2.678424000	-2.725390000
1	1.553413000	-4.950497000	1.199157000
1	1.673922000	-5.420398000	0.615252000
1	-1.745557000	-4.045062000	3.514565000
1	-2.330171000	-3.582877000	3.367741000
1	-4.404581000	-3.249337000	0.274453000
1	-4.462305000	-3.504910000	-0.435920000

Table S4. XYZ Coordinates of the (MgO)_n, n=1-10 clusters with H₂ molecules optimized at a def2-TZVP/ωB97X-D3 level theory.

MgO-(H₂)₉

12	-0.856714000	1.702598000	-2.474180000
8	-0.050021000	1.367256000	-0.986812000
1	-0.523560000	0.980468000	1.901859000
1	-0.373006000	1.072251000	1.167125000
1	1.742365000	2.791278000	-1.618308000
1	2.190484000	3.295020000	-1.961425000
1	-0.389266000	4.017467000	-3.342271000
1	-0.899030000	3.887090000	-3.880146000
1	1.575000000	-0.023067000	-1.726212000
1	2.062686000	-0.504973000	-2.048695000
1	-2.509863000	-0.056083000	-3.050388000
1	-2.702996000	0.372068000	-3.639021000
1	0.680020000	0.881002000	-4.269369000
1	0.197357000	1.153611000	-4.778652000
1	-1.419975000	-1.432938000	-0.923639000
1	-1.019587000	-0.795947000	-0.846391000
1	-2.557953000	1.463893000	-0.206576000
1	-3.305190000	1.535972000	-0.268348000
1	-0.705357000	4.273062000	0.003878000
1	-0.485403000	3.563140000	-0.130213000

(MgO)₂-(H₂)₁₃

12	-1.120279000	-0.467699000	0.859515000
12	0.790671000	-1.153495000	-0.494827000
8	-0.620211000	0.010971000	-0.872208000
8	0.284412000	-1.635143000	1.240440000
1	2.111928000	-0.692131000	-2.474230000
1	1.498783000	-0.251542000	-2.462139000
1	2.003880000	-1.505762000	2.647764000
1	2.636706000	-1.426709000	3.055600000
1	-0.709063000	-2.688842000	3.833709000
1	-0.369159000	-2.480738000	3.189845000
1	-2.518807000	-1.605479000	2.222646000
1	-3.055196000	-1.166380000	1.927207000
1	2.516347000	-0.079183000	0.656418000
1	2.750115000	0.260317000	0.026840000
1	-1.201075000	-0.006971000	-2.990282000
1	-1.340727000	-0.095586000	-3.729552000
1	2.204088000	-2.838373000	0.037970000
1	2.568253000	-2.777230000	-0.622122000
1	-2.784631000	-1.246854000	-1.206019000
1	-0.824722000	0.919494000	2.827150000
1	-0.328534000	0.349994000	2.820692000
1	0.167548000	-2.966777000	-2.061145000
1	-0.305151000	-2.386265000	-2.142350000
1	-0.178806000	-3.842752000	0.900207000
1	-0.306374000	-4.555675000	0.683489000
1	-2.778395000	1.288873000	0.806039000

1	-3.374582000	-1.675366000	-1.018744000
1	-2.346320000	1.253460000	0.181876000
1	0.353696000	1.904231000	-1.511761000
1	0.779092000	2.493271000	-1.725183000

(MgO)₃-(H₂)₁₂

12	0.330814000	1.399260000	0.463172000
12	-1.195616000	-0.149376000	-1.557131000
12	-0.358014000	-1.445250000	0.999051000
8	0.485844000	0.037162000	1.675160000
8	-0.460255000	1.486334000	-1.188802000
8	-1.249587000	-1.706332000	-0.583477000
1	-1.419119000	1.801121000	-3.340282000
1	-1.802648000	1.592120000	-3.955648000
1	-3.308545000	-0.854213000	-2.042176000
1	-3.426262000	-0.246905000	-2.471723000
1	-2.097445000	-3.346045000	-1.879462000
1	-2.404874000	-3.831984000	-2.368579000
1	-0.325177000	4.432261000	-1.730004000
1	-0.399101000	3.682757000	-1.671122000
1	-0.277556000	3.297382000	1.702871000
1	-0.550256000	3.457031000	1.020360000
1	2.000957000	2.182699000	3.164546000
1	1.667545000	1.542435000	2.940371000
1	-1.187864000	-1.297211000	3.134074000
1	-1.621478000	-1.906302000	3.036703000
1	-1.112491000	-4.101602000	1.386305000
1	-1.296399000	-3.754318000	0.742569000
1	1.324414000	-2.960591000	1.868936000
1	1.487524000	-2.247721000	2.056019000
1	-0.670851000	-1.562689000	-3.284207000
1	-0.618670000	-0.952863000	-3.722412000
1	-4.064794000	-2.242324000	0.618463000
1	-3.397034000	-2.142806000	0.284562000
1	2.326200000	2.636080000	0.184157000
1	1.960953000	2.690477000	-0.471861000

(MgO)₄-(H₂)₁₄

12	-1.385261000	-0.164235000	-2.080492000
12	0.631899000	-1.044168000	1.886378000
12	-0.189913000	-2.751303000	-0.671413000
12	-0.540698000	1.567199000	0.475161000
8	0.537006000	-2.622393000	0.986637000
8	0.288302000	0.743923000	1.870292000
8	-1.310028000	1.409950000	-1.167800000
8	-0.995203000	-1.940339000	-2.079731000
1	-1.018067000	0.878197000	-4.121593000
1	-0.955208000	0.164642000	-4.350512000

1	-3.550567000	-0.528623000	-2.894655000
1	-3.626134000	0.189133000	-2.683689000
1	-2.181784000	-2.648531000	-4.745132000
1	-1.858114000	-2.565905000	-4.068077000
1	0.245127000	-4.992346000	-0.820799000
1	-0.079207000	-4.903785000	-1.493820000
1	1.717173000	-4.331011000	3.160586000
1	1.420698000	-3.988175000	2.556821000
1	2.494117000	-0.621873000	3.182909000
1	2.609890000	-1.360489000	3.100073000
1	-0.299842000	-2.030205000	3.816600000
1	-0.394070000	-1.307235000	3.999774000
1	-0.620332000	1.614767000	4.612580000
1	-0.398297000	1.406889000	3.921935000
1	2.504405000	2.511178000	2.907266000
1	1.952129000	2.054927000	2.670161000
1	0.861569000	3.432915000	0.526660000
1	0.502792000	3.563428000	-0.121326000
1	-3.935796000	2.903375000	-1.344559000
1	-3.264153000	2.560509000	-1.320475000
1	-0.824687000	3.148477000	-2.538873000
1	-0.631577000	3.706080000	-3.009092000
1	-3.560978000	-0.147909000	0.852481000
1	-3.254878000	0.309609000	0.344637000
1	-1.816476000	2.822154000	1.964119000
1	-2.172789000	3.023931000	1.333327000

(MgO)₅-(H₂)₁₆

12	3.523657000	-0.278601000	-1.672339000
12	-1.674301000	0.616166000	-0.823335000
12	3.197132000	0.735967000	1.457333000
12	0.515748000	-0.384889000	-3.075795000
12	-0.019292000	1.305268000	1.992076000
8	-1.460204000	1.060526000	0.920220000
8	2.315764000	-0.594201000	-2.982358000
8	-1.128165000	0.093215000	-2.473525000
8	1.743300000	1.245079000	2.411990000
8	4.094005000	0.172758000	-0.016006000
1	-0.175137000	-2.659924000	-3.572028000
1	0.574941000	-2.703365000	-3.545821000
1	-2.595266000	-1.268373000	-3.580178000
1	-3.038481000	-1.762521000	-3.938237000
1	-3.562872000	-0.757564000	-0.335078000
1	-3.433387000	-0.938288000	-1.053129000
1	3.245729000	-0.819003000	-5.023860000
1	3.552635000	-0.886015000	-5.710114000
1	5.688420000	-0.620330000	-2.402772000
1	5.323379000	-0.779087000	-3.041174000
1	6.974849000	-0.178175000	0.760065000
1	6.259214000	-0.096795000	0.534334000

1	3.921083000	-0.657631000	3.239796000
1	4.407650000	-0.874382000	2.709656000
1	2.245911000	2.951792000	4.827556000
1	2.141935000	2.509386000	4.224621000
1	-1.064060000	0.777309000	4.071483000
1	-0.334941000	0.823642000	4.249414000
1	-2.311737000	-1.590553000	2.390521000
1	-2.171277000	-0.950972000	2.019896000
1	5.036882000	2.066096000	2.098746000
1	4.542086000	2.295439000	2.616015000
1	-0.226252000	3.502964000	2.905785000
1	-0.880338000	3.432924000	2.542417000
1	0.503596000	-1.391974000	0.352952000
1	1.044854000	-1.697961000	-0.063253000
1	0.516534000	-0.296696000	-5.413545000
1	-0.186674000	-0.064968000	-5.282348000
1	-3.331176000	2.256261000	-0.978467000
1	-3.311721000	2.080506000	-1.709219000
1	-2.522520000	1.820557000	-4.568858000
1	-2.181412000	1.381836000	-4.059434000

(MgO)₆-(H₂)₁₇

12	0.248729000	-2.081973000	-0.613938000
12	0.787655000	-0.550505000	2.176528000
12	2.323920000	-0.553173000	0.004102000
12	-1.728309000	0.246511000	0.361613000
12	0.371213000	1.781688000	0.950428000
12	-0.191048000	0.249703000	-1.812715000
8	1.975221000	0.801358000	1.293989000
8	-0.696676000	1.653096000	-0.623152000
8	1.391776000	-0.812824000	-1.644484000
8	-1.368564000	-1.114802000	-0.933938000
8	1.293436000	-1.961571000	0.982037000
8	-0.787665000	0.520280000	2.004927000
1	-3.277855000	-0.725065000	1.898626000
1	-3.623489000	-1.016651000	1.298450000
1	-2.164170000	-0.176535000	-3.093362000
1	-2.071881000	0.384232000	-3.587811000
1	0.997992000	0.694932000	-3.762267000
1	0.494227000	1.209597000	-3.981159000
1	-0.674466000	-4.127553000	-1.541122000
1	-1.187513000	-3.576340000	-1.576774000
1	3.879272000	-2.894328000	2.342338000
1	3.210799000	-2.766274000	2.018600000
1	2.207296000	-0.201605000	4.197689000
1	2.430890000	0.215885000	3.609830000
1	0.027235000	3.566975000	2.578064000
1	-0.368485000	2.960572000	2.784215000
1	-1.596179000	3.366020000	-2.934865000

1	-1.372983000	3.029184000	-2.296793000
1	-3.268114000	1.734448000	-0.476565000
1	-3.836891000	1.317248000	-0.212170000
1	4.456587000	-1.456939000	-0.463686000
1	4.064120000	-1.519682000	-1.102055000
1	3.103916000	1.033741000	-2.078356000
1	3.572662000	1.576860000	-1.858681000
1	-4.224563000	-1.927141000	-1.427330000
1	-3.491102000	-1.769517000	-1.339579000
1	2.206238000	3.241808000	0.653234000
1	1.781119000	3.805142000	0.390099000
1	-3.289835000	2.139788000	2.965170000
1	-2.670329000	1.728987000	2.848153000
1	-0.760628000	0.371460000	5.091282000
1	-0.893427000	0.471023000	4.356200000
1	1.967476000	-4.023637000	-0.126294000
1	1.972233000	-4.501315000	-0.708434000
1	0.268661000	-2.180404000	3.972625000
1	0.559312000	-2.542262000	3.379648000

(MgO)₇-(H₂)₁₆

12	0.884781000	-0.552440000	1.257953000
12	-0.388033000	-2.752526000	0.523998000
12	0.540944000	-1.533885000	-1.635084000
12	-1.917770000	-0.659762000	-0.009231000
12	-0.446333000	2.207361000	0.233153000
12	-0.739661000	1.374131000	-2.237377000
12	1.645696000	1.468378000	-1.156004000
8	1.354454000	-2.034605000	0.071237000
8	1.167651000	1.231654000	0.730541000
8	0.806743000	0.175088000	-2.365704000
8	-0.924602000	-1.222366000	1.586921000
8	0.290533000	2.811987000	-1.454253000
8	-1.249243000	-2.137093000	-1.100754000
8	-1.825506000	1.110920000	-0.625726000
1	-3.469424000	-1.166215000	1.640496000
1	-4.049287000	-1.025852000	1.180770000
1	-2.471670000	3.605750000	1.067764000
1	-2.653067000	3.021810000	0.626504000
1	0.242615000	4.447457000	0.280570000
1	0.085450000	4.605672000	1.003048000
1	-0.241971000	4.199547000	-3.145497000
1	-0.503609000	4.545354000	-3.765711000
1	2.947709000	1.208902000	-3.061081000
1	3.478408000	1.698441000	-2.844035000
1	1.273936000	-4.414714000	0.437259000
1	0.839280000	-5.015627000	0.584123000
1	-0.733150000	-4.075402000	2.739458000
1	-0.885698000	-3.335945000	2.768632000

1	-0.128710000	1.091246000	-4.463367000
1	-0.667593000	1.542059000	-4.736748000
1	2.208192000	-0.408087000	3.278628000
1	2.217070000	0.263623000	2.939798000
1	-1.471731000	1.554160000	2.939692000
1	-1.398312000	0.859085000	2.654288000
1	-2.905090000	2.120494000	-2.629280000
1	-2.760207000	2.350275000	-3.332288000
1	-2.020644000	-4.265058000	-0.261665000
1	-1.969377000	-4.787398000	0.282229000
1	3.272524000	2.387300000	0.243295000
1	3.740364000	2.601198000	-0.308250000
1	-2.160099000	-1.100905000	-3.051661000
1	-2.392554000	-0.697345000	-3.645605000
1	-0.048705000	-3.267765000	-3.058091000
1	0.616105000	-3.242707000	-3.410806000
1	3.352759000	-0.878649000	-0.514952000
1	3.921962000	-0.426451000	-0.718533000

(MgO)₈-(H₂)₁₆

12	-0.132863000	0.202203000	-0.051826000
8	0.039680000	-0.984511000	-1.537837000
8	1.757742000	0.015333000	0.512871000
12	1.864164000	-1.313673000	-0.860926000
8	-0.826937000	-0.398812000	1.624546000
12	-1.853445000	-1.981553000	1.724492000
8	-1.716086000	-3.284794000	0.234866000
12	-0.356236000	-2.783152000	-0.974604000
8	1.520937000	-3.161443000	-0.466848000
12	-1.382496000	-4.597877000	1.584020000
8	0.399070000	-5.014099000	2.136026000
12	1.623741000	-3.787306000	1.313614000
8	-1.709711000	-3.331875000	3.076876000
12	1.057755000	-0.762769000	2.120694000
8	1.491292000	-2.473433000	2.790323000
12	0.128583000	-3.609068000	3.506891000
1	3.068134000	0.899097000	-1.362505000
1	3.334960000	0.843834000	-2.064760000
1	4.065423000	-0.991000000	0.500826000
1	4.542412000	-1.495935000	0.212326000
1	3.698064000	-3.722404000	2.341182000
1	3.961639000	-4.247690000	1.870864000
1	0.865361000	-5.116962000	5.260186000
1	0.858067000	-5.479431000	4.599159000
1	0.655932000	-0.323063000	-3.617036000
1	0.954072000	-0.139723000	-4.285982000
1	-0.673428000	-2.716148000	-3.273015000
1	-0.882447000	-3.438575000	-3.306006000
1	1.250471000	-7.819895000	2.673595000

1	1.046593000	-7.108562000	2.520278000
1	-3.208196000	-5.197576000	2.856013000
1	-3.376455000	-5.817331000	2.457475000
1	-3.815518000	-1.903470000	0.473181000
1	-4.107046000	-1.363322000	0.909738000
1	0.225156000	2.615876000	-0.332857000
1	0.849943000	2.272686000	-0.085927000
1	0.801732000	0.688427000	4.098109000
1	0.155701000	0.675438000	3.711459000
1	-0.344234000	-2.567856000	5.769524000
1	-0.960517000	-2.624729000	5.338313000
1	3.111651000	-2.483834000	-2.368252000
1	3.370447000	-1.845963000	-2.674400000
1	0.759654000	-5.244162000	-1.516351000
1	0.273392000	-5.715724000	-1.842629000
1	-1.009569000	-6.750954000	0.775156000
1	-1.683288000	-6.747979000	0.438890000
1	-2.152034000	1.232162000	-1.095765000
1	-1.844624000	0.721888000	-1.557288000

(MgO)₉-(H₂)₁₈

8	0.382673961	0.646028243	0.222934255
12	2.124933542	1.110846358	1.216316950
8	3.932870373	0.261473736	0.728515955
12	3.943485967	-1.092399422	-0.826117376
8	2.249915546	-1.617991802	-1.871071572
12	0.482147604	-0.720476597	-1.316215142
12	0.268494917	-0.890735948	1.407765855
8	1.778373640	-0.426753612	2.469848936
8	0.189807050	-2.193337529	0.021422592
12	1.906537727	-2.887018587	-0.418181405
8	3.548869446	-2.560079479	0.495400498
12	3.397313355	-1.232491659	1.855229781
12	0.931770562	1.969303409	-1.091241157
8	2.471366770	2.558468877	-0.135046255
8	0.883540967	0.789272267	-2.583132943
12	4.058819123	1.643664226	-0.656068835
12	2.582115459	-0.007678529	-2.937399973
8	4.237595193	0.421143534	-2.107052717
1	0.622674979	0.293494431	5.135775980
1	0.944491038	0.100615383	4.479945158
1	2.001660729	2.352371719	3.203167206
1	2.138095130	2.916369615	2.724872821
1	2.554313140	5.331366771	0.938821885
1	2.561953572	4.632853257	0.649458367
1	4.029999119	-1.670270356	4.214815591
1	3.370097599	-1.307377651	4.175838440
1	5.170842788	-5.032024143	-0.029368233
1	4.781568337	-4.408097460	0.143011715

1	0.369263403	4.170498787	-0.869483015
1	-0.255109840	4.018650315	-1.261468448
1	2.153375095	1.425667161	-4.789048046
1	2.844695630	1.310476664	-5.062112105
1	2.174652615	-4.888316906	0.858804976
1	1.463941758	-5.069819584	0.695171406
1	2.103002830	-4.127165606	-2.364572623
1	1.953133327	-4.777054715	-2.016509205
1	2.618020367	-1.851270854	-4.360385114
1	2.811387181	-1.455647760	-4.970642060
1	6.031445712	-2.227577223	2.435888367
1	5.622343782	-2.553633260	1.895439039
1	5.899407390	-2.336512231	-1.337871618
1	5.979592345	-1.726898842	-1.771020587
1	5.777057285	1.942315958	0.870262505
1	6.051286523	2.554548025	0.527954949
1	5.241590522	3.405524612	-2.027723219
1	5.229757180	2.743476727	-2.386538267
1	-1.641339390	-1.334578718	2.712046655
1	-1.692070629	-1.806497139	2.128529856
1	-1.434861972	-3.695935937	-0.176042230
1	-1.985695892	-4.207916923	-0.253349451
1	-1.468738633	-1.664008433	-2.188752454
1	-1.381265246	-1.130815131	-2.711876075
1	-0.458248471	0.812554369	-4.365644056
1	-0.898737755	0.779823795	-4.978822304

(MgO)₁₀-(H₂)₁₈

8	2.515034205	1.666758213	-1.135737944
8	-0.923990438	2.785593753	-1.270026008
8	2.501710523	-1.929867996	-0.396944881
8	-3.167561431	-0.020319540	-0.608352528
8	-0.964474987	-2.833759717	-0.118392670
12	-2.472727246	-1.718248107	-0.177609505
12	0.915741491	-2.897489845	-0.067167138
12	0.960742818	2.733447444	-1.199028846
12	-2.400709825	1.683960046	-0.872329192
12	2.924024703	-0.113691254	-0.670645485
12	2.496240395	2.030024669	0.860389435
12	-0.832880771	3.114263519	0.738422404
12	2.477825456	-1.482507731	1.570838407
12	-3.014455813	0.380668186	1.378836505
12	-0.879777490	-2.377344160	1.858203641
8	-2.480370939	-1.376076640	1.811439046
8	0.997295693	-2.590886250	1.938989824
8	1.044782782	3.222414375	0.752970089
8	-2.404418319	2.142252418	1.089412138
8	3.046404664	0.290865725	1.312717625
1	1.572854459	4.551964830	-2.573211125

1	2.201703628	4.142500658	-2.540035435
1	-0.450684900	2.493922243	-3.655130669
1	-0.055480648	2.360967349	-4.280209543
1	-0.132730858	-0.714909251	-1.876966952
1	0.048196737	-0.050101098	-2.171510692
1	0.556320783	-4.095642745	-2.104322256
1	1.298595185	-4.012398150	-2.184904901
1	-1.629267293	5.496377982	0.264216812
1	-1.563646689	5.097972389	-0.370305298
1	-0.276753650	0.600904826	2.654803854
1	0.449928372	0.544767891	2.481302493
1	-1.172129675	-1.728887902	4.322570757
1	-0.472278662	-1.991409743	4.385305589
1	1.612878096	-4.512174484	4.176562420
1	1.474383137	-4.022576935	3.618920976
1	4.362556946	3.115254824	-0.097335705
1	4.598016971	3.400471399	0.557762770
1	5.011861092	-0.609953626	-1.615512197
1	4.962112744	0.121429025	-1.778752666
1	4.434263819	-2.981017854	1.953372904
1	4.262981357	-2.962885992	1.221127859
1	-5.535654521	0.361324748	1.519688320
1	-5.310891009	0.265191934	0.808633967
1	-3.669829135	0.761390928	3.723315708
1	-3.496664402	1.444067340	3.460934126
1	-5.092111328	-0.303942537	-1.770241314
1	-5.748237809	-0.388875895	-2.133076616
1	-4.281802199	2.274269446	-2.097746199
1	-3.855402374	2.870349682	-2.263220421
1	1.621591566	-4.892369570	1.049988712
1	1.730978227	-5.282378410	0.416172452
1	-1.190791416	-4.489883762	2.883897797
1	-1.906336255	-4.265678963	2.855536245
1	-4.318044110	-2.869993265	0.725858659
1	-4.543022177	-3.112751031	0.050509131

Table S5. Harmonic frequencies (ω) of the ground state structures of the $(\text{MgO})_n$, $n=1-10$ clusters with H_2 at a def2-TZVP/BP86/D3 level theory.

MgO-(H₂)_n								
4.1	17.99	25.96	33	39.32	43.38	58.95	60.77	67.15
73.58	81.78	92.97	96.93	103.65	106.88	128.71	134.07	151.06
164.84	185.94	190.2	201.17	214.19	219.5	223.99	232.2	245.03
247.56	295.66	416.93	431.01	432.49	446.51	510.21	531.57	535.95
539.77	543.64	556.31	567.22	577.9	594.94	604.07	607.02	815.38
3983.09	3988.01	4000.08	4018.99	4040.92	4057.94	4159.14	4179.15	4179.83

(MgO)₂-(H₂)₁₃

17.57	27.85	30.97	33.86	48.79	51.09	51.93	65.8	72.23
80.02	85.61	95.1	98.92	111.36	114.49	121.85	132.83	153.43
156.67	163.61	172.6	176.96	188.81	197.88	210.09	214.44	221.34
224.78	232.78	238.4	245.47	254.11	257.19	269.83	280.13	291.91
296.37	310.81	316.11	325.79	343.48	402.1	426.19	448.39	483.79
484.14	486.17	514.57	542.22	554.97	559.98	562.73	567.42	578.16
584.73	589.67	601.1	605.16	607.34	617.61	620.46	632.58	648.83
691.7	725.82	734.69	748.6	772.41	804.46	807.63	870.93	3911.54
3968.83	3982.59	4002.8	4007.73	4012.99	4018.33	4022.68	4024.61	4031.33
4052.14	4082.09	4164.36						

(MgO)₃-(H₂)₁₂

11.07	20.13	23.91	46.27	50.01	52.46	57.18	59.89	63.32
66.06	72.53	79.25	87.7	92.83	109.54	120.42	128.49	138.82
163.69	165.63	171.22	173.03	179.88	183.67	187.39	197.68	198.96
205.95	209.58	227.59	232.19	233.61	246.81	257.53	263.02	265.24
268.59	276.68	291.26	297.36	303.1	341.67	427.67	451.18	452.35
478.01	485.43	492.34	495.28	503.69	506.16	513.07	525.16	531.77
537.85	539.27	562.99	566.76	581.11	586.04	712.96	714.05	742.2
745.44	748.44	752.39	761.8	767.08	780.53	786.82	787.93	805.89
3989.98	4016.62	4018.4	4030.54	4035.49	4044.68	4055.22	4061.61	4068.44
4077.66	4080.12	4101.68						

(MgO)₄-(H₂)₁₄

10.55	15.2	15.53	19.42	21.92	25.78	27.05	31.07	32.47
34.13	38.05	38.65	45.33	49.36	52.85	55.15	62.46	65.16
69.05	77.82	79.57	83.3	86.16	86.81	92.34	96.84	116.79
120.77	124.38	139.25	144.56	145.67	163.94	185.04	186.95	197.19
198.86	209.65	220.51	226.43	240.02	247.6	250.99	255.33	269.92
301.29	319.69	322.87	336.21	337.55	338.94	342.17	345.05	356.49
360.96	362.38	369.02	372.77	376.6	417.8	430.61	437.03	500.94
504.42	506.77	508.15	516.74	523.56	529.41	530.64	559.65	571.39
579.38	582.92	584.86	585.22	665.01	696	699.94	706.3	717.4
719.65	723.33	728.67	744.07	823.2	827.23	843.45	4052.77	4053.73
4055.76	4058.4	4064.42	4068.17	4129.97	4130.65	4158.24	4161.34	4168.78
4174.54	4184.89	4185.02						

(MgO)₅-(H₂)₁₆

7.86	11.1	16.55	18.08	21.07	24.54	30.63	34.32	35.06
39.02	40.32	42.38	44.22	46.42	50.91	51.34	53.4	57.66
59.32	60.4	62.67	65.17	66.02	71.07	74.79	76.29	81.44
85.45	86.02	99.2	103.08	105.57	115.16	120.92	124.77	132.1
133.38	137.02	143.81	146	151.46	154.37	195.24	199.05	205.89
209.42	214.92	215.11	226.79	228.73	239.39	241.64	245.92	250.54
254.32	269.46	294.36	296.36	303.38	314.6	317.61	323.43	325.51
343.95	353.24	355.72	356.46	359.01	373.09	378.49	379.56	398.54
399.7	413.55	431.15	440.55	486.34	510.02	518.99	526.12	532.37
532.97	561.75	576.92	579.28	584.3	588.43	590.08	607.05	609.62
679.74	687.22	692.06	695.29	701.02	706.27	714.75	715.33	718.43
785.66	787.83	873.02	879.57	886.21	4044.56	4046.99	4047.86	4051.17
4055.82	4056.86	4134.35	4151.87	4152.28	4162.87	4163.61	4169.57	4179.54
4181.64	4183.08	4186.06						

(MgO)₆-(H₂)₁₇

30.05	42.34	43.55	54.67	58.7	63.6	70.14	73.05	76.2
77.14	78.23	80.82	87.87	92.27	92.89	94.96	98.77	102.9
103.25	107.4	114.29	121.73	124.61	129.26	133.61	134.76	137.15
139.31	145.24	152.37	163.31	165.28	180.12	184.58	189.07	191.79
196.26	198.4	200.66	204.57	210.49	215.2	220.37	228.32	231.69
236.04	240.3	243.32	250.02	255.46	264.97	275.24	278.36	287.48
291.83	300.55	308.01	313.39	316.31	325.39	361.22	364	367.34
378.51	382.71	388.86	397.7	402.71	404.2	408.08	413.85	415.9
430.01	451.89	452.83	463.09	473.85	480.77	496.73	497.46	500.63
502.72	520.18	526.06	541.19	543.53	566.01	569.93	599.95	600.47
608.31	610.54	616.58	626.5	641.51	643.95	647.39	660.45	699.86
743.81	748.48	750.32	751.55	756.98	758.11	768.02	815.35	858.22
864.49	881.31	905.34	985.92	1004.34	1168.8	1314.99	2630.29	3365.56
3628.3	3767.52	3861.18	4022.62	4039.57	4044.37	4057.77	4070.53	4082.34
4103.16	4103.85	4121.12	4128.51	4131.99	4136.61			

(MgO)₇-(H₂)₁₆

23.4	40.85	51.27	55.06	70.36	80.03	82.57	83.94	86
88.34	91.82	93.23	95.43	101.56	103.93	104.19	106.95	118.03
120.67	128.58	130.58	139.02	147.05	148.57	150.41	156.51	158.78
163.59	168.96	169.33	173.95	175.04	176.34	190	197.12	204.46

212.08	223.71	226.77	228.26	232.71	233.47	234.42	235.86	246.32
249.61	252.42	255.76	259.35	265.95	273.15	273.73	276.18	281.69
285.26	292.58	294.04	303	313.27	319.32	322.77	367.75	387.95
405.93	411.37	415.26	420.96	421.9	423.09	425.19	432.83	439.54
449.4	451.18	457.37	458.47	463.15	471.7	475.18	479.37	500.98
505.14	506.1	517.35	523.02	529.34	532.56	533.26	537.96	539.78
541.04	541.65	551.37	560.13	570.35	572.87	578.79	579.65	580.78
587.43	619.92	662.09	663.55	694.91	733.95	736.81	741.28	755.87
768.49	770.34	773.84	778.35	778.67	783.85	793.54	821.91	3948.35
3953.61	3956.49	3961	3976.52	3981.16	3986.86	3996.88	4039.7	4047.74
4057.94	4062.3	4072.07	4099.94	4109.21	4126.24			

(MgO)₈-(H₂)₁₆

24.31	26.57	30.78	39.26	55	64.14	67.84	70.72	74.7
81.74	85.46	88.02	88.56	94.82	98.09	101.48	105.71	107.05
109.2	110.27	112.71	113.42	116.72	118.1	119.84	121.67	126.06
128.59	143.48	147.2	151.6	175.15	176.32	178.41	181.16	184.93
186.29	192.25	203.65	209.38	210.95	214.54	223.22	235.96	236.86
239.3	252.82	254.37	258.64	264.36	270.01	273.6	277.07	286.03
286.55	291.35	296.41	299.65	300.9	305.04	311.39	315.79	317.52
324.96	359.58	374.51	396.34	404.66	410.21	414.01	415.97	419.38
421.96	428.57	432.93	435.7	437.53	439.03	440.38	446.35	459.1
460.58	464.78	468.03	473.46	476.18	495.21	499.52	501.82	511.03
512.84	519.38	523.33	527.83	534.3	551.98	555.77	569.43	570.96
585.38	591.26	598.75	608.58	613.49	616.43	619.18	667.01	670.62
673.14	693.25	710.44	713.67	742.36	754.08	756.03	757.42	764.58
775.79	786.23	797.95	811.75	830.19	4018.24	4041.97	4058.57	4059.1
4069.49	4073.52	4078.29	4081.3	4089.56	4102.67	4110.37	4115.81	4116.77
4118.16	4126.01	4157.74						

(MgO)₉-(H₂)₁₈

8.81	16.1	20.52	22.61	23.58	25.82	26.59	29.03	43.32
46.01	47.88	61.92	64.29	65.49	67.3	68.45	69.63	70.73
72.23	73.87	79.34	81.63	82.74	84.6	87.84	91.45	91.64
98.26	99.38	99.77	104.25	106.08	115.29	119.4	167.7	170.56
175.36	183.5	188.28	207.57	211.97	214.11	215.7	218.7	222.99
228.1	235.24	237.72	238.88	242.82	247.42	248.7	253.11	255.28
258.53	261.71	266.96	269.28	269.4	274.43	281.26	283.51	285.64
294.19	300	303.18	311.98	318.22	321.31	333.24	337.29	342.05
345.15	348.16	357.6	362.05	368.87	374.14	375.9	379.53	383.49
383.89	385.49	389.91	393.41	414.61	416.26	423.9	425.33	428.7
432.52	436.44	438.74	450.37	454.58	456.59	466.97	489.75	492.63
496.65	502.5	516.07	517.5	520.27	537.05	538.58	556.08	557.88
563.13	569.53	570.58	572.11	572.58	573.99	578.47	583.9	587.23
591.75	639.54	643.2	646.79	651.33	653.59	657.47	665.4	668.78

681.4	699.65	707.57	713.78	731.91	739.58	740.13	746.36	747.58
749.99	753.21	773.27	4009.86	4016.03	4021.4	4023.76	4029.98	4041.07
4067.91	4072.12	4084.23	4100.6	4107.7	4110.42	4114.79	4140.72	4150.98
4156.02	4164.35	4167.25						

(MgO)₁₀-(H₂)₁₈

7.16	17.31	21.38	30.87	33.4	34.46	35.5	37.25	42.26
44.54	44.99	50.63	57.48	61.14	63.62	66.73	68.52	70.43
74.49	78.67	81.32	83.71	89.45	93.6	96.05	97.45	100.12
101.96	111.67	114	115.61	118.6	121.87	123.53	123.91	127.01
140.79	144.09	145.71	163.09	176.57	179.71	180.67	184.36	190.83
196.93	203.57	205.65	209.97	213.16	217.54	227.53	228.62	230.98
240.49	243.84	250.15	253.56	256.23	261.7	267.17	268.59	270.83
273.19	276.32	279.33	281.95	284.83	293.54	297.17	299.29	301.21
308.2	310.52	313.88	322.04	325.98	327.02	331.51	332.85	335.34
338.14	352.34	355.08	362.32	367.25	368.85	370.45	372.43	376.16
377.68	381.64	382.48	387.33	388.68	393.9	397.86	399.91	404.9
408.97	410.36	423.55	426.31	432.49	434.54	438.27	440.56	443.75
449.16	461.13	461.47	482.99	513.75	517.55	530.83	543.04	554.67
562.98	565.74	568.85	574.36	585.57	660.38	671.27	673.77	690.48
691.93	694.32	695.89	705.28	709.17	714.88	717.9	718.53	722.87
725.36	726.48	733.7	735.54	744.58	748.42	753.55	762.33	771.24
3937.42	4007.48	4035.29	4046.54	4077.98	4085.08	4086.22	4097.69	4105.55
4110.22	4112.22	4121.65	4122	4128.71	4160.28	4161.53	4186.2	4186.96