Understanding the hydrolysis mechanism of ethyl acetate catalyzed by an aqueous molybdocene: A computational chemistry investigation

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Supporting Information

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Computational Details: B3LYP is a three-parameter hybrid DFT functional that combines the Becke's nonlocal exchange functional,[1] the Hartree-Fock exchange energy, the nonlocal correlation functional of Lee, Yang, and Parr (LYP),[2] and the Vosko-Wilk-Nusair (VWN) fitting to the correlation energy derived from the local spin density approximation.[3,4] VDZ (VTZ) is the correlation consistent double-ζ (triple-ζ) basis set augmented by diffuse functions aug-cc-pVDZ (aug-cc-pVTZ) here used for the non-metal atoms,[5,6] plus aug-cc-pVDZ-PP (aug-cc-pVTZ-PP) for Mo,[7] in which the valence electrons are represented explicitly by aug-cc-pVDZ (aug-cc-pVTZ) while the core electrons are modelled by the corresponding double-ζ (triple-ζ) Stuttgart-Koln energy-consistent relativistic pseudopotential. Solvent effects were taken into account on molecular geometries and energies from the outset. To that end, we used the Polarizable Continuum Model (PCM) approach of Tomasi and co-workers[8-11] together with the integral equation formalism model[12-14] and the Bondi radii.[15] A relative permittivity of 78.39 was considered in the PCM computations to simulate the water solvent used in the experiments on the ethyl acetate hydrolysis catalyzed by molybdocenes.

Geometry optimizations were performed without constraints using the Schlegel's algorithm[16] at the PCM-B3LYP/VDZ level of theory. The character of all first-order saddle points and local minima on the potential energy surface (PES) was confirmed by means of analytical calculations of harmonic vibrational frequencies. Intrinsic reaction coordinate (IRC) computations with the Hessian-based predictor-corrector integrator method were performed to verify the expected connections between the first-order saddle points and local minima on the PES.[17,18] To obtain more accurate energies of the stationary points, PCM-B3LYP/VTZ single-point energy calculations on the PCM-B3LYP/VDZ optimized geometries were done and identified in the text as PCM-B3LYP/VTZ//PCM-B3LYP/VDZ computations.

M06 is a hybrid meta generalized gradient approximation (HM-GGA) functional that is parameterized for both transition metals and nonmetals with a percentage of Hartree-Fock exchange of 27%.[19] BP86 and G96LYP are GGA methods. The first is composed of the Becke's nonlocal exchange functional[1] and the Perdew 1986 correlation functional,[20] while the second combines the exchange functional proposed by Gill in 1996 (G96)[21] with the LYP correlation functional.[2] B3PW91 is a hybrid GGA functional as B3LYP with the same percentage of Hartree-Fock exchange (20%) that uses the Perdew and Wang 1991 correlation functional[22] instead of the LYP one, but retains the three parameters derived for B3LYP.

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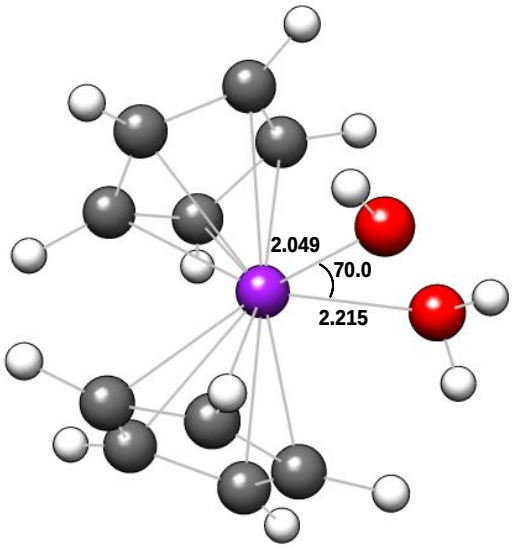

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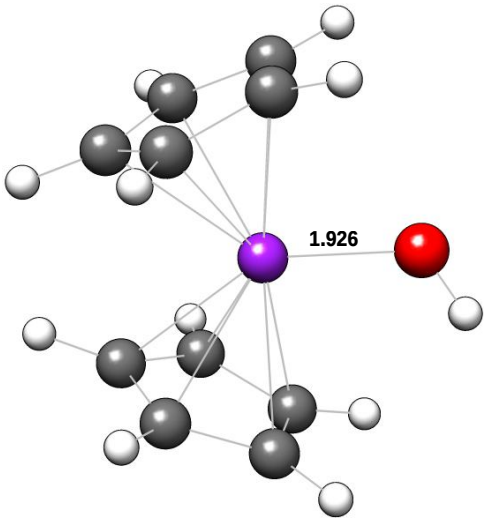

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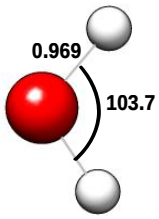

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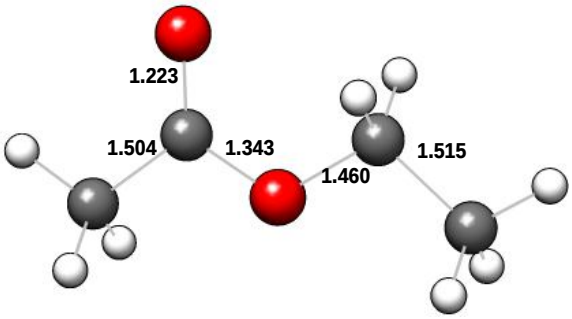

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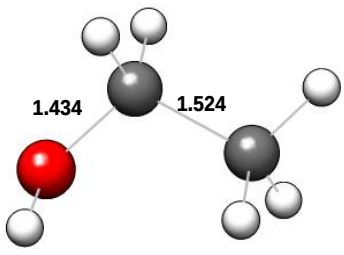

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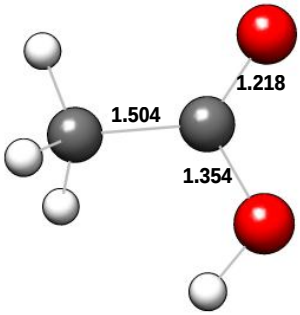

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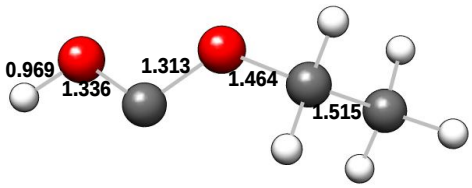

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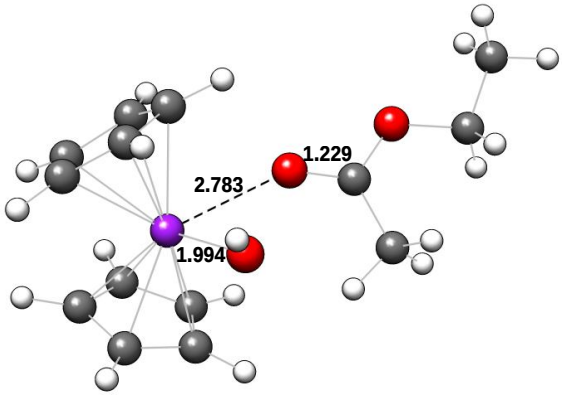

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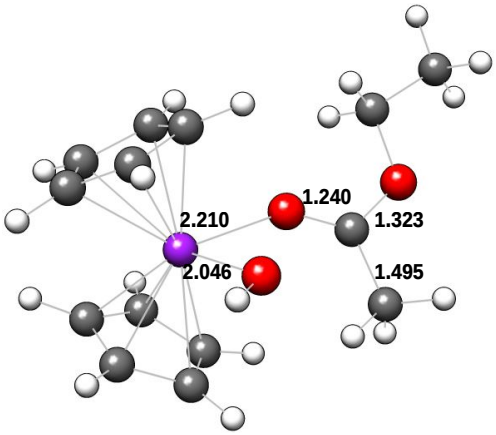

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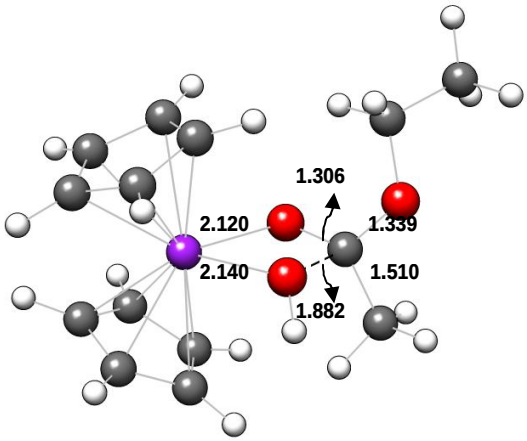

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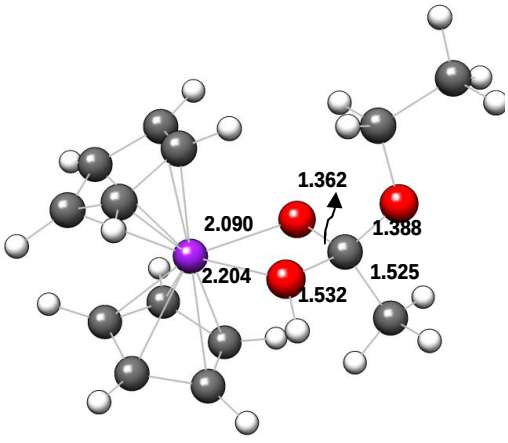

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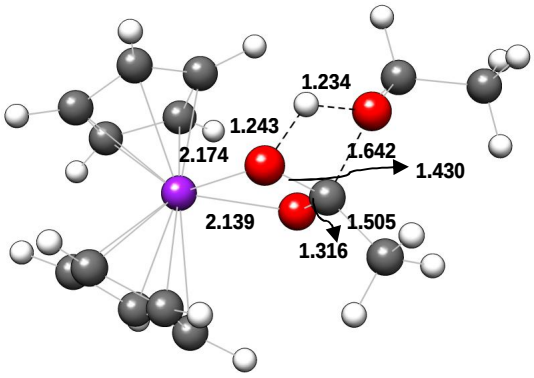

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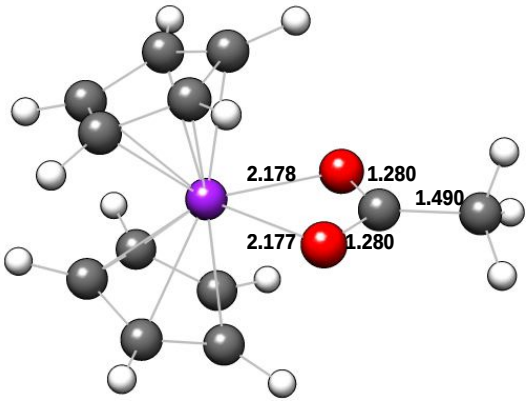

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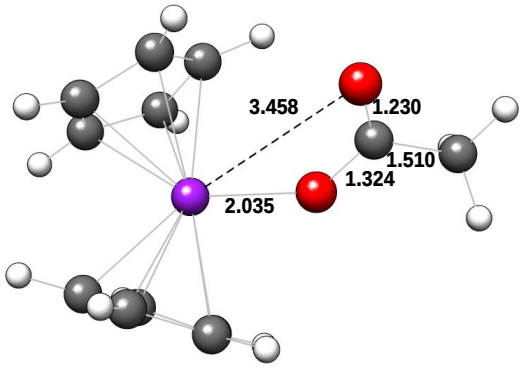

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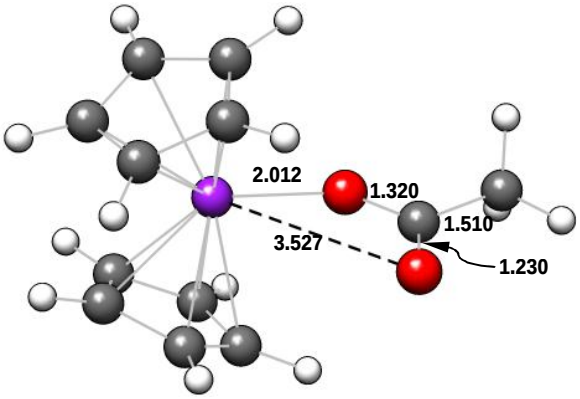

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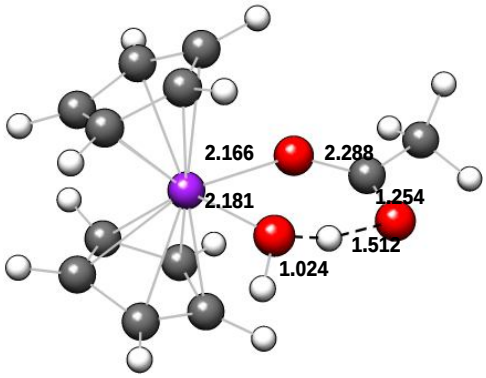

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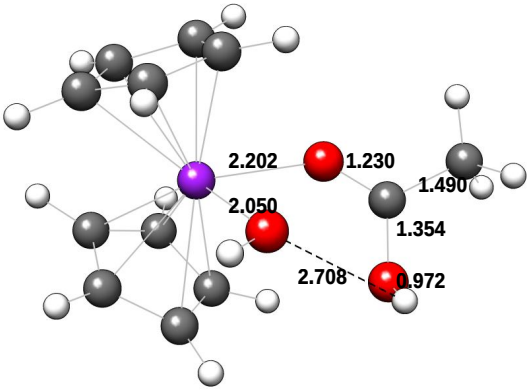

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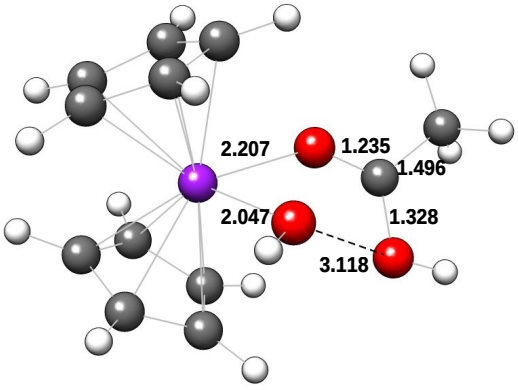

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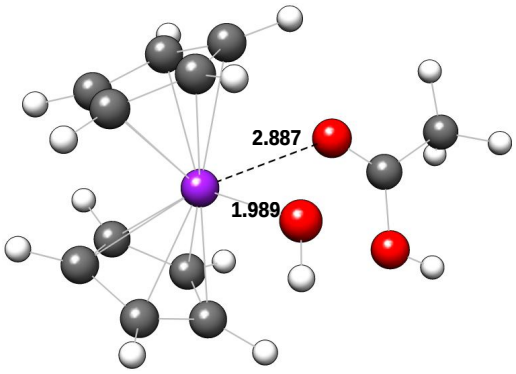

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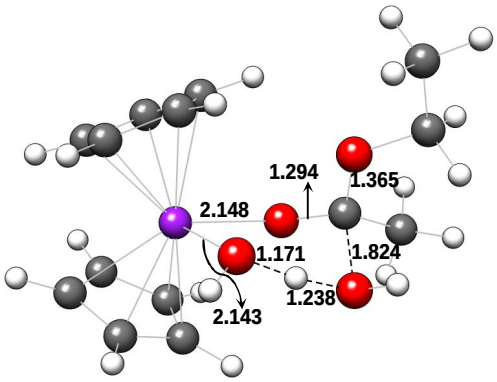

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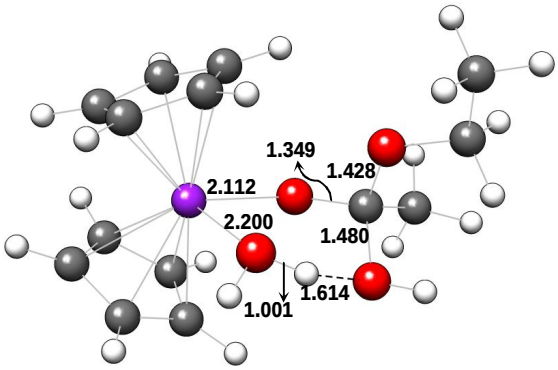

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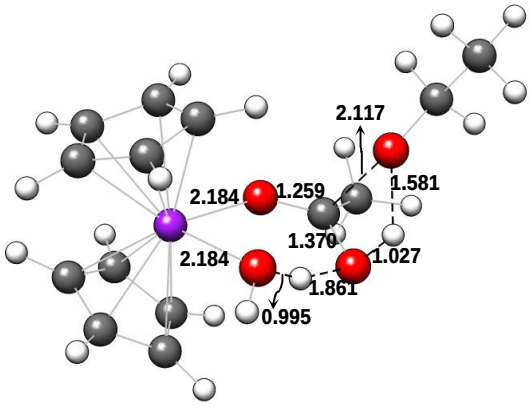

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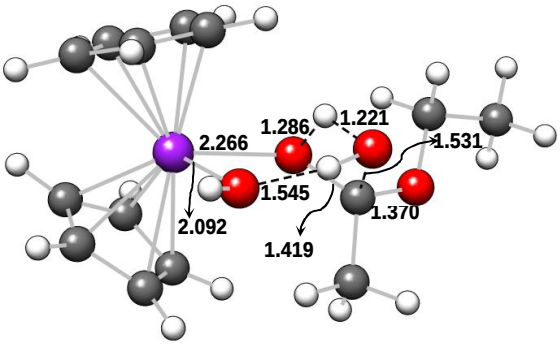

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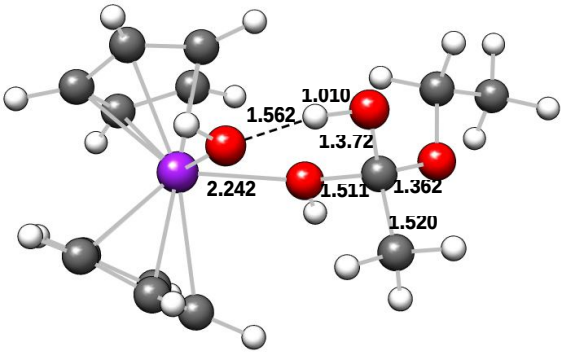

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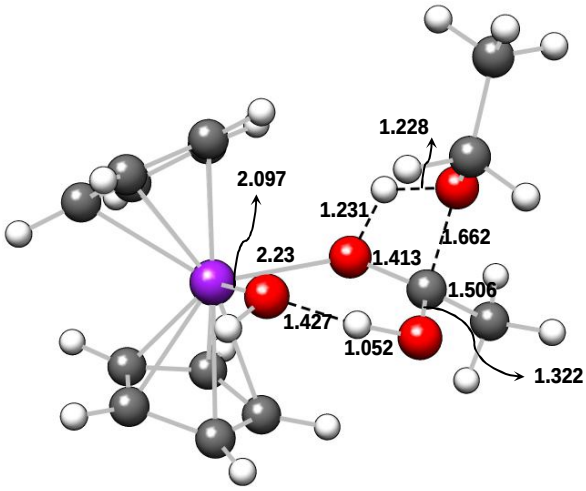

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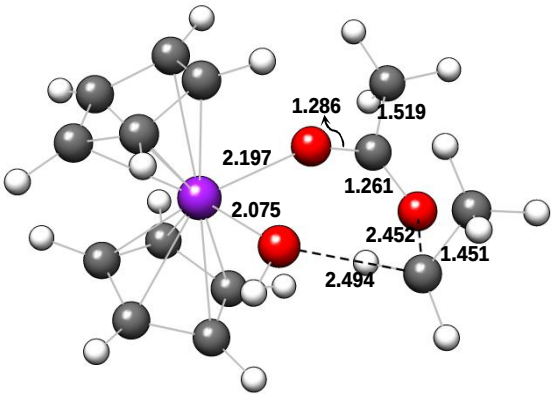

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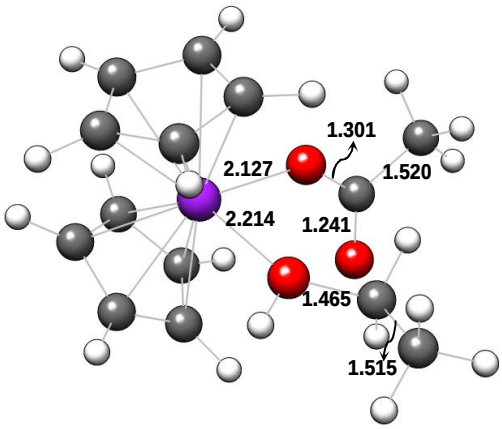

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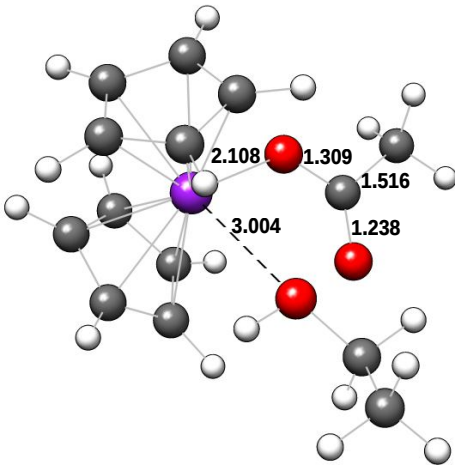

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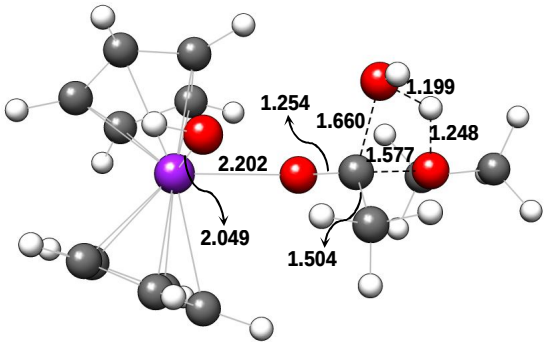

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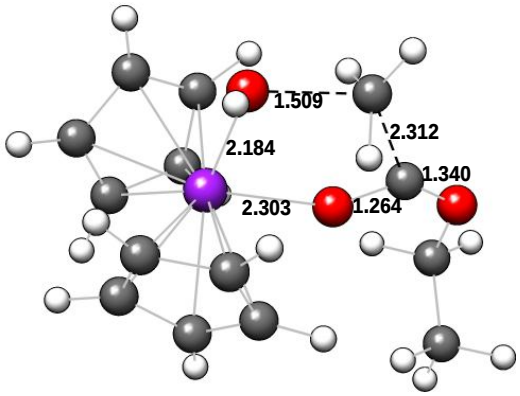

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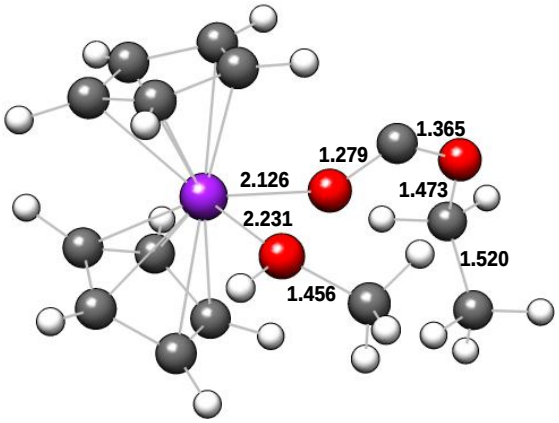

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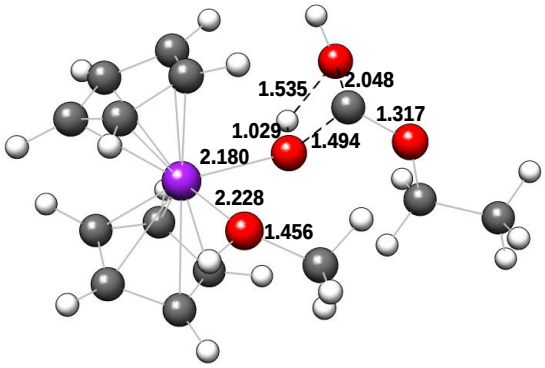

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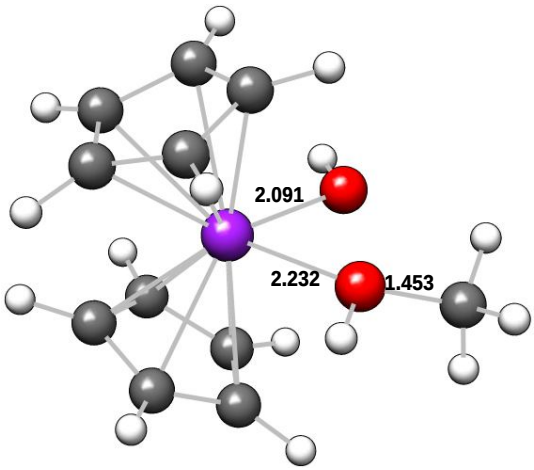

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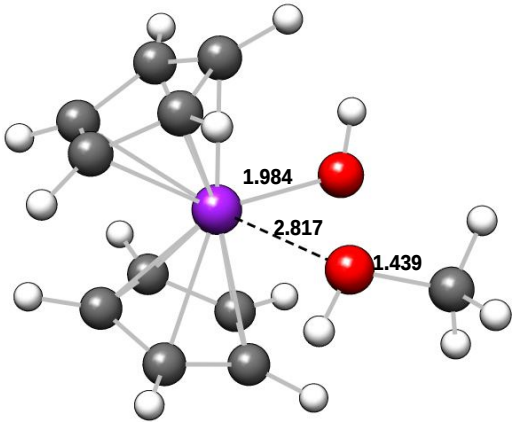

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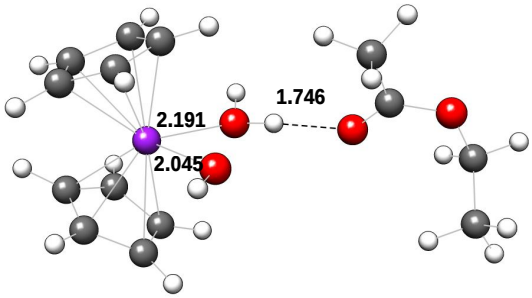

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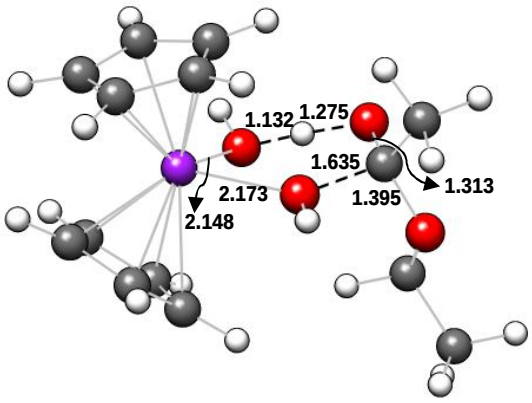

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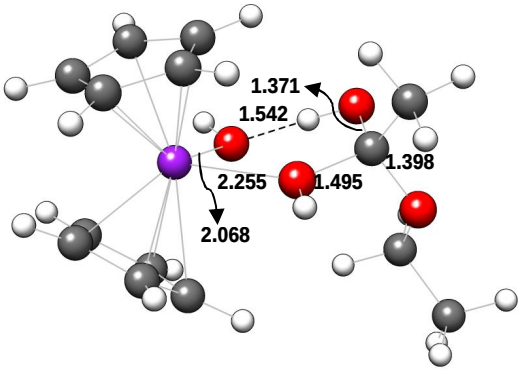

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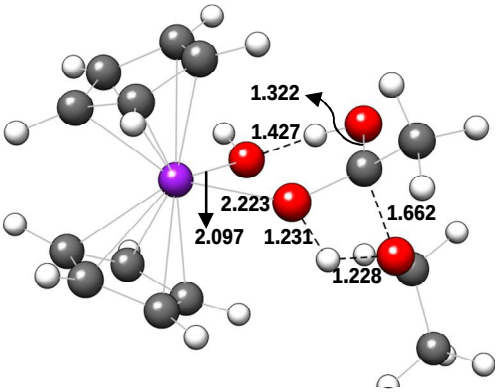

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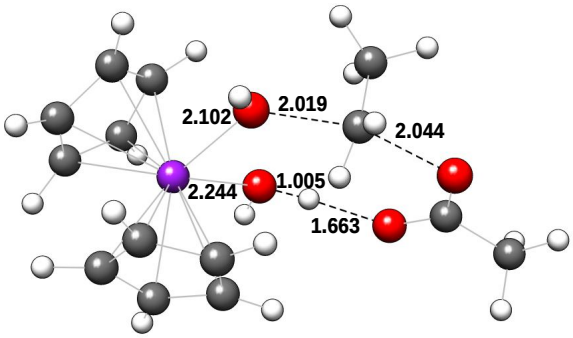

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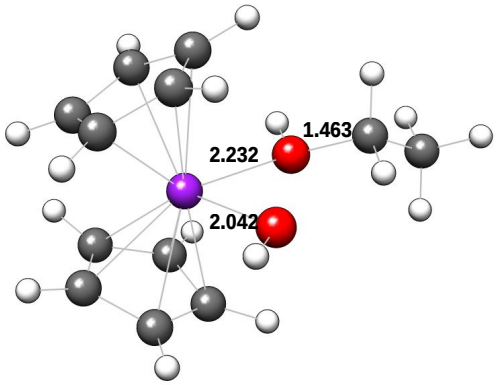

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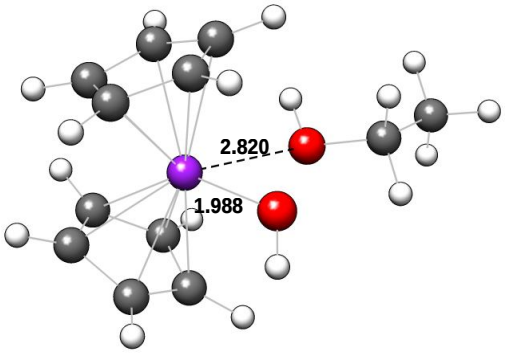

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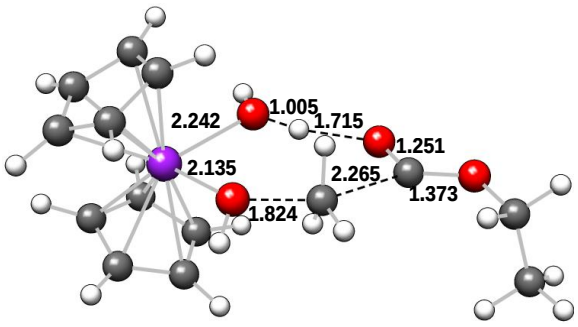

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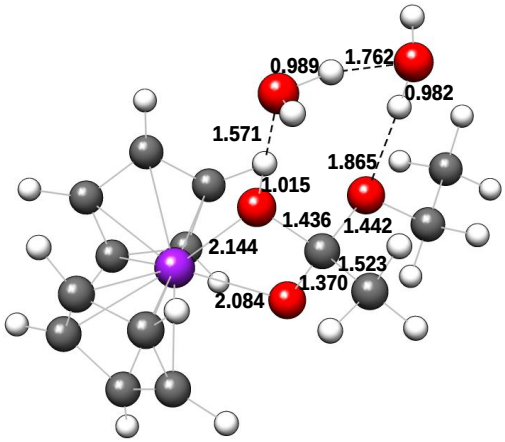

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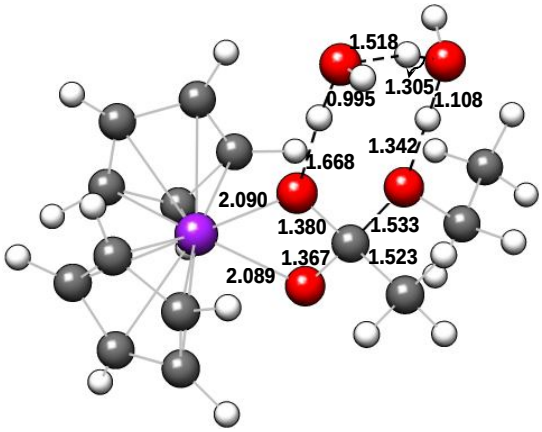

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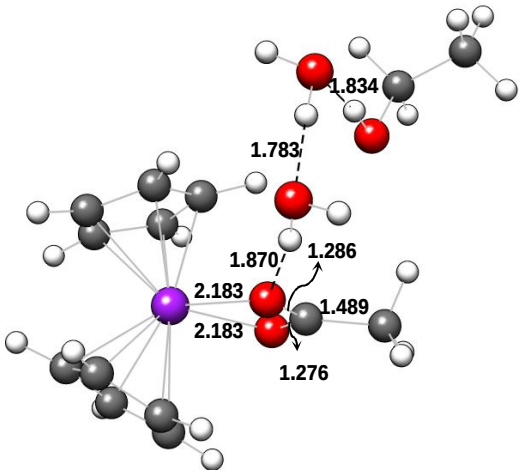

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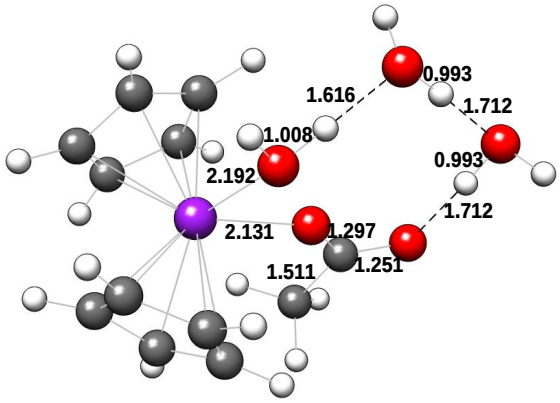

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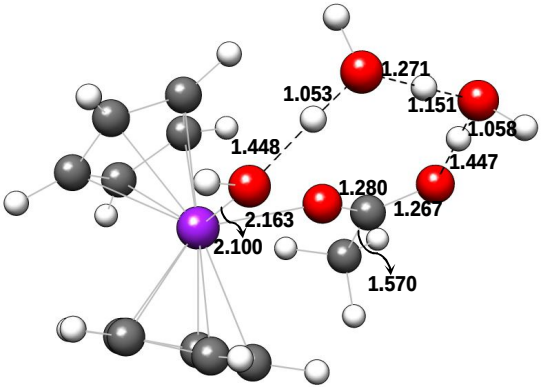
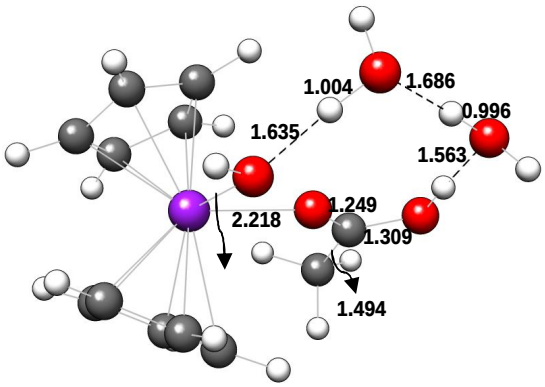
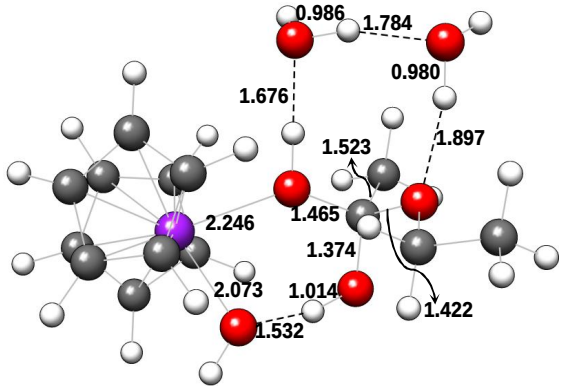


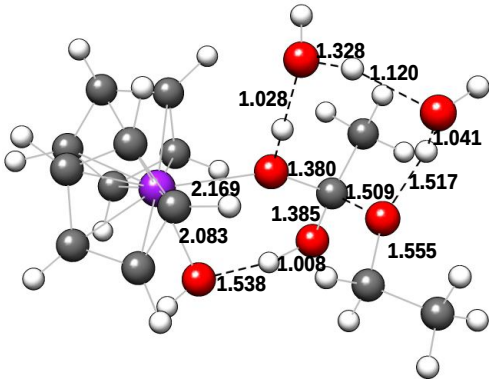
TS4-OH1-2WAT



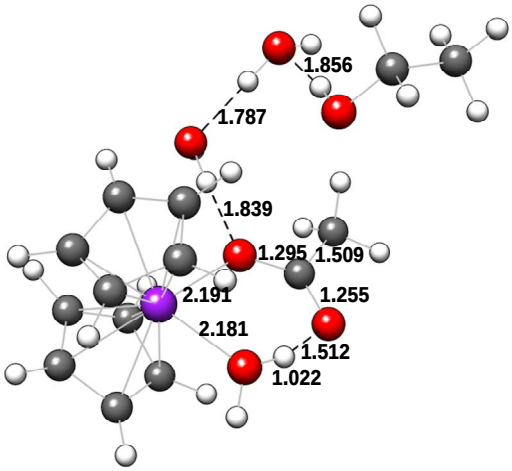
I6-OH1-2WAT



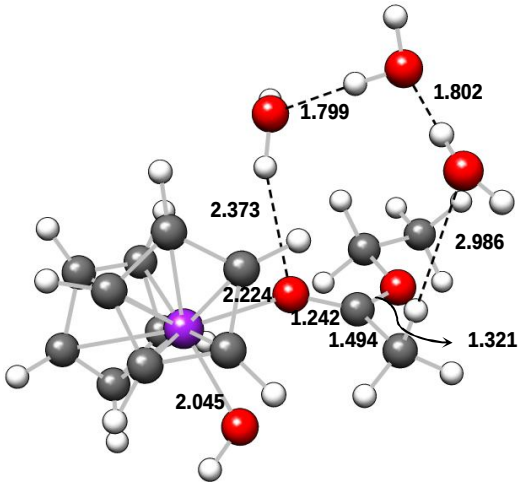
I1-OH1’-2WAT



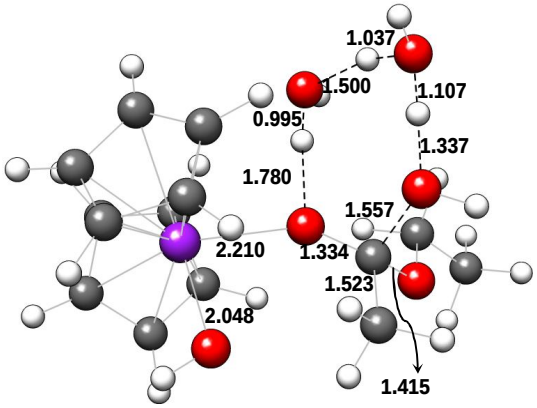
TS2-OH1’-2WAT



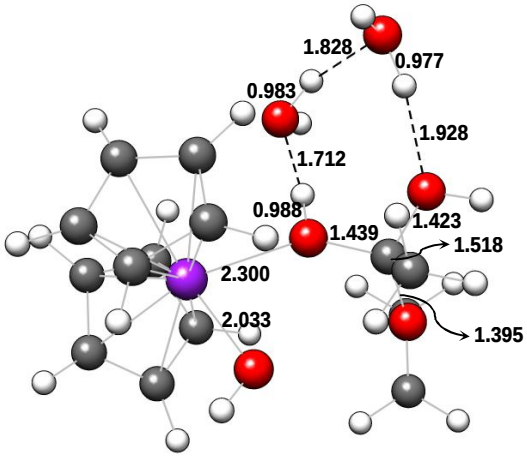
I5-OH1’-2WAT



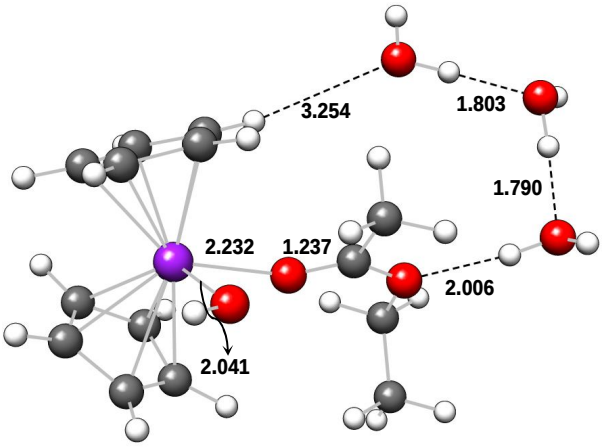
I1-W2-2WAT



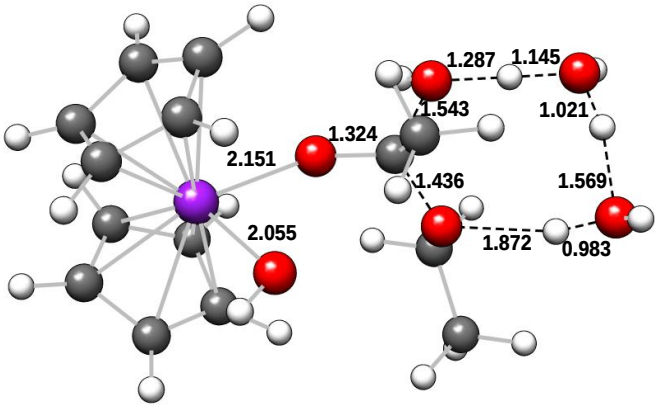
TS1-W2-2WAT



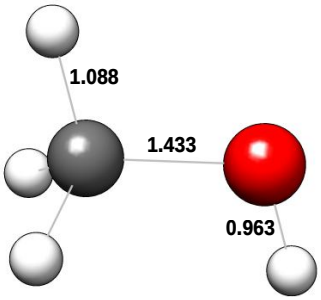
I2-W2-2WAT



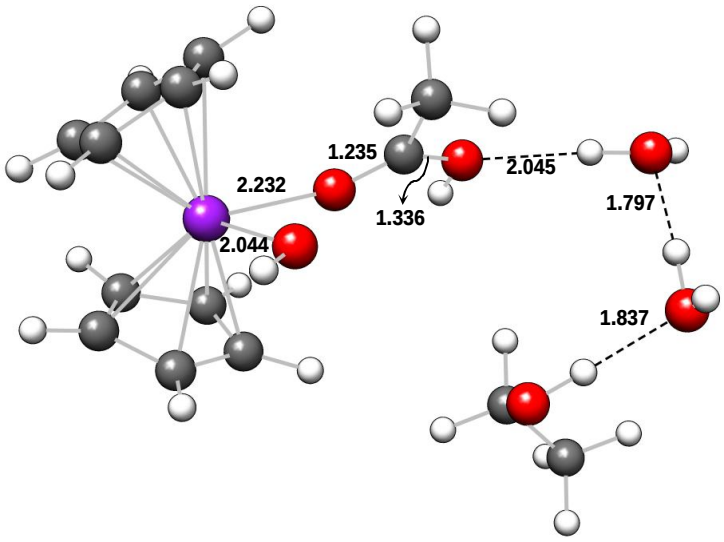
I1-W3-2WAT



TS1-W3-2WAT



methanol



I6-W3-2WAT

Figure S1. PCM-B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo) optimized geometries of the critical structures involved in the reaction mechanisms found for the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate.

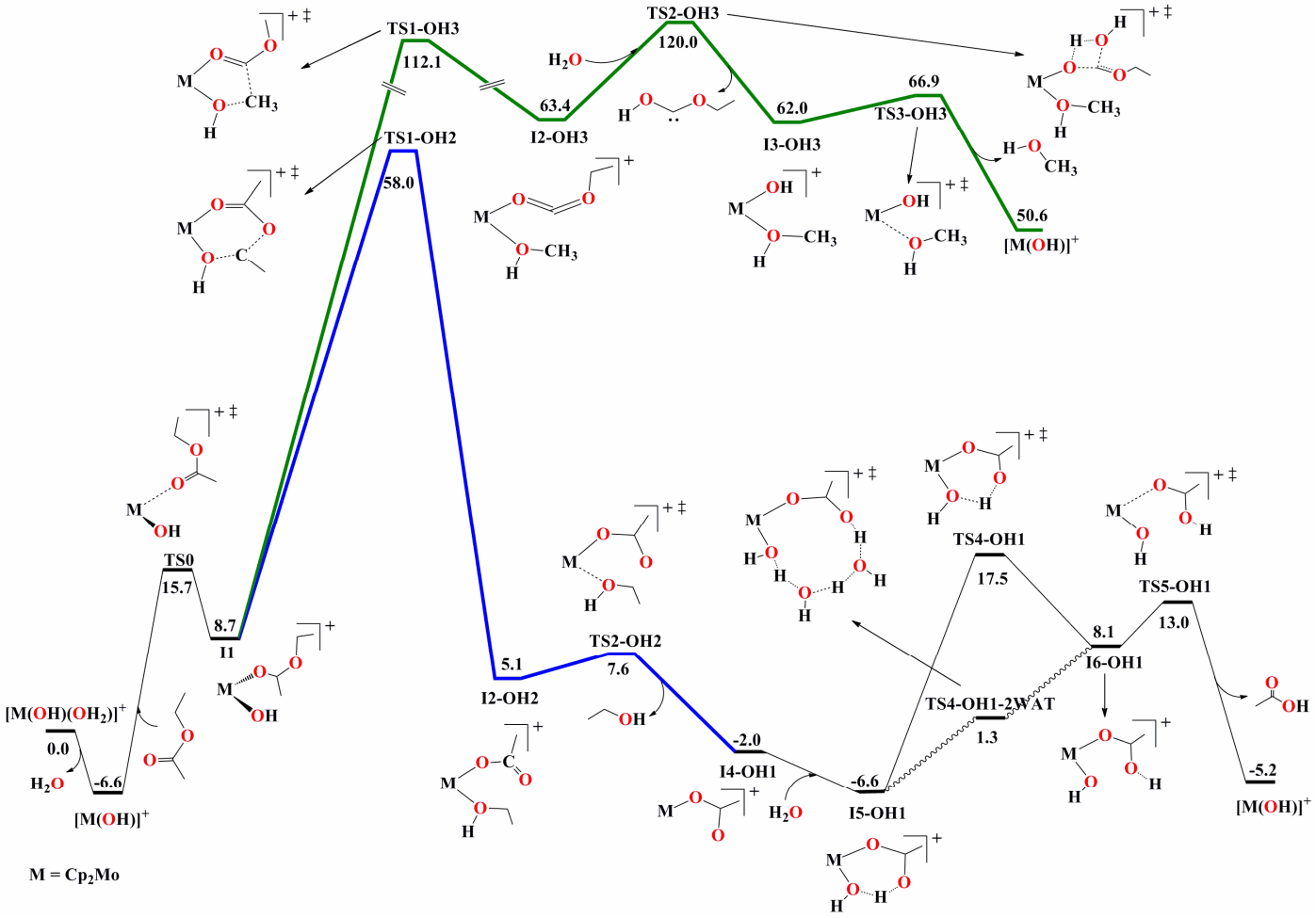


Figure S2. Gibbs energy profile in water solution of the reaction mechanisms starting with the water ligand release followed by the hydroxo ligand attack (OH2, blue line, and OH3, green line) for the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate at the PCM-B3LYP/aug-cc-pVTZ (aug-cc-pVTZ-PP for Mo)// PCM-B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo) level of theory.

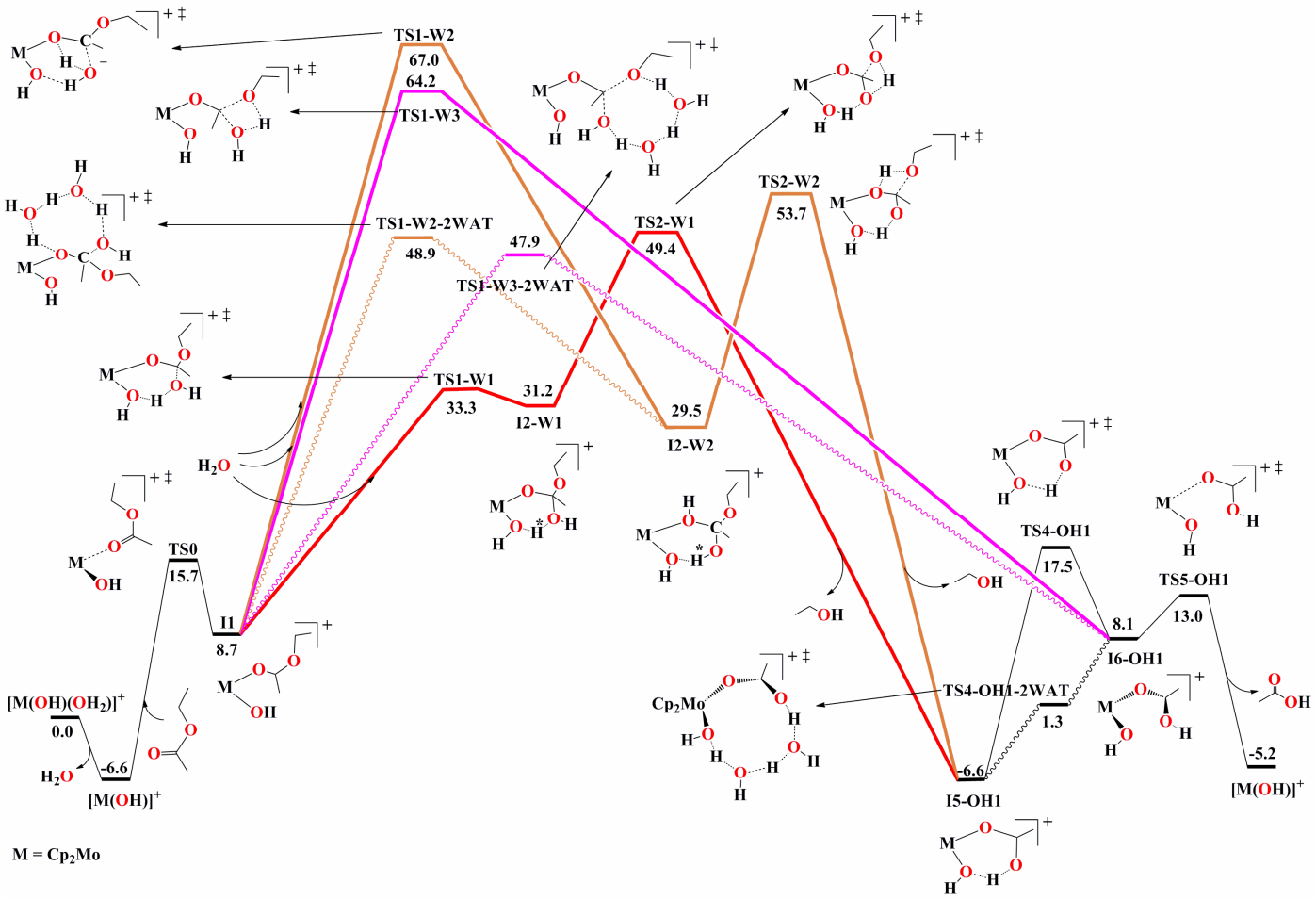


Figure S3. Gibbs energy profile in water solution of the reaction mechanisms starting with the water ligand release followed by the attack of an external water molecule (W1, red line, W2, orange lines, and W3, pink lines) for the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate at the PCM-B3LYP/aug-cc-pVTZ (aug-cc-pVTZ-PP for Mo)// PCM-B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo) level of theory.

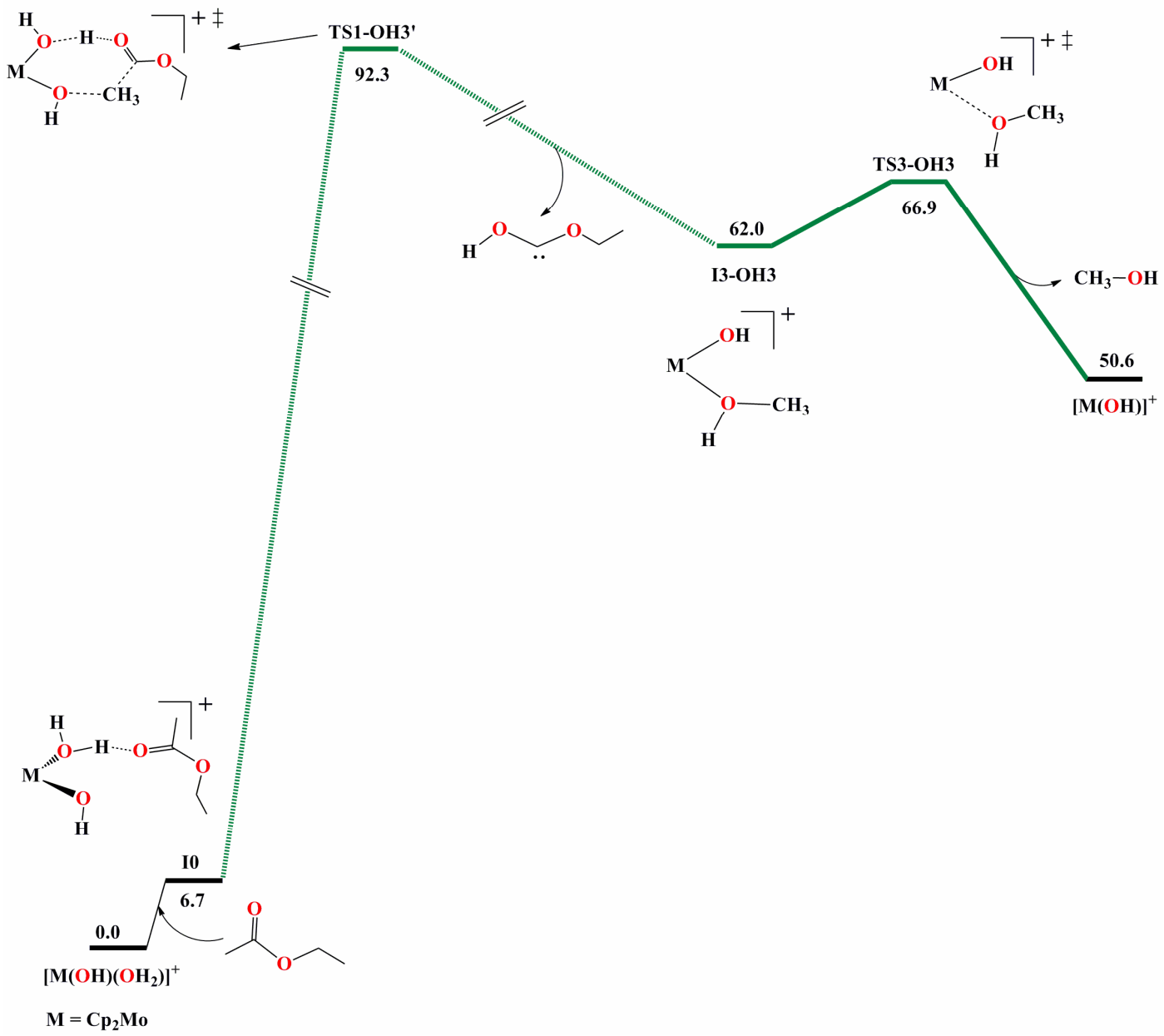


Figure S4. Gibbs energy profile in water solution of the reaction mechanism starting without the water ligand release OH3' for the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate at the PCM-B3LYP/aug-cc-pVTZ (aug-cc-pVTZ-PP for Mo)// PCM-B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo) level of theory.

Description of the reaction mechanisms not included in the manuscript:

The OH2 mechanism (continuous blue line in Figure S2). **I1** proceeds through the $O_{hydroxo}$ attack on $C_{methylenic}$ via the TS **TS1-OH2** (58.0 kcal/mol) leading to the intermediate **I2-OH2** (5.1 kcal/mol). At this species, the original single $C_{carbonyl}$-$O_{ethoxyl}$ bond is clearly cleaved while the ethanol ligand is formed. The next step is for the elimination of the ethanol ligand via the TS **TS2-OH2** (7.6 kcal/mol) giving rise to the intermediate **I4-OH1**, which in turn evolves to the separate products via **I5-OH1** as explained for OH1.

The OH3 mechanism (continuous green line in Figure S2). **I1** becomes the intermediate **I2-OH3** (63.4 kcal/mol) via the TS **TS1-OH3** (112.1 kcal/mol) for the $O_{hydroxo}$ attack on C_{methyl}. At **I2-OH3**, the C_{methyl}-$C_{carbonyl}$ bond is completely broken while a new $O_{hydroxo}$-C_{methyl} bond is formed. From **I2-OH3**, we could not find any significant TS or intermediate for the formation of acetic acid and ethanol. Instead, our theoretical exploration reveals that **I2-OH3** undergoes the addition of an external water molecule to the initial carbonyl bond via the TS **TS2-OH3** (120.0 kcal/mol) leading to CH_3CH_2OCOH and the intermediate **I3-OH3** (62.0 kcal/mol). **I3-OH3** proceeds through the cleavage of the methanol ligand via the TS **TS3-OH3** (66.9 kcal/mol) to give methanol, thus recovering the catalyst (50.6 kcal/mol). The high instability of this mechanism can be attributed to the formation of the carbene species CH_3CH_2OCOH (Schreiner, P. R.; Reisenauer, H. P. *Angew. Chem. Int. Ed.* **2008**, *47*, 7071-7074).

The W1 mechanism (continuous red line in Figure S3). **I1** evolves through the TS **TS1-W1** (33.3 kcal/mol) for the attack on $C_{carbonyl}$ of an external water molecule simultaneously interacting with the hydroxo ligand to give rise to the six-membered metallocycle **I2-W1** (31.2 kcal/mol). This species connects to the intermediate **I5-OH1** (-6.6 kcal/mol) via the TS **TS2-W1** (49.4 kcal/mol) for a hydrogen migration from the incoming water oxygen atom to $O_{ethoxyl}$. Then, **I5-OH1** becomes the separate products as mentioned for OH1.

The W2 mechanism (continuous orange line in Figure S3). The process starts with the addition of an external water molecule to the carbonyl bond of **I1** via the TS **TS1-W2** (67.0 kcal/mol) leading to the six-membered metallocycle **I2-W2** (29.5 kcal/mol). This intermediate differs from **I2-W1** in the position of a hydrogen atom of the incoming water molecule being 0.7 kcal/mol more stable than it. At **I2-W2** this hydrogen atom, which is identified by the asterisk symbol, is bonded to $O_{carbonyl}$ whereas it remains linked to

the incoming water at **I2-W1**. As happened for **I2-W1**, **I2-W2** becomes **I5-OH1** first and then evolves to the separate products as previously described. **TS2-W2** (53.7 kcal/mol) is the TS for the transformation **I2-W2** → **I5-OH1** and implies a H shift from $O_{carbonyl}$ to $O_{ethoxyl}$.

The W3 mechanism (continuous pink line in Figure S3). This reaction pathway implies the addition of an external water molecule to the single $C_{carbonyl}$-$O_{ethoxyl}$ bond of the ester ligand to afford ethanol and **I6-OH1** via the TS **TS1-W3** (64.2 kcal/mol). Subsequently, **I6-OH1** leads to the products as indicated for OH1.

The mechanism OH3' (discontinuous green line in Figure S4). This mechanism initiates with the $O_{hydroxo}$ attack on C_{methyl} combined with a hydrogen transfer from the water ligand to $O_{carbonyl}$ and the cleavage of the C_{methyl}-$C_{carbonyl}$ bond via the TS **TS1-OH3'** (92.3 kcal/mol). This TS connects the separate reactants with the intermediate **I3-OH3** (62.0 kcal/mol) after eliminating the CH_3CH_2OCOH molecule. Finally, **I3-OH3** undergoes the methanol ligand release as discussed for OH3 in Figure S2, thus recovering the $[Cp_2Mo(OH)]^+$ complex (50.6 kcal/mol).

Table S1. PCM-B3LYP/VDZ and PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energies with electrostatic and non-electrostatic solute-solvent interactions ($G_{\text{PCM-B3LYP/VDZ}}$ and $G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$, respectively), PCM-B3LYP/VDZ thermal Gibbs energy correction in water solution ($G^{\text{therm}}{}_{\text{PCM-B3LYP/VDZ}}$), and Gibbs energy in water solution ($G^{\text{sol}}{}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b,c,d]

Species	$G_{\text{PCM-B3LYP/VDZ}}$	$G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$	$G^{\text{therm}}{}_{\text{PCM-B3LYP/VDZ}}$	$G^{\text{sol}}{}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$
$[Cp_2Mo(OH)(OH_2)]^+$	-607.329093	-607.467830	0.169599	-607.298231
$[Cp_2Mo(OH)]^+$	-530.870295	-530.988974	0.146592	-530.842382
H_2O	-76.454991	-76.476646	0.003365	-76.473281
ethyl acetate	-307.758858	-307.843240	0.084290	-307.758950
ethanol	-155.073232	-155.118026	0.053708	-155.064318
acetic acid	-229.135085	-229.196084	0.034363	-229.161721
CH_3CH_2OCOH	-268.367445	-268.439266	0.059192	-268.380074
methanol	-115.750532	-115.784906	0.027802	-115.757104
TS0	-838.611757	-838.812908	0.250150	-838.562758
I1	-838.627056	-838.827800	0.253964	-838.573836
I1-W2-2WAT	-1068.003995	-1068.266764	0.309662	-1067.957102
I1-W3-2WAT	-1068.003488	-1068.267103	0.306419	-1067.960684
TS1-OH1	-838.605724	-838.804442	0.256440	-838.548002
I2-OH1	-838.609588	-838.807613	0.259482	-838.548131
I2-OH1-2WAT	-991.537429	-991.776996	0.301102	-991.475894
TS2-OH1	-838.570007	-838.767698	0.253174	-838.514524
TS2-OH1-2WAT	-991.525341	-991.765074	0.297572	-991.467502
I3-OH1	-683.570025	-683.726796	0.178526	-683.548270
I3-OH1-2WAT	-991.567836	-991.810077	0.290136	-991.519941
TS3-OH1	-683.544117	-683.701752	0.176965	-683.524787
I4-OH1	-683.550077	-683.707861	0.178221	-683.529640
I5-OH1	-760.026669	-760.204041	0.200656	-760.003385
I5-OH1-2WAT	-912.948192	-913.166888	0.245884	-912.921004
TS4-OH1	-759.987243	-760.165262	0.200302	-759.964960
TS4-OH1-2WAT	-912.932576	-913.151521	0.24307	-912.908451
I6-OH1	-760.003063	-760.181066	0.201076	-759.979990
I6-OH1-2WAT	-912.940139	-913.158824	0.246836	-912.911988
TS5-OH1	-759.994361	-760.172569	0.200478	-759.972091
TS1-W1	-915.058164	-915.277368	0.276295	-915.001073
I2-W1	-915.067124	-915.285865	0.281398	-915.004467
TS2-W1	-915.031562	-915.251319	0.275814	-914.975505
TS1-W2	-915.006178	-915.223973	0.276587	-914.947386
TS1-W2-2WAT	-1067.953895	-1068.213764	0.320668	-1067.893096
I2-W2	-915.068780	-915.287516	0.280410	-915.007106
I2-W2-2WAT	-1067.978098	-1068.238128	0.321634	-1067.916494
TS2-W2	-915.025825	-915.243945	0.275349	-914.968596

TS1-OH2	-838.541962	-838.741889	0.246630	-838.495259
I2-OH2	-838.632090	-838.832400	0.252824	-838.579576
TS2-OH2	-838.618394	-838.819120	0.250354	-838.568766
TS1-W3	-915.004188	-915.223625	0.271860	-914.951765
TS1-W3-2WAT	-1067.957671	-1068.218287	0.320189	-1067.898098
I6-W3-2WAT	-1067.999292	-1068.262937	0.311177	-1067.951760
TS1-OH3	-838.462928	-838.661794	0.252703	-838.409091
I2-OH3	-838.540315	-838.739876	0.253247	-838.486629
TS2-OH3	-914.918279	-915.136818	0.273841	-914.862977
I3-OH3	-646.622684	-646.773778	0.195536	-646.578242
TS3-OH3	-646.611436	-646.762838	0.192299	-646.570539
I0	-915.092144	-915.314222	0.270720	-915.043502
TS1-OH1'	-915.061692	-915.280607	0.276482	-915.004125
I1-OH1'	-915.066892	-915.285672	0.280574	-915.005098
I1-OH1'-2WAT	-1067.993307	-1068.252869	0.322145	-1067.930724
TS2-OH1'	-915.025825	-915.243943	0.275353	-914.968590
TS2-OH1'-2WAT	-1067.971598	-1068.230815	0.321570	-1067.909245
I5-OH1'-2WAT	-1068.025063	-1068.287530	0.314241	-1067.973289
TS1-OH2'	-915.035767	-915.255413	0.274645	-914.980768
I1-OH2'	-685.945472	-686.107296	0.221177	-685.886119
TS2-OH2'	-685.934297	-686.096267	0.217613	-685.878654
TS1-OH3'	-914.962051	-915.181816	0.274698	-914.907118

[a]All the magnitudes are given in hartree. [b]Thermodynamic contributions are computed at a temperature of 298.15 K and a pressure of 1 atm. [c]$G^{sol}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}} = G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}} + G^{therm}_{\text{PCM-B3LYP/VDZ}}$. [d]VTZ = aug-cc-pVTZ (aug-cc-pVTZ-PP for Mo); VDZ = aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo).

Table S2. Relative PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energy with electrostatic and non-electrostatic solute-solvent interactions ($\Delta G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$), PCM-B3LYP/VDZ thermal Gibbs energy correction ($\Delta G^{\text{therm}}{}_{\text{PCM-B3LYP/VDZ}}$), PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}{}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$), and PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}{}_{\text{corr}}$) computed at the standard concentration of 1 *M* (55.5 *M* for water) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b]

Species	$\Delta G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$	$\Delta G^{\text{therm}}{}_{\text{PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}{}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}{}_{\text{corr}}$
$[Cp_2Mo(OH)(H_2O)]^+$ + ethyl acetate	0.0	0.0	0.0	0.0
$[Cp_2Mo(OH)]^+$ + ethyl acetate + H_2O	1.4	-12.3	-10.9	-6.6
TS0 + H_2O	13.5	-0.2	13.3	15.7
I1 + H_2O	4.2	2.2	6.3	8.7
TS1-OH1 + H_2O	18.8	3.7	22.5	24.9
I2-OH1 + H_2O	16.8	5.6	22.4	24.8
TS2-OH1 + H_2O	41.9	1.7	43.5	45.9
I3-OH1 +H_2O + ethanol	-6.5	-11.5	-18.0	-13.7
TS3-OH1 + H_2O + ethanol	9.2	-12.5	-3.3	1.0
I4-OH1 + H_2O + ethanol	5.4	-11.7	-6.3	-2.0
I5-OH1 + ethanol	-6.9	0.3	-6.6	-6.6
TS4-OH1 + ethanol	17.4	0.1	17.5	17.5
I6-OH1 + ethanol	7.5	0.6	8.1	8.1
TS5-OH1 + ethanol	12.8	0.2	13.0	13.0
TS1-W1	21.1	14.1	35.2	33.3
I2-W1	15.8	17.3	33.1	31.2
TS2-W1	37.5	13.8	51.3	49.4
TS1-W2	54.7	14.2	68.9	67.0
I2-W2	14.8	16.6	31.4	29.5
TS2-W2	42.1	13.5	55.6	53.7
TS1-OH2 + H_2O	58.1	-2.4	55.6	58.0
I2-OH2 + H_2O	1.3	1.4	2.7	5.1
TS2-OH2	9.6	-0.1	9.5	7.6
TS1-W3	54.9	11.3	66.1	64.2
TS1-OH3 + H_2O	108.3	1.4	109.7	112.1
I2-OH3 + H_2O	59.3	1.7	61.0	63.4
TS2-OH3	109.3	12.5	121.9	120.0
I3-OH3 + CH_3CH_2OCOH	61.5	0.5	62.0	62.0
TS3-OH3 + CH_3CH_2OCOH	68.4	-1.5	66.9	66.9
I0	-2.0	10.6	8.6	6.7
TS1-OH1'	19.1	14.2	33.3	31.4
I1-OH1'	15.9	16.7	32.7	30.8
TS2-OH1'	42.1	13.5	55.6	53.7
TS1-OH2'	34.9	13.0	47.9	46.0
I1-OH2' + acetic acid	4.8	1.0	5.9	5.9
TS2-OH2' + acetic acid	11.7	-1.2	10.5	10.5
TS1-OH3'	81.1	13.1	94.2	92.3
$[Cp_2Mo(OH)]^+$ + ethanol + acetic acid	5.0	-12.1	-7.1	-5.2
$[Cp_2Mo(OH)]^+$ + CH_3CH_2OCOH + methanol	61.4	-12.7	48.7	50.6

[a]All the thermodynamic magnitudes are given in kcal/mol at a temperature of 298.15 K and a pressure of 1 atm. [b]$\Delta G^{\text{sol}}{}_{\text{corr}} = \Delta G^{\text{sol}}{}_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$ + (1.9 kcal/mol) Δn + (4.3 kcal/mol) Δm, where Δn and Δm are the changes in the number of non-water components and water molecules for each transformation along the reaction mechanisms found, respectively.

Table S3. PCM-B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP for Mo) optimized cartesian coordinates of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate.

$[Cp_2Mo(OH)(OH_2)]^+$

C	2.220212	0.636121	-0.106763
C	1.895988	-0.186168	-1.246450
C	1.547444	-1.460996	-0.742120
C	1.660741	-1.438800	0.689713
C	2.102976	-0.156958	1.075961
Mo	-0.004811	0.166908	0.033647
C	-1.668626	-0.889165	-1.212572
C	-2.336382	0.212286	-0.596125
C	-2.300695	0.047334	0.807026
C	-1.593031	-1.148053	1.109396
C	-1.233511	-1.747560	-0.151100
H	2.506017	1.681843	-0.140513
H	1.940101	0.103977	-2.290544
H	1.230144	-2.309392	-1.337473
H	1.425297	-2.261435	1.357218
H	2.255518	0.185328	2.093464
H	-1.573471	-1.073140	-2.276893
H	-2.740605	1.074669	-1.115618
H	-2.667216	0.765429	1.532011
H	-1.426786	-1.568291	2.095141
H	-0.760847	-2.714441	-0.268317
O	-0.091347	1.745848	1.337021
H	-0.086803	1.486051	2.265569
O	-0.209171	2.064639	-1.089865
H	-0.044816	2.756260	-0.422504
H	0.364156	2.240762	-1.849440

$[Cp_2Mo(OH)]^+$

C	-1.415430	-1.552198	0.124649
C	-1.699221	-0.889135	-1.115816
C	-2.245334	0.382415	-0.792184
C	-2.258191	0.522361	0.622247
C	-1.729477	-0.667131	1.208512
Mo	0.001116	0.270189	-0.005680
C	2.258236	0.397345	0.771013
C	2.276175	0.493596	-0.644136
C	1.736559	-0.708862	-1.194375
C	1.423337	-1.564048	-0.086929
C	1.702032	-0.862516	1.132095
O	0.079916	2.194681	-0.026283
H	2.575428	1.368459	-1.212860
H	1.666142	-0.961042	-2.246409
H	1.059022	-2.580119	-0.163138
H	1.573242	-1.243054	2.139498
H	2.539268	1.184740	1.463914
H	-1.571179	-1.299666	-2.111404
H	-2.528876	1.148732	-1.507795
H	-2.563121	1.410843	1.167146
H	-1.662179	-0.890162	2.267189
H	-1.054571	-2.566912	0.229860
H	-0.737461	2.712290	-0.041531

H_2O

O	-0.024248	0.000000	-0.017137
H	0.025062	0.000000	0.950263
H	0.904123	0.000000	-0.293580

ethyl acetate

C	-1.022840	0.243368	-0.079113
C	-2.225362	-0.658623	-0.040793
O	-1.060398	1.458117	-0.215401
O	0.123463	-0.443283	0.055370
C	1.367895	0.319275	0.034525
C	2.508204	-0.663470	0.201401
H	-3.136929	-0.065261	-0.152566
H	-2.248005	-1.205192	0.911427
H	-2.158499	-1.399210	-0.848904
H	1.334632	1.051397	0.850559
H	1.425003	0.855508	-0.920573
H	3.458356	-0.112348	0.188931
H	2.432110	-1.198787	1.157292
H	2.522672	-1.395078	-0.617514

ethanol

C	5.672813	-0.844888	-0.631210
C	4.496646	-1.368735	0.184115
O	3.301979	-0.602654	-0.023918
H	4.311184	-2.428296	-0.045710
H	4.709978	-1.298505	1.255004
H	6.576826	-1.428131	-0.422881
H	5.471503	-0.917299	-1.707267
H	5.877410	0.203601	-0.389237
H	3.034807	-0.679046	-0.966070

acetic acid

C	4.131683	0.385674	-0.335127
C	2.777777	-0.252385	-0.186444
O	1.731707	0.232087	-0.581033
O	2.729103	-1.454932	0.433241
H	4.794446	-0.277647	-0.908105
H	3.612205	-1.750672	0.707202
H	4.031633	1.345708	-0.848511
H	4.582600	0.536422	0.655574

CH_3CH_2OCOH

C	6.709847	-0.353915	-1.024043
C	5.723355	-0.642549	0.083503
O	4.706642	0.404099	0.126001
C	3.490657	0.063366	-0.204321
O	2.762006	1.170879	-0.106577
H	1.850392	0.952552	-0.340554
H	6.197580	-0.620734	1.062065
H	5.216202	-1.594727	-0.053361
H	7.176057	0.622039	-0.889375
H	7.493573	-1.112145	-1.009675
H	6.221380	-0.380874	-1.998091

TS0

C	1.748074	1.973255	0.757624
C	0.416719	2.387460	0.425113
C	0.213701	2.202488	-0.977906
C	1.395835	1.658236	-1.523182
C	2.343829	1.518894	-0.462893
Mo	0.577037	0.107213	0.144548
C	2.315429	-1.442768	0.488414
C	2.079125	-1.275557	-0.923602
C	0.760261	-1.723892	-1.231995
C	0.199452	-2.195243	0.003925
C	1.161942	-2.050168	1.036223
O	-0.540300	0.161351	1.794860
O	-1.995963	-0.198350	-0.871728
C	-3.155241	0.129388	-0.630471
O	-4.117752	-0.604719	-1.205815
C	-5.535075	-0.304086	-0.996004
C	-6.329971	-1.377948	-1.708474
C	-3.541425	1.279427	0.252540
H	-0.708864	2.386515	-1.518253
H	1.543824	1.356866	-2.554962
H	3.358283	1.150977	-0.563889
H	2.234277	2.053674	1.723265
H	-0.324056	2.755968	1.124860
H	0.301861	-1.771558	-2.212656
H	-0.815322	-2.554860	0.139128
H	1.008951	-2.281921	2.085510
H	3.224440	-1.187791	1.022423
H	2.795307	-0.890619	-1.639547
H	-0.324909	-0.438957	2.518093
H	-4.205995	1.967817	-0.284088
H	-4.085873	0.910664	1.131931
H	-2.642139	1.805759	0.574804
H	-5.736847	-0.303443	0.081103
H	-5.742030	0.690024	-1.408971
H	-6.110264	-2.370316	-1.293409
H	-7.400658	-1.174968	-1.573664
H	-6.110488	-1.381970	-2.784095

I1

C	-0.168975	0.230959	0.381018
C	0.085341	0.193599	1.782285
C	1.471399	0.008595	1.989226
C	2.121295	-0.090325	0.724311
C	1.098820	0.014751	-0.271799
Mo	1.188007	2.068683	0.718664
C	0.826880	2.657854	-1.588792
C	2.226134	2.380121	-1.419407
C	2.760408	3.299501	-0.490654
C	1.675526	4.151478	-0.072145
C	0.496593	3.766700	-0.781866
O	-0.145825	3.027085	1.938917
H	1.969601	-0.001813	2.952219
H	3.176878	-0.270955	0.554713
H	1.239925	-0.102070	-1.338721
H	-1.138685	0.307692	-0.098068
H	-0.647634	0.366508	2.561722
H	3.789987	3.352307	-0.156256
H	1.741884	4.949445	0.658113
H	-0.489239	4.204485	-0.673107
H	0.140100	2.097139	-2.214391
H	2.773578	1.577828	-1.901270
H	-1.036918	2.987205	1.570486
O	2.445169	2.841745	2.363675
C	1.520754	2.334062	4.571424
H	1.323645	3.014246	5.406127
H	0.593000	2.051188	4.073851
H	2.017672	1.440496	4.975869
C	2.447418	2.984850	3.595240
O	3.363444	3.743756	4.174093
C	4.354028	4.415133	3.323485
H	3.809635	5.044832	2.611588
H	4.902398	3.640930	2.775879
C	5.253463	5.222331	4.233596
H	6.005428	5.735882	3.619998
H	4.680851	5.979796	4.784385
H	5.774934	4.574536	4.949890

TS1-OH1

C	2.577565	1.150003	0.832407
C	1.603334	2.139411	0.515508
C	1.336557	2.092672	-0.873546
C	2.129612	1.067092	-1.459889
C	2.930026	0.512369	-0.404032
Mo	0.764751	-0.080218	0.040321
C	2.083376	-2.018404	0.452924
C	1.602027	-2.146530	-0.893613
C	0.195260	-2.214856	-0.848818
C	-0.202060	-2.094408	0.519065
C	0.975231	-1.985973	1.335431
O	-0.728749	0.519611	1.450324
H	0.598943	2.688652	-1.398725
H	2.183437	0.815519	-2.513079
H	3.709772	-0.225864	-0.536410
H	3.020982	0.970077	1.805337
H	1.116778	2.791241	1.233535
H	-0.466996	-2.275696	-1.705470
H	-1.218600	-2.091819	0.886567
H	1.012094	-1.926978	2.416937
H	3.123966	-1.957455	0.749112
H	2.215506	-2.155069	-1.788722
H	-0.489159	1.224356	2.067209
O	-1.071179	0.490591	-0.852490
C	-1.937101	2.540519	0.211840
H	-2.459536	2.941822	-0.667714
H	-2.522082	2.780991	1.105003
H	-0.953977	3.004139	0.278107
C	-1.853524	1.043090	0.034852
O	-3.058154	0.510214	0.275413
C	-3.397091	-0.843398	-0.148334
H	-3.228732	-1.502670	0.711096
H	-2.739700	-1.132147	-0.971666
C	-4.856635	-0.845792	-0.559055
H	-5.146081	-1.868199	-0.837453
H	-5.500275	-0.518147	0.267650
H	-5.022539	-0.189813	-1.423482

I2-OH1

C	2.556422	1.124406	0.892540
C	1.592657	2.119481	0.562513
C	1.377903	2.102384	-0.837170
C	2.191559	1.087963	-1.413410
C	2.955193	0.512665	-0.338902
Mo	0.762500	-0.087823	-0.006488
C	2.065218	-2.032284	0.459570
C	1.692384	-2.107034	-0.925493

C	0.286013	-2.187293	-0.998995
C	-0.216934	-2.123018	0.336027
C	0.891422	-2.036814	1.249025
O	-0.927725	0.531778	1.264486
H	0.661991	2.709170	-1.378582
H	2.286210	0.858447	-2.468774
H	3.737010	-0.226413	-0.456201
H	2.957820	0.919579	1.878527
H	1.075330	2.748808	1.279604
H	-0.304854	-2.227430	-1.907379
H	-1.258418	-2.154040	0.620911
H	0.840498	-2.018829	2.331791
H	3.078263	-1.965860	0.838885
H	2.375809	-2.083044	-1.767924
H	-0.844664	1.175399	1.984725
O	-1.014582	0.510278	-0.930631
C	-1.867837	2.565256	0.128753
H	-2.347572	2.894513	-0.799978
H	-2.494977	2.866113	0.975591
H	-0.895359	3.050227	0.214613
C	-1.753770	1.044887	0.080766
O	-3.060854	0.589541	0.180045
C	-3.376528	-0.804463	-0.034224
H	-3.120721	-1.366532	0.874236
H	-2.789528	-1.184678	-0.876933
C	-4.865681	-0.898704	-0.312723
H	-5.144940	-1.953080	-0.442609
H	-5.447938	-0.488784	0.523396
H	-5.128784	-0.353742	-1.229044

TS2-OH1

C	-2.545360	1.169676	-0.863726
C	-1.578429	2.129870	-0.446078
C	-1.416832	2.037018	0.957389
C	-2.267815	1.011257	1.451339
C	-2.995679	0.498211	0.322262
Mo	-0.814021	-0.113126	0.014367
C	-2.048291	-2.058365	-0.647696
C	-1.837993	-2.144407	0.769766
C	-0.449097	-2.196897	1.015572
C	0.207075	-2.122644	-0.259164
C	-0.791498	-2.053158	-1.290370
O	0.761781	0.664533	-1.266100
H	-0.701061	2.598104	1.547843
H	-2.395247	0.722180	2.488560
H	-3.788266	-0.237668	0.368854
H	-2.921031	1.027505	-1.870826
H	-1.008337	2.777640	-1.103279
H	0.030040	-2.264264	1.985886
H	1.274779	-2.175181	-0.419590
H	-0.615467	-2.003918	-2.359274
H	-3.011665	-1.979471	-1.139875
H	-2.616960	-2.138700	1.524918
H	1.745888	-0.074561	-1.441326
O	1.014201	0.511678	0.932390
C	2.137690	2.413824	-0.098599
H	2.874144	2.476428	0.710701
H	2.617507	2.663463	-1.049976
H	1.330464	3.127705	0.101138
C	1.575046	1.018926	-0.144505
O	2.767317	0.081028	-0.773746
C	3.476146	-0.872205	0.057004
H	3.548901	-1.797172	-0.527641
H	2.870995	-1.064370	0.951659
C	4.850579	-0.338409	0.420474
H	5.375609	-1.083153	1.034898
H	5.448854	-0.146988	-0.479877
H	4.770319	0.590622	0.999910

I3-OH1

C	-0.361093	-1.726576	-0.110519
C	0.916722	-2.044253	0.471488
C	1.915445	-2.013588	-0.553136
C	1.233663	-1.678967	-1.768603
C	-0.155676	-1.528715	-1.492837
Mo	1.117017	0.116146	-0.284381
C	1.088563	2.220838	0.709975
C	2.392396	1.713680	0.980344
C	2.262932	0.536998	1.747988
C	0.858699	0.335096	1.991473
C	0.120174	1.376677	1.346851
O	0.285375	1.330160	-1.889565
C	1.432087	1.504266	-2.432056
C	1.620923	2.339302	-3.651403
O	2.409028	0.929778	-1.836130
H	-0.911740	-1.221081	-2.207906
H	-1.307413	-1.657987	0.415253
H	1.089859	-2.305981	1.508049
H	2.964501	-2.264038	-0.445440
H	1.700104	-1.539487	-2.737855
H	-0.951014	1.536249	1.390743
H	0.866997	3.092234	0.103296
H	3.320511	2.112899	0.584444
H	3.072120	-0.096779	2.094615
H	0.430996	-0.454890	2.596481
H	1.815638	3.373376	-3.331066
H	2.484192	1.983393	-4.223365
H	0.712708	2.328172	-4.262676

TS3-OH1

C	0.373499	1.526156	1.332994
C	1.611175	2.155538	0.950286
C	2.697192	1.354942	1.401679
C	2.159953	0.204500	2.024697
C	0.728700	0.328339	2.016815
Mo	1.395059	0.178375	-0.217804
C	0.096796	-1.221135	-1.688183
C	-0.329853	-1.439127	-0.356539
C	0.784775	-1.970631	0.372151
C	1.922505	-2.027892	-0.496662
C	1.475362	-1.558460	-1.776985
O	2.639324	1.101051	-1.537705
C	2.592287	1.326443	-2.841571
C	3.905309	1.803517	-3.415062
H	-0.501140	-0.781213	-2.479961
H	-1.324385	-1.257003	0.036018
H	0.768364	-2.301629	1.403474
H	2.899724	-2.432480	-0.259121
H	2.091949	-1.456948	-2.662923
H	-0.626705	1.921569	1.196918
H	1.699984	3.071412	0.374277
H	3.749660	1.540669	1.213867
H	2.727044	-0.619843	2.444095
H	0.031465	-0.376206	2.454495
H	4.209810	2.728705	-2.907318
H	4.684017	1.052423	-3.226224
H	3.810538	1.983581	-4.489856
O	1.575050	1.188654	-3.519824

I4-OH1

C	-0.855339	-1.524231	1.325639
C	-0.093441	-2.235323	0.355595
C	-0.801632	-2.232094	-0.872525
C	-2.028178	-1.528605	-0.697106
C	-2.075043	-1.118559	0.676191
Mo	-0.372670	0.057866	-0.284047
C	0.039949	2.077789	0.839837
C	-1.271232	1.685673	1.198600
C	-2.084105	1.685391	0.016126
C	-1.277366	2.042299	-1.088825
C	0.052365	2.268613	-0.577229
O	1.613715	-0.135845	-0.542254
C	2.709306	-0.248480	0.185877
C	3.974252	-0.295274	-0.637404
H	0.887243	2.166833	1.510380
H	-1.604791	1.423383	2.197137
H	-3.135293	1.422239	-0.027037
H	-1.603115	2.139776	-2.118744
H	0.920378	2.529752	-1.173548
H	-0.601018	-1.383247	2.369869
H	0.900630	-2.641307	0.509488
H	-0.427963	-2.625310	-1.814015
H	-2.802478	-1.386372	-1.442406
H	-2.906980	-0.623699	1.161413
H	3.902489	-1.094820	-1.386019
H	4.089516	0.654361	-1.177911
H	4.841833	-0.460097	0.007944
O	2.696901	-0.307451	1.414798

I5-OH1

C	-2.005358	1.941836	0.420629
C	-2.076838	1.461325	-0.934103
C	-0.806375	1.679484	-1.570102
C	0.020835	2.340339	-0.613653
C	-0.708300	2.501936	0.587261
Mo	-0.574932	0.129542	0.122128
C	-1.681439	-1.507794	-1.257479
C	-2.489958	-1.240012	-0.097712
C	-1.763213	-1.610107	1.058836
C	-0.477645	-2.083263	0.611430
C	-0.459177	-2.048975	-0.821925
C	2.577588	-0.263994	0.309853
O	2.594456	-0.371339	1.564333
C	3.871739	-0.366586	-0.463035
O	0.257685	0.338478	2.127593
H	0.328188	-2.434676	1.246288
H	0.379424	-2.316792	-1.454661
H	-1.958874	-1.298186	-2.285344
H	-3.491998	-0.826114	-0.106575
H	-2.117146	-1.559098	2.082725
H	1.062016	2.608595	-0.755716
H	-0.308363	2.903191	1.512046
H	-2.806062	1.939444	1.151856
H	-2.957237	1.055209	-1.415866
H	-0.549041	1.451894	-2.598400
H	4.574011	-1.023529	0.061067
H	-0.215796	-0.097379	2.847773
H	1.220248	-0.006973	2.080416
H	3.695491	-0.723640	-1.482827
H	4.317406	0.637418	-0.519380
O	1.521843	-0.044611	-0.394320

TS4-OH1

C	-1.961627	1.565314	-1.041248
C	-0.630835	2.033562	-1.009732
C	-0.293172	2.252304	0.374239
C	-1.440009	1.949737	1.173891
C	-2.457270	1.500400	0.304685
Mo	-0.582874	0.003846	0.153139
C	-0.768828	-2.356102	0.665035
C	-0.196604	-2.258001	-0.623551
C	-1.111270	-1.583595	-1.487360
C	-2.268055	-1.279161	-0.703773
C	-2.043137	-1.723353	0.650545
O	0.451727	-0.117913	1.919216
C	2.601447	-0.357560	-0.137451
C	3.913125	0.210472	-0.558285
O	2.636344	-1.554735	0.493325
H	0.796420	-2.595552	-0.896010
H	-0.975895	-1.393666	-2.546286
H	-3.182926	-0.832622	-1.072250
H	-2.748880	-1.672654	1.472415
H	-0.274113	-2.759571	1.540938
H	0.014993	2.193893	-1.865576
H	0.666171	2.592122	0.747138
H	-1.501370	2.001737	2.255076
H	-3.439365	1.147291	0.601404
H	-2.507761	1.270400	-1.930278
H	4.401916	-0.505275	-1.234332
H	2.762292	-1.449537	1.451591
H	-0.152469	-0.179858	2.669037
O	1.533398	0.179688	-0.427739
H	3.782290	1.175847	-1.053118
H	4.557550	0.309590	0.326103

I6-OH1

C	-1.820415	1.573238	-1.013408
C	-0.482832	2.036166	-1.111563
C	-0.073506	2.387230	0.224304
C	-1.168322	2.175327	1.108636
C	-2.237464	1.640829	0.362963
Mo	-0.405561	0.101472	0.148201
C	-0.461326	-2.244000	0.545375
C	0.030445	-2.105096	-0.776625
C	-0.954113	-1.456997	-1.565929
C	-2.079672	-1.213642	-0.714319
C	-1.772777	-1.683546	0.610365
O	0.459107	0.014994	2.001095
C	2.819120	-0.294947	-0.047125
C	4.135443	0.278352	-0.467979
O	2.809605	-1.463562	0.583536
H	1.020793	-2.390029	-1.113941
H	-0.874010	-1.209578	-2.618776
H	-3.029869	-0.796243	-1.023561
H	-2.440925	-1.694335	1.464301
H	0.096324	-2.647594	1.381840

H	0.100656	2.143597	-2.018745
H	0.910082	2.738229	0.515548
H	-1.149840	2.307319	2.184675
H	-3.201530	1.331723	0.753289
H	-2.429848	1.232929	-1.841909
H	4.647403	-0.433993	-1.129374
H	3.711310	-1.809045	0.692178
H	-0.212433	-0.059355	2.690082
O	1.751041	0.276707	-0.289162
H	3.982736	1.228536	-0.984255
H	4.766843	0.426548	0.418911

TS5-OH1

C	2.143441	-1.107801	-1.048537
C	0.880749	-1.725032	-1.297443
C	0.495036	-2.373390	-0.078937
C	1.493342	-2.149205	0.897614
C	2.501234	-1.325847	0.332255
Mo	0.576363	-0.006155	0.226845
C	0.076466	2.188962	0.556485
C	-0.186649	1.987471	-0.844254
C	1.031441	1.667691	-1.466653
C	2.057536	1.671672	-0.463641
C	1.479768	2.022917	0.791156
O	-0.241648	-0.238571	2.025004
C	-3.189605	-0.220984	-0.150294
C	-4.491333	-0.838790	-0.574998
O	-3.249377	0.961549	0.489313
H	-1.158703	2.027008	-1.323579
H	1.165500	1.403730	-2.510556
H	3.108756	1.469387	-0.635457
H	2.008428	2.168200	1.726705
H	-0.668839	2.436104	1.303680
H	0.352132	-1.762223	-2.243150
H	-0.442786	-2.893124	0.088777
H	1.441415	-2.458717	1.935612
H	3.406331	-0.987077	0.824583
H	2.745541	-0.582420	-1.779618
H	-5.025281	-0.152105	-1.246104
H	-4.168964	1.258027	0.586041
H	-0.035034	0.416186	2.703816
O	-2.095039	-0.727425	-0.351805
H	-4.303423	-1.787620	-1.083213
H	-5.123887	-1.004471	0.308018

TS1-W1

C	-2.532754	-1.157994	1.184134
C	-1.676553	-2.006407	0.399148
C	-1.967129	-1.779302	-0.988683
C	-2.946040	-0.766802	-1.053787
C	-3.298727	-0.387234	0.286437
Mo	-0.965605	0.108664	-0.012850
C	-2.008545	1.998099	-0.727669
C	-0.982711	1.734486	-1.700293
C	0.263496	1.934366	-1.050593
C	0.023720	2.264792	0.303581
C	-1.385756	2.302874	0.530849
O	0.180837	-0.156675	1.777784
C	1.993301	-1.034779	-0.389642
C	4.038969	0.195584	0.123206
H	-1.488626	-2.261334	-1.833488
H	-3.348058	-0.327427	-1.960878
H	-4.015595	0.378961	0.561102
H	-2.578117	-1.107937	2.266654
H	-0.951432	-2.710707	0.789511
H	1.239546	1.769761	-1.490010
H	0.788371	2.396975	1.059687
H	-1.885416	2.587398	1.450062
H	-3.072193	2.018205	-0.928632
H	-1.132952	1.486421	-2.745099
H	4.547926	-0.111297	-0.798720
H	-0.335404	-0.239801	2.587549
O	1.806108	-1.829233	1.241468
H	0.977647	-1.005781	1.652276
H	2.626345	-1.748342	1.749765
O	0.765367	-0.908850	-0.777339
C	4.395904	1.622126	0.493078
H	3.890471	1.927284	1.418421
H	5.480362	1.691596	0.650687
H	4.118300	2.315774	-0.311409
H	4.314057	-0.498478	0.928492
O	2.604086	0.147512	-0.087947
C	2.803461	-2.087952	-1.114807
H	3.082176	-1.693811	-2.101888
H	3.712060	-2.358949	-0.569967
H	2.182048	-2.977552	-1.247318

I2-W1

C	-2.521247	-1.104136	1.232179
C	-1.635445	-1.986422	0.515159
C	-1.909148	-1.855649	-0.885310
C	-2.899977	-0.865657	-1.035123
C	-3.285258	-0.409208	0.272722
Mo	-0.959134	0.119638	-0.004267
C	-2.044093	1.971417	-0.757581
C	-1.012351	1.703769	-1.727530
C	0.229680	1.952317	-1.089081
C	-0.014682	2.306623	0.257456
C	-1.426154	2.323943	0.487360
O	0.192367	-0.022078	1.864846
C	1.977693	-1.091556	-0.320193
C	4.040899	0.138615	0.245486
H	-1.396707	-2.371134	-1.688998
H	-3.292110	-0.491750	-1.975363
H	-4.025086	0.354359	0.485740
H	-2.595348	-0.991286	2.308575
H	-0.907068	-2.654120	0.960023
H	1.208675	1.791842	-1.522807
H	0.748785	2.475440	1.008012
H	-1.928873	2.619075	1.401546
H	-3.107642	1.963624	-0.959553
H	-1.160321	1.425325	-2.765063
H	4.624741	-0.221200	-0.613688
H	-0.323084	-0.180935	2.665975
O	1.824729	-1.784306	0.978891
H	0.876748	-0.746889	1.771795
H	2.694304	-1.995531	1.348928
O	0.744206	-0.839195	-0.805238
C	4.449037	1.557024	0.605211
H	3.888753	1.917634	1.478067
H	5.520456	1.580853	0.845774
H	4.269249	2.238552	-0.237306
H	4.228990	-0.536318	1.095192
O	2.640315	0.151590	-0.084055
C	2.752486	-2.009649	-1.269739
H	2.944814	-1.481243	-2.211307
H	3.707945	-2.333316	-0.840752
H	2.141800	-2.895829	-1.473114

TS2-W1

C	-2.284735	2.180246	0.046517
C	-1.890383	1.890045	-1.306008
C	-0.482381	1.853154	-1.362164
C	0.007542	2.084232	-0.029882
C	-1.121156	2.321170	0.829928
Mo	-1.082569	0.111150	0.079662
C	-3.190352	-0.573964	-0.399748
C	-2.962205	-0.900945	0.981708
C	-1.978963	-1.933069	1.000595
C	-1.582107	-2.212657	-0.327884
C	-2.308688	-1.366441	-1.214500
O	0.070277	-0.067461	1.926027
O	1.898992	-1.644862	0.955663
C	1.806742	-1.251853	-0.358687
C	2.659891	-1.984175	-1.350335
O	0.767113	-0.675704	-0.773437
O	3.252921	0.138466	0.316989
C	4.462335	0.391895	-0.348997
C	5.274342	1.497826	0.333688
H	-0.801280	-2.908376	-0.615250
H	-2.253556	-1.368078	-2.297176
H	-3.940143	0.115154	-0.768452
H	-3.486899	-0.494183	1.838829
H	-1.550224	-2.385031	1.889329
H	1.049927	2.098033	0.268277
H	-1.088095	2.531348	1.893151
H	-3.305581	2.251889	0.406397
H	-2.565169	1.705521	-2.135214
H	0.117805	1.642371	-2.239937
H	4.267832	0.697456	-1.397965
H	-0.418712	-0.257586	2.737768
H	0.771492	-0.761274	1.795830
H	2.752343	-1.108261	1.149738
H	5.519922	1.215070	1.368394
H	6.216817	1.677378	-0.206409
H	4.705969	2.439559	0.359408
H	5.094611	-0.518637	-0.406427
H	2.825836	-1.368092	-2.239811
H	3.613014	-2.285348	-0.909984
H	2.105094	-2.886301	-1.650112

TS1-W2

C	1.604707	1.437469	-1.658622
C	2.788839	1.042662	-0.954149
C	2.713128	1.536556	0.396755
C	1.505658	2.287052	0.486581
C	0.833763	2.222235	-0.756375
Mo	1.066341	-0.049881	0.067688
C	0.647273	-2.261678	0.409042
C	1.934317	-2.021560	0.994483
C	2.814865	-1.688891	-0.056010
C	2.090254	-1.747378	-1.295180
C	0.758301	-2.112351	-1.017523
O	0.242340	0.180236	1.976460
O	-1.162394	0.025115	-0.335585
C	-2.202467	0.616726	0.427963
O	-2.123420	-0.459581	1.514427
O	-3.420558	0.531736	-0.193110
C	-3.773420	-0.694009	-0.895398
C	-5.205308	-0.541404	-1.369004
C	-2.054148	2.010098	0.988342
H	-0.137773	2.649555	-0.973443
H	1.370875	1.234559	-2.697647
H	3.627912	0.510299	-1.383648
H	3.470540	1.436910	1.166302
H	1.126057	2.761448	1.384056
H	-0.037828	-2.235222	-1.743146
H	-0.241773	-2.562056	0.951546
H	2.182617	-2.067776	2.048811
H	3.859170	-1.417899	0.055322
H	2.494147	-1.515338	-2.274838
H	0.867556	0.046607	2.697115
H	-2.901887	2.205434	1.653826
H	-1.123401	2.109917	1.545898
H	-2.086337	2.731597	0.165062
H	-3.674260	-1.543397	-0.208300
H	-3.086084	-0.830187	-1.737604
H	-5.500434	-1.446189	-1.917210
H	-5.890169	-0.411210	-0.520727
H	-5.305547	0.319421	-2.043482
H	-1.482204	-0.849970	0.551475
H	-1.252609	-0.207879	2.013230

I2-W2

C	1.578711	1.560928	-1.575550
C	2.734686	0.960421	-0.978925
C	2.785962	1.332585	0.412774
C	1.692560	2.215356	0.639245
C	0.957920	2.348087	-0.559659
Mo	0.938701	-0.009800	0.027518
C	0.214732	-2.153577	0.200455
C	1.505213	-2.149952	0.820252
C	2.455340	-1.858262	-0.182240
C	1.765175	-1.725873	-1.435086
C	0.386232	-1.913837	-1.210223
O	0.190806	0.213350	1.947189
O	-1.246530	0.353604	-0.318340
C	-2.430206	0.659612	0.569883
O	-2.299077	-0.166590	1.657173
O	-3.569782	0.375161	-0.159129
C	-3.857816	-1.023105	-0.432020
C	-5.002400	-1.064473	-1.426273
C	-2.429660	2.144327	0.897260
H	0.032428	2.902599	-0.670016
H	1.275934	1.493693	-2.614471
H	3.478919	0.369458	-1.497581
H	3.557187	1.063218	1.125855
H	1.412864	2.642020	1.595597
H	-0.398189	-1.873260	-1.957271
H	-0.730835	-2.311679	0.704618
H	1.713685	-2.296118	1.874230
H	3.522617	-1.735156	-0.030831
H	2.225031	-1.485848	-2.387441
H	0.817053	-0.010554	2.644340
H	-3.294505	2.362612	1.534130
H	-1.511560	2.400913	1.434400

H	-2.497658	2.741621	-0.019545
H	-4.129732	-1.519012	0.507277
H	-2.958929	-1.502222	-0.838986
H	-5.261351	-2.110964	-1.636816
H	-5.892347	-0.564147	-1.021338
H	-4.722751	-0.579922	-2.371369
H	-1.429465	0.717577	-1.196702
H	-1.344794	-0.071501	1.975055

TS2-W2

C	0.347126	-1.327246	-2.063750
C	-0.003316	-2.045130	-0.867885
C	1.204905	-2.374247	-0.166755
C	2.277128	-1.822516	-0.902937
C	1.747938	-1.181282	-2.073734
Mo	0.835942	-0.070238	-0.132793
C	1.078982	2.297836	0.285918
C	1.832348	1.897353	-0.857184
C	2.829519	0.978345	-0.388086
C	2.650834	0.781098	1.028207
C	1.577014	1.626355	1.425622
O	-0.265729	-0.553140	1.584313
O	-2.021526	1.167929	1.480451
C	-2.196346	1.252431	0.173015
C	-2.785254	2.552941	-0.305910
O	-1.179825	0.713155	-0.647228
O	-3.224803	0.089536	-0.421298
C	-3.737553	-0.893276	0.511778
C	-4.580301	-1.900913	-0.250217
H	0.229238	2.970203	0.277283
H	1.719336	2.272319	-1.868063
H	3.620529	0.547519	-0.988859
H	3.263556	0.167297	1.679094
H	1.154313	1.686237	2.422499
H	-0.340907	-0.937176	-2.805687
H	-1.007115	-2.310232	-0.556516
H	1.282358	-2.923189	0.764660
H	3.324296	-1.860240	-0.621940
H	2.325912	-0.639212	-2.814716
H	0.281814	-0.757282	2.351069
H	-3.694760	2.775325	0.263336
H	-2.055945	3.354864	-0.135712
H	-3.019512	2.497203	-1.373029
H	-4.336910	-0.349122	1.252036
H	-2.900050	-1.382466	1.024444
H	-4.982995	-2.639849	0.455976
H	-5.421283	-1.408906	-0.756188
H	-3.975880	-2.431913	-0.997704
H	-2.102652	-0.062229	-0.897081
H	-1.300145	0.426199	1.670958

TS1-OH2

C	-0.413161	2.407268	-0.377294
C	0.031391	2.098486	0.927362
C	-1.048688	1.522316	1.661556
C	-2.181418	1.510409	0.782541
Mo	-0.703468	0.023059	-0.100070
C	-2.821358	-1.049656	-0.454724
C	-2.391745	-1.410669	0.871262
C	-1.181731	-2.121609	0.766128
C	-0.844178	-2.184952	-0.630365
C	-1.881055	-1.549936	-1.386275
O	0.361719	0.130393	-1.877065
H	1.048703	2.214763	1.285731
H	-1.030441	1.211301	2.699931
H	-3.187383	1.215040	1.052606
H	-2.415349	2.181973	-1.365275
H	0.212205	2.796749	-1.172642
H	-0.595214	-2.512302	1.589505
H	0.043512	-2.649152	-1.044001
H	-1.920994	-1.435555	-2.463084
H	-3.709989	-0.477257	-0.698416
H	-2.895418	-1.144946	1.794492
H	-0.112083	0.626621	-2.556041
O	1.243797	-0.583236	0.717098
C	2.821898	-1.132079	2.393769
C	2.410144	-0.309971	1.185100
O	3.177641	0.605612	0.783115
C	2.774986	0.710051	-1.633470
H	3.148343	1.618097	-2.115637
H	1.983879	0.821316	-0.928860
C	3.378320	-0.552369	-2.019202
H	3.232118	-0.667714	-3.109614
H	4.474463	-0.466520	-1.916797
H	2.988323	-1.419443	-1.483244
H	2.185908	-2.012582	2.532989
C	-1.779181	2.030595	-0.500290
H	2.707392	-0.480577	3.273856
H	3.877084	-1.417736	2.325688

I2-OH2

C	0.332273	1.921740	1.244436
C	-0.380073	2.394316	0.113286
C	0.491433	2.396977	-1.001228
C	1.786644	1.978762	-0.529966
Mo	0.451062	0.148444	-0.313689
C	2.407580	-0.685156	-1.444582
C	1.461216	-0.283723	-2.450661
C	0.305541	-1.080202	-2.316625
C	0.507140	-1.946042	-1.191614
C	1.831001	-1.714886	-0.675704
O	0.184163	-0.983391	1.569865
H	-1.439226	2.616586	0.095220
H	0.242918	2.702490	-2.011606
H	2.691311	1.960961	-1.124715
H	2.502592	1.370376	1.521767
H	-0.095015	1.750148	2.226506
H	-0.594433	-1.004970	-2.915639
H	-0.206646	-2.665474	-0.806944
H	2.293284	-2.221309	0.163915
H	3.391593	-0.256514	-1.291383
H	1.609431	0.510319	-3.175052
H	0.914826	-0.830997	2.184609
O	-1.642384	-0.192597	-0.474104
C	-3.972665	-0.551782	-0.486586
C	-2.760656	0.165436	0.085236
O	-2.880829	0.992485	1.002489
C	-1.004158	-1.387357	2.325075
H	-1.483952	-0.484660	2.717101
H	-1.662050	-1.858435	1.591679
C	-0.616739	-2.351191	3.428351
H	0.069916	-1.879577	4.145340
H	-1.524480	-2.644325	3.973055
H	-0.146868	-3.255653	3.021146
H	-4.897514	-0.101362	-0.112891
C	1.691047	1.663628	0.865198
H	-3.938194	-1.607653	-0.182183
H	-3.955298	-0.521881	-1.583226

TS2-OH2

C	0.721803	-1.327438	1.994076
C	-0.089181	-0.201340	2.310785
C	0.674709	0.977819	2.133400
C	1.990609	0.617148	1.712252
C	2.023912	-0.822891	1.663141
Mo	0.657766	-0.110830	0.003443
O	-2.089455	-1.291052	-0.282445
C	-3.452547	-0.981729	0.085592
C	-4.388126	-2.154546	-0.167087
C	1.863242	-1.905633	-1.029331
C	2.641998	-0.703891	-1.166893
C	1.907145	0.219599	-1.942124
C	0.642898	-0.384068	-2.241356
C	0.635426	-1.720319	-1.694236
O	0.066041	1.842186	-0.525774
C	-1.055645	2.448654	-0.232016
O	-1.930020	1.992048	0.515797
C	-1.190937	3.810884	-0.884270
H	0.300374	1.988733	2.244284
H	2.825639	1.290469	1.554807
H	2.900842	-1.425167	1.461686
H	0.429679	-2.369745	2.053796
H	-1.148285	-0.232310	2.547364
H	2.221078	1.222831	-2.206665
H	-0.167570	0.078685	-2.794200
H	-0.172478	-2.439445	-1.762777
H	2.157576	-2.787947	-0.470950
H	3.626426	-0.534795	-0.743682
H	-1.784443	-2.025493	0.269010
H	-3.489820	-0.671986	1.140784
H	-3.728588	-0.119913	-0.532999
H	-4.105206	-3.022229	0.447088
H	-5.417353	-1.870787	0.097571
H	-4.370180	-2.449858	-1.225592
H	-2.181804	4.231956	-0.688448
H	-1.024995	3.728786	-1.966219
H	-0.421431	4.484117	-0.481689

TS1-W3

C	-1.318770	-1.004175	-1.933716
C	-2.535116	-0.651436	-1.261364
C	-2.625222	-1.402992	-0.035652
C	-1.478084	-2.251007	0.003263
C	-0.690011	-2.006156	-1.144640
Mo	-0.870142	0.074807	0.115085
C	-0.217431	2.152969	0.820810
C	-1.519383	1.992292	1.383715
C	-2.440418	1.896284	0.322063
C	-1.715751	2.047599	-0.909935
C	-0.343104	2.215189	-0.613469
O	-0.358118	-0.571227	1.990870
O	1.309598	-0.169377	-0.083424
C	2.238585	-0.727614	0.548327
O	2.796207	0.223257	1.788962
O	3.651209	-0.460330	-0.084859
C	3.706198	0.308746	-1.328920
C	5.164793	0.505859	-1.690945
C	2.216256	-2.158990	1.010921
H	0.274195	-2.455442	-1.354336
H	-0.968591	-0.618152	-2.884593
H	-3.293523	0.023721	-1.636607
H	-3.450573	-1.400315	0.667725
H	-1.209611	-2.914246	0.817015
H	0.457026	2.372925	-1.327248
H	0.708752	2.213391	1.379831
H	-1.750375	1.882126	2.437298
H	-3.506999	1.719199	0.414242
H	-2.148424	2.023311	-1.903390
H	-1.144553	-0.647069	2.544690
H	3.141962	-2.422516	1.530554
H	1.352720	-2.298139	1.667033
H	2.111536	-2.798945	0.126547
H	3.190848	1.263239	-1.178819
H	3.172109	-0.278443	-2.082837
H	5.219716	1.075195	-2.628628
H	5.690764	1.073711	-0.912211
H	5.671009	-0.456740	-1.837875
H	3.716645	0.141438	0.950272
H	2.966138	-0.305454	2.585788

TS1-OH3

C	0.879141	1.978446	1.377630
C	-0.120680	2.223857	0.408769
C	0.456219	2.120630	-0.884320
C	1.860134	1.860749	-0.695446
Mo	0.805236	0.002566	0.053363
C	2.644265	-0.966185	-1.163986
C	1.614035	-0.565000	-2.091068
C	0.442537	-1.306240	-1.815780
C	0.744159	-2.153380	-0.692149
C	2.112517	-1.965489	-0.326350
O	1.062210	-0.862010	2.042565
H	-1.175580	2.364262	0.618056
H	-0.050257	2.255131	-1.833582
H	2.607911	1.818177	-1.476933
H	3.091498	1.600338	1.180680
H	0.711481	1.946408	2.449106
H	-0.498371	-1.241198	-2.348926
H	0.057613	-2.846681	-0.217991
H	2.624034	-2.442548	0.501105
H	3.649129	-0.560783	-1.109646
H	1.723183	0.178932	-2.871964
H	1.515017	-0.247863	2.635683
O	-1.481494	-0.260924	0.110481
C	-0.863608	-1.094985	2.594404
C	-2.383079	-0.639277	0.911866
O	-3.634356	-0.712257	0.437417
C	-3.941054	-0.346990	-0.962315
H	-4.819591	-0.955197	-1.200579
H	-3.100420	-0.651203	-1.592380
C	-4.238874	1.137073	-1.078157
H	-4.499998	1.372968	-2.119490
H	-5.087142	1.416044	-0.439290
H	-3.366297	1.739629	-0.795035
H	-0.799746	-1.839517	1.828993
H	-1.029913	-1.458268	3.614097

H	-0.929080	-0.035168	2.450081
C	2.125245	1.743507	0.710746

I2-OH3

C	0.485403	2.419871	0.463870
C	-0.298320	2.093388	-0.667531
C	0.556284	1.572924	-1.684907
C	1.893819	1.610443	-1.156873
Mo	0.741202	0.036441	0.022104
C	2.892854	-0.931516	-0.244315
C	2.122724	-1.330198	-1.391839
C	1.028880	-2.092687	-0.942994
C	1.089616	-2.143798	0.489551
C	2.274584	-1.447325	0.917192
O	0.088270	0.039110	2.150781
H	-1.379065	2.155954	-0.720751
H	0.264766	1.280689	-2.687323
H	2.794155	1.359026	-1.703352
H	2.688465	2.264941	0.852054
H	0.100429	2.781782	1.412058
H	0.243154	-2.510646	-1.561833
H	0.366155	-2.633724	1.130362
H	2.625074	-1.330653	1.936644
H	3.791657	-0.324760	-0.267427
H	2.334269	-1.062073	-2.421658
H	0.743015	0.494150	2.696028
O	-1.301053	-0.469385	-0.279944
C	-1.238125	0.258461	2.710584
C	-1.975492	-1.531055	-0.051316
O	-3.268710	-1.422442	-0.477469
C	-3.769415	-0.212652	-1.147599
H	-4.574076	-0.582907	-1.792693
H	-2.972780	0.205468	-1.770777
C	-4.297014	0.806333	-0.150170
H	-4.726532	1.659417	-0.694655
H	-5.085901	0.367593	0.475180
H	-3.497271	1.179945	0.500795
H	-1.850671	-0.603972	2.443464
H	-1.134898	0.327064	3.797514
H	-1.673124	1.178385	2.305992
C	1.844977	2.108738	0.188856

TS2-OH3

C	0.774929	2.322988	-0.182122
C	-0.002909	1.796676	-1.240141
C	0.842026	1.020968	-2.092081
C	2.163537	1.097184	-1.537002
Mo	0.882525	-0.103758	-0.086784
C	2.977322	-1.189152	-0.046408
C	2.219566	-1.844659	-1.078916
C	1.094836	-2.440448	-0.481569
C	1.119758	-2.129028	0.917006
C	2.317059	-1.377984	1.190807
O	0.165182	0.442238	1.950540
H	-1.075338	1.913395	-1.348394
H	0.555332	0.532303	-3.016249
H	3.057739	0.682041	-1.984936
H	2.952271	2.126155	0.313400
H	0.394088	2.910947	0.646451
H	0.315286	-2.984977	-1.000320
H	0.370261	-2.425919	1.641129
H	2.652618	-1.022464	2.158667
H	3.902046	-0.642331	-0.191991
H	2.462100	-1.852965	-2.136256
H	0.875558	0.901613	2.416922
O	-1.210838	-0.612845	-0.418409
C	-1.116215	0.949326	2.419857
C	-2.089720	-1.584223	0.299840
O	-3.246161	-1.007992	0.553890
C	-3.763312	0.178498	-0.161852
H	-3.740340	-0.046995	-1.232145
H	-3.098967	1.021228	0.048988
C	-5.170134	0.421943	0.341300
H	-5.585328	1.302739	-0.167491
H	-5.820358	-0.437186	0.130605
H	-5.174456	0.614931	1.422408
H	-1.848204	0.150817	2.298091
H	-1.008824	1.200574	3.479215
H	-1.409051	1.835016	1.846212
C	2.115239	1.876976	-0.329259
O	-2.362344	-2.246832	-1.618362
H	-1.386934	-1.103847	-1.305595
H	-1.917479	-3.104164	-1.594788

I3-OH3

C	-3.426694	1.022169	-0.155280
C	-3.707614	-0.328326	-0.458187
C	-3.021843	-0.680166	-1.669518
C	-2.333159	0.460258	-2.135020
C	-2.549964	1.510829	-1.190249
Mo	-1.363146	-0.054075	-0.040469
C	-1.797755	-2.199461	0.593128
C	-1.580690	-1.466116	1.803246
C	-0.199895	-1.096969	1.812971
C	0.413518	-1.574094	0.633154
C	-0.566473	-2.234389	-0.157675
O	0.276938	0.810486	-0.893494
O	-0.945247	1.705011	1.268955
C	0.281951	2.453980	1.477795
H	1.438077	-1.379037	0.337362
H	-0.400152	-2.742023	-1.101444
H	-2.716886	-2.694921	0.307790
H	-2.301097	-1.287404	2.593833
H	0.286670	-0.494077	2.573264
H	-1.703615	0.509224	-3.016512
H	-2.122589	2.505611	-1.241489
H	-3.807369	1.585121	0.689664
H	-4.316025	-0.996267	0.141377
H	-3.018707	-1.661153	-2.133617
H	-1.419987	1.628352	2.106517
H	0.558704	0.326530	-1.679292
H	0.652241	2.741701	0.494196
H	1.024447	1.834886	1.995288
H	0.039986	3.340687	2.073245

TS3-OH3

O	0.977404	-0.253930	1.769899
O	2.276348	-1.032016	-0.808193
Mo	-0.147311	0.029069	0.160127
H	4.327507	-1.417472	-0.667883
H	0.645007	2.505470	1.857407
H	-1.940106	2.304985	1.119815
H	-1.980090	1.714692	-1.535056
H	0.572789	1.514622	-2.401703
H	2.181831	1.984143	-0.268117
H	-2.353933	-1.062287	1.887733
H	-0.262529	-2.707377	1.297169
H	0.139501	-2.649289	-1.365118
H	-1.609953	-0.919286	-2.439092
H	-3.132314	0.073076	-0.435537
H	2.368641	-0.556571	-1.644882
H	0.643110	-0.832537	2.466644
H	3.384824	-1.479507	0.851619
H	3.786295	0.101807	0.121724
C	-1.075975	2.144468	0.484384
C	-1.094224	1.825456	-0.922533
C	0.251920	1.714812	-1.385661
C	1.096845	2.023579	-0.270978
C	0.285057	2.306517	0.853977
C	-0.829802	-2.110782	0.591204
C	-0.627120	-2.102283	-0.829296
C	-1.540711	-1.192805	-1.391259
C	-2.323714	-0.639411	-0.322941
C	-1.905412	-1.220842	0.913548
C	3.521221	-0.942963	-0.091907

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C	2.771176	1.652402	1.098773
C	1.550739	2.334745	0.852278
C	1.329711	2.380053	-0.541767
C	2.427384	1.750655	-1.210501
C	3.334264	1.325273	-0.187205
Mo	1.458316	0.039924	0.025272
C	3.135637	-1.562444	0.668733
C	3.131683	-1.481748	-0.764269
C	1.860116	-1.876041	-1.236315
C	1.065323	-2.199468	-0.077865
C	1.873252	-2.031809	1.089345
O	-0.120084	0.096272	1.323942
O	-0.360413	0.167970	-1.189521
H	0.437434	2.767109	-1.021729
H	2.578317	1.684660	-2.282192
H	4.308046	0.879460	-0.345214
H	3.228876	1.477586	2.066291
H	0.851449	2.671667	1.609330
H	1.550724	-1.941291	-2.273820
H	0.030479	-2.519600	-0.090670
H	1.556429	-2.177683	2.115923
H	3.962185	-1.287136	1.315664
H	3.958307	-1.147758	-1.380865
H	0.171676	0.105253	2.243287
H	-1.256278	0.004535	-0.801671
H	-0.351851	-0.184144	-2.088146
C	-3.766043	-0.771154	-0.097174
O	-2.984806	0.054611	-0.563263
C	-3.368395	-2.098912	0.478008
H	-2.371988	-2.374808	0.124251
H	-3.348699	-2.009628	1.573299
H	-4.100108	-2.869585	0.213041
O	-5.083278	-0.563765	-0.033605
C	-5.614526	0.715881	-0.508161
H	-6.631561	0.469758	-0.828327
H	-5.026502	1.036748	-1.373258
C	-5.613878	1.752187	0.600948
H	-4.593200	1.990773	0.924862
H	-6.081098	2.672863	0.224781
H	-6.192165	1.399778	1.464933

TS1-OH1'

C	-1.269547	1.644517	-1.465544
C	-0.141928	2.153118	-0.758579
C	-0.501842	2.353378	0.593275
C	-1.863469	1.973990	0.770468
C	-2.348417	1.567325	-0.521064
Mo	-0.827056	-0.001177	0.120445
C	-2.488870	-1.381468	-0.945359
C	-2.924801	-1.084166	0.391326
C	-1.988275	-1.623378	1.303281
C	-0.944731	-2.232594	0.524365
C	-1.283464	-2.102905	-0.864690
O	1.137732	-0.426377	-0.703731
O	0.487851	-0.002744	1.818984
H	0.174322	2.662223	1.382479
H	-2.441728	2.052090	1.684309
H	-3.370971	1.302351	-0.758424
H	-1.322592	1.428440	-2.526738
H	0.852662	2.287969	-1.169438
H	-2.049987	-1.580942	2.385344
H	-0.061700	-2.721540	0.918632
H	-0.689192	-2.448122	-1.703113
H	-2.985540	-1.067633	-1.857770
H	-3.820358	-0.534240	0.657786
H	1.167300	-0.391249	-1.668787
H	1.385954	-0.647769	1.574964
H	0.079476	-0.260565	2.654146
C	2.495855	-1.173220	-0.183639
O	2.333817	-1.359248	1.105796
C	2.612176	-2.425279	-1.039935
H	3.512577	-2.968238	-0.725865
H	1.738520	-3.064517	-0.881997
H	2.705474	-2.179616	-2.104476
O	3.503668	-0.292434	-0.578497
C	3.713499	0.871636	0.251407
H	4.014427	0.548275	1.255920
C	4.794764	1.714042	-0.400253
H	4.487278	2.048461	-1.400362
H	4.987314	2.602060	0.217134
H	5.731826	1.147983	-0.490477
H	2.771211	1.429297	0.332121

I1-OH1'

C	-1.209717	1.701899	-1.499711
C	-0.186016	2.241050	-0.656303
C	-0.722509	2.473482	0.629297
C	-2.077428	2.052945	0.641401
C	-2.390270	1.611138	-0.696485
Mo	-0.912027	0.091032	0.138164
C	-2.585686	-1.303255	-0.906443
C	-3.007791	-1.005247	0.433108
C	-2.060501	-1.545523	1.335093
C	-1.021343	-2.141326	0.549968
C	-1.368311	-2.005946	-0.841374
O	1.132977	-0.373440	-0.690978
O	0.341406	0.153183	1.782029
H	-0.159394	2.812819	1.491107
H	-2.767495	2.121729	1.475138

H	-3.369626	1.307661	-1.044030
H	-1.123958	1.478302	-2.557203
H	0.848939	2.394861	-0.941925
H	-2.104424	-1.493342	2.417282
H	-0.130742	-2.622508	0.936106
H	-0.785206	-2.356509	-1.685370
H	-3.094675	-0.994690	-1.813278
H	-3.899737	-0.451772	0.706848
H	1.148387	-0.294439	-1.655032
H	1.560975	-0.741183	1.482385
H	-0.116312	0.163753	2.630266
C	2.382961	-1.079181	-0.271989
O	2.263182	-1.342840	1.068223
C	2.538102	-2.353487	-1.085775
H	3.429384	-2.886294	-0.735075
H	1.658567	-2.988977	-0.944235
H	2.660627	-2.121356	-2.150256
O	3.454355	-0.242447	-0.598966
C	3.641824	0.937402	0.217825
H	3.929858	0.627796	1.230667
C	4.728146	1.776660	-0.428673
H	4.430578	2.099545	-1.435447
H	4.909637	2.671241	0.182353
H	5.667983	1.213023	-0.501892
H	2.697036	1.491985	0.277204

TS2-OH1’

C	-0.657600	1.971829	-1.255669
C	-0.062775	2.229721	0.028056
C	-1.112700	2.334313	1.000903
C	-2.330946	2.096381	0.326147
C	-2.049854	1.877331	-1.064900
Mo	-0.943227	0.146901	0.205685
C	-2.207319	-1.427772	-0.939589
C	-3.035111	-0.695833	-0.024148
C	-2.619386	-0.997683	1.322245
C	-1.573430	-1.957487	1.220827
C	-1.320877	-2.214492	-0.145931
O	0.891393	-0.470755	-0.887156
O	0.452200	-0.014554	1.761981
H	-0.995003	2.535410	2.059480
H	-3.313666	2.065565	0.784688
H	-2.781795	1.636251	-1.828509
H	-0.131107	1.838439	-2.194303
H	0.996592	2.344792	0.226411
H	-3.066725	-0.625281	2.237147
H	-1.005861	-2.365037	2.050162
H	-0.544356	-2.867278	-0.526871
H	-2.287613	-1.439142	-2.020642
H	-3.870634	-0.064223	-0.298397
H	1.826844	0.317179	-1.026164
H	1.399003	-0.993360	1.335483
H	0.051674	-0.068352	2.637241
C	1.973913	-1.285222	-0.484973
O	2.014832	-1.645822	0.785996
C	2.365787	-2.361085	-1.462962
H	3.331008	-2.789126	-1.169945
H	1.606005	-3.152424	-1.440717
H	2.433008	-1.952168	-2.475404
O	2.992533	-0.018773	-0.833978
C	3.728312	0.573233	0.264941
H	4.387464	-0.206814	0.665403
H	3.027088	0.882023	1.050106
C	4.524411	1.756044	-0.257931
H	3.857999	2.526168	-0.668868
H	5.094986	2.199370	0.569622
H	5.230086	1.442144	-1.038196

TS1-OH2’

C	-2.021864	1.281955	-1.597108
C	-0.774804	1.919676	-1.345689
C	-0.688005	2.224259	0.032137
C	-1.885302	1.795434	0.679809
C	-2.725716	1.237508	-0.341023
Mo	-0.960850	-0.171558	-0.135213
C	-2.757890	-1.732668	-0.499335
C	-2.756198	-1.375680	0.893341
C	-1.527167	-1.777238	1.458050
C	-0.745471	-2.364862	0.400730
C	-1.534030	-2.365005	-0.795455
O	0.606300	-0.593099	-1.470759
O	0.776337	0.020149	1.271578
H	0.178161	2.653030	0.524910
H	-2.136690	1.931423	1.725630
H	-3.744470	0.895984	-0.207346
H	-2.399883	0.961347	-2.561566
H	0.016142	2.072847	-2.071507
H	-1.228633	-1.659044	2.494008
H	0.262475	-2.751703	0.495512
H	-1.224551	-2.729395	-1.768219
H	-3.556326	-1.526467	-1.204540
H	-3.556888	-0.865470	1.417334
H	0.323878	-0.557036	-2.393420
H	0.458031	0.244595	2.156213
H	1.610808	0.567179	1.149994
C	2.461605	0.187247	-1.305601
O	4.009354	1.416516	-0.784558
C	3.915372	1.814545	0.427083
C	4.999828	2.748763	0.934355
H	5.448961	2.324938	1.842351
H	5.775064	2.912649	0.179235
H	4.544671	3.710790	1.207745
O	2.989673	1.493374	1.231230
C	3.146118	-1.097091	-0.953367
H	3.026311	-1.347052	0.105457
H	2.733891	-1.908645	-1.563815
H	4.214563	-1.021379	-1.186470
H	1.953579	0.822892	-0.617527
H	2.502449	0.530368	-2.334965

I1-OH2’

C	-1.712165	-2.487973	-0.304444
C	-2.771860	-1.724523	0.228317
C	-2.406958	-1.295021	1.548190
C	-1.127100	-1.811922	1.846951
C	-0.673343	-2.525947	0.692978
Mo	-0.797792	-0.355164	0.027415
C	-2.511398	1.135696	-0.177066
C	-1.898781	1.040700	-1.466569
C	-0.595392	1.621134	-1.339454
C	-0.410545	2.054436	-0.007980
C	-1.571064	1.730160	0.741579
O	1.079429	-0.204276	0.816620
O	0.519070	-1.075125	-1.624526
C	1.924838	-0.813035	-1.933014
C	2.516795	-1.964567	-2.723066
H	0.507162	2.467268	0.395560
H	-1.746183	1.954683	1.788088
H	-3.530011	0.859315	0.064318
H	-2.357551	0.679045	-2.379986
H	0.152694	1.673657	-2.123559
H	-0.572525	-1.652561	2.764881
H	0.289106	-3.012864	0.586638
H	-1.686407	-2.955586	-1.282580
H	-3.692797	-1.474512	-0.286665
H	-3.007067	-0.663662	2.195429
H	0.021647	-1.154010	-2.449935
H	1.054514	0.121259	1.724687
H	2.474364	-2.899966	-2.149917
H	1.992069	-2.105370	-3.678425
H	3.569428	-1.738558	-2.943492
H	2.404851	-0.686934	-0.962537
H	1.981775	0.131650	-2.489275

TS2-OH2’

C	-1.610680	-2.498187	-0.014374
C	-2.771443	-1.752847	0.265928
C	-2.623643	-1.148808	1.558039
C	-1.379970	-1.552782	2.110274
C	-0.733106	-2.363717	1.124076
Mo	-0.859527	-0.283231	0.239797
C	-2.584067	1.141499	-0.259032
C	-1.827435	0.974125	-1.460139
C	-0.555512	1.590093	-1.232472
C	-0.525855	2.110344	0.082436
C	-1.757140	1.803419	0.722277
O	1.011897	-0.080299	0.880655
O	0.690236	-1.470074	-1.795098
C	2.085641	-1.151809	-2.000449
C	2.632648	-1.789653	-3.267961
H	0.333446	2.569892	0.558128
H	-2.054199	2.096281	1.723414
H	-3.615727	0.846760	-0.112476
H	-2.172837	0.533857	-2.388872
H	0.275850	1.599442	-1.930981
H	-0.993862	-1.284191	3.087567
H	0.249829	-2.812978	1.215255
H	-1.412227	-3.063209	-0.917648
H	-3.611649	-1.611209	-0.405647
H	-3.346074	-0.495587	2.035702
H	0.188877	-1.146190	-2.556763
H	1.233789	-0.461635	1.739492
H	2.527497	-2.882710	-3.236900
H	2.109178	-1.408354	-4.156668
H	3.699662	-1.545383	-3.370703
H	2.600057	-1.535309	-1.112665
H	2.215152	-0.060120	-2.025032

TS1-OH3’

C	-1.708556	1.752405	-1.609787
C	-0.365590	2.049376	-1.238733
C	-0.331832	2.366378	0.138022
C	-1.655521	2.281646	0.666013
C	-2.514017	1.937137	-0.431165
Mo	-1.218274	0.116865	-0.045363
C	-3.347352	-0.842835	-0.563648
C	-3.345637	-0.565959	0.847119
C	-2.322708	-1.326247	1.446482
C	-1.658693	-2.058452	0.402587
C	-2.326267	-1.777048	-0.838185
O	0.311470	-0.765564	-1.245646
O	0.320279	-0.094910	1.571175
H	0.566303	2.566964	0.712698
H	-1.960761	2.511455	1.680679
H	-3.594546	1.879899	-0.392045
H	-2.064407	1.513424	-2.605815
H	0.501487	1.974450	-1.886288
H	-2.060622	-1.326788	2.498934
H	-0.812042	-2.722716	0.533145
H	-2.071070	-2.178019	-1.812130
H	-4.009547	-0.392404	-1.295576
H	-4.000267	0.132703	1.356993
H	0.244981	-0.536065	-2.182272
H	0.009488	0.297426	2.397688
H	1.314587	0.047039	1.554631
C	2.044194	-0.645715	-0.687040
H	1.862422	-1.371576	0.086507
H	1.986055	0.412035	-0.497207
O	3.009844	0.151595	1.789295
O	5.036528	-0.274030	1.083343
C	5.890047	-0.694897	-0.011695
H	6.638047	-1.362855	0.433074
H	5.282068	-1.266003	-0.724587
C	6.550001	0.500167	-0.678989
H	7.131519	1.084893	0.046847
H	7.232921	0.150058	-1.466321
H	5.797687	1.156029	-1.138354
H	2.562203	-0.979712	-1.580880
C	3.690008	-0.244549	0.816903

I2-OH1-2WAT

Mo	-1.132089	0.170263	-0.030523
O	0.378208	-0.183819	-1.422393
O	0.703828	-0.697019	0.659140
O	2.465883	0.178100	-0.453101
O	1.935422	-1.704984	2.697266
C	-2.877246	-0.740960	-1.269214
C	-3.331751	-0.449027	0.065026
C	-2.636817	-1.298462	0.986761
C	-1.798874	-2.149037	0.206228
C	-1.951320	-1.815793	-1.159253
C	-0.046389	2.141729	0.288506
C	-0.744459	1.892660	1.520222
C	-2.125755	1.961892	1.240610
C	-2.292125	2.260779	-0.151600
C	-1.012694	2.391026	-0.740766
C	1.351600	-0.721758	-0.621911
C	1.793340	-2.122698	-1.023215
C	3.225826	0.474108	-1.651459
C	4.010083	1.751793	-1.413465
H	-1.387748	-2.247677	-1.978473
H	-3.235155	-0.288749	-2.187383
H	-4.101466	0.267105	0.324000
H	-2.775624	-1.339389	2.061227
H	-1.102255	-2.881141	0.600391
H	-0.805734	2.616605	-1.780729

H	1.028352	2.132372	0.157679
H	-0.296411	1.676781	2.484120
H	-2.927168	1.774269	1.947335
H	-3.241102	2.352306	-0.668981
H	1.185437	-1.081804	1.465838
H	2.196665	-2.104244	-2.041881
H	2.568043	-2.491018	-0.340323
H	0.934969	-2.800903	-1.000017
H	2.530288	0.594090	-2.491124
H	3.902405	-0.364117	-1.869633
H	4.609968	1.980065	-2.304880
H	3.334531	2.595960	-1.222700
H	4.692389	1.643225	-0.559700
H	2.849806	-1.388795	2.493000
H	2.001570	-2.668781	2.646561
O	4.182017	-0.572196	1.678281
H	3.651955	-0.227874	0.927309
H	4.539419	0.206892	2.125358

TS2-OH1-2WAT

Mo	-1.097079	0.132290	-0.072744
O	0.402241	-0.193153	-1.489834
O	0.628214	-0.847302	0.584826
O	2.489301	0.079775	-0.425789
O	1.792507	-1.474349	2.870494
C	-2.979658	-0.567963	-1.309572
C	-3.320431	-0.438230	0.080758
C	-2.583032	-1.411458	0.832426
C	-1.826127	-2.165994	-0.114465
C	-2.072587	-1.655929	-1.411240
C	0.053862	2.121697	0.169694
C	-0.337589	1.784687	1.500506
C	-1.746361	1.795218	1.559333
C	-2.234894	2.164898	0.261914
C	-1.125912	2.373874	-0.609491
C	1.267030	-0.821493	-0.637961
C	1.765860	-2.179473	-1.114349
C	3.332530	0.321954	-1.581529
C	4.153446	1.579019	-1.348023
H	-1.580059	-1.982943	-2.320540
H	-3.381113	0.015889	-2.130860
H	-4.051214	0.245966	0.492518
H	-2.655672	-1.598263	1.898050
H	-1.125423	-2.956957	0.127218
H	-1.167030	2.714359	-1.638390
H	1.073706	2.149873	-0.192665
H	0.329962	1.493551	2.305117
H	-2.353925	1.536583	2.421159
H	-3.277297	2.284300	-0.009916
H	1.247457	-1.382347	2.038450
H	2.240149	-2.098664	-2.098910
H	2.487915	-2.592155	-0.398997
H	0.912321	-2.861057	-1.196704
H	2.673851	0.440429	-2.449797
H	3.984381	-0.547558	-1.745319
H	4.781398	1.763866	-2.230247
H	3.503054	2.450512	-1.195105
H	4.814959	1.469422	-0.477598
H	2.982689	-0.720147	2.304585
H	1.957879	-2.421371	2.985415
O	3.647251	-0.188287	1.716061
H	3.146310	-0.064995	0.735949
H	3.780097	0.687231	2.117767

I3-OH1-2WAT

Mo	1.387512	-0.084626	-0.154266
O	0.285035	1.258796	-1.475643
O	-0.088281	1.308179	0.649718
O	-3.634486	-0.079378	-0.628861
O	-1.634302	0.901167	2.990106
C	3.505708	0.334527	-0.995377
C	3.604137	-0.427701	0.220008
C	3.127447	0.376556	1.312870
C	2.772934	1.640886	0.767006
C	3.001058	1.615502	-0.634213
C	-0.421354	-1.399464	-0.457091
C	0.085557	-1.755496	0.841446
C	1.355391	-2.338233	0.650843
C	1.630475	-2.378628	-0.759304
C	0.531462	-1.820949	-1.449159
C	-0.370762	1.779825	-0.512485
C	-1.393526	2.843052	-0.710447
C	-4.718867	-0.680951	-1.350320
C	-6.083448	-0.176960	-0.893575
H	2.764249	2.418606	-1.323856
H	3.812292	0.017874	-1.985701
H	4.013172	-1.426956	0.306145
H	3.094193	0.092525	2.358481
H	2.332145	2.465417	1.317208
H	0.436664	-1.710338	-2.523524
H	-1.381624	-0.931616	-0.653806
H	-0.402757	-1.574991	1.792354
H	2.027783	-2.671953	1.434023
H	2.540956	-2.754571	-1.213404
H	-1.128315	1.173358	2.197358
H	-1.331297	3.246603	-1.724757
H	-2.386024	2.399253	-0.551886
H	-1.249546	3.636186	0.032416
H	-4.668670	-1.778165	-1.257199
H	-4.555142	-0.429190	-2.406710
H	-6.877513	-0.643434	-1.494931
H	-6.261547	-0.428789	0.161751
H	-6.155856	0.913608	-1.010625
H	-2.829377	-0.293994	2.421388
H	-2.060900	1.709311	3.306888
O	-3.495600	-0.919932	2.050285
H	-3.652137	-0.402018	0.297761
H	-3.085417	-1.793505	2.125478

I5-OH1-2WAT

C	-1.049173	-2.310591	-0.698267
C	-2.296472	-1.597906	-0.736078
C	-2.605593	-1.134339	0.588444
C	-1.567745	-1.614824	1.439716
C	-0.627086	-2.327379	0.661456
Mo	-0.704537	-0.065894	-0.194770
C	0.221314	1.056806	-2.078499
C	-0.118061	1.968251	-1.029028
C	-1.550367	1.975323	-0.877936
C	-2.064914	1.032457	-1.797794
C	-0.969920	0.457693	-2.531008
O	-0.493873	0.975680	1.722575
O	1.446123	2.598209	2.395626
O	3.522914	-0.596126	0.429071
C	2.408819	-0.815083	-0.096785
O	1.352253	-0.206142	0.345314
C	2.312206	-1.820087	-1.221292
H	-3.491201	-0.588681	0.894835
H	-1.468857	-1.399243	2.497975
H	0.298091	-2.751945	1.035570
H	-0.566813	-2.809879	-1.529840
H	-2.925391	-1.486839	-1.610354
H	-2.127238	2.591798	-0.197572
H	-3.111947	0.783778	-1.926132
H	-1.050217	-0.320008	-3.283550
H	1.222469	0.827117	-2.424495
H	0.586265	2.564843	-0.460849
H	2.060734	-2.800467	-0.791743
H	0.296077	1.574902	1.903981
H	1.532589	-1.555475	-1.940438
H	3.282196	-1.906016	-1.720128
H	-1.283200	1.462847	1.993733
H	1.529917	3.375251	1.826447
H	2.335094	2.156614	2.377016
O	3.824195	1.313454	2.318131
H	4.030896	0.872551	3.153088
H	3.687648	0.582098	1.659717

TS4-OH1-2WAT

C	-0.783562	-2.074835	-0.491851
C	-2.040172	-1.394552	-0.599423
C	-2.420450	-0.912230	0.704092
C	-1.416879	-1.352334	1.610980
C	-0.418886	-2.044063	0.888969
Mo	-0.509173	0.185885	-0.027653
C	0.379302	1.261710	-1.948690
C	0.084783	2.201675	-0.905598
C	-1.339006	2.244477	-0.723637
C	-1.899310	1.299756	-1.615084
C	-0.838720	0.694548	-2.369667
O	-0.255423	1.196951	1.795297
O	1.655290	2.622880	2.545872
O	3.767327	-0.270715	0.554359
C	2.638464	-0.541627	0.047576
O	1.588172	0.047836	0.482353
C	2.576618	-1.587542	-1.035826
H	-3.331634	-0.381881	0.958058
H	-1.371365	-1.111503	2.666953
H	0.503951	-2.429953	1.308672
H	-0.253333	-2.582933	-1.288143
H	-2.631074	-1.306752	-1.502618
H	-1.884567	2.871776	-0.027903
H	-2.954233	1.065471	-1.706883
H	-0.955834	-0.093114	-3.106762
H	1.364946	1.007111	-2.320798
H	0.814883	2.785869	-0.358235
H	2.315727	-2.550458	-0.573447
H	0.857446	2.034217	2.189986
H	1.807845	-1.348660	-1.775764
H	3.555520	-1.688351	-1.513461
H	-1.085878	1.580525	2.101828
H	1.654203	3.447886	2.039861
H	2.772903	2.029548	2.426080
O	3.792054	1.502557	2.322330
H	4.041368	1.100600	3.168267
H	3.749534	0.737888	1.591742

I6-OH1-2WAT

C	-0.967425	-2.308150	-0.666180
C	-2.222677	-1.633339	-0.797921
C	-2.633415	-1.156844	0.500354
C	-1.650274	-1.597046	1.427410
C	-0.631839	-2.278233	0.723494
Mo	-0.712505	-0.046768	-0.184792
C	0.181892	1.029359	-2.097583
C	-0.102342	1.967702	-1.046623
C	-1.523758	2.025864	-0.864972
C	-2.096023	1.091515	-1.760452
C	-1.043484	0.482539	-2.523016
O	-0.457436	0.932268	1.628365
O	1.417952	2.596736	2.442016
O	3.617825	-0.566072	0.436394
C	2.444354	-0.801428	-0.094314
O	1.440503	-0.191019	0.328111
C	2.437616	-1.840266	-1.168414
H	-3.552661	-0.631613	0.735264
H	-1.629707	-1.361113	2.485249
H	0.283586	-2.661991	1.162118
H	-0.418393	-2.813473	-1.451533
H	-2.795821	-1.542025	-1.712142
H	-2.061489	2.650494	-0.160896
H	-3.153457	0.867853	-1.851725
H	-1.170023	-0.298352	-3.265624
H	1.163969	0.768382	-2.475235
H	0.633783	2.540515	-0.495188
H	2.174592	-2.803068	-0.706464
H	0.703496	1.990551	2.081010
H	1.683637	-1.605189	-1.923480
H	3.431287	-1.928797	-1.615424
H	-1.299286	1.277637	1.949590
H	1.413583	3.375798	1.870257
H	2.876066	1.752876	2.369067
O	3.720329	1.230035	2.288760
H	3.885789	0.861567	3.167325
H	3.578954	0.132173	1.184743

I1-OH1'-2WAT

C	1.338683	1.761803	1.525316
C	0.383992	2.247562	0.585987
C	1.027905	2.468123	-0.650863
C	2.403921	2.115162	-0.523857
C	2.598590	1.713214	0.846327
Mo	1.307506	0.118680	-0.150492
C	2.785182	-1.175169	1.242502
C	3.452790	-0.927355	-0.004319
C	2.706005	-1.531584	-1.040193
C	1.546213	-2.120825	-0.441638
C	1.614864	-1.914561	0.983196
O	-0.848513	-0.395719	0.211533
O	0.481042	0.117509	-2.051785
H	0.534681	2.766536	-1.568316
H	3.170835	2.219348	-1.283224
H	3.549429	1.462944	1.299665
H	1.154193	1.528518	2.567409
H	-0.678934	2.356455	0.771148
H	2.953197	-1.521281	-2.095931

H	0.757167	-2.643358	-0.968426
H	0.892099	-2.250533	1.717769
H	3.106707	-0.813082	2.213146
H	4.370889	-0.363668	-0.130759
H	-0.725935	-0.825089	-2.006915
H	1.137035	0.113398	-2.757792
C	-1.918408	-1.122973	-0.474960
O	-1.483281	-1.442284	-1.736709
C	-2.291450	-2.379077	0.299157
H	-3.050244	-2.928712	-0.268970
H	-1.402815	-3.007529	0.414364
H	-2.694618	-2.130282	1.285974
O	-3.073822	-0.293464	-0.486778
C	-3.025223	0.890093	-1.322086
H	-2.626105	0.612421	-2.304009
H	-2.354003	1.626269	-0.861736
C	-4.434206	1.440468	-1.450240
H	-4.842742	1.728911	-0.472928
H	-4.413596	2.333425	-2.089585
H	-5.103044	0.701318	-1.910497
O	-1.484812	0.010102	2.776078
H	-1.079394	-0.292198	1.178364
H	-1.317547	-0.751246	3.348004
O	-4.124382	0.318936	2.101715
H	-3.899710	0.058062	1.184476
H	-2.466521	0.084893	2.717867
H	-4.753319	-0.349102	2.406463

TS2-OH1'-2WAT

C	1.264125	1.821312	1.430904
C	0.282695	2.254228	0.492884
C	0.899623	2.446165	-0.760631
C	2.287348	2.133060	-0.647658
C	2.514637	1.781079	0.729848
Mo	1.247730	0.115122	-0.176963
C	2.776645	-1.106770	1.255159
C	3.433545	-0.852583	0.004469
C	2.708797	-1.496456	-1.023714
C	1.572679	-2.124042	-0.412732
C	1.640110	-1.898337	1.006296
O	-0.799018	-0.414300	0.307252
O	0.418221	0.026929	-2.086115
H	0.382650	2.698130	-1.679329
H	3.038080	2.233007	-1.423960
H	3.478022	1.571917	1.177517
H	1.106667	1.625847	2.485288
H	-0.779729	2.341424	0.688988
H	2.960699	-1.500401	-2.078494
H	0.805085	-2.687994	-0.927905
H	0.925549	-2.241859	1.744991
H	3.081553	-0.714560	2.219950
H	4.329975	-0.257228	-0.130982
H	-0.742668	-0.970554	-1.937965
H	1.092224	0.016485	-2.774564
C	-1.782839	-1.166524	-0.301271
O	-1.474841	-1.570156	-1.589938
C	-2.185115	-2.395412	0.515743
H	-2.963916	-2.955128	-0.014891
H	-1.303586	-3.035204	0.632755
H	-2.558149	-2.120726	1.507872
O	-3.048272	-0.347065	-0.358412
C	-3.034415	0.787696	-1.257001
H	-2.545533	0.484906	-2.188945
H	-2.454668	1.603641	-0.804355
C	-4.467633	1.219804	-1.520093
H	-4.975737	1.512046	-0.590900
H	-4.465206	2.087108	-2.194759
H	-5.039462	0.411840	-1.996135
O	-1.420086	0.188752	2.727753
H	-1.071956	-0.107174	1.807303
H	-1.277993	-0.550756	3.336312
O	-3.708088	0.481031	1.957811
H	-3.549039	0.111926	0.997941
H	-2.707756	0.339326	2.440260
H	-4.374286	-0.071983	2.396422

I5-OH1'-2WAT

C	0.507498	1.643927	1.405707
C	-0.324186	1.803751	0.257919
C	0.450361	2.354035	-0.790329
C	1.783722	2.545636	-0.332423
C	1.809407	2.135205	1.046389
Mo	1.465401	0.246561	-0.159561
C	2.961327	-0.565911	1.540693
C	3.740943	0.052126	0.501421
C	3.535896	-0.660147	-0.701600
C	2.589417	-1.706317	-0.417143
C	2.271552	-1.656783	0.983194
O	-0.303007	-1.043245	-0.059163
O	1.093187	0.068158	-2.306700
H	0.103633	2.516736	-1.804953
H	2.603455	2.980115	-0.893555
H	2.653189	2.231108	1.718098
H	0.198447	1.279842	2.378384
H	-1.361209	1.492047	0.171243
H	4.006893	-0.451846	-1.656318
H	2.207385	-2.430713	-1.128164
H	1.573700	-2.302067	1.504144
H	2.893507	-0.224471	2.568402
H	4.375168	0.923672	0.620933
H	0.444195	-0.714001	-2.415592
H	1.868432	-0.083103	-2.862664
C	-0.891070	-1.780493	-0.946149
O	-0.602674	-1.776879	-2.167896
C	-1.986392	-2.681927	-0.431773
H	-2.369503	-3.310886	-1.239918
H	-1.601511	-3.308498	0.382673
H	-2.798601	-2.066306	-0.024202
O	-3.661839	0.898406	-0.233918
C	-4.914061	1.464584	-0.648285
H	-4.691510	2.071151	-1.536632
H	-5.295726	2.143830	0.131729
C	-5.959540	0.405983	-0.980313
H	-6.198083	-0.201015	-0.094977
H	-6.887080	0.887150	-1.323540
H	-5.600329	-0.261657	-1.776330
O	-1.202676	-1.174090	2.608320
H	-0.852030	-1.171194	1.690836
H	-1.136203	-2.095130	2.896110
O	-3.828950	-0.348541	2.303674
H	-3.786200	0.458745	0.633495
H	-2.915292	-0.692929	2.437327
H	-4.383158	-1.138606	2.246630

I1-W2-2WAT

C	-1.396306	1.367209	1.677865
C	-2.544989	0.542399	1.786947
C	-3.446378	0.855881	0.709166
C	-2.868644	1.896961	-0.044219
C	-1.595302	2.194320	0.515620
Mo	-1.388019	-0.004068	-0.183737
C	-0.215121	-2.138517	-0.248029
C	-1.066552	-2.025184	-1.378250
C	-2.418082	-1.910101	-0.927744
C	-2.372058	-1.970049	0.506972
C	-1.007377	-2.091506	0.923971
O	-1.267029	0.719116	-2.092995
O	0.698734	0.750633	-0.337719
C	1.647722	0.803547	-1.137513
O	3.701962	-3.296370	-0.777914
O	2.649108	1.640685	-0.931995
C	2.598993	2.531627	0.234920
C	3.847268	3.385402	0.203038
C	1.822611	-0.048402	-2.351737
H	-0.887230	2.912535	0.118986
H	-0.556175	1.399304	2.361475
H	-2.717505	-0.197627	2.559252
H	-4.398243	0.373831	0.512788
H	-3.279416	2.325142	-0.951684
H	-0.646941	-2.143703	1.944960
H	0.868254	-2.187273	-0.272682
H	-0.739382	-1.982960	-2.409710
H	-3.307031	-1.877274	-1.547628
H	-3.236138	-1.974217	1.159994
H	-2.108914	0.618271	-2.553760
H	2.512526	0.426839	-3.053662
H	2.249642	-1.011521	-2.036790
H	0.847568	-0.221578	-2.811330
H	2.550534	1.904972	1.130710
H	1.683691	3.127995	0.158254
H	3.832866	4.059008	1.070092
H	4.751083	2.765559	0.261986
H	3.887251	3.995405	-0.708410
O	1.786358	-0.540157	2.511368
H	1.280118	-0.201217	1.756545
H	3.212721	-1.507569	1.995509
H	3.797608	-2.827465	0.080528
O	3.989823	-2.021674	1.681340
H	4.174675	-2.656919	2.385809
H	4.135479	-2.719932	-1.420605
H	2.039752	0.249693	3.009326

TS1-W2-2WAT

C	-0.986821	-1.367119	-1.803727
C	-2.379007	-1.137244	-1.578980
C	-2.782755	-1.853160	-0.393153
C	-1.644386	-2.568309	0.060310
C	-0.548361	-2.258433	-0.772520
Mo	-1.271440	-0.145806	0.160554
C	-0.980967	2.235953	-0.151193
C	-1.457837	1.913161	1.160200
C	-2.772833	1.352131	1.039567
C	-3.064667	1.297190	-0.351530
C	-1.959706	1.849977	-1.081392
O	-1.018891	-0.778520	2.091476
O	0.925845	0.084080	0.219495
C	1.942984	0.095130	1.082890
O	2.639467	1.475277	0.897220
O	2.937608	-0.877919	0.826723
C	3.341860	-1.095090	-0.538386
C	4.465961	-2.116087	-0.530716
C	1.684453	0.024155	2.582479
H	0.470557	-2.593800	-0.616207
H	-0.398616	-1.003477	-2.637308
H	-3.031730	-0.567080	-2.227532
H	-3.781301	-1.895837	0.028042
H	-1.594713	-3.164736	0.964038
H	-1.874770	1.904493	-2.161571
H	-0.003942	2.639900	-0.387828
H	-0.917781	2.075882	2.084772
H	-3.430130	1.055144	1.848939
H	-3.985172	0.922707	-0.783812
H	-1.881832	-1.014590	2.453469
H	2.636476	0.133070	3.115708
H	1.005926	0.824393	2.886894
H	1.233694	-0.937208	2.835132
H	3.680858	-0.146330	-0.975984
H	2.488697	-1.463983	-1.121000
H	4.790657	-2.310002	-1.562075
H	5.329169	-1.748364	0.040024
H	4.130430	-3.065085	-0.090788
O	1.355146	0.984652	-2.352798
H	1.173666	0.532682	-1.484896
H	2.262679	2.063552	-1.841652
H	2.767496	2.143308	-0.253294
O	2.853640	2.657551	-1.229998
H	2.452724	3.539995	-1.172405
H	3.483528	1.453816	1.373714
H	1.819455	0.336346	-2.900305

I2-W2-2WAT

C	1.106648	-0.973514	2.008630
C	2.470031	-0.915833	1.596298
C	2.676664	-1.872769	0.535104
C	1.451810	-2.556950	0.350183
C	0.486058	-1.995491	1.215419
Mo	1.199386	-0.178778	-0.171289
C	1.179101	2.218783	-0.251878
C	1.355919	1.636688	-1.552461
C	2.617725	0.960183	-1.580493
C	3.183140	1.099410	-0.282807
C	2.299755	1.886591	0.527539
O	0.469148	-1.094500	-1.833393
O	-1.041185	0.316423	-0.007687
C	-2.245860	0.240287	-0.791489
O	-3.152767	1.072228	-0.077963
O	-2.712219	-1.072388	-0.871164
C	-3.230862	-1.670889	0.341975
C	-3.345514	-3.165765	0.107821
C	-2.026395	0.743573	-2.206494
H	-0.561014	-2.271211	1.244769
H	0.643748	-0.405809	2.806950
H	3.235260	-0.288603	2.035957
H	3.610783	-2.071950	0.021099
H	1.256420	-3.306333	-0.408538
H	2.444481	2.127125	1.575429

H	0.309663	2.771626	0.086104
H	0.653886	1.702082	-2.373015
H	3.064848	0.451337	-2.426926
H	4.135843	0.690918	0.034798
H	1.173532	-1.507969	-2.347248
H	-2.977959	0.691268	-2.747972
H	-1.693032	1.785605	-2.171094
H	-1.278556	0.127776	-2.711098
H	-4.212884	-1.234059	0.565183
H	-2.558648	-1.448413	1.180401
H	-3.770925	-3.642451	1.001149
H	-4.007004	-3.377325	-0.743238
H	-2.361983	-3.611886	-0.090516
O	-1.264475	1.484126	2.416764
H	-1.220649	0.695947	0.897381
H	-1.688758	2.325739	2.137247
H	-2.764239	2.874325	0.488251
O	-2.530202	3.585888	1.114758
H	-1.924499	4.161332	0.627823
H	-4.001788	1.058698	-0.544866
H	-1.896456	1.070885	3.021500

methanol

C	-1.667908	1.247069	-0.001356
H	-1.293406	0.226008	-0.023015
H	-1.306388	1.737101	0.905079
H	-2.759502	1.222998	0.015471
O	-1.177260	1.898513	-1.179260
H	-1.499010	2.806259	-1.179752

I1-W3-2WAT

C	2.050954	1.322917	-1.601496
C	3.237866	0.561675	-1.392110
C	3.791409	0.905458	-0.104790
C	2.974763	1.920597	0.443000
C	1.897657	2.159014	-0.443538
Mo	1.674704	-0.125152	0.154494
C	0.566239	-2.177263	-0.458751
C	1.013836	-2.216945	0.898209
C	2.444248	-2.150371	0.911610
C	2.856431	-2.054126	-0.452208
C	1.696144	-2.072532	-1.293146
O	1.248727	0.391172	2.082813
O	-0.426635	0.613639	0.009048
C	-1.528531	0.497657	0.559216
O	-3.629196	-2.693005	-1.351128
O	-2.579865	1.175214	0.108648
C	-2.426229	2.088013	-1.037297
C	-2.171657	3.500864	-0.549731
C	-1.844251	-0.396873	1.713247
H	1.068987	2.831963	-0.254249
H	1.428928	1.327369	-2.489115
H	3.674584	-0.129405	-2.101953
H	4.691007	0.492477	0.338751
H	3.088637	2.359901	1.427745
H	1.688534	-1.976265	-2.373660
H	-0.467763	-2.169570	-0.787293
H	0.376611	-2.282378	1.770569
H	3.090797	-2.218899	1.779108
H	3.883915	-2.005297	-0.793046
H	2.011627	0.260214	2.659269
H	-2.734985	-0.047244	2.240861
H	-2.040239	-1.404487	1.319559
H	-0.978753	-0.434176	2.378540
H	-3.382109	2.002082	-1.561482
H	-1.621870	1.710478	-1.672203
H	-2.105263	4.166924	-1.420733
H	-2.992227	3.847558	0.090661
H	-1.230431	3.564392	0.009933
O	-5.442108	0.861409	0.817124
H	-4.486148	1.004262	0.709364
H	-5.831364	-0.703547	0.040622
H	-4.469097	-2.314138	-1.006550
O	-5.992190	-1.578460	-0.380954
H	-6.639087	-1.407431	-1.077923
H	-3.560571	-3.559042	-0.927549
H	-5.584435	0.852389	1.774323

TS1-W3-2WAT

C	2.709024	1.486831	-1.371886
C	3.257536	1.644886	-0.055844
C	2.240062	2.116638	0.799298
C	1.043640	2.228975	0.016739
C	1.349978	1.859163	-1.337308
Mo	1.488140	-0.003255	0.107754
C	1.856305	-2.243167	0.965340
C	3.059931	-1.476064	0.937934
C	3.343657	-1.212653	-0.448549
C	2.291775	-1.767628	-1.250570
C	1.397779	-2.420078	-0.358517
O	0.471164	0.086547	1.891514
O	-0.525282	-0.271257	-0.601453
C	-1.712952	-0.591943	-0.110873
C	-1.836934	-1.692164	0.934189
O	-2.495889	-1.148639	-1.318029
O	-2.477287	0.519559	0.382701
C	-2.619558	1.659345	-0.498733
C	-3.019703	2.867189	0.330407
O	-5.121253	-0.061095	1.127541
O	-4.907621	-1.336997	-1.097374
H	0.080232	2.555029	0.386200
H	0.659877	1.837949	-2.172688
H	3.241526	1.103446	-2.235909
H	4.276872	1.417840	0.237265
H	2.342128	2.333806	1.856510
H	2.223837	-1.748581	-2.332736
H	0.472783	-2.906151	-0.644815
H	1.334117	-2.566956	1.858204
H	3.688046	-1.229478	1.787011
H	4.236578	-0.733336	-0.828917
H	1.099991	0.218166	2.611407
H	-2.891857	-1.915321	1.126813
H	-1.350340	-2.600710	0.569559
H	-1.349887	-1.359660	1.852755
H	-3.389527	1.431932	-1.250089
H	-1.671068	1.830847	-1.017512
H	-3.135893	3.737124	-0.330086
H	-3.975069	2.698912	0.844733
H	-2.253551	3.100786	1.081268
H	-4.166073	0.172631	1.112867
H	-5.131554	-0.862025	-0.221494
H	-3.778949	-1.212430	-1.245792
H	-5.392089	-0.895475	-1.813027
H	-2.168167	-0.688595	-2.107114
H	-5.245028	-0.614361	1.911637

I6-W3-2WAT

C	1.211324	1.881117	-1.345608
C	2.605980	1.961741	-1.156603
C	2.864467	2.222522	0.231133
C	1.626440	2.328228	0.902496
C	0.595634	2.085719	-0.058719
Mo	1.720137	0.114751	0.111468
C	2.364550	-2.187549	-0.352939
C	2.656483	-1.929457	1.005644
C	3.581051	-0.848467	1.079576
C	3.889772	-0.478669	-0.280366
C	3.109184	-1.285025	-1.167861
O	0.509024	-0.217788	1.724566
O	-0.178397	-0.607813	-0.812609
C	-1.050111	-1.466767	-0.648580
O	-2.121573	-1.455966	-1.447040
O	-3.713989	1.466531	1.081034
C	-3.739347	1.978061	-0.260019
C	-5.033874	2.714652	-0.587216
C	-1.050083	-2.586300	0.334987
H	-0.468738	2.064503	0.144625
H	0.700317	1.688950	-2.282018
H	3.358915	1.811140	-1.922477
H	3.845143	2.308611	0.686941
H	1.488195	2.509454	1.962331
H	3.124802	-1.258999	-2.251627
H	1.648663	-2.916617	-0.716468
H	2.184610	-2.415296	1.851760
H	4.039073	-0.449989	1.978084
H	4.630285	0.253363	-0.577165
H	0.952292	0.023503	2.547099
H	-2.061697	-2.734411	0.726342
H	-0.759202	-3.505135	-0.194369
H	-0.346837	-2.371751	1.139236
H	-3.576862	1.156594	-0.977609
H	-2.883072	2.661060	-0.336998
H	-4.992155	3.113254	-1.611704
H	-5.898188	2.038965	-0.518586
H	-5.189447	3.553666	0.105698
O	-5.572814	-0.638628	1.305395
H	-4.375331	0.746005	1.151845
H	-5.328546	-1.325005	0.644187
H	-3.968956	-2.193656	-0.974732
O	-4.819897	-2.498217	-0.618680
H	-5.416211	-2.508480	-1.380297
H	-2.056868	-0.713380	-2.075367
H	-5.503580	-1.079663	2.162713

Table S4. PCM-DFT/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ}$; DFT = B3LYP, B3LYP-D3, M06, BP86, G96LYP, B3PW91) for the structures involved in the most significant steps found along the intramolecular nucleophilic hydroxo attack mechanism: the intramolecular hydroxo attack on the carbonyl carbon atom of the Mo-coordinated ester, the ethanol formation, and the acetic acid formation.[a,b,c,d]

Species	B3LYP	B3LYP-D3	M06	BP86	G96LYP	B3PW91
$[Cp_2Mo(OH)(OH_2)]^+$	-607.298231	-607.360429	-606.878408	-607.3808683	-607.021869	-607.135806
$[Cp_2Mo(OH)]^+$	-530.842382	-530.895997	-530.457067	-530.9239685	-530.590295	-530.708933
H_2O	-76.473281	-76.473855	-76.429633	-76.47296907	-76.456561	-76.443111
ethyl acetate	-307.758950	-307.774073	-307.550488	-307.7510716	-307.631270	-307.634993
ethanol	-155.064318	-155.071423	-154.950026	-155.0567635	-154.989100	-155.002687
acetic acid	-229.161721	-229.168884	-229.022424	-229.1610689	-229.093221	-229.069451
TS1-OH1	-838.548002	-838.634533	-837.970162	-838.6274025	-838.158084	-838.293465
I2-OH1	-838.548131	-838.634805	-837.973538	-838.6257481	-838.154450	-838.295522
I2-OH1-2WAT	-991.475894	-991.571085	-990.818187	-991.552879	-991.038399	-991.161514
TS2-OH1	-838.514524	-838.601061	-837.937983	-838.6001646	-838.127386	-838.263796
TS2-OH1-2WAT	-991.467502	-991.563553	-990.808671	-991.5523552	-991.034544	-991.155581
I3-OH1	-683.548270	-683.614821	-683.074552	-683.6315289	-683.241278	-683.356119
TS5-OH1	-759.972091	-760.041579	-759.456320	-760.0533301	-759.645047	-759.745615

[a]All the magnitudes are given in hartree. [b]Thermodynamic magnitudes were computed at a pressure of 1 atm and a temperature of 298.15 K. [c]B3LYP results are given for comparison purposes. [d]$G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ} = G_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ} + G^{therm}_{PCM\text{-}B3LYP/VDZ}$.

Table S5. Relative PCM-DFT/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ}$; DFT = B3LYP, B3LYP-D3, M06, BP86, G96LYP, B3PW91) and PCM-DFT/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution (ΔG^{sol}_{corr}) computed at the standard concentration of 1 *M* (55.5 *M* for water) for the structures involved in the most significant steps found along the intramolecular nucleophilic hydroxo attack mechanism: the intramolecular hydroxo attack on the carbonyl carbon atom of the Mo-coordinated ester, the ethanol formation, and the acetic acid formation.[a,b,c,d]

	$\Delta G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ}$						ΔG^{sol}_{corr}					
Species	B3LYP	B3LYP-D3	M06	BP86	G96LYP	B3PW91	B3LYP	B3LYP-D3	M06	BP86	G96LYP	B3PW91
$[Cp_2Mo(OH)(H_2O)]^+$ + ethyl acetate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$[Cp_2Mo(OH)]^+$ + ethyl acetate + H_2O	-10.9	-5.9	-5.2	-10.1	-15.7	-10.2	-6.6	-1.6	-0.9	-5.8	-11.4	-5.9
TS1-OH1 + H_2O	22.5	16.4	18.3	19.8	24.2	21.5	24.9	18.8	20.7	22.2	26.6	23.9
I2-OH1 + H_2O	22.4	16.2	16.1	20.8	26.4	20.2	24.8	18.6	18.5	23.2	28.8	22.6
TS2-OH1 + H_2O	43.5	37.4	38.5	36.9	43.4	40.1	45.9	39.8	40.9	39.3	45.8	42.5
TS2-OH1-2WAT + H_2O	27.7	20.9	22.1	21.2	28.9	23.9	30.1	23.3	24.5	23.6	31.3	26.3
I3-OH1 + H_2O + ethanol	-18.0	-16.1	-15.9	-18.4	-21.2	-19.5	-13.7	-11.8	-11.6	-14.1	-16.9	-15.2
TS5-OH1 + ethanol	13.0	13.5	14.2	13.7	11.9	14.1	13.0	13.5	14.2	13.7	11.9	14.1
$[Cp2Mo(OH)]^+$ + ethanol + acetic acid	-7.1	-1.1	-0.4	-6.2	-12.2	-6.4	-5.2	0.8	1.5	-4.3	-10.3	-4.5

[a]All the values are given in kcal/mol at a temperature of 298.15 K and a pressure of 1 atm. [b]B3LYP results are also given for comparison purposes. [c]$\Delta G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ} = \Delta G_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ} + \Delta G^{therm}_{PCM\text{-}B3LYP/VDZ}$. [d]$\Delta G^{sol}_{corr} = \Delta G^{sol}_{PCM\text{-}DFT/VTZ//PCM\text{-}B3LYP/VDZ}$ + (1.9 kcal/mol) Δn + (4.3 kcal/mol) Δm, where Δn and Δm are the changes in the number of non-water components and water molecules for each transformation along the reaction mechanisms found, respectively.

Comments on Table S5: We recomputed the energy barrier of the most relevant steps found for OH1, that is, the tetrahedral intermediate formation ($[Cp_2Mo(OH)]^+$ + H_2O + ethyl acetate → **TS1-OH1**), the tetrahedral intermediate cleavage ($[Cp_2Mo(OH)]^+$ + H_2O + ethyl acetate → **TS2-OH1-2WAT**), and the acetic acid formation (**I3-OH1** → **TS5-OH1**) at the PCM-DFT/VTZ//PCM-B3LYP/VDZ (DFT = B3LYP-D3, M06, BP86, G96LYP, B3PW91) levels of theory. As seen in Table S5, the Gibbs energy barrier for the tetrahedral intermediate formation is lower than the B3LYP one by 11.1 (B3LYP-D3), 9.9 (M06), 3.5 (BP86), and 1.7 (B3PW91) kcal/mol, while a rise of 6.5 kcal/mol was found for G96LYP. A similar trend was found when analyzing the Gibbs energy barrier values for the tetrahedral intermediate cleavage. Specifically, B3LYP-D3, M06, BP86, and B3PW91 reduce such an energy barrier by 11.8, 11.3, 7.3, and 4.5 kcal/mol, respectively, while an increase of 6.0 kcal/mol was found for G96LYP. It is interesting to note that the functionals involving dispersion energy correction terms (B3LYP-D3 and M06) provoke a greater reduction of the Gibbs energy barriers. Concerning the acetic acid elimination step, the discrepancy between B3LYP and the remaining functionals used is notably lesser. B3LYP-D3 and M06 stabilize the corresponding Gibbs energy barrier by 1.4 and 1.1 kcal/mol, respectively, while values of 1.1, 2.1, and 2.6 kcal/mol were obtained for BP86, G96LYP, and B3PW91. So, on the one hand, we find that the tetrahedral intermediate cleavage is clearly more energy-demanding than the tetrahedral intermediate formation. On the other hand, as happened for B3LYP, the tetrahedral intermediate cleavage remains as the rate-determining step with Gibbs energy barriers of 29.4, 42.7, and 32.2 kcal/mol for BP86, G96LYP, and B3PW91, respectively. However, the Gibbs energy barrier of such a step with B3LYP-D3 (24.9 kcal/mol) and M06 (25.4 kcal/mol) is 0.4 kcal/mol lower in energy than that found for the acetic acid elimination step at both DFT methods. As a consequence, we note that the tetrahedral intermediate cleavage and the acetic acid formation compete to be the rate-determining step of the overall process. Taken as reference the Gibbs energy barrier (25.1 kcal/mol) deduced from the experimental kinetic constant for $[Cp'_2Mo(OH)(OH_2)]^+$-catalyzed hydrolysis of ethyl acetate using the thermodynamic formulation of TST, we conclude that B3LYP-D3 and M06 give the best agreement with experiment.

Table S6. PCM-B3LYP/VDZ and PCM-M06/VTZ//PCM-B3LYP/VDZ Gibbs energies with electrostatic and non-electrostatic solute-solvent interactions ($G_{\text{PCM-B3LYP/VDZ}}$ and $G_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$, respectively), PCM-B3LYP/VDZ thermal Gibbs energy correction in water solution ($G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$), and Gibbs energy in water solution ($G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b,c]

Species	$G_{\text{PCM-B3LYP/VDZ}}$	$G_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$	$G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$	$G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$
$[Cp_2Mo(OH)(OH_2)]^+$	-607.329093	-607.048007	0.169599	-606.878408
$[Cp_2Mo(OH)]^+$	-530.870295	-530.603659	0.146592	-530.457067
H_2O	-76.454991	-76.432998	0.003365	-76.429633
ethyl acetate	-307.758858	-307.634778	0.084290	-307.550488
ethanol	-155.073232	-155.003734	0.053708	-154.950026
acetic acid	-229.135085	-229.056787	0.034363	-229.022424
TS0	-838.611757	-838.229126	0.250150	-837.978976
I1	-838.627056	-838.248066	0.253964	-837.994102
TS1-OH1	-838.605724	-838.226602	0.256440	-837.970162
I2-OH1	-838.609588	-838.233020	0.259482	-837.973538
I2-OH1-2WAT	-991.5374294	-991.119289	0.301102	-990.818187
TS2-OH1	-838.570007	-838.191157	0.253174	-837.937983
TS2-OH1-2WAT	-991.5253413	-991.106243	0.297572	-990.808671
I3-OH1	-683.570025	-683.253078	0.178526	-683.074552
I3-OH1-2WAT	-991.5678364	-991.140584	0.290136	-990.850448
TS3-OH1	-683.544117	-683.222706	0.176965	-683.045741
I4-OH1	-683.550077	-683.229310	0.178221	-683.051089
I5-OH1	-760.026669	-759.689857	0.200656	-759.489201
I5-OH1-2WAT	-912.9481918	-912.572309	0.245884	-912.326425
TS4-OH1	-759.987243	-759.653106	0.200302	-759.452804
TS4-OH1-2WAT	-912.9325764	-912.555224	0.24307	-912.312154
I6-OH1	-760.003063	-759.668874	0.201076	-759.467798
I6-OH1-2WAT	-912.9401389	-912.563401	0.246836	-912.316565
TS5-OH1	-759.994361	-759.656798	0.200478	-759.456320
I1-OH1'	-915.066892	-914.6705356	0.280574	-914.389962
I1-OH1'-2WAT	-1067.993307	-1067.559035	0.322145	-1067.236890
TS2-OH1'	-915.025825	-914.626187	0.275353	-914.350834
TS2-OH1'-2WAT	-1067.971598	-1067.536645	0.32157	-1067.215075
I5-OH1'-2WAT	-1068.025063	-1067.580674	0.314241	-1067.266433
TS1-OH2'	-915.035767	-914.634097	0.274645	-914.359452

[a]All the magnitudes are given in hartree. [b]Thermodynamic contributions are computed at a temperature of 298.15 K and a pressure of 1 atm. [c]$G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}} = G_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}} + G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$.

Table S7. Relative PCM-M06/VTZ//PCM-B3LYP/VDZ Gibbs energy with electrostatic and non-electrostatic solute-solvent interactions ($\Delta G_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$), PCM-B3LYP/VDZ thermal Gibbs energy correction ($\Delta G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$), PCM-M06/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$), and PCM-M06/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}_{\text{corr}}$) computed at the standard concentration of 1 *M* (55.5 *M* for water) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b]

Species	$\Delta G_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$	$\Delta G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}_{\text{corr}}$
$[Cp_2Mo(OH)(H_2O)]^+$ + ethyl acetate	0.0	0.0	0.0	0.0
$[Cp_2Mo(OH)]^+$ + ethyl acetate + H_2O	7.1	-12.3	-5.2	-0.9
TS0 + H_2O	13.0	-0.2	12.8	15.2
I1 + H_2O	1.1	2.2	3.3	5.7
TS1-OH1 + H_2O	14.5	3.7	18.2	20.6
I2-OH1 + H_2O	10.5	5.6	16.1	18.5
TS2-OH1 + H_2O	36.8	1.7	38.5	40.9
I3-OH1 + H_2O + ethanol	-4.4	-11.5	-15.9	-11.6
TS3-OH1 + H_2O + ethanol	14.7	-12.5	2.2	6.5
I4-OH1 + H_2O + ethanol	10.5	-11.7	-1.2	3.1
I5-OH1 + ethanol	-6.8	0.3	-6.5	-6.5
TS4-OH1 + ethanol	16.3	0.1	16.4	16.4
I6-OH1 + ethanol	6.4	0.6	7.0	7.0
TS5-OH1 + ethanol	14.0	0.2	14.2	14.2
I1-OH1'	7.7	16.7	24.4	22.5
TS2-OH1'	35.5	13.5	49.0	47.1
TS1-OH2'	30.6	13.0	43.6	41.7
$[Cp2Mo(OH)]^+$ + ethanol + acetic acid	11.7	-12.1	-0.4	1.5

[a]All the thermodynamic magnitudes are given in kcal/mol at a temperature of 347.15 K and a pressure of 1 atm. [b]$\Delta G^{\text{sol}}_{\text{corr}} = \Delta G^{\text{sol}}_{\text{PCM-M06/VTZ//PCM-B3LYP/VDZ}}$ + (1.9 kcal/mol) Δn + (4.3 kcal/mol) Δm, where Δn and Δm are the changes in the number of non-water components and water molecules for each transformation along the reaction mechanisms found, respectively.

Table S8. PCM-B3LYP/VDZ and PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energies with electrostatic and non-electrostatic solute-solvent interactions ($G_{\text{PCM-B3LYP/VDZ}}$ and $G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$, respectively), dispersion energy correction (E_{disp}), PCM-B3LYP/VDZ thermal Gibbs energy correction in water solution ($G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$), and Gibbs energy in water solution ($G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}}$) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b,c]

Species	$G_{\text{PCM-B3LYP/VDZ}}$	$G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$	E_{disp}	$G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$	$G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}}$
$[Cp_2Mo(OH)(OH_2)]^+$	-607.329093	-607.467830	-0.062198	0.169599	-607.360429
$[Cp_2Mo(OH)]^+$	-530.870295	-530.988974	-0.053615	0.146592	-530.895997
H_2O	-76.454991	-76.476646	-0.000574	0.003365	-76.473855
ethyl acetate	-307.758858	-307.843240	-0.015123	0.084290	-307.774073
ethanol	-155.073232	-155.118026	-0.007105	0.053708	-155.071423
acetic acid	-229.135085	-229.196084	-0.007163	0.034363	-229.168884
TS0	-838.611757	-838.812908	-0.079497	0.250150	-838.642256
I1	-838.627056	-838.827800	-0.083401	0.253964	-838.657237
TS1-OH1	-838.605724	-838.804442	-0.086530	0.256440	-838.634533
I2-OH1	-838.609588	-838.807613	-0.086674	0.259482	-838.634805
I2-OH1-2WAT	-991.5374294	-991.7769957	-0.095191	0.301102	-991.571085
TS2-OH1	-838.570007	-838.767698	-0.086537	0.253174	-838.601061
TS2-OH1-2WAT	-991.5253413	-991.7650735	-0.096051	0.297572	-991.563553
I3-OH1	-683.570025	-683.726796	-0.066550	0.178526	-683.614821
I3-OH1-2WAT	-991.5678364	-991.8100766	-0.086090	0.290136	-991.606031
TS3-OH1	-683.544117	-683.701752	-0.064762	0.176965	-683.589548
I4-OH1	-683.550077	-683.707861	-0.065045	0.178221	-683.594684
I5-OH1	-760.026669	-760.204041	-0.073859	0.200656	-760.077244
I5-OH1-2WAT	-912.9481918	-913.1668883	-0.084245	0.245884	-913.005249
TS4-OH1	-759.987243	-760.165262	-0.072743	0.200302	-760.037703
TS4-OH1-2WAT	-912.9325764	-913.1515211	-0.084865	0.24307	-912.993316
I6-OH1	-760.003063	-760.181066	-0.072258	0.201076	-760.052248
I6-OH1-2WAT	-912.9401389	-913.1588237	-0.083325	0.246836	-912.995313
TS5-OH1	-759.994361	-760.172569	-0.069489	0.200478	-760.041579
I1-OH1'	-915.066892	-915.285672	-0.091480	0.280574	-915.096578
I1-OH1'-2WAT	-1067.993307	-1068.252869	-0.102921	0.322145	-1068.033645
TS2-OH1'	-915.025825	-915.243943	-0.091791	0.275353	-915.060381
TS2-OH1'-2WAT	-1067.971598	-1068.230815	-0.105105	0.32157	-1068.014350
I5-OH1'-2WAT	-1068.025063	-1068.28753	-0.095250	0.314241	-1068.068539
TS1-OH2'	-915.035767	-915.255413	-0.091674	0.274645	-915.072442

[a]All the magnitudes are given in hartree. [b]Thermodynamic contributions are computed at a temperature of 298.15 K and a pressure of 1 atm. [c]$G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}} = G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}} + E_{disp} + G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$.

Table S9. Relative PCM-B3LYP/VTZ//PCM-B3LYP/VDZ Gibbs energy with electrostatic and non-electrostatic solute-solvent interactions ($\Delta G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$), dispersion energy correction (ΔE_{disp}), PCM-B3LYP/VDZ thermal Gibbs energy correction ($\Delta G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$), PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}}$), and PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ Gibbs energy in water solution ($\Delta G^{\text{sol}}_{\text{corr}}$) computed at the standard concentration of 1 *M* (55.5 *M* for water) of the critical structures involved in the $[Cp_2Mo(OH)(OH_2)]^+$-catalyzed neutral hydrolysis of ethyl acetate.[a,b]

Species	$\Delta G_{\text{PCM-B3LYP/VTZ//PCM-B3LYP/VDZ}}$	ΔE_{disp}	$\Delta G^{\text{therm}}_{\text{PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}}$	$\Delta G^{\text{sol}}_{\text{corr}}$
$[Cp_2Mo(OH)(H_2O)]^+$ + ethyl acetate	0.0	0.0	0.0	0.0	0.0
$[Cp_2Mo(OH)]^+$ + ethyl acetate + H_2O	1.4	5.0	-12.3	-5.9	-1.6
TS0 + H_2O	13.5	-1.7	-0.2	11.5	13.9
I1 + H_2O	4.2	-4.2	2.2	2.1	4.5
TS1-OH1 + H_2O	18.8	-6.1	3.7	16.4	18.8
I2-OH1 + H_2O	16.8	-6.2	5.6	16.2	18.6
TS2-OH1 + H_2O	41.9	-6.1	1.7	37.4	39.8
I3-OH1 + H_2O + ethanol	-6.5	1.9	-11.5	-16.1	-11.8
TS3-OH1 + H_2O + ethanol	9.2	3.1	-12.5	-0.2	4.1
I4-OH1 + H_2O + ethanol	5.4	2.9	-11.7	-3.4	0.9
I5-OH1 + ethanol	-6.9	-2.3	0.3	-8.9	-8.9
TS4-OH1 + ethanol	17.4	-1.6	0.1	15.9	15.9
I6-OH1 + ethanol	7.5	-1.3	0.6	6.8	6.8
TS5-OH1 + ethanol	12.8	0.5	0.2	13.5	13.5
I1-OH1'	15.9	-8.9	16.7	23.8	21.9
TS2-OH1'	42.1	-9.1	13.5	46.5	44.6
TS1-OH2'	34.9	-9.0	13.0	38.9	37.0
$[Cp2Mo(OH)]^+$ + ethanol + acetic acid	5.0	5.9	-12.1	-1.1	0.8

[a]All the thermodynamic magnitudes are given in kcal/mol at a temperature of 298.15 K and a pressure of 1 atm. [b]$\Delta G^{\text{sol}}_{\text{corr}} = \Delta G^{\text{sol}}_{\text{PCM-B3LYP-D3/VTZ//PCM-B3LYP/VDZ}} + \Delta E_{disp}$ + (1.9 kcal/mol) Δn + (4.3 kcal/mol) Δm, where Δn and Δm are the changes in the number of non-water components and water molecules for each transformation along the reaction mechanisms found, respectively.

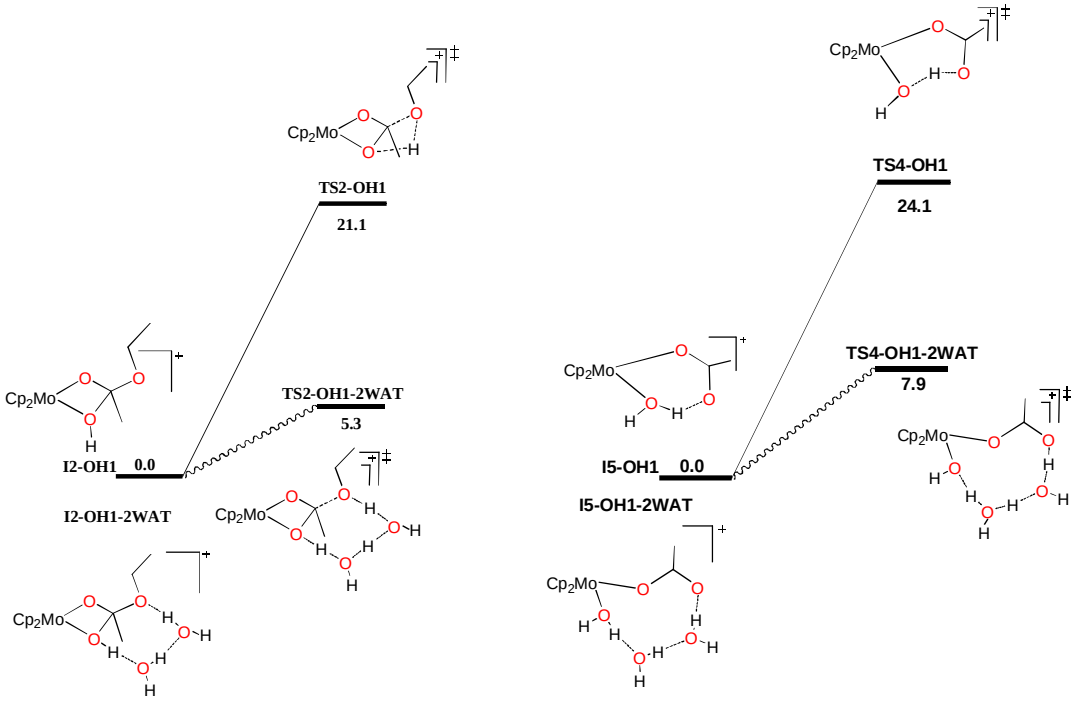

Figure S5. Schematic Gibbs energy profiles in water solution for the hydrogen migrations found along the OH1 mechanism both in the absence and in the presence of two explicit water molecules at the PCM-B3LYP/VTZ//PCM-B3LYP/VDZ level of theory.

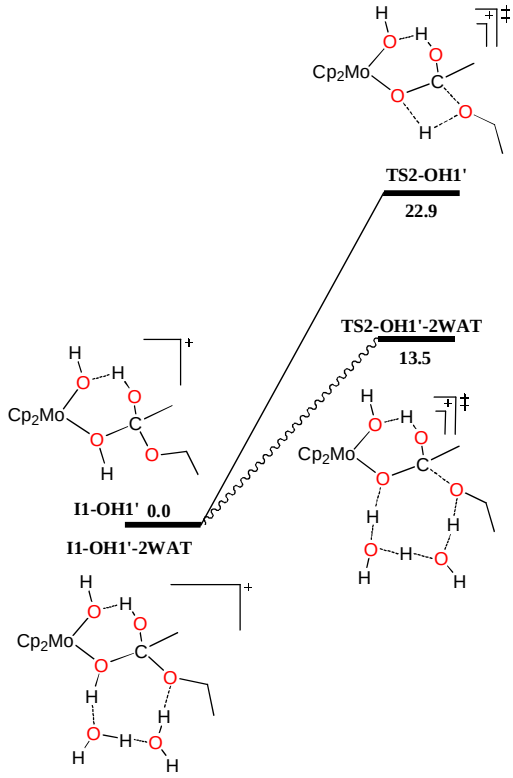

Figure S6. Schematic Gibbs energy profiles in water solution for the hydrogen migration found along the OH1' mechanism both in the absence and in the presence of two explicit water molecules at the PCM-B3LYP/VTZ//PCM-B3LYP/VDZ level of theory.

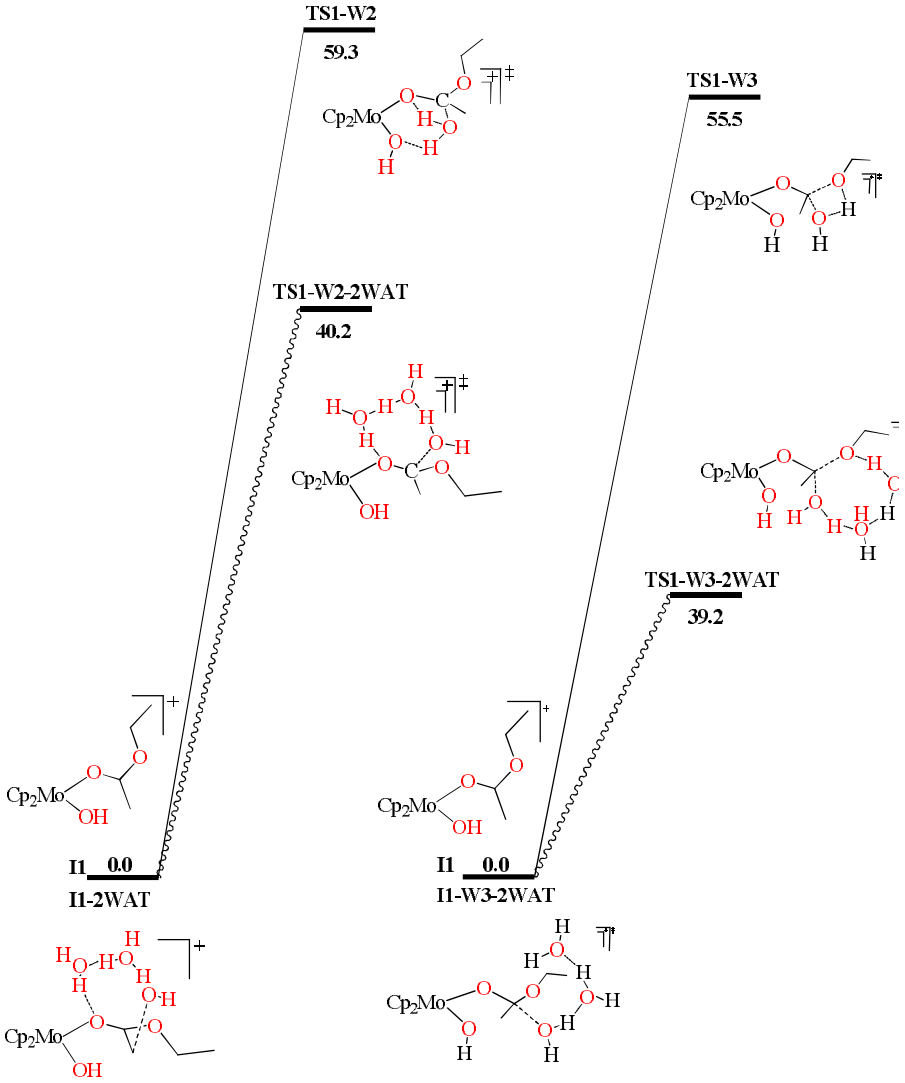

Figure S7. Schematic Gibbs energy profiles in water solution for the water addition found along the W2 and W3 mechanisms both in the absence and in the presence of two explicit water molecules at the PCM-B3LYP/VTZ//PCM-B3LYP/VDZ level of theory.

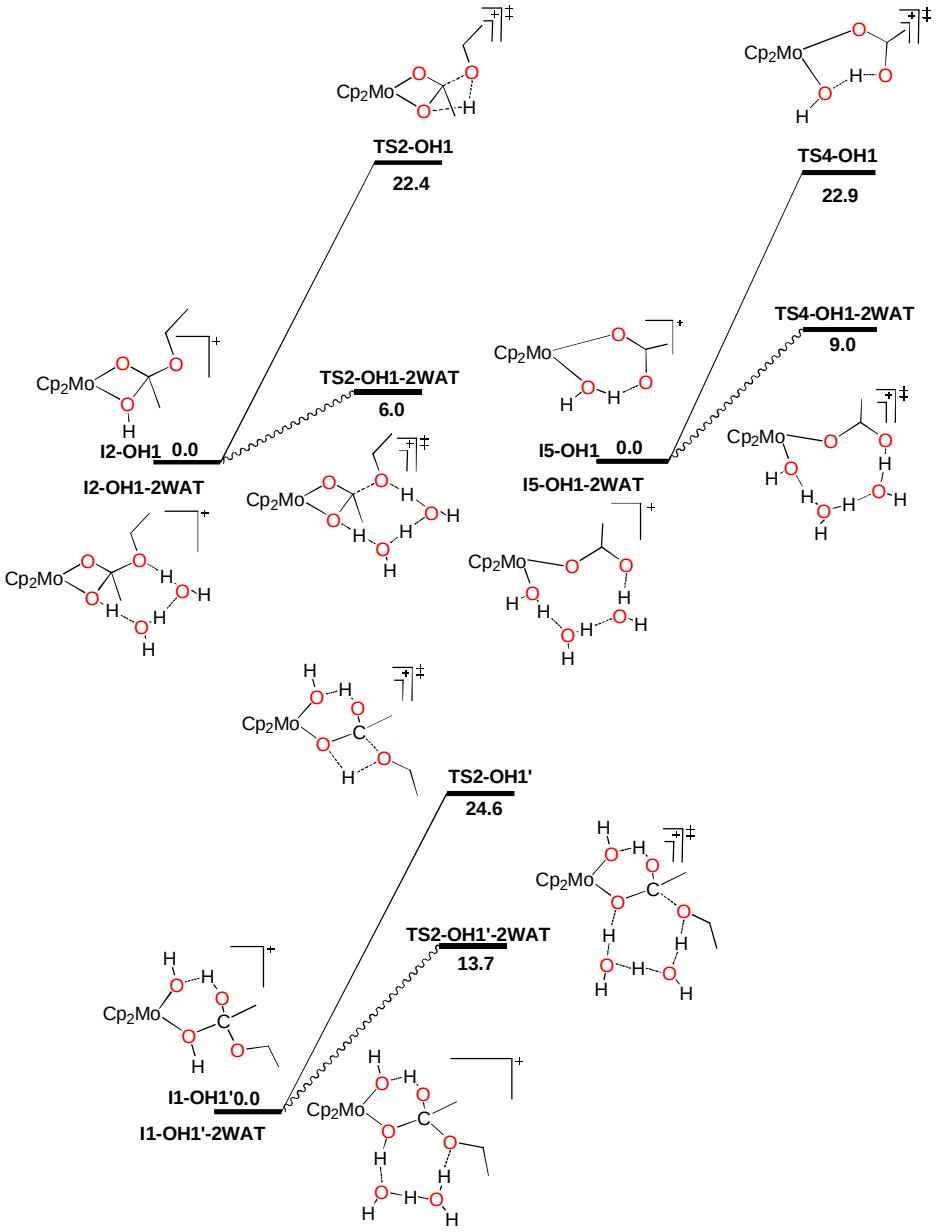

Figure S8. Schematic Gibbs energy profiles in water solution for the water addition found along the OH1 and OH1' mechanisms both in the absence and in the presence of two explicit water molecules at the PCM-M06/VTZ//PCM-B3LYP/VDZ level of theory.

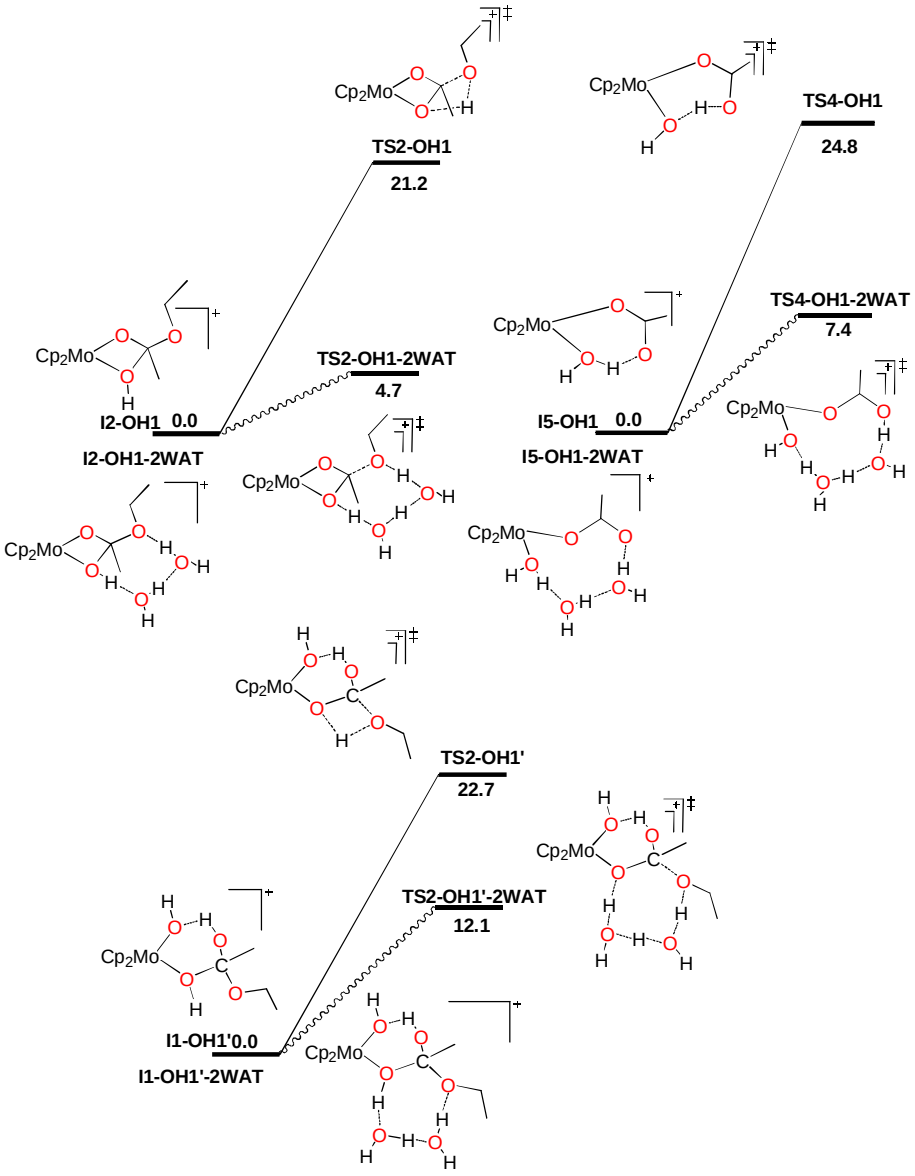

Figure S9. Schematic Gibbs energy profiles in water solution for the water addition found along the OH1 and OH1' mechanisms both in the absence and in the presence of two explicit water molecules at the PCM-B3LYP-3D/VTZ//PCM-B3LYP/VDZ level of theory.