

SUPPORTING INFORMATION

Mechanism of CO₂ Hydration: Porous Metal Oxide Nanocapsule Catalyst Can Mimic the Biological Carbonic Anhydrase Role

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Computational Details

The Amsterdam Density Functional (ADF) program package¹ version 2012.01 has been used throughout. The Perdew, Burke and Ernzerhof (PBE)² gradient corrected exchange and correlation functionals were used in the calculations. The choice of this functional is due to the fairly accurate description it provides of hydrogen bonds,³ an aspect which is crucial to this work. The ZORA^{4, 5} scalar relativistic Hamiltonian was employed with a triple zeta Slater type orbital⁶ (STO) augmented with one polarization function (TZP) for molybdenum, and double zeta STO type functions augmented with d functions on the remaining elements. A small frozen core was used for all the elements (1s² shell for O and C, and 3d¹⁰ shell for Mo) except hydrogen. The geometry optimizations were performed via the numerical integration scheme of Versluis and Ziegler.⁷ Stationary points were located with a 5.0 digit integration accuracy whereas partial and full analytic hessian calculations were done with 7.0 digit integration accuracy. The COSMO⁸ implicit solvation scheme was used throughout. The imaginary frequencies related to the reaction coordinate were followed by a small fraction of their coordinate displacement in either direction and subsequently re-optimized to achieve the reactant and product. Partial hessian calculations were performed on the reaction site, i.e. the eight atoms present in the ensemble {CO₂+OH₂+OH⁻} for **2a**, **2b**, **TS2b**, and **2c**. For the remainder of the steps seven atoms {HCO₃⁻+OH⁻} were used to compute the partial hessian. Electronic and free energies of reactions leading to a formal loss of a proton were calculated via an explicit Brønsted type equilibrium between two water molecules and the Zundel cation (H₅O₂⁺).

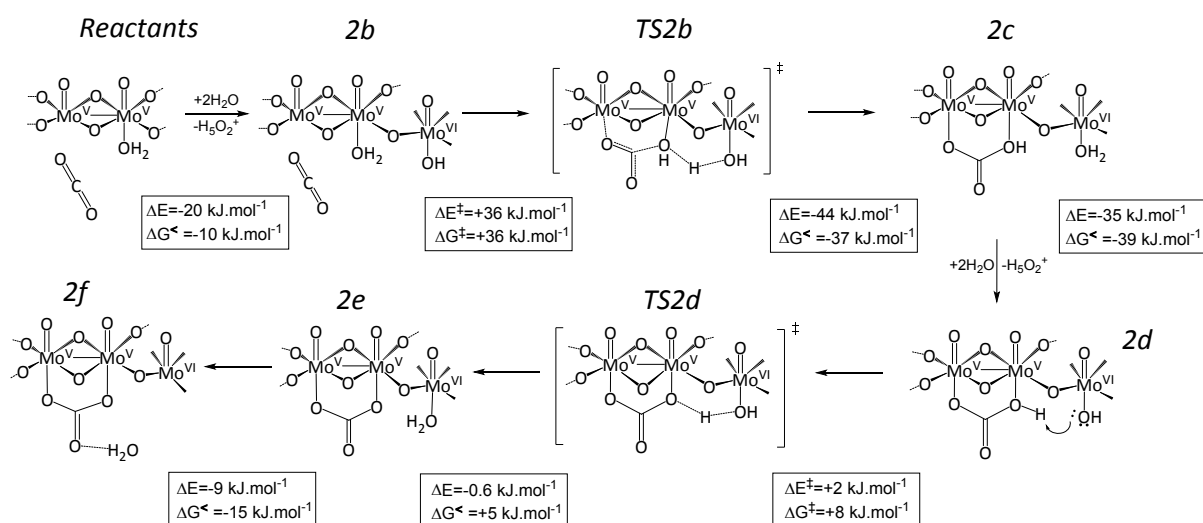
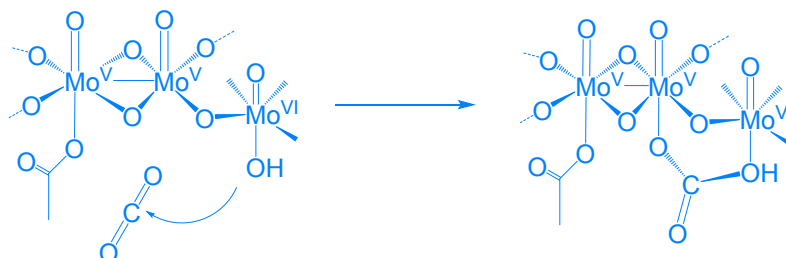
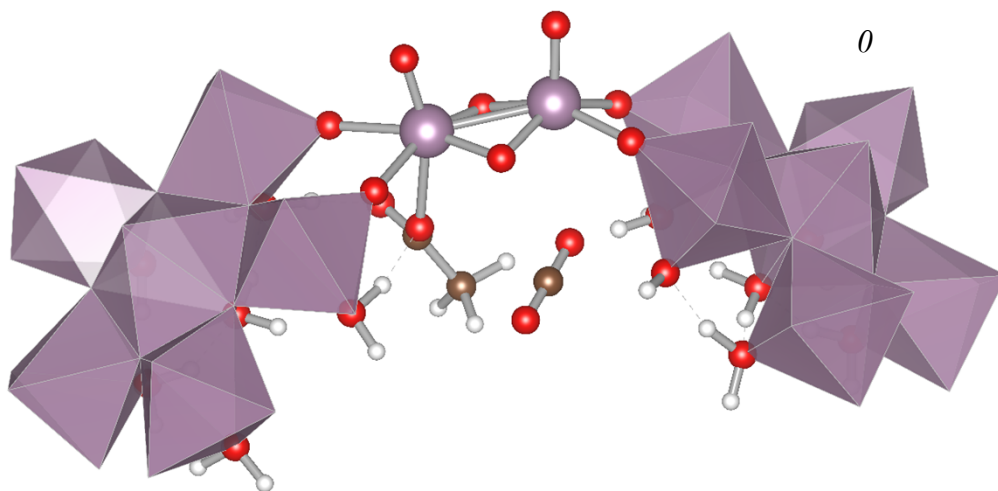


Figure S1 - Calculated mechanistic steps of the catalysed CO₂ hydration presented in Figure 2 of the accompanying paper.

Optimised geometries in xyz coordinates:



1) Mo(VI) pathway (Depicted in blue colour in Figure 2)



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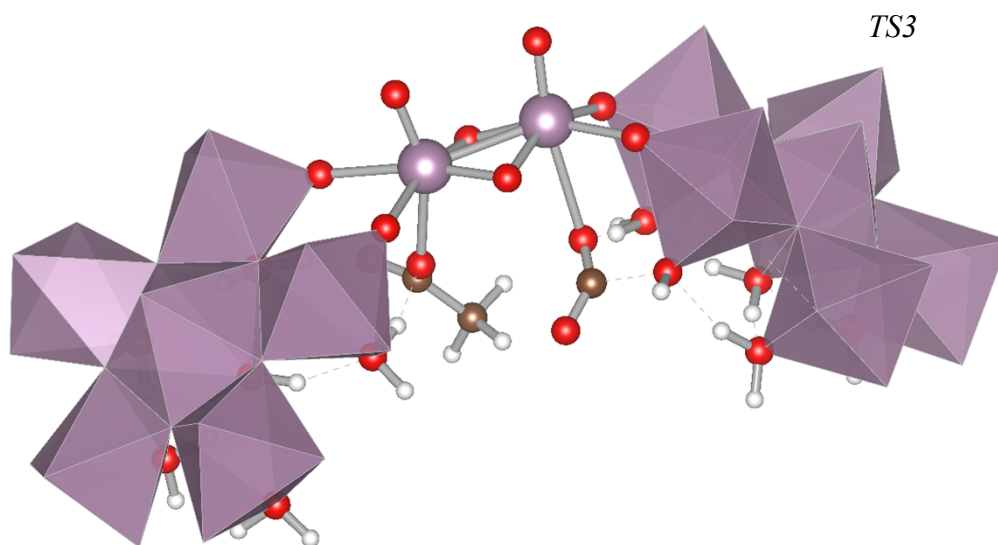
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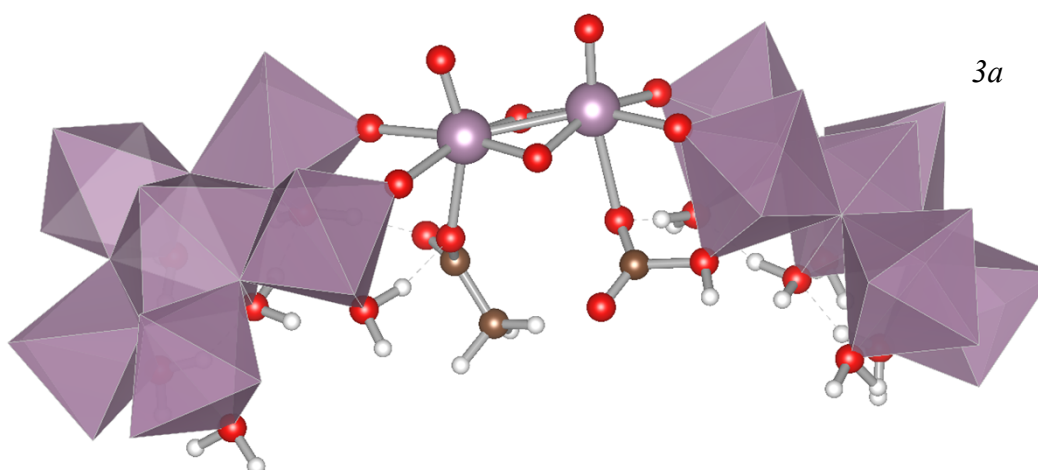
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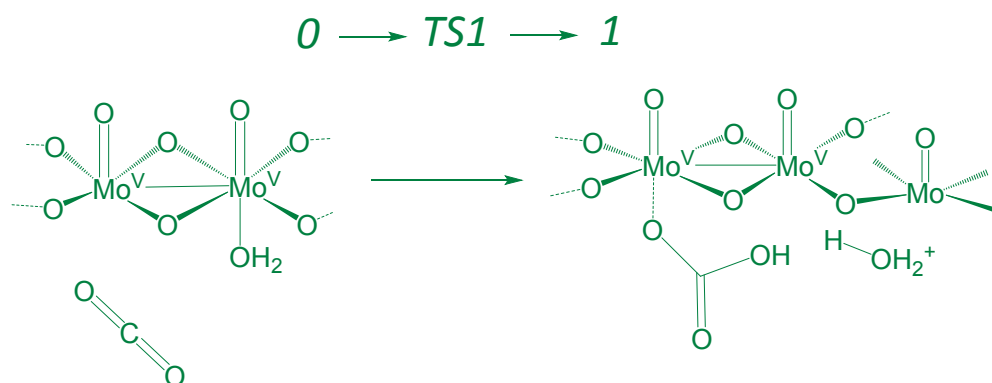
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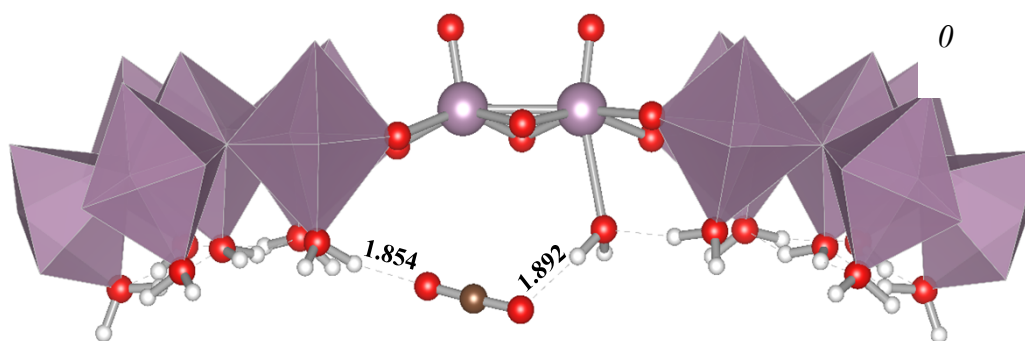
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H	10.635000000	-0.383900000	3.904900000
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H	-3.866500000	-1.850300000	4.260600000
H	4.613000000	1.626800000	4.544500000
H	5.764300000	0.533400000	4.381900000
O	7.358400000	-2.598900000	-2.707500000
H	8.163100000	-3.057500000	-2.359600000
H	7.108400000	-3.117000000	-3.509500000
O	4.140100000	-1.379900000	-1.695100000
H	3.259500000	-1.441600000	-1.193900000
H	3.997000000	-1.827900000	-2.559600000
O	6.215500000	-1.753700000	0.053100000
H	5.611100000	-1.724800000	0.860400000
O	8.363600000	-3.045000000	0.703400000
H	8.532000000	-4.002500000	0.543200000
O	7.431800000	-2.008400000	3.011300000
H	7.624400000	-2.495900000	3.846800000
O	4.691600000	-1.285000000	2.195000000
H	5.230000000	-1.746200000	2.884100000
H	3.737100000	-1.700200000	2.152800000
H	7.842600000	-2.563900000	2.280200000
H	5.582500000	-1.827100000	-0.719100000
H	7.470600000	-2.825600000	0.296500000
O	-2.737900000	-2.116400000	-2.261100000
O	-4.519400000	-4.068400000	-0.848200000
H	-3.818800000	-3.859400000	-0.139600000
O	-5.043400000	-4.321300000	-3.773500000
H	-5.448700000	-5.218000000	-3.698200000
O	-5.795800000	-6.320500000	-0.699200000
H	-5.501600000	-7.140000000	-1.161000000

O	-2.936200000	-3.090200000	0.953700000
H	-2.476200000	-3.643700000	1.626700000
O	-5.248800000	-5.580600000	1.827700000
H	-5.075100000	-6.236400000	2.542700000
H	-4.098400000	-3.868200000	-1.718200000
H	-2.639600000	-2.324800000	-3.223000000
H	-2.216100000	-2.604700000	0.395600000
H	-5.422900000	-6.118700000	1.000700000
H	-5.116900000	-5.604500000	-0.896600000
H	-4.550800000	-4.356900000	-4.628400000
C	2.028100000	-2.388900000	0.637400000
C	1.606400000	-3.656200000	-0.040900000
H	1.296800000	-4.406200000	0.697400000
H	0.826700000	-3.464000000	-0.787500000
H	2.487300000	-4.057000000	-0.573200000
C	-1.382800000	-2.047600000	-1.775000000
O	-0.483700000	-2.300000000	-2.555400000
O	-1.347300000	-1.735400000	-0.525600000



2) Aqua ligand pathway (Depicted in green colour in Figure 2)



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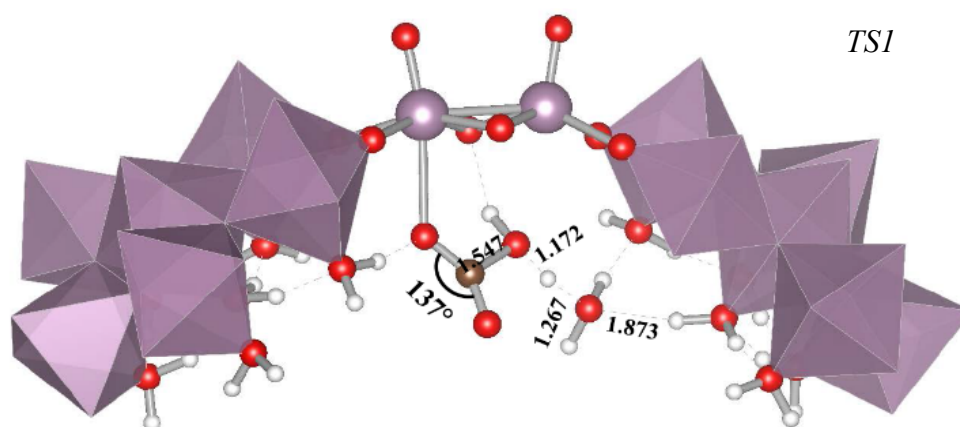
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Mo	0.130700000	0.843400000	-1.344400000
O	1.294600000	-0.111500000	-2.791500000
Mo	1.969300000	0.291400000	-4.417500000
O	2.293300000	1.949600000	-4.278400000
Mo	0.118500000	0.831100000	1.275900000
O	-0.622700000	-1.542700000	1.760900000
O	-1.328900000	0.779800000	-0.039000000
O	1.333000000	0.036000000	-0.039300000
O	-1.327200000	0.523000000	-2.790100000
Mo	-1.863400000	0.891100000	-4.476900000
O	-1.886900000	0.442200000	-6.555800000
Mo	-3.129100000	0.333800000	-8.243900000
O	-3.791600000	-0.580700000	-9.763800000

O	3.795100000	-0.417600000	-4.486200000
O	0.036400000	0.363300000	-5.160800000
Mo	0.031600000	0.384000000	-7.212100000
O	0.132300000	2.041400000	-7.568100000
O	1.936100000	0.122400000	-6.554800000
Mo	3.165100000	-0.153600000	-8.201100000
O	3.671800000	-1.242300000	-9.720500000
O	1.327500000	0.041000000	2.813500000
Mo	1.962000000	0.448100000	4.444400000
O	1.920100000	0.224200000	6.586800000
Mo	3.151000000	-0.108100000	8.219700000
O	4.513900000	-0.193000000	6.984900000
O	-1.312100000	0.941100000	2.817100000
Mo	-1.874400000	1.030900000	4.512400000
O	-3.801000000	0.708100000	4.532300000
O	0.606600000	2.447200000	1.481000000
O	3.806600000	-0.234600000	4.526200000
O	0.032200000	0.534900000	5.192600000
Mo	0.010200000	0.412900000	7.243600000
O	0.054900000	2.050700000	7.689800000
O	2.286400000	2.108800000	4.311900000
O	-3.807800000	0.764100000	-4.533700000
O	-1.689400000	2.574300000	-4.613900000
O	-1.866900000	2.697900000	4.859900000
O	-1.899700000	0.422300000	6.574600000
Mo	-3.157100000	0.215100000	8.215800000
O	-3.800700000	-0.852800000	9.642100000
O	-1.197000000	-0.393900000	8.677400000
Mo	-0.109100000	-1.101500000	10.291700000
O	-1.353800000	-2.484300000	10.617200000
O	1.156500000	-0.335400000	8.769100000
O	1.475100000	-1.593300000	11.123500000

O	-0.658600000	0.108700000	11.341200000
O	-4.524900000	0.353000000	6.984500000
O	-3.076800000	1.750200000	8.937500000
O	3.406700000	1.414500000	8.924000000
O	3.671500000	-1.258700000	9.690200000
O	-1.184500000	-0.321200000	-8.683000000
Mo	-0.104700000	-1.015600000	-10.313200000
O	-1.401800000	-2.345100000	-10.664700000
O	1.170800000	-0.327000000	-8.760200000
O	3.448700000	1.394300000	-8.834500000
O	4.527100000	-0.308500000	-6.966200000
O	-4.514300000	0.448200000	-7.026300000
O	-2.963400000	1.910700000	-8.854700000
O	1.465900000	-1.533400000	-11.152200000
O	-0.624000000	0.230300000	-11.335600000
H	-4.026200000	-0.336300000	10.456300000
H	-4.363900000	0.506600000	5.974000000
H	-4.070500000	-0.089900000	4.016500000
H	-2.079600000	-2.244900000	11.247000000
H	2.342500000	-1.683800000	10.605300000
H	4.178300000	-0.752400000	10.374700000
H	-3.962800000	0.012000000	-10.538500000
H	-4.367800000	0.614000000	-6.022400000
H	-4.171200000	-0.018000000	-4.051400000
H	-2.112700000	-2.064800000	-11.295300000
H	2.336400000	-1.644400000	-10.643800000
H	4.172900000	-0.708200000	-10.388000000
H	4.333000000	-0.342100000	5.972800000
H	4.440700000	0.431700000	4.161500000
H	4.439300000	0.231100000	-4.107000000
H	4.348000000	-0.507100000	-5.971200000
H	0.148400000	-2.157700000	1.775800000

H	-1.282400000	-1.996300000	1.181700000
O	-3.128400000	-1.991100000	-7.541200000
H	-2.888200000	-2.579400000	-8.296500000
H	-4.042400000	-2.282200000	-7.307000000
O	-2.179300000	-1.551800000	-4.564700000
H	-1.927400000	-2.043800000	-3.745500000
H	-3.048700000	-1.931500000	-4.826000000
O	-0.304900000	-1.994400000	-6.645700000
H	0.308200000	-2.222500000	-5.881500000
O	0.526900000	-2.975300000	-8.897400000
H	0.272900000	-3.858600000	-9.255400000
O	2.762300000	-2.446400000	-7.454000000
H	3.564300000	-3.010000000	-7.569800000
O	1.698500000	-2.096500000	-4.929000000
H	2.268600000	-2.377400000	-5.705000000
H	1.879000000	-2.748300000	-4.210700000
H	2.058000000	-2.862700000	-8.040600000
H	-1.215500000	-2.074900000	-6.260000000
H	0.038800000	-2.862400000	-8.025300000
O	-1.861200000	-1.379700000	4.200100000
H	-1.429000000	-1.564100000	3.316800000
O	-0.319500000	-1.960000000	6.634100000
H	0.109800000	-2.183900000	5.762900000
O	-3.008900000	-2.094700000	7.344000000
H	-2.976700000	-2.730700000	8.099400000
O	0.601300000	-3.010700000	8.826400000
H	0.372700000	-3.913900000	9.149700000
O	1.696700000	-1.938800000	4.875500000
H	2.212300000	-2.222100000	5.689800000
O	2.775600000	-2.373700000	7.375700000
H	3.595500000	-2.919000000	7.444800000
H	-1.298900000	-2.097000000	6.532500000

H	-2.642500000	-1.975500000	4.236500000
H	1.995400000	-2.542100000	4.155400000
H	2.100600000	-2.829100000	7.969100000
H	0.124400000	-2.882100000	7.950800000
H	-3.831400000	-2.353700000	6.862900000
C	-1.806900000	-2.794700000	-1.112000000
O	-1.244200000	-2.627200000	-2.123900000
O	-2.337500000	-2.932700000	-0.079300000



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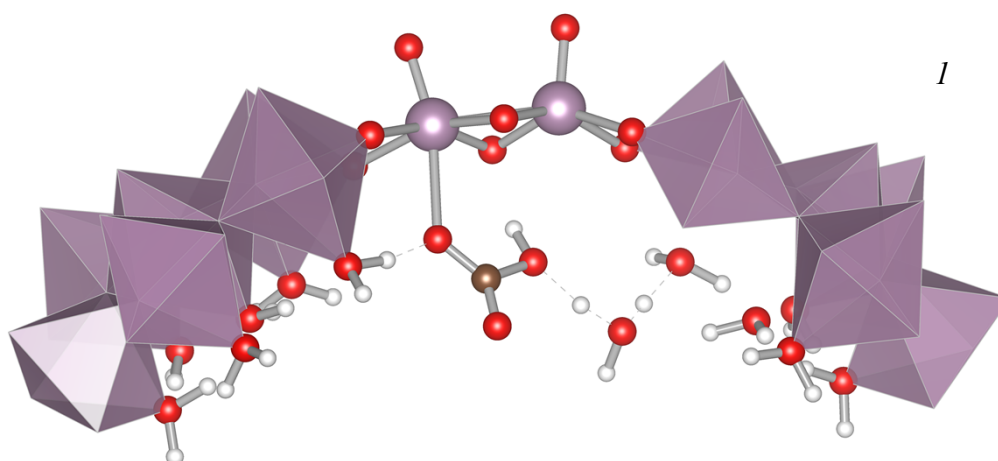
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Mo	0.712800000	2.148700000	-1.317700000
O	1.778600000	1.105500000	-2.789100000
Mo	2.249400000	1.035800000	-4.520100000
O	2.604500000	2.650300000	-4.899100000
Mo	0.734800000	2.297200000	1.325000000
O	0.318700000	-0.679900000	0.865700000
O	-0.699800000	2.400100000	0.000400000
O	1.876200000	1.330100000	0.047000000
O	-0.784500000	2.173300000	-2.765100000

Mo	-1.551500000	1.908300000	-4.366400000
O	-1.871200000	0.705400000	-6.083000000
Mo	-3.337300000	0.014800000	-7.403100000
O	-4.259000000	-1.422800000	-8.229500000
O	4.085000000	0.318600000	-4.646200000
O	0.235200000	1.060600000	-5.034600000
Mo	-0.073600000	0.181900000	-6.855600000
O	0.007300000	1.490600000	-7.937700000
O	1.906100000	0.079200000	-6.397900000
Mo	2.848100000	-0.951700000	-7.941800000
O	3.101400000	-2.567000000	-8.987900000
O	1.755000000	1.230400000	2.807800000
Mo	2.131200000	1.245400000	4.570800000
O	1.800600000	0.256200000	6.393700000
Mo	2.843000000	-0.520200000	8.055900000
O	4.347500000	-0.136800000	7.080700000
O	-0.802400000	1.999900000	2.638900000
Mo	-1.710200000	1.457300000	4.100200000
O	-3.067700000	0.388000000	3.351600000
O	1.317100000	3.863900000	1.599900000
O	4.048100000	0.885800000	4.771300000
O	0.069000000	0.843400000	4.902700000
Mo	-0.186100000	0.125500000	6.806300000
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O	2.114600000	2.889600000	4.960000000
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Mo	-3.428200000	-0.443300000	7.169400000
O	-4.000100000	-1.910100000	8.213500000
O	-1.478200000	-1.148800000	7.701400000

Mo	-0.561100000	-2.328700000	9.135000000
O	-1.688600000	-3.801000000	8.810500000
O	0.829500000	-1.028900000	8.137000000
O	0.948600000	-2.989100000	9.984100000
O	-1.346900000	-1.570100000	10.427300000
O	-4.809900000	-0.097300000	5.949300000
O	-3.580200000	0.874300000	8.210200000
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O	-1.525100000	-1.017000000	-7.654100000
Mo	-0.732000000	-2.407600000	-8.967200000
O	-2.091400000	-3.663500000	-8.602800000
O	0.792200000	-1.219300000	-8.063000000
O	3.014900000	0.211600000	-9.166900000
O	4.374500000	-0.717600000	-6.947900000
O	-4.528400000	0.913600000	-6.307600000
O	-3.158400000	1.054100000	-8.735300000
O	0.691100000	-3.368400000	-9.659000000
O	-1.342800000	-1.635400000	-10.348400000
H	-4.387200000	-1.657100000	9.089800000
H	-5.072500000	-0.822400000	5.329200000
H	-3.994700000	0.730900000	3.409900000
H	-2.506400000	-3.831500000	9.369400000
H	1.889500000	-2.823100000	9.647900000
H	3.606400000	-1.724200000	10.072100000
H	-4.479100000	-1.242800000	-9.177800000
H	-4.254600000	1.286800000	-5.390300000
H	-3.760900000	1.275900000	-3.337100000
H	-2.877700000	-3.610000000	-9.203000000
H	1.658500000	-3.231000000	-9.372000000
H	3.455600000	-2.356500000	-9.888700000
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H	4.582900000	1.718100000	4.803500000
H	4.741200000	1.057800000	-4.677300000
H	4.360500000	-0.390800000	-5.952900000
H	1.181100000	-0.324700000	0.495200000
H	0.464300000	-1.524200000	1.665300000
O	-3.514200000	-1.627800000	-5.635300000
H	-3.279000000	-2.531800000	-5.951800000
H	-4.463900000	-1.717000000	-5.381000000
O	-1.794100000	-0.375900000	-3.419800000
H	-1.302900000	-0.416400000	-2.524500000
H	-2.665000000	-0.821100000	-3.307600000
O	-0.332500000	-1.644000000	-5.230200000
H	0.490800000	-1.668600000	-4.651800000
O	0.003600000	-3.570700000	-6.905000000
H	-0.320400000	-4.494800000	-6.789500000
O	2.524800000	-2.764800000	-6.339000000
H	3.251700000	-3.431600000	-6.374800000
O	2.022500000	-1.370200000	-4.069600000
H	2.435400000	-1.986500000	-4.746000000
H	2.286600000	-1.702300000	-3.179700000
H	1.677500000	-3.273900000	-6.541100000
H	-1.033300000	-1.318000000	-4.581200000
H	-0.329600000	-3.037100000	-6.116800000
O	0.625400000	-2.281400000	2.668500000
H	0.794900000	-3.208200000	2.364000000
O	-0.411900000	-2.081100000	5.315200000
H	-0.160100000	-2.249300000	4.368900000
O	-3.073400000	-2.418500000	5.690700000
H	-3.279000000	-3.251400000	6.183800000
O	0.509600000	-3.578900000	7.236600000
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O	2.514800000	-1.231100000	4.097500000

H	2.639200000	-1.757000000	4.954600000
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H	3.602100000	-2.962300000	6.560600000
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H	1.478300000	-1.966900000	3.141300000
H	3.382500000	-1.303100000	3.630600000
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H	0.094200000	-3.242000000	6.381200000
H	-3.554100000	-2.526200000	4.834000000
C	-0.631300000	-0.964500000	-0.316600000
O	-0.311300000	-0.237400000	-1.291300000
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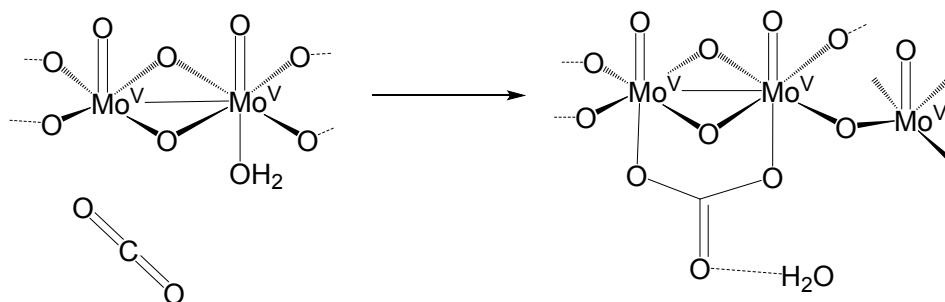
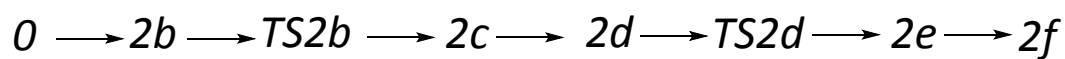
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O	1.786680000	1.119233000	-2.812533000
Mo	2.241034000	1.041720000	-4.533825000
O	2.598744000	2.654916000	-4.925231000
Mo	0.636317000	2.309689000	1.350374000
O	0.943353000	-1.236890000	0.185213000
O	-0.793803000	2.380802000	0.001109000

O	1.763991000	1.269869000	0.118165000
O	-0.828420000	2.186818000	-2.791958000
Mo	-1.571239000	1.906417000	-4.400254000
O	-1.876279000	0.711078000	-6.119807000
Mo	-3.334698000	0.064657000	-7.482027000
O	-4.258993000	-1.302809000	-8.419830000
O	4.069335000	0.302133000	-4.653564000
O	0.224905000	1.059234000	-5.050675000
Mo	-0.074652000	0.212833000	-6.893535000
O	0.022409000	1.545801000	-7.943975000
O	1.898990000	0.088355000	-6.426234000
Mo	2.853618000	-0.931745000	-7.963657000
O	3.099821000	-2.539617000	-9.024441000
O	1.667157000	1.318376000	2.855273000
Mo	2.107250000	1.276183000	4.601865000
O	1.812605000	0.280310000	6.439635000
Mo	2.861240000	-0.565370000	8.043961000
O	4.346440000	-0.227618000	7.024341000
O	-0.883537000	1.909934000	2.642089000
Mo	-1.724389000	1.448817000	4.175546000
O	-2.998825000	0.182695000	3.527066000
O	1.207348000	3.886957000	1.573172000
O	3.986327000	0.717329000	4.704858000
O	0.059480000	1.001882000	5.027250000
Mo	-0.165858000	0.157696000	6.902410000
O	-0.256851000	1.524667000	7.904094000
O	2.249734000	2.908714000	5.009434000
O	-3.505279000	1.843705000	-4.148446000
O	-1.452009000	3.406423000	-5.194482000
O	-2.389943000	2.913086000	4.700526000
O	-1.987655000	0.395196000	6.043996000
Mo	-3.443290000	-0.463837000	7.202514000

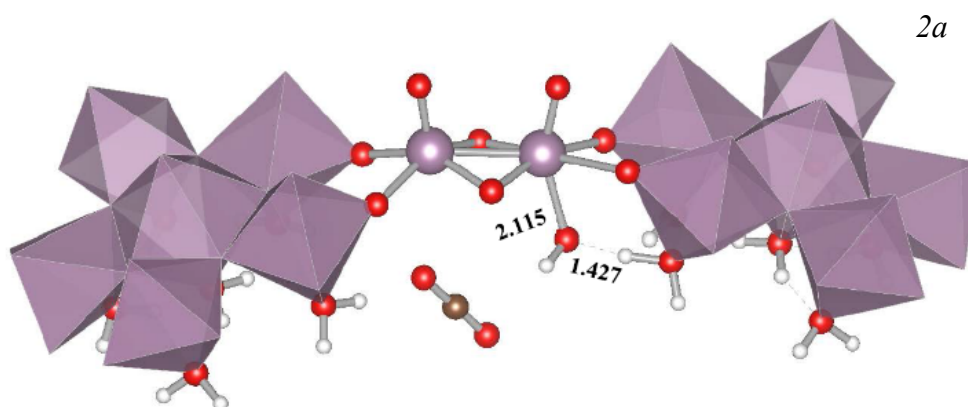
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O	-1.882948000	-3.480499000	9.415591000
O	0.864072000	-1.069714000	8.156327000
O	0.940529000	-2.911664000	10.057903000
O	-1.075913000	-1.096267000	10.621167000
O	-4.778591000	0.155597000	6.041600000
O	-3.690301000	0.603328000	8.483766000
O	2.910327000	0.665388000	9.203467000
O	3.266895000	-2.138950000	9.082645000
O	-1.519376000	-0.946919000	-7.753822000
Mo	-0.719485000	-2.336322000	-9.059683000
O	-2.117873000	-3.559367000	-8.714729000
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O	3.051683000	0.243392000	-9.173213000
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O	-3.132661000	1.189550000	-8.741220000
O	0.698966000	-3.316794000	-9.729879000
O	-1.291355000	-1.548372000	-10.448543000
H	-4.567094000	-2.124994000	8.643587000
H	-4.953275000	-0.350682000	5.209501000
H	-3.763618000	0.522426000	2.998121000
H	-2.563409000	-3.414569000	10.131530000
H	1.881579000	-2.747283000	9.713196000
H	3.758747000	-1.918310000	9.915172000
H	-4.469608000	-1.053488000	-9.354405000
H	-4.255609000	1.282021000	-5.430966000
H	-3.788006000	1.274930000	-3.392551000
H	-2.890280000	-3.481897000	-9.330307000
H	1.664759000	-3.189412000	-9.428453000

H	3.461727000	-2.325382000	-9.921126000
H	4.321051000	0.090707000	6.026515000
H	4.607361000	1.487148000	4.653038000
H	4.736455000	1.031875000	-4.671961000
H	4.344564000	-0.397269000	-5.948751000
H	1.419566000	-0.340822000	0.162386000
H	0.628814000	-1.791003000	1.478058000
O	-3.469367000	-1.708676000	-5.867884000
H	-3.288335000	-2.582191000	-6.287944000
H	-4.392771000	-1.801057000	-5.531493000
O	-1.809498000	-0.360541000	-3.444888000
H	-1.259200000	-0.355997000	-2.573129000
H	-2.678774000	-0.770082000	-3.231413000
O	-0.377540000	-1.638759000	-5.291746000
H	0.435953000	-1.663697000	-4.701834000
O	-0.033623000	-3.539341000	-6.996512000
H	-0.361670000	-4.464720000	-6.905861000
O	2.484254000	-2.759113000	-6.384250000
H	3.204856000	-3.433205000	-6.410331000
O	1.977301000	-1.376172000	-4.107936000
H	2.381953000	-1.984073000	-4.797756000
H	2.271232000	-1.713117000	-3.229677000
H	1.635718000	-3.258484000	-6.605140000
H	-1.093108000	-1.321532000	-4.655905000
H	-0.373611000	-3.022242000	-6.200473000
O	0.360455000	-2.092330000	2.470947000
H	0.315399000	-3.082774000	2.477314000
O	-0.170012000	-1.823281000	5.510238000
H	-1.132750000	-1.996902000	5.303657000
O	-2.934781000	-1.991352000	5.293619000
H	-3.436607000	-2.840868000	5.244727000
O	0.021493000	-3.720887000	7.491480000

H	0.700269000	-4.324923000	7.878592000
O	2.226171000	-1.212759000	3.963351000
H	2.397381000	-1.771832000	4.789323000
O	2.789847000	-2.444093000	6.292074000
H	3.709942000	-2.800279000	6.213278000
H	0.044911000	-2.583668000	6.115670000
H	1.139472000	-1.807126000	3.116904000
H	3.061291000	-1.291429000	3.439580000
H	2.249293000	-3.252195000	6.453411000
H	-0.726583000	-4.337172000	7.293496000
H	-3.121633000	-1.515800000	4.442160000
C	-0.145329000	-1.216631000	-0.708174000
O	-0.233536000	-0.140508000	-1.420600000
O	-0.868298000	-2.199758000	-0.732465000



3) Hydroxo pathway (Depicted in black colour in Figure 2). The starting material is 0 as in the previous section.



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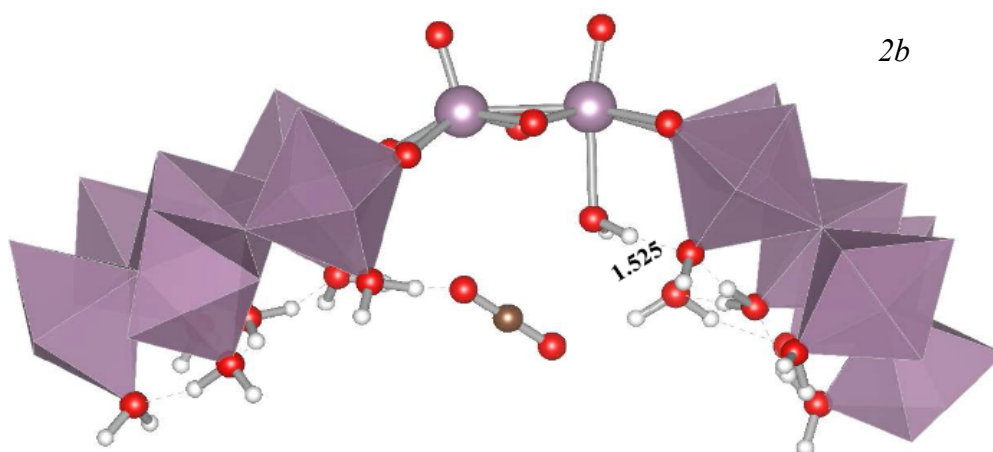
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Mo	0.186710000	1.186791000	-1.449596000
O	-0.652590000	-1.992302000	-1.705336000
O	1.331540000	0.210978000	-2.881879000
Mo	1.976534000	0.458677000	-4.547160000
O	2.347908000	2.114372000	-4.551944000
Mo	0.042062000	0.915657000	1.161033000
O	-1.018062000	-0.863788000	1.586270000
O	-1.328691000	1.139844000	-0.204209000
O	1.334837000	0.279895000	-0.122360000
O	-1.244695000	0.968091000	-2.900025000

Mo	-1.838867000	1.052290000	-4.600551000
O	-1.902248000	0.380387000	-6.629535000
Mo	-3.180654000	0.163237000	-8.254971000
O	-3.850028000	-0.886463000	-9.683150000
O	3.794760000	-0.307627000	-4.592434000
O	0.044013000	0.502692000	-5.279025000
Mo	0.005824000	0.335981000	-7.323704000
O	0.071899000	1.966490000	-7.795420000
O	1.915569000	0.123471000	-6.671167000
Mo	3.139506000	-0.287838000	-8.280443000
O	3.612860000	-1.499997000	-9.718992000
O	1.181247000	0.101926000	2.761307000
Mo	1.875333000	0.144152000	4.405269000
O	1.823469000	-0.303000000	6.571732000
Mo	3.076626000	-0.455158000	8.163357000
O	4.508221000	-0.905876000	7.022971000
O	-1.397098000	1.434658000	2.973024000
Mo	-1.857331000	1.147935000	4.635426000
O	-3.814646000	0.847371000	4.660865000
O	0.516504000	2.518383000	1.581424000
O	3.367360000	-1.046321000	4.334300000
O	0.012392000	0.493002000	5.252874000
Mo	-0.021183000	0.153989000	7.296762000
O	0.145415000	1.782157000	7.765014000
O	2.606323000	1.676267000	4.518760000
O	-3.780125000	0.792279000	-4.593415000
O	-1.767771000	2.709777000	-4.969484000
O	-1.880358000	2.709925000	5.348411000
O	-1.916518000	0.222205000	6.665261000
Mo	-3.190498000	0.028759000	8.251874000
O	-3.858831000	-1.101955000	9.624171000
O	-1.233708000	-0.625706000	8.753323000

Mo	-0.167598000	-1.266342000	10.389715000
O	-1.404995000	-2.602714000	10.891091000
O	1.127480000	-0.577770000	8.835669000
O	1.424415000	-1.765255000	11.192553000
O	-0.660641000	0.034991000	11.364797000
O	-4.533167000	0.224289000	7.006913000
O	-3.100928000	1.540111000	9.028266000
O	3.477852000	1.167961000	8.449480000
O	3.576890000	-1.126677000	9.941309000
O	-1.227319000	-0.465507000	-8.732245000
Mo	-0.154611000	-1.243746000	-10.327509000
O	-1.434950000	-2.607978000	-10.600024000
O	1.130194000	-0.470091000	-8.831387000
O	3.438357000	1.205682000	-9.031318000
O	4.496642000	-0.372056000	-7.042374000
O	-4.529584000	0.291586000	-7.003719000
O	-3.095091000	1.704535000	-8.963866000
O	1.414093000	-1.792151000	-11.155666000
O	-0.686048000	-0.059931000	-11.415773000
H	-4.089871000	-0.615659000	10.454259000
H	-4.342675000	0.485141000	6.002955000
H	-4.095177000	0.152031000	4.019526000
H	-2.074891000	-2.313200000	11.559643000
H	2.344105000	-1.616740000	10.752513000
H	3.980695000	-0.413382000	10.494542000
H	-4.068478000	-0.361354000	-10.493866000
H	-4.355359000	0.503841000	-6.002918000
H	-4.081178000	0.065309000	-3.996566000
H	-2.142951000	-2.374739000	-11.252283000
H	2.274594000	-1.897957000	-10.627937000
H	4.135200000	-1.028990000	-10.416979000
H	4.432840000	-1.796515000	6.593954000

H	4.234031000	-0.577494000	4.410132000
H	4.452418000	0.330320000	-4.219265000
H	4.311612000	-0.464833000	-6.018443000
H	-1.806798000	-0.889948000	0.999398000
O	-3.039997000	-2.146957000	-7.389786000
H	-2.999411000	-2.785841000	-8.142209000
H	-3.870478000	-2.398921000	-6.919451000
O	-1.949619000	-1.377592000	-4.238564000
H	-1.607192000	-1.657668000	-3.355289000
H	-2.779633000	-1.895774000	-4.346500000
O	-0.349978000	-2.005733000	-6.646231000
H	0.089807000	-2.200853000	-5.771144000
O	0.524287000	-3.127524000	-8.819940000
H	0.252562000	-4.031472000	-9.105448000
O	2.710643000	-2.514084000	-7.350029000
H	3.522349000	-3.074167000	-7.392783000
O	1.615611000	-1.951316000	-4.844303000
H	2.151878000	-2.293996000	-5.618363000
H	1.864791000	-2.522047000	-4.079413000
H	2.037921000	-2.978000000	-7.935840000
H	-1.326316000	-2.145823000	-6.531269000
H	0.067137000	-2.948734000	-7.942335000
O	-1.834086000	-1.094102000	3.928576000
H	-1.558254000	-1.038967000	2.894960000
O	-0.384879000	-2.170842000	6.682621000
H	0.047038000	-2.383535000	5.797859000
O	-3.066999000	-2.275544000	7.294354000
H	-3.185416000	-2.943581000	8.011921000
O	0.360519000	-3.205781000	8.943121000
H	0.032653000	-4.089772000	9.230025000
O	0.897932000	-2.183583000	4.392369000
H	1.556615000	-2.874781000	4.141201000

O	2.798029000	-2.773413000	7.962387000
H	3.527087000	-3.289192000	8.380265000
H	-1.368239000	-2.311841000	6.600469000
H	-2.607467000	-1.696217000	3.990251000
H	0.189584000	-2.218185000	3.705526000
H	1.953204000	-3.098532000	8.409840000
H	-0.005564000	-3.031158000	8.018627000
H	-3.831148000	-2.443300000	6.692835000
C	-0.746502000	-2.907391000	-0.971960000
O	-0.834199000	-3.809362000	-0.240738000



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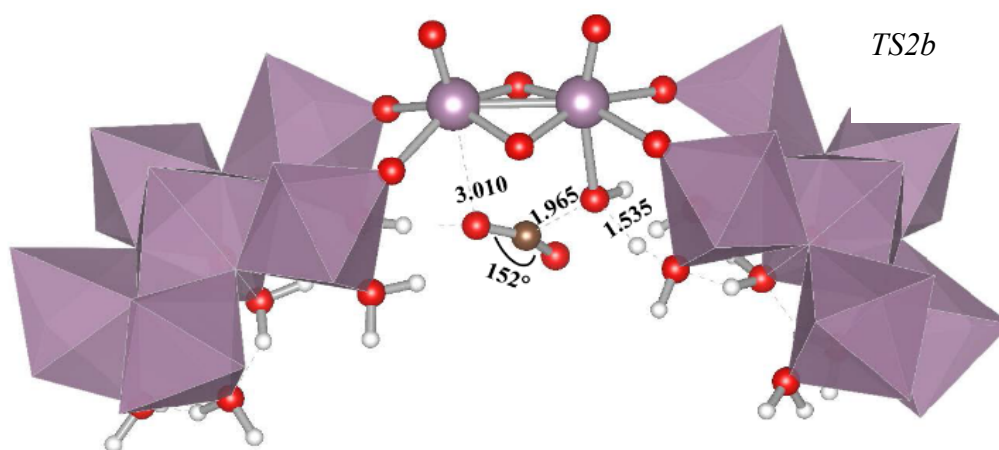
O	6.626900000	-0.742600000	-7.340900000
Mo	6.790100000	-0.095100000	-5.770300000
O	6.926600000	0.417100000	-3.442600000
O	8.243300000	-1.480200000	-5.143400000
Mo	8.907800000	-2.707200000	-4.021500000
O	9.288000000	-4.044600000	-5.022200000
Mo	6.766500000	2.496700000	-6.322500000
O	6.449600000	3.328400000	-2.582500000
O	5.413900000	1.291900000	-5.604900000
O	8.195200000	1.244700000	-5.846600000

O	5.500800000	-1.511000000	-4.862300000
Mo	5.010900000	-2.995300000	-3.989700000
O	5.134700000	-4.127100000	-2.186400000
Mo	3.982000000	-5.218900000	-0.839200000
O	3.413000000	-5.641600000	0.966900000
O	10.791400000	-2.276900000	-3.649700000
O	6.958500000	-3.309300000	-3.465200000
Mo	7.076500000	-4.573900000	-1.820400000
O	7.143100000	-6.082100000	-2.608100000
O	8.930700000	-3.985700000	-2.259200000
Mo	10.245100000	-4.864800000	-0.925000000
O	10.889800000	-5.155700000	0.843900000
O	8.142200000	3.940800000	-5.799600000
Mo	8.812500000	5.614400000	-5.788300000
O	8.837200000	7.651400000	-5.121100000
Mo	10.167100000	9.171100000	-4.643000000
O	11.312700000	7.802600000	-4.207600000
O	5.493800000	4.034700000	-5.734100000
Mo	4.952400000	5.744400000	-5.905200000
O	3.079200000	5.835800000	-5.371600000
O	6.651100000	2.554000000	-8.014000000
O	10.665300000	5.512300000	-5.146000000
O	6.898000000	6.378800000	-5.615200000
Mo	6.993900000	8.425600000	-5.429400000
O	7.095300000	8.832500000	-7.078500000
O	9.096100000	5.962800000	-7.425900000
O	3.340800000	-2.414700000	-3.198800000
O	4.611900000	-4.155900000	-5.161400000
O	4.803600000	5.972200000	-7.579900000
O	5.045500000	7.841100000	-5.400700000
Mo	3.857800000	9.501700000	-5.142700000
O	3.363500000	11.018000000	-4.032900000

O	5.858600000	9.945700000	-4.696600000
Mo	7.041000000	11.622500000	-4.394000000
O	5.647400000	12.259900000	-3.342800000
O	8.207400000	9.909700000	-4.707900000
O	8.611100000	12.448700000	-3.848400000
O	6.772000000	12.280000000	-5.938200000
O	2.427800000	8.349000000	-5.293500000
O	3.854400000	10.277100000	-6.655800000
O	10.674400000	9.632700000	-6.195200000
O	10.654200000	10.731600000	-3.613500000
O	5.941100000	-5.208700000	-0.224100000
Mo	7.235200000	-5.556300000	1.447800000
O	5.645300000	-5.842000000	2.359700000
O	8.271000000	-4.856100000	-0.180700000
O	10.265700000	-6.475600000	-1.473400000
O	11.576600000	-4.039900000	-1.907300000
O	2.567400000	-4.382200000	-1.688100000
O	3.933000000	-6.773200000	-1.517000000
O	8.401900000	-4.742800000	2.690600000
O	7.880800000	-7.123300000	1.365100000
H	2.919100000	11.709800000	-4.585700000
H	2.529300000	7.325200000	-5.235300000
H	2.873800000	5.364500000	-4.528000000
H	4.699200000	11.942900000	-3.521900000
H	9.420300000	11.913600000	-3.560500000
H	11.313300000	11.288200000	-4.102900000
H	3.064900000	-6.566500000	1.033300000
H	2.710100000	-3.536700000	-2.261300000
H	3.571600000	-1.700000000	-2.514800000
H	4.721400000	-5.688600000	1.963700000
H	9.145700000	-5.322000000	2.994700000
H	11.122400000	-6.102600000	1.013000000

H	11.199000000	6.840400000	-4.596700000
H	10.760100000	4.896800000	-4.377700000
H	10.909400000	-1.373000000	-3.273300000
H	11.382600000	-3.289300000	-2.592100000
O	4.076400000	-3.099400000	0.412800000
H	4.865300000	-3.094800000	1.042600000
H	3.281100000	-2.976200000	0.984700000
O	4.603700000	-1.071700000	-1.275700000
H	4.447200000	-0.153000000	-0.953100000
H	4.255800000	-1.671700000	-0.546600000
O	7.018200000	-2.389500000	-0.798200000
H	7.757400000	-1.859300000	-1.372500000
O	6.497700000	-3.216200000	1.582000000
H	6.887300000	-2.715600000	0.790900000
O	10.106100000	-2.692800000	0.097800000
H	11.015300000	-2.337400000	0.242200000
O	8.556200000	-1.231300000	-2.368200000
H	9.317900000	-0.872300000	-1.863200000
H	7.637500000	-0.167100000	-2.959900000
H	9.740200000	-2.759900000	1.010900000
H	6.189200000	-1.860800000	-0.967900000
H	6.735900000	-2.719200000	2.399500000
O	5.155300000	5.689100000	-3.407800000
H	5.419100000	4.815600000	-3.024900000
O	6.740700000	7.851300000	-3.101500000
H	7.631800000	7.878200000	-2.653800000
O	4.084700000	8.636700000	-2.928900000
H	5.045800000	8.551900000	-2.694200000
O	7.599800000	10.665000000	-1.946700000
H	7.944600000	11.435200000	-1.433300000
O	8.463200000	5.356600000	-3.382200000
H	9.106800000	5.751800000	-2.751000000

O	9.252400000	8.659500000	-2.434500000
H	9.912900000	8.401200000	-1.749200000
H	6.420000000	6.906600000	-3.057000000
H	4.403200000	6.001400000	-2.849600000
H	8.262300000	4.468600000	-3.006400000
H	8.762700000	9.460900000	-2.063500000
H	6.821700000	10.367200000	-1.417800000
H	3.669900000	9.173200000	-2.213500000
C	6.146600000	2.565200000	-1.742000000
O	5.839800000	1.803000000	-0.916300000
H	6.070900000	0.139400000	-3.053100000



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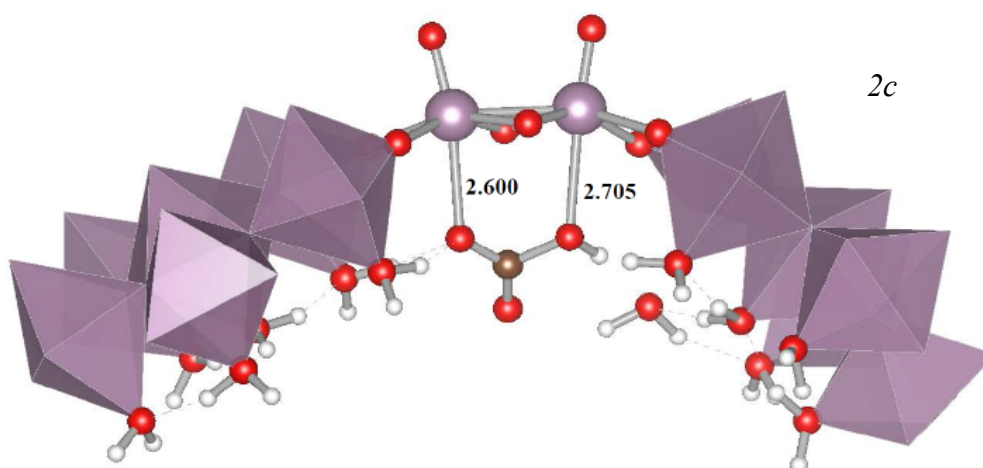
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Mo	23.740400000	-1.312900000	-13.786300000
O	23.874000000	-0.896200000	-11.534800000
O	25.233000000	-2.742400000	-13.203500000
Mo	25.951300000	-4.051300000	-12.238600000
O	26.167700000	-5.339700000	-13.330800000
Mo	23.735700000	1.232700000	-14.507100000

O	23.703700000	1.642800000	-11.525100000
O	22.357500000	0.058400000	-13.756000000
O	25.151500000	-0.008100000	-13.928400000
O	22.449300000	-2.774200000	-12.846700000
Mo	22.046800000	-4.320900000	-12.060800000
O	22.245800000	-5.470300000	-10.281900000
Mo	21.152700000	-6.621100000	-8.922400000
O	20.635600000	-7.032800000	-7.103300000
O	27.832000000	-3.608400000	-11.931000000
O	24.024600000	-4.542500000	-11.538800000
Mo	24.210000000	-5.854100000	-9.958900000
O	24.327000000	-7.337900000	-10.781100000
O	26.045600000	-5.176300000	-10.435700000
Mo	27.409500000	-6.086100000	-9.121900000
O	28.117400000	-6.413600000	-7.390200000
O	25.135600000	2.688100000	-14.121700000
Mo	25.835800000	4.341800000	-13.992200000
O	25.873400000	6.327900000	-13.205300000
Mo	27.238600000	7.808100000	-12.681900000
O	28.347800000	6.401400000	-12.278800000
O	22.468700000	2.799500000	-14.074200000
Mo	21.960100000	4.526100000	-14.050800000
O	20.129100000	4.591900000	-13.380800000
O	23.653800000	1.168200000	-16.199400000
O	27.685600000	4.176200000	-13.341100000
O	23.919600000	5.108700000	-13.778100000
Mo	24.041600000	7.139700000	-13.461500000
O	24.100800000	7.617800000	-15.093100000
O	26.149100000	4.787800000	-15.601200000
O	20.257400000	-3.959100000	-11.369500000
O	21.812900000	-5.463000000	-13.292300000
O	21.719100000	4.907000000	-15.686200000

O	22.092100000	6.572400000	-13.382400000
Mo	20.925000000	8.230000000	-13.032100000
O	20.485600000	9.725000000	-11.867700000
O	22.949500000	8.645700000	-12.637000000
Mo	24.159800000	10.307500000	-12.387200000
O	22.792300000	10.985500000	-11.326600000
O	25.293400000	8.582200000	-12.722900000
O	25.752400000	11.119700000	-11.873200000
O	23.881300000	10.956300000	-13.933700000
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O	20.878900000	9.053800000	-14.519900000
O	27.755000000	8.293100000	-14.223800000
O	27.759800000	9.329200000	-11.614900000
O	23.134900000	-6.534700000	-8.350400000
Mo	24.466300000	-6.903700000	-6.723600000
O	22.915300000	-7.282100000	-5.781300000
O	25.453500000	-6.126400000	-8.360800000
O	27.423100000	-7.673400000	-9.733500000
O	28.700900000	-5.208800000	-10.104700000
O	19.688200000	-5.873100000	-9.754700000
O	21.181700000	-8.181900000	-9.586800000
O	25.645500000	-6.069100000	-5.507000000
O	25.167400000	-8.441200000	-6.868900000
H	20.022300000	10.431800000	-12.385000000
H	19.589500000	6.062600000	-13.157200000
H	19.974000000	4.063800000	-12.561300000
H	21.844600000	10.634700000	-11.437400000
H	26.546200000	10.571500000	-11.575100000
H	28.431800000	9.880300000	-12.092600000
H	20.310800000	-7.965300000	-7.022300000
H	19.765700000	-5.049800000	-10.380800000
H	20.297900000	-3.136500000	-10.809600000

H	21.982600000	-7.089800000	-6.132200000
H	26.416200000	-6.629700000	-5.235600000
H	28.374000000	-7.358100000	-7.242000000
H	28.223400000	5.460200000	-12.721300000
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H	27.978200000	-2.676100000	-11.641100000
H	28.476400000	-4.520100000	-10.844700000
O	21.201700000	-4.465300000	-7.749000000
H	21.962800000	-4.458400000	-7.089200000
H	20.388500000	-4.320500000	-7.208100000
O	21.851500000	-2.481000000	-9.534900000
H	21.762600000	-1.539400000	-9.248900000
H	21.419400000	-3.024500000	-8.813200000
O	24.146600000	-3.684900000	-8.844700000
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H	23.995900000	-4.041600000	-7.220000000
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H	28.069000000	-3.509300000	-7.977400000
O	25.719500000	-2.314600000	-10.481500000
H	26.466400000	-1.827000000	-10.065400000
H	25.059700000	-1.608700000	-10.869500000
H	26.910300000	-4.067500000	-7.109400000
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H	22.753200000	3.244200000	-11.428300000
O	23.806800000	6.421500000	-11.159600000
H	24.698100000	6.481500000	-10.710500000
O	21.217900000	7.321600000	-10.862500000
H	22.179900000	7.120300000	-10.702400000
O	24.726500000	9.338500000	-9.962200000

H	25.112300000	10.092400000	-9.453700000
O	25.472300000	3.881500000	-11.622800000
H	26.128300000	4.109300000	-10.925300000
O	26.297200000	7.269400000	-10.489900000
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H	21.648300000	4.230700000	-10.895600000
H	25.168400000	2.968000000	-11.401900000
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H	23.937900000	9.083500000	-9.426400000
H	20.915500000	7.883800000	-10.112000000
C	23.285800000	0.809700000	-10.757100000
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H	23.140300000	-1.423100000	-11.157300000



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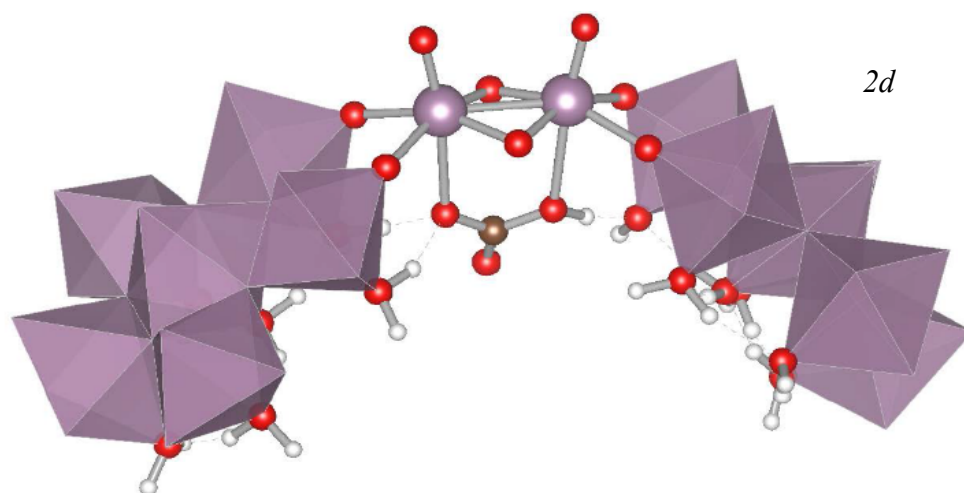
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Mo	8.916600000	-2.742300000	-4.039800000
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O	5.524100000	-1.413800000	-4.797800000
Mo	5.006000000	-2.912100000	-3.952000000
O	5.134800000	-4.018600000	-2.150800000
Mo	3.971700000	-5.091700000	-0.786700000
O	3.424500000	-5.455600000	1.032800000
O	10.796700000	-2.338900000	-3.720200000
O	6.960800000	-3.174400000	-3.379600000
Mo	7.078700000	-4.450300000	-1.777600000
O	7.186800000	-5.950800000	-2.564000000
O	8.943400000	-3.809900000	-2.233500000
Mo	10.257500000	-4.751900000	-0.869300000
O	10.919400000	-5.049100000	0.879500000
O	8.158000000	3.950700000	-6.119400000
Mo	8.821200000	5.601100000	-5.911700000
O	8.815200000	7.570200000	-5.085400000
Mo	10.156700000	9.058100000	-4.532400000
O	11.278100000	7.661500000	-4.133500000
O	5.432200000	4.028200000	-6.155200000
Mo	4.929200000	5.740400000	-6.024600000
O	3.092100000	5.772500000	-5.357000000
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Mo	6.980600000	8.361800000	-5.358500000
O	7.050000000	8.869700000	-6.981200000
O	9.188100000	6.099000000	-7.496500000

O	3.276800000	-2.383000000	-3.249600000
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O	4.660800000	6.210300000	-7.636500000
O	5.041100000	7.776600000	-5.298900000
Mo	3.854500000	9.412200000	-4.955100000
O	3.369500000	10.892400000	-3.785100000
O	5.866400000	9.846500000	-4.519100000
Mo	7.049400000	11.520200000	-4.244400000
O	5.654900000	12.181400000	-3.207900000
O	8.206900000	9.810900000	-4.588000000
O	8.629200000	12.335800000	-3.698600000
O	6.792300000	12.178800000	-5.791400000
O	2.427800000	8.262000000	-5.139900000
O	3.826700000	10.252600000	-6.434000000
O	10.688300000	9.562100000	-6.064300000
O	10.654300000	10.578000000	-3.448700000
O	5.950700000	-5.070700000	-0.186600000
Mo	7.241100000	-5.464400000	1.477200000
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O	8.285000000	-4.694400000	-0.150900000
O	10.218000000	-6.347400000	-1.453000000
O	11.595200000	-3.946600000	-1.852100000
O	2.554500000	-4.294000000	-1.657600000
O	3.937000000	-6.661500000	-1.425200000
O	8.416100000	-4.665000000	2.706700000
O	7.904100000	-7.017400000	1.318500000
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H	2.539500000	7.234300000	-5.129500000
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H	4.713400000	11.819800000	-3.333900000
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H	4.746000000	-5.572000000	2.022800000
H	9.171300000	-5.237600000	2.997000000
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H	10.971000000	-1.402300000	-3.457400000
H	11.416800000	-3.261400000	-2.603400000
O	4.072000000	-2.907900000	0.348500000
H	4.803800000	-2.925900000	1.037800000
H	3.242700000	-2.751400000	0.861100000
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H	4.619000000	0.090000000	-1.228000000
H	4.317200000	-1.374700000	-0.680100000
O	7.004400000	-2.232000000	-0.698100000
H	7.772500000	-1.708800000	-1.082700000
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H	6.844900000	-2.584000000	0.950800000
O	10.122300000	-2.556600000	0.104700000
H	11.032800000	-2.202300000	0.245500000
O	8.806800000	-0.924900000	-2.192700000
H	9.559900000	-0.710500000	-1.591200000
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O	5.349100000	5.232200000	-3.625800000
H	5.778700000	4.308500000	-3.606000000
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H	7.605200000	7.618400000	-2.628900000

O	4.125800000	8.491800000	-2.788400000
H	5.079800000	8.250900000	-2.631900000
O	7.572800000	10.531700000	-1.842900000
H	7.944700000	11.286500000	-1.325900000
O	8.409400000	5.011400000	-3.594300000
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C	6.196600000	2.021800000	-3.045800000
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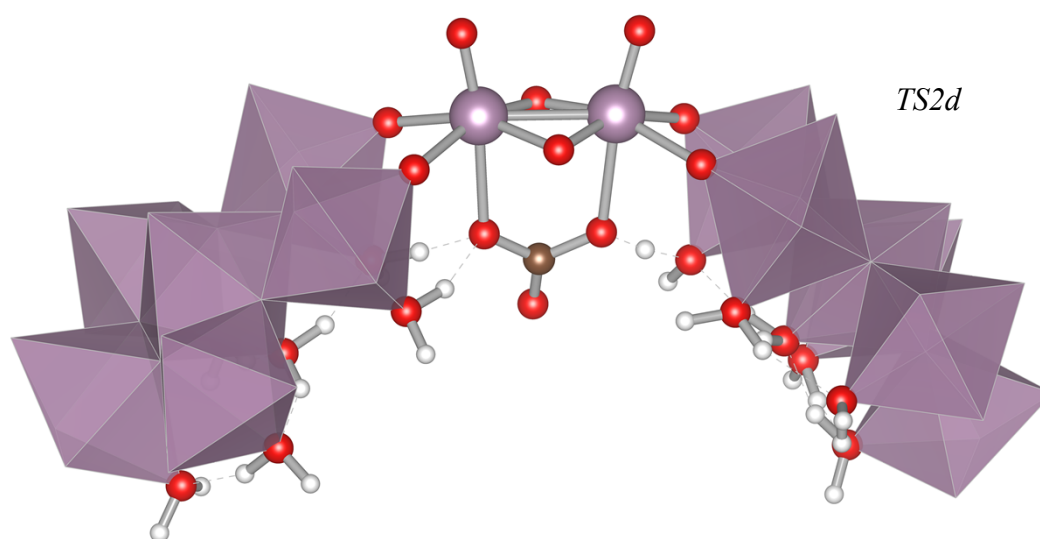
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Mo	-0.077300000	1.296800000	-1.614000000
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O	-1.368800000	-2.542800000	0.082100000
Mo	-1.864700000	-3.673500000	1.385300000
O	-1.665600000	-4.856000000	3.231900000
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O	3.952000000	-3.649900000	1.115600000
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Mo	0.261600000	-5.357300000	3.461600000
O	0.214300000	-6.918800000	2.776900000
O	2.137100000	-4.940800000	2.788800000
Mo	3.456300000	-5.892100000	4.099000000
O	4.295500000	-5.943700000	5.799400000
O	1.283600000	2.863500000	-1.415000000
Mo	1.890500000	4.513300000	-1.076700000
O	1.818700000	6.417400000	-0.100900000
Mo	3.095700000	7.831700000	0.709000000
O	4.237900000	6.426400000	0.957900000
O	-1.443800000	2.889100000	-1.545100000
Mo	-1.986200000	4.579800000	-1.329300000
O	-3.858800000	4.525900000	-0.753100000
O	-0.021700000	1.185600000	-3.315100000
O	3.734700000	4.352200000	-0.354400000
O	-0.059400000	5.202300000	-0.920000000

Mo	-0.029800000	7.188100000	-0.340300000
O	0.098400000	7.874600000	-1.893100000
O	2.295400000	5.130400000	-2.612000000
O	-3.704800000	-3.266400000	1.979300000
O	-2.340700000	-5.091700000	0.547900000
O	-2.205000000	5.156500000	-2.915800000
O	-1.958000000	6.565200000	-0.446000000
Mo	-3.202100000	8.117800000	0.029200000
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Mo	0.635000000	-6.116800000	6.756700000
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O	3.239400000	-7.546400000	3.787200000
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H	-4.029600000	3.920800000	0.007100000

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H	4.143700000	5.512900000	0.409000000
H	3.817400000	3.596300000	0.275900000
H	4.207300000	-2.755200000	1.448600000
H	4.564900000	-4.671100000	2.152500000
O	-2.528700000	-3.662800000	5.752200000
H	-1.725300000	-3.625600000	6.349800000
H	-3.295200000	-3.458500000	6.337000000
O	-1.379900000	-2.050400000	2.851600000
H	-2.093900000	-1.653400000	3.396800000
O	0.305500000	-3.140900000	4.356600000
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O	-0.021300000	-3.776600000	6.816800000
H	0.231000000	-3.332400000	5.937300000
O	3.756800000	-3.492500000	4.727500000
H	4.724500000	-3.306400000	4.801200000
O	2.305100000	-2.155200000	2.853600000
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H	2.356900000	-1.181800000	2.707200000
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H	-1.163100000	3.069900000	1.018200000

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H	-2.042600000	6.785200000	2.289200000
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H	0.639000000	9.512000000	4.102500000
O	1.450100000	3.812400000	1.180500000
H	2.118200000	3.761800000	1.899100000
O	2.079000000	6.963400000	2.743700000
H	2.717700000	6.621600000	3.412200000
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C	-0.644100000	0.955400000	1.683400000
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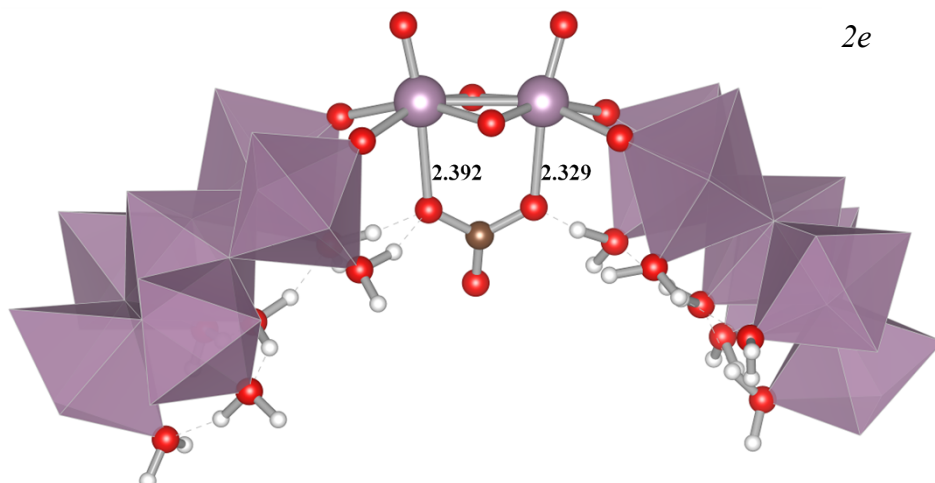


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O	1.927200000	-5.122600000	-0.187800000
Mo	-0.051800000	1.304800000	-1.658300000
O	-0.232200000	1.815000000	0.690000000
O	-1.466800000	0.059800000	-1.110700000
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O	-1.371400000	-2.554800000	0.082700000
Mo	-1.871500000	-3.696400000	1.365300000
O	-1.676800000	-4.761600000	3.257700000
Mo	-2.781800000	-5.638700000	4.742100000
O	-3.184300000	-5.977300000	6.627900000
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O	0.106600000	-4.143500000	1.799900000
Mo	0.241900000	-5.322100000	3.477100000
O	0.144800000	-6.886800000	2.810000000
O	2.117800000	-4.954400000	2.785300000
Mo	3.427900000	-5.935200000	4.083400000
O	4.275400000	-6.004900000	5.777800000
O	1.305800000	2.879700000	-1.473100000
Mo	1.899200000	4.525200000	-1.095200000
O	1.813800000	6.416000000	-0.089100000
Mo	3.078600000	7.814300000	0.761100000
O	4.216200000	6.406100000	0.997900000
O	-1.420800000	2.896700000	-1.621500000
Mo	-1.973800000	4.578600000	-1.373200000
O	-3.848300000	4.504400000	-0.800700000
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O	3.741700000	4.364300000	-0.355000000
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Mo	-0.035100000	7.182100000	-0.329500000
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H	-3.542500000	-6.893000000	6.743400000
H	-4.132600000	-4.104200000	3.199400000
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H	4.442100000	-6.926400000	6.098300000
H	4.125500000	5.495600000	0.430200000
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H	4.240200000	-2.830600000	1.403100000
H	4.550200000	-4.757700000	2.116500000
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O	0.029500000	-3.708700000	6.838500000
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O	3.809200000	-3.545900000	4.700600000
H	4.783200000	-3.390300000	4.761800000
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H	3.082800000	-2.419500000	3.493900000
H	2.419600000	-1.205300000	2.689900000
H	3.487700000	-3.351300000	5.613800000
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H	0.408700000	-3.173600000	7.573800000

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H	-2.057200000	6.717700000	2.279900000
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H	0.536900000	9.422000000	4.174000000
O	1.440400000	3.789100000	1.138600000
H	2.110000000	3.709200000	1.852900000
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H	1.496000000	7.616600000	3.241700000
H	-0.529100000	8.332400000	3.897200000
H	-3.367900000	7.383700000	2.886500000
C	-0.575200000	0.915000000	1.615000000
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H	-0.779300000	-1.097200000	2.148600000



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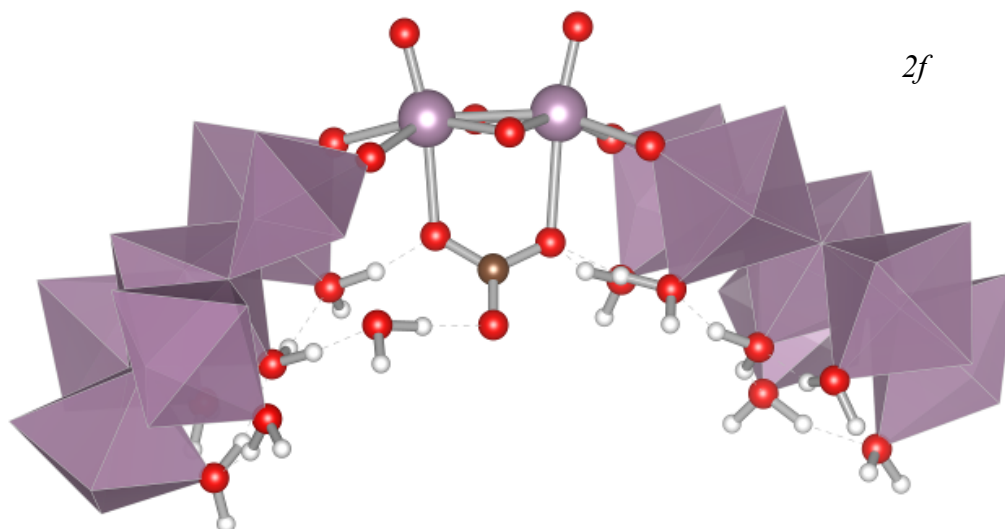
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O	1.406200000	-2.387600000	0.178400000
Mo	2.023300000	-3.838200000	1.003600000
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O	0.169600000	-6.881600000	2.796000000

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Mo	3.433300000	-5.907000000	4.121400000
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Mo	1.883400000	4.551600000	-1.153900000
O	1.807200000	6.437100000	-0.139800000
Mo	3.083700000	7.837300000	0.689200000
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O	3.650600000	8.622900000	-0.709200000

O	3.488700000	9.185200000	2.026000000
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H	2.621900000	-5.948700000	8.191000000
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H	4.247000000	-2.764200000	1.467600000
H	4.562800000	-4.692700000	2.181700000
O	-2.505300000	-3.614000000	5.789600000
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O	3.785200000	-3.514100000	4.753800000
H	4.757300000	-3.356200000	4.838300000
O	2.329400000	-2.151500000	2.902900000
H	3.051600000	-2.390900000	3.551900000
H	2.383700000	-1.179500000	2.747200000
H	3.440100000	-3.312200000	5.656900000
H	-0.429100000	-2.577100000	3.958400000
H	0.354700000	-3.246900000	7.628500000
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H	-1.117100000	3.025800000	0.933400000
O	-0.368100000	6.123900000	1.796700000
H	0.507300000	6.053900000	2.267000000
O	-2.988300000	6.900900000	2.137000000
H	-2.027700000	6.701300000	2.306800000
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H	-0.865800000	-1.161100000	2.245700000
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Mo	6.870000000	-0.142800000	-5.999100000
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Mo	8.902700000	-2.731200000	-4.068800000
O	9.134500000	-4.116500000	-5.033600000
Mo	6.797400000	2.421500000	-6.647400000
O	6.711200000	2.771300000	-4.180500000
O	5.425800000	1.159900000	-6.045800000
O	8.263300000	1.200300000	-6.223800000
O	5.534600000	-1.459100000	-4.994000000
Mo	5.002900000	-2.782600000	-3.933400000
O	5.130400000	-3.861200000	-2.093500000
Mo	3.953900000	-4.888500000	-0.734300000
O	3.399000000	-5.312400000	1.086300000
O	10.784600000	-2.303600000	-3.715300000
O	6.966000000	-3.092500000	-3.385700000

Mo	7.062200000	-4.328200000	-1.730700000
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O	8.932100000	-3.733100000	-2.184200000
Mo	10.234000000	-4.657200000	-0.835500000
O	10.893800000	-4.972000000	0.918900000
O	8.178700000	3.954000000	-6.424400000
Mo	8.819400000	5.580600000	-6.040800000
O	8.794900000	7.489100000	-5.056300000
Mo	10.134000000	8.935200000	-4.423200000
O	11.246500000	7.518400000	-4.086400000
O	5.450000000	4.002700000	-6.377800000
Mo	4.928400000	5.687800000	-6.109400000
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O	2.417300000	8.116800000	-5.040700000

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O	2.538700000	-4.082500000	-1.605400000
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H	9.392100000	11.612500000	-3.185000000
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H	2.668800000	-3.272700000	-2.233700000
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H	4.701900000	-5.385300000	2.057400000
H	9.131000000	-5.108100000	3.073800000
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H	10.726300000	4.669600000	-4.679900000
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H	5.419500000	0.245100000	-2.026200000
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O	7.022900000	-2.138800000	-0.727400000
H	7.812700000	-1.656900000	-1.119400000
O	6.502700000	-2.951600000	1.669800000
H	6.861400000	-2.440500000	0.874100000
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H	10.962100000	-2.079800000	0.281200000
O	8.624400000	-0.882000000	-2.456400000
H	9.379500000	-0.353100000	-2.112600000
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H	6.247500000	-1.577900000	-1.101000000
H	6.760100000	-2.453200000	2.479800000
O	5.375400000	4.989400000	-3.768300000
H	5.809700000	4.056000000	-3.820200000
O	6.702500000	7.322300000	-3.073600000
H	7.581400000	7.370900000	-2.602600000
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O	7.526000000	10.298600000	-1.676500000
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H	3.881600000	8.799300000	-1.914300000
C	6.515600000	1.700400000	-3.424600000
O	5.848500000	1.750900000	-2.359400000

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Supporting information for this article is given via a link at the end of
the document

1. E. J. Baerends, J. Autschbach, A. Bérces, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. F. Guerra, S. J. A. van Gisbergen, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, F. E. Harris, P. v. d. Hoek, H. Jacobsen, L. Jensen, G. van Kessel, F. Kootstra, E. van Lenthe, D. A. McCormack, A. Michalak, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. G. Snijders, M. Sola, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, O. Visser, F. Wang, E. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev and T. Ziegler, <http://www.scm.com>, *Scientific Computing and Modelling* ADF-2012.01.
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